Neutron Resonance Theory for Nuclear Reactor Applications: Modern Theory and Practices.

Nuclear Engineering Division

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Neutron Resonance Theory for Nuclear Reactor Applications: Modern Theory and Practices.

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TABLE OF CONTENTS

Contents

TABLE OF CONTENTS.....	1
INTRODUCTION LIST OF FIGURES	5
LIST OF FIGURES.....	5
LIST OF TABLES.....	6
<i>FOREWORD</i>	7
INTRODUCTION	9
References	17
Chapter IBASIC RESULTS OF RESONANCE REACTIONS THEORY	
.....	18
I.1 Potential Scattering	18
I.2 Reaction Channels and Cross Sections	24
I.3 Resonance Collision Matrix	28
I.4 One-Level Approximation.....	35
I.5 Doppler Broadening of Resonances	41
I.6 Resonance Interference.....	48
I.7 Some Transformations of Collision Matrix	58
I.8 Multilevel Formulae for Resonance Cross Sections	66
I.9 Pole representation of Cross Sections.....	77
I.9.1 Appendix I.A1 Outgoing Wave Functions and Their Boundary Factors	82
I.9.2 Appendix I.A2 Doppler Functions	85
I.9.3 Appendix I.A3 Unitary Property of U-Matrix	86
References	90

Chapter II	UNRESOLVED	RESONANCES	92
II.1	Average Cross Sections		93
II.2	Statistical Distributions of Resonance Parameters		102
II.3	Resonance Ladder Method		109
References			116
Chapter III	RESONANCE	SELF-SHIELDING	EFFECTS
			118
III.1	General Remarks on the Physical Meaning of Self-Shielding Effect		119
III.2	Slowing-Down Theory for Infinite Homogeneous Media		122
III.2.1	Kinematics of Elastic Scattering and Scattering Kernel		123
III.2.2	Characteristics of Slowing-Down Equation		126
III.2.3	Concept of Placzek Oscillations		129
III.2.4	Traditional Treatment of Neutron Slowing-Down Problems in Presence of Resonances		135
III.3	Resonance Integrals and Their Applications		140
III.3.1	Traditional Resonance Integral Concept		140
III.3.2	Fast Reactor Considerations		148
III.3.3	Generalization of Resonance Integrals		150
III.3.4	Applications in Conjunction to Effective Cross Section Approach		158
III.4	Continuous Energy Approach		160
III.5	Doppler Reactivity		163
References			166
Chapter IV	RESONANCE	ABSORPTION	IN
			HETEROGENEOUS
			MEDIA
			168
IV.1	Fundamental Equations in Lattice Physics		170

IV.1.1	Integral Transport Equation	170
IV.1.2	Collision Probability and Interface Current Approaches	171
IV.2	General Features of Collision and Transmission Probabilities	173
IV.2.1	General Remarks of Collision and Transmission Probabilities in an Isolated Lump	173
IV.2.2	General Features of Traditional Treatment of Collision Probability in a Closely Packed Lattice	177
IV.2.3	General Features of Collision Probabilities in a Cell with Many Regions	184
IV.3	Traditional Collision Probability Method for a Two-Region Cell	189
IV.3.1	Fundamental Equations.....	190
IV.3.2	Historical Notes on the Resonance Treatment for an Isolated Lump	192
IV.3.3	Nordheim's Method for Treating Resonance Absorption in a Two-Region Cell	196
IV.3.4	Equivalence Relation and Rational Approximations	197
IV.3.5	Equivalence Relation Based Resonance Integrals for Two-Region Cells	200
IV.3.6	Multiple-Term Rational Approximations.....	202
IV.4	Recent Collision Probability Methods for a Multiple-Region Cell with Many Resonant Isotopes	204
IV.4.1	Discretized Slowing-Down Equation for a Multi-Region Cell	205
IV.4.2	Collision Probabilities for Practical Geometries	206
IV.5	Interface-Current Method for a Multi-Region Cell With Many Resonant Isotopes	206
IV.5.1	Neutron Transport in a Generic Unit Cell.....	207
IV.5.2	Collision and Transmission Probabilities for Geometries of Practical Interest	209
	REFERENCES.....	217
	Chapter V STATISTICAL TREATMENT OF UNRESOLVED RESONANCES	222
V.1	Nature of the Problem.....	222

V.2	Existing Methods---Basis and Problems	223
V.2.1	Methods Based on Distributions of Resonance Parameters	223
V.2.2	Method Based on Conditional Distributions of Cross Sections	232
V.3	Recent Advances in the Treatment of Unresolved Resonances.....	237
V.3.1	Method Based on Information Theory	237
V.3.2	Method Based on Characteristic Function	243
	References	247

INTRODUCTION LIST OF FIGURES

Figure 1 Neutron Spectrum in LWR Pin Cell around ^{238}U resonance at 6.672 eV	13
Figure 2 Spatial Flux Distribution in LWR in Pin Cell around ^{238}U resonance at 6.672 eV	14

LIST OF FIGURES

Figure I. 1 Symmetric and Anti-Symmetric Natural Line Shape Functions	37
Figure I. 2 Porter-Thomas Distributions for n Channels.....	39
Figure I. 3 Symmetric and Anti-Symmetric Doppler-Broadened Line Shape Functions	43
Figure I. 4 Total Cross Section of ^{238}U at 300K	49
Figure I. 5 Total Cross Section of ^{235}U at 300K	49
Figure I. 6 Total Cross Section of ^{239}Pu at 300K.....	50
Figure I. 7 Illustration of Interference Effect of Two Interacting Resonances	51
Figure I. 8 Illustrative Example of Constructive and Destructive Interferences	55
Figure II. 1 Fluctuation Factor for Multi-Channel Radioactive Capture	96
Figure II. 2 Three Channel Probability Distribution Function ($\beta_1 = 1 - \beta$, $\beta_2 = \beta_3 = \beta$)	105
Figure II. 3 Fluctuation Factor for Two-Channel Problem.....	108
Figure III. 1 Velocities and Scattering Angles in C- and L-Systems.....	125
Figure III. 2 Placzek Function in a Mixture of Fast Reactor Composition.....	132
Figure III. 3 Placzek Oscillations in the Presence of a Breit-Wigner Resonance	135
Figure IV. 1 Escape Probabilities from a Lump.....	177
Figure IV. 2 Schematic Illustration of Neutron Transport in a Medium with Multiple Absorbers.....	179

Figure IV. 3 Schematic Illustration of Carlivik's Approach	187
Figure IV. 4 Neutron Path in Annular Geometry	211
Figure V. 1 Analytical pdf for Kapur-Peierls Level Spacing Using Two Levels	230

LIST OF TABLES

Table I. 1 External functions and their factors on the boundary of nucleus	21
Table IV. 1 Geometric Parameters for Three Most Commonly Considered Configurations.....	183
Table V. 1 Average Spacing and Variances for Various Cases.....	230

Photo by Sharon Hwang Jaster

FOREWORD

For 44 years, Richard Hwang provided the mathematical basis and computational capabilities for nuclear resonance cross section calculations at Argonne National Laboratory, the nation's lead laboratory for peaceful nuclear energy development. These cross sections represent the probability of neutron-induced nuclear reactions mathematically, physically, and computationally, and are of particular importance in fast neutron reactors where fast neutrons born from fission are not quickly slowed to far lower thermal energies, as they are in today's water-cooled commercial power reactors. The fast neutrons consequently have very many reactions in the resonance range. Although relatively uncommon in the world today, fast reactors will ultimately provide a way to convert used nuclear fuel to energy while decreasing the volume of nuclear waste and the period of its toxicity from about 300,000 years to a few hundred years. They will also extend the uranium resource base by almost one hundred times, fueling a large fraction of the world's energy consumption for many thousands of years. In the bargain, fast reactors are expected to be considerably safer than today's already-safe commercial power plants.

Because computers are now orders of magnitude more powerful than 30 years ago, nuclear engineers are performing ever-more detailed calculations of nuclear reactor designs, and will soon be solving, all at once, the several important equations describing reactor behavior during operation. The important details in physics calculations include the temperature distribution within each fuel pin -- until now approximated by an average. The fuel temperature affects the resonance cross section strongly, so it is crucial to solve the governing equations with a model that reflects the full complexity of the physics involved. This extension is what Dr. Hwang's work has enabled.

The effects of fuel temperature on neutron cross sections occur because of "Doppler broadening", the microscopic nuclear physics equivalent of the familiar frequency (tonal pitch) shift one hears when passed by a high-speed vehicle or aircraft. The use of more detailed neutron cross section data has made computer memory the limiting constraint on accurate Doppler broadening calculations in reactor physics.

During the 1980s, long before massively parallel computing shifted the computational bottleneck from computation to storage, Dr. Hwang proposed a rigorous pole representation that carried out Doppler broadening while reducing the amount of computer memory required by a factor between 10 and 100. This development was far ahead of its time. It is particularly important on today's massively parallel supercomputers, where data transfer and memory limitations can seriously hobble computational

performance. He saw, using his prodigious mathematical talent and his keen physical insight that the solution to Doppler broadening could be produced analytically instead of iteratively. This he did by recasting the relevant equations in terms of momentum instead of the traditional energy-based prescription. He implemented his method in his WHOPPER code, versions of which have been in use in ANL's ETOE cross section processing code and MIT's OpenMC code. OpenMC, a very advanced multi-physics code still under development, will simultaneously model both the detailed reactor physics and the reactor thermal-hydraulics that affects reactor physics behavior.

Much of Dr. Hwang's work has had a lasting impact on the field of computational reactor physics. He generalized the traditional resonance integral concept to accommodate interference of neighboring resonances and the multilevel resonance formalism. He studied the effects of crystalline binding on Doppler broadening, and made widely-adopted original contributions to the theory of statistical treatment of the self-shielding effects in the unresolved resonance range. He developed efficient numerical algorithms for treating the self-shielded resonance cross sections in both the resolved and the unresolved regions, all incorporated in ANL's MC²-2 and MC²-3 codes. Working as a reactor physicist, he developed an accurate method for computing the transmission probabilities in annular cell geometry for the integral transport theory, as well as a rational approximation for cells with complex geometries. He contributed further to the field of fast reactor physics by computation and analysis of the Doppler effects for liquid metal-cooled fast breeder reactors, fast critical assemblies, and space reactors. He also developed a method for treating sensitivity analysis and data adjustment, along with introduction of the vector space concept to assess the results of data adjustment.

For this work, he received the 2004 American Nuclear Society Eugene P. Wigner Reactor Physicist Award for outstanding contributions to the advancement of the field of reactor physics. The fruits of his work can also be found in numerous other computer codes, among them:

- MATDIAG code (in collaboration with P. A. Moldauer): Conversion of statistically generated R-matrix parameters to the Kapur-Peierls type parameters.
- SUPERW-code: A rigorous analytical method for treating Doppler-broadening of cross sections.
- IMPLIC-code: An exceedingly accurate numerical method based on the generalized Gauss-Hermite quadrature applicable to arbitrary interval for computing Doppler-broadening of cross sections.

This report is based on unpublished manuscripts of five chapters written by Richard Hwang for a book which he co-authored with Russian physicist Dr. Alexander Lukyanov. It summarized his work and publications in resonance theory. Dr. Lukyanov's portion of the book resides in Sophia, Bulgaria, and is under the jurisdiction of the National Laboratory there. The editors of this volume were privileged to work with Dr. Hwang during his decades at Argonne, before his death in 2008. They are Richard's former student and colleague, Dr. Luiz Leal (formerly of Oak Ridge National Laboratory, now at IRSN), Dr. Won Sik Yang (formerly at Argonne National Laboratory, now at Purdue University), and Dr. Roger Blomquist (Argonne). They, with help from administrative staff at Argonne, have integrated the chapters to form this report.

Dr. Roger N. Blomquist

INTRODUCTION

The neutron resonance phenomena constitute one of the most fundamental subjects in nuclear physics as well as in reactor physics. It is the area where the concepts of nuclear interaction and the treatment of the neutronic balance in reactor fuel lattices become intertwined. The latter requires the detailed knowledge of resonance structures of many nuclides of practical interest to the development of nuclear energy.

The most essential element in reactor physics is to provide an accurate account of the intricate balance between the neutrons produced by the fission process and neutrons lost due to the absorption process as well as those leaking out of the reactor system. The presence of resonance structures in many major nuclides obviously plays an important role in such processes. There has been a great deal of theoretical and practical interest in resonance reactions since Fermi's discovery of resonance absorption of neutrons as they were slowed down in water. The resonance absorption became the center of attention when the question was raised as to the feasibility of the self-sustaining chain reaction in a natural uranium-fueled system. The threshold of the nuclear era was crossed almost eighty years ago[1] when Fermi and Szilard observed that a substantial reduction in resonance absorption is possible if the uranium was made into the form of lumps instead of a homogeneous mixture with water. In the West, the first practical method for estimating the resonance escape probability in a reactor cell was pioneered by Wigner et al[2,3] in early forties.

A great deal of work in this area began to emerge in the fifties and most notably was the work by Chernick et al[4,5] that provided a concise description of resonance absorption in a two-region cell as neutrons are slowed down by the elastic scattering process. At approximately the same time, this type of problem was also examined in Russia; the most representative work was that of Gourevitch and Pomeranchouk[6]. A collection of work that followed can be found in a book edited by Marchuk[7]. Because of the general lack of good quality data and computing facilities, these earlier investigations were primarily based relatively simple models with focus on the single level Breit-Wigner resonance alone.

Practical needs have since provided the motivation for better understanding of the resonance phenomena exhibited by neutron cross sections and their effects on various reactor physics parameters of practical interest. Thus, resonance theory involves essentially two rather diverse subject areas. One deals with nuclear reaction theory and pertinent nuclear data that lead to concise specification of the energy behavior of the microscopic cross sections while the other concerns with problems resulting from applying the microscopic quantities to the macroscopic reactor systems. The general theories of the former are described in great detail by Lane and Thomas[8] and also in the more recent book by Lynn[9], whereas those of the latter are discussed by Weinberg and Wigner[10]. The macroscopic nature has two major consequences, namely, the Doppler-broadening of cross sections resulting from the thermal motion of the target nuclei and the self-shielding effects whereby the reaction rates can be strongly dependent on the macroscopic properties such as composition, geometric configuration and operating temperature of a reactor. Obviously, these two subject areas each have a substantial theoretical base that is of interest in its own right. It is quite apparent that there is practical need for a book that concentrates on the relevant theoretical foundations and methodologies pertinent to the treatment of resonance absorption in reactor applications alone. In particular, a book that accounts for the state-of-art developments in these fields will be of interest to reactor physics communities around

the globe.

One earlier book with similar objectives is that by Dresner[11] published in 1960. It provided an excellent summary of a great deal of pioneer work carried out in the U.S. The primary interest at the time was focused on issues directly related to the development of the light water reactors. Another excellent book of its kind by Lukyanov[12] (in Russian) was published in 1974. A second book by the same author[13] with emphasis on the applied reaction theory to supplement the former was published in 1978. These books encompass a large body of Russian work in resonance theory little known in the West. Clearly, our knowledge in these areas has been significantly enhanced by many recent theoretical developments along with the availability of large quantities of high resolution resonance data for the past 20 years. Much of the recent advances can be attributed to the much improved cooperation among the scientific communities around the globe. Our perception of resonance theory and its applications has obviously changed accordingly. In light of these recent developments, it is apparent that time has come for a new book to provide an adequate account on these subjects crucial to reactor applications.

To set the tone for the detailed discussions in chapters that follow, we shall begin with some important developments that have significant impact on our perception of resonance absorption in Section I.1. In Section I.2, the conceptual aspects of the self-shielding effects will be addressed. Because the dependence on composition, operating temperature and geometric configuration of a reactor cell, the self-shielding effect can be considered as a generic term to represent the macroscopic nature of the problems involved.

1. General Remark on the Status of the Field in Past Three Decades

With no loss of generality, two different philosophies must be applied to the treatment of resonance absorption according to whether the deterministic resonance data are available or not. The energy range in which resonance data for a given nuclide are experimentally resolved, is generally referred to as the resolved energy region for that nuclide. The calculations in the resolved energy range, in principle, can be carried out deterministically. In contrast, the relatively high energy region where resolved resonance data are unavailable due to the resolution problems resulting from the difficulties of instrument resolution as well as the Doppler-broadening of resonances, is referred to as the unresolved energy region. The latter requires the statistical treatment on the basis of statistical distributions of resonance parameters deduced from nuclear spectroscopy. One key factor directly responsible for the dramatic improvement of resonance data and the related methodologies for treating resonance absorption in the resolved and unresolved energy ranges was the emergence of the fast reactor development. In contrast to the light water reactors in which the attention was primarily focused on a handful of low-lying and well-isolated U^{238} resonances, the resonance contributions from those of all major actinides as well as structural materials over considerably large energy span must also be taken into account. The development of such a system has motivated great advances in the areas of nuclear data and method development. Another factor that has had immeasurable impact on these fields is the significant advances in the new generation computers. The availability of modern computing facilities makes possible the processing of a large quantity of resonance data and the investigation of the extremely complex problems unimaginable in the earlier days. Last but not least is the closer collaboration among the scientific communities around the globe that allows extensive exchange of ideas for the benefit of all concerned.

In the general area of nuclear data, one notable milestone was the formation of the Cross Section Evaluation Working Group' (CSWEG) by the U. S. Atomic Energy Commission in 1966. The function of

such a group was to provide a reference data base which would replace many of the individual data libraries then in use and thus provide a common point of reference for comparison of research results in the reactor physics communities. The CSWEG activities have produced six versions of the 'Evaluated Nuclear Data File' generally referred to as ENDF/B files since 1967. From the perspective of resonance theory, the ENDF/B 6[14] released in 1990 is particularly noteworthy. It reflects especially the most astounding improvement in our knowledge of resonance data in the resolved energy ranges. Two special features that have a profound impact on the reactor applications are the dramatic expansion of the resolved energy region and the availability of the R-matrix parameters in the Reich-Moore form for most of major nuclides of practical interest. The SAMMY-code[15] developed at Oak Ridge National Laboratory was instrumental in the evaluations of these new data. The impact of the vastly improved resonance data will be further addressed in the later chapters where appropriate. Other similar files provided by research centers around the globe have also emerged since the conception of the ENDF/B files. The most notable files include JENDL by Japanese Atomic Energy Research Institute, JEF by western European nuclear data communities, BROND by IPPE at Obninsk and CENDL by Chinese Nuclear Data Center in Beijing. Through the much improved cooperation among the nuclear data communities, it is possible to mobilize a concerted effort toward the common goal. The international nuclear data conferences are held and sponsored by various research centers biannually as an effective means to exchange ideas on the subject of mutual interest.

From the perspectives of reactor physics methodologies, the emergence of fast reactor development has also presented a special challenge especially in the treatment of resonance absorption. Unlike the relatively simple scenario assumed in the thermal reactor applications, one is confronted by the resonances from many nuclides that are present not only in the fuel but also in the cladding, supporting structures and the coolant in the resolved as well as the unresolved regions. In addition, it is well-known that the validity of the traditional single level Breit-Wigner approximation exclusively used in the past is questionable for many nuclides with closely spaced levels. The accurate estimation of the combined self-shielding effects resulting from resonances of numerous nuclides is not only essential in estimation of the criticality of a reactor but also from the point of view of reactor safety considerations. The latter manifests itself through the Doppler reactivity effect crucial to the fast reactor development. The related subjects will be addressed in Chapters III and IV that follow. The availability of new resolved resonance data in the much expanded energy regions provides the data base needed for many meaningful calculations. Furthermore, a large body of work on the statistical treatment of resonance absorption in the unresolved ranges is now available, as one shall see in Chapter V.

The availability of high resolution data given in the form of the Reich-Moore parameters has also made necessary a conceptual change in our traditional thinking especially in conjunction with the resonance integral concept on the basis of the isolated Breit-Wigner resonances. This motivates the development of the rigorous pole representation[16] with its parameters obtainable from a given set of the Reich-Moore parameters whereby the resonance cross sections are representable as a linear combination of the Breit-Wigner-like terms. Thus, the traditional resonance integral concept remains practically intact provided that the overlap effect is accounted for in the calculations. The detail account of this development will be presented in Chapters II and III.

Last, but certainly not least, is the impact attributed to the vastly improved computational facilities which makes possible the examination of extremely complex problems unimaginable in the past. These problems can now be treated with rigor at little cost especially if one uses exceedingly efficient yet inexpensive work stations. One example is the routine use of the rigorous method for treating the slowing-down problem in multi-region cells over a large energy span containing many resonances as one

shall see in Chapters III and IV. Another example is the far more routine use of the Monte Carlo methods in reactor applications using huge numbers of particle histories, which is not included in our discussions.

In the following section, the conceptual aspects of the self-shielding effects will be addressed. The emphasis is on the connection between the microscopic cross sections and the macroscopic quantities in the reactor physics calculations downstream.

2. Self-Shielding Effects in Perspective

The self-shielding effect is a phenomenon directly attributed to the localized fluctuations in neutron cross sections resulting from the resonance structures on the averaged reaction rates of a reactor cell over energy and space. The most common scenario in reactor applications is a system consisting of fuel lumps surrounded by moderators with light weight and relatively 'smooth' cross sections. Qualitatively, the presence of the resonances in the cross sections of the heavy nuclei will give rise to the localized perturbation of neutron flux in energy and in space. The degree of the impact is obviously dependent upon the relative concentration of the resonant nuclide under consideration with respect to other background material in the system and the geometric configuration of the fuel cell. In the limit of infinitely dilute concentration of resonant absorber, the neutron flux is virtually constant in energy and in space. Since the flux and the resonance absorption cross section are usually anti-correlated, the magnitude of the absorption rate per atom ($\langle \sigma_a \phi \rangle$) for the system with finite dilution is usually smaller than that for the infinitely dilute system.

In the earlier days of reactor development essentially focused on thermal reactors with low enrichment fuel, a reactor lattice is usually assumed to be composed of a handful of light nuclide with relatively constant cross sections serving as coolant and/or moderator and cladding along with fuel element dominated by U^{238} . A few low-lying resonances of the latter are substantially responsible for the absorption rates over the resonance energy range which, in turn, determines the fraction of neutrons that can reach the thermal energy via the elastic scattering. Two commonly considered scenarios in reactor applications were usually restricted to either the infinite homogeneous medium or infinite lattice consisting of repeated cells with fuel lumps surrounded by cladding and moderator. The resonance effect in the former attributed to the flux depression in energy alone is generally referred to as the energy self-shielding effect whereas the energy and spatial self-shielding effects are inseparable in the latter. Such effects can be best illustrated graphically for the simplest cases involving a single Breit-Wigner resonance.

Figure 1 Neutron Spectrum in LWR Pin Cell around ^{238}U resonance at 6.672 eV

Fig. 1 shows the behavior of the neutron flux as a function of energy in the vicinity of the ^{238}U resonance at 6.672 eV in a 'homogenized' system typical of light water reactor composition. Also shown here is the macroscopic total cross section as a function of energy. The significant flux depression within the extent of the resonance in question clearly indicates the existence of severe energy self-shielding effect. The actual absorption rate is far less than what can be expected if the flux depression were not present.

Figure 2 Spatial Flux Distribution in LWR in Pin Cell around 238U resonance at 6.672 eV

Fig. 2 shows the flux distribution in a realistic light water reactor (LWR) cell consisting of a fuel pin with 3% enrichment with zirconium clad imbedded in water. Here, the energy and space dependence of flux become intertwined. The results shown were computed via the use of the integral transport theory code RABBLE using many spatial meshes in the vicinity of the resonance at 6.672eV. For illustration purposes, the radial distributions of flux given correspond to the energy at the resonance peak, 3 and 10 Doppler widths away respectively. The significant flux depression near the resonance peak which leads to the spatial self-shielding effect is quite evident. The fact that a substantial reduction in absorption rate is possible upon making the uranium into the form of lumps is one of the key factors leading to the successful demonstration of the first self-sustained chain reactions. The quick recovery of the flux in energy as well as in space reflects the characteristics of the sharp resonance considered.

Thus, for the simple cases described, a quantity traditionally referred to as the shielding factor defined below is widely used as measure of the degree of the resonance self-shielding effect

$$f_x = \frac{\langle \sigma_x(E) \phi(E, r) \rangle_{E,r}}{\langle \sigma_x(E) \rangle_{E,r} \phi_{asym}} \quad (1)$$

where ϕ_{asym} is the asymptotic flux in absence of the resonance. Physically, the numerator and the denominator can be identified as the resonance integrals for the finite and the infinite dilution of the resonance absorber respectively. As long as the resonances are well-isolated and the flux recovers between them, the concept of the self-shielding effect in conjunction with the resonance integrals is quite easy to visualize without ambiguity.

Since early 60's, advances in three major areas in the previous section have had significant impacts on our perceptions as well as the methodologies for treating the self-shielding effects. First, the emergence of the liquid metal fast breeder reactor development cast the traditional resonance treatment into

different light. Here, the focus is no longer on the question of how many high energy neutrons can survive resonance absorption to reach the thermal energy. Instead, it is the intricate neutronic balance over an extremely large energy span ranging from high keV region down to thermal energy with numerous number of nuclide that exhibit resonance behavior. Thus, unlike the oversimplified model adopted earlier, one must also deal with resonances of many other actinides, structural isotopes, as well as coolant in addition to those of U^{238} in both the resolved and the unresolved energy regions. Of particular concern are the estimation of the Doppler coefficient and the sodium void coefficient, both crucial to reactor safety. Both these quantities require accurate resonance treatment. Furthermore, it is also note-worthy that several zero-power assemblies such as ZPR-3, ZPR-6, ZEBRA, and ZPPR were constructed in the course of the fast reactor development for the purpose of providing the experiments to verify various reactivity coefficients of practical interest. The geometric configurations of the cells in these assemblies are far more complex than what was envisioned in the earlier reactor programs. Consequently, our perception of self-shielding effects must be modified accordingly in order to accommodate the situation involving the mutual self-shielding effect of all resonances as well as the spatial effects in the more complicated cells.

Secondly, there have been continuous and relentless efforts in the international nuclear data communities in recent years to systematically improve the neutron physics data base. The most recent improvements in resonance data through dramatic extension of the resolved resonance range and the introduction of the R-matrix parameters are particularly remarkable. Thus, while the elimination of the long-standing difficulty of applying the Breit-Wigner approximation to the closely spaced resonances enhances the rigor of the resonance cross section as a function of energy, it also makes necessary the modification of the traditional resonance integral concept based on isolated resonances.

Thirdly, the amazing progress in our computational capabilities provides strong motivations for reactor physicists to venture into the much more rigorous of the resonance effects in reactor lattices unimaginable before. One noticeable consequence is the availability of both the deterministic and Monte Carlo codes for treating the lattice physics problems on a continuous energy basis whereby the continuous nature of neutron flux in energy is preserved. It is important to realize, however, that the former is generally not free from simplified assumptions while the latter is only useful as a bench-mark tool but still too costly for routine applications in spite of the high-speed computing facilities now in existence. The most commonly used method for reactor neutronic calculations today are still based on the multigroup concept. It is, therefore, useful to cast the self-shielding concept within the context of the multigroup approach.

One essential principle of the multigroup approach is the separation of the fine structure effect treatment from the global neutronic calculations of the entire reactor. This can be best accomplished by first computing a set of effective group cross sections for each nuclide and reaction type at a given location of the reactor lattice,

$$\tilde{\sigma}_x = \frac{\langle \sigma_x(E) \phi(E, r) \rangle_{E,r}}{\langle \phi(E, r) \rangle_{E,r}} \quad (2)$$

over the energy group with width much greater than the extent of resonances for the actinides. From practical point of view, it is clearly impossible to maintain the rigor of the flux in great detail throughout the entire reactor especially when many zones are present. Thus, it is a common practice that the actual

flux $\phi(E, r)$ is usually replaced by $\tilde{\phi}(E, r)$ with close resemblance in shape, typically taken as that of the repeated cell in an infinite lattice. For reactors with multiple zones with different composition, the effective resonance cross sections are treated separately first before they are collapsed into desirable structures more readily amenable to diffusion theory or S_N -codes. It is note-worthy that $\tilde{\sigma}_x$, unlike the reaction rate, is more susceptible to the multigroup approach without the recourse of the potentially troublesome renormalization of neutron source if the heterogeneous nature of the reactor is considered.

Within the context of the effective cross section concept, the self-shielding effect can be viewed as a measure of correlation between the microscopic cross section and the neutron flux in energy and in space at a given temperature. With no loss of generality, the self-shielding effect can be defined as:

$$f_x = \frac{\tilde{\sigma}_x}{\langle \sigma_x(E) \rangle_E} = 1 + \frac{\text{COV}[\sigma_x(E), \phi(E, r)]}{\langle \sigma_x(E) \rangle_E \langle \phi(E, r) \rangle_{E, r}} \quad (3)$$

where the covariance signifies the degree of correlation between σ_x and ϕ . All averages here also implicitly include those over statistical properties of cross sections if resonances are unresolved, and can be cast either into the form of the usual Riemann integrals or Lebesgue integrals.

Conceptually, such a description provides a plausible basis for much of the discussions that follow. The main difference among various methods in practical applications is the rigor by which such a correlation is treated. For the resolved resonance energy range, the degree of correlation is clearly deterministic and multi-variant in nature. Many existing methodologies are implicitly built around the premise that the correlation defined in Eq. (3) is short range in nature with respect to space and/or energy. In the limit of an isolated resonance, such correlations are certainly short-ranged as clearly illustrated in Fig. I.1 and Fig. I.2. Generally speaking, in a highly heterogeneous cell with well-separated fuel regions sandwiched between substantial amounts of moderators, the spatial correlation is obviously localized and thus the use of $\phi(E, r)$ for the infinite repeated lattice in the self-shielding calculations is warranted. On the other hand, in a closely spaced lattice consisting of fuel lumps with different composition, such an assumption may not necessarily be justified. The preservation of the rigor in energy correlation is also a primary concern. If the energy dependence of resonance cross sections can always be specified concisely by a linear combination of the Doppler-broadened line shape functions characterized by the relatively short-range fluctuations with respect to their peaks, the covariance defined by Eq. (3) can also be viewed as a superposition of short-ranged terms. Many methods based on the traditional resonance integral approach, in effect, took advantage of such behavior. For the unresolved resonance energy range, the statistical properties of the widths and level spacing of resonances must also be considered in the determination of the self-shielding effect. It is quite natural that the mutual self-shielding effects of neighboring resonances exhibit strikingly different characteristics depending on whether they belong to the same or different spin sequences. More discussions will be given in the later sections.

From Eq. (1), it is quite obvious that estimation of the self-shielding effects requires accurate descriptions of the cross section and the neutron flux as a function of energy at a given location and temperature in a reactor system. The general theories that account for the behavior of these quantities are well-known. The energy dependence of neutron cross sections is generally specified by the R-matrix

theory while their temperature dependence attributed to the thermal motion of the nuclei is characterized by the Doppler-broadening process according to the Maxwell-Boltzmann distribution. On the other hand, the neutron flux distribution resulting from the slow-down and transport processes of neutrons is, in principle, described by the Boltzmann's transport equation as a function of the macroscopic cross sections at a given location and temperature in the system under consideration. The utilization of these theories in the practical applications is by no means simple. To facilitate their applications constitutes one of the most fundamental problems in reactor physics. There have been many advances on this subject in the past decade due primarily to the availability of the high resolution data and the significant improvement in our computational capability. In the following sections, an overview of this subject will be presented.

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Chapter I BASIC RESULTS OF RESONANCE REACTIONS THEORY

The analysis of resonance neutron cross section data is usually a determination of level parameters – energies and resonance widths and an appropriate physical interpretation if it is of special interest. Such an interpretation up to now does not surpass the framework of traditional idea about Niels Bohr compound resonances. Now, the new information about fine energy structure of neutron cross sections in the permanently enlarged resolved resonance energy region and the problem of evaluating the corresponding data require more and more common and sophisticated mathematical methods for parameterization of these cross sections. The formal theory of nuclear resonance reactions contains the principles for improvement of such methods. The theoretical description here is mathematically rigorous and does not contain any essential restrictions about the reaction mechanism, in spite of being mostly adapted for the compound resonances [1-6].

First of all, this theory treats the kinematics of binary reactions (with formation of two particles only) in a stationary non-relativistic approach. The relations between cross sections and the elements of the so-called “collision matrix $\mathbf{U}$ ” are universal for both resonance and non-resonance processes and reflect the basic physical conservation laws for total energy, angular momentum and parity, the balance of the intensities of all possible reactions at given energy, and time invariance of description and summation rules for quantum momenta [1,4,7,8].

The analytic properties of $\mathbf{U}$ -matrix provide its complete pole expansion in the complex plane of the energy E (or momentum $k \propto \sqrt{E}$) [9,10], poles and residues being associated with the observed resonances and their widths. Different forms of representation here correspond to their typical schemes (formalism of resonance theory) for parameterization of the resonance cross sections, and these in the general case are related reciprocally [4]. So, to have a general idea about the methods used in practice for the so-called “multilevel analysis” of resonance cross sections, taking into account the mutual influence (interference) of levels in a wide energy interval, it is sufficient to consider the physical principles of construction, e.g., Wigner’s $\mathbf{R}$ -matrix theory, and to establish the algorithms of transformation of the results of this theory to the schemes of other formalism.

I.1 Potential Scattering

The basic principles of nuclear reaction theory in stationary non-relativistic approach can be illustrated with the example of elastic scattering of two spinless particles. This classical problem of quantum mechanics is reduced to the consideration of motion of one particle with effective mass of $\mu = M_1 M_2 / (M_1 + M_2)$ in the central force potential $V(r)$, depending only on the relative distance between particles [11]. The solution of the corresponding Schrödinger equation in spherical coordinates is written as a sum:

$$\Psi(\vec{r}, E) = \sum_{lm} u_l(r, E) [i^l Y_{lm}(\theta, \phi)] \quad , \quad (I.1.1)$$

where Y_{lm} ’s are the orthonormal wave functions of the angular orbital momentum operator (spherical functions), and $u_l(r, E)$ ’s are the radial solutions satisfying the equation:

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{du_l}{dr} \right) - \frac{l(l+1)}{r^2} u_l + \left(k^2 - 2\mu \frac{V(r)}{\hbar^2} \right) u_l = 0 \quad (1.1.2)$$

where $k^2 = 2\mu E / \hbar^2$ [1]. The solutions of Eq. (1.1.2) depend on the form of potential $V(r)$.

a) For the free motion ($V = 0$), two independent solutions are given by the spherical Bessel function $j_l(kr)$ and the spherical Neumann function $n_l(kr)$ [13]. In this case, the following functions are more convenient:

$$F_l(kr) = kr j_l(kr), \quad G_l(kr) = -kr n_l(kr) \quad (1.1.3)$$

of which the asymptotes for $kr \gg 1$ are [4,11]:

$$F_l(kr) \rightarrow \sin(kr - \pi l / 2), \quad G_l(kr) \rightarrow \cos(kr - \pi l / 2).$$

In the scattering problem, the following complex combinations of these functions are also useful:

$$I_l = G_l - iF_l = kr[j_l(kr) - in_l(kr)], \quad O_l = I_l^* = G_l + iF_l. \quad (1.1.4)$$

The corresponding asymptotes to the incoming (I_l) and outgoing (O_l) waves are given by

$$I_l \rightarrow \exp[-i(kr - \pi l / 2)], \quad O_l \rightarrow \exp[i(kr - \pi l / 2)].$$

The Wronskian of this pair of solutions is

$$I_l \frac{dO_l}{dr} - O_l \frac{dI_l}{dr} = 2ik \quad (1.1.5)$$

which does not depend on r (see Appendix.I.A at the end of this chapter).

The radial solutions in the case of free motion can be presented by using these functions as

$$u_l(r) = r^{-1} [A_l I_l(kr) - B_l O_l(kr)] \quad (1.1.6)$$

From the condition of regularity at $r = 0$, it follows $A_l = B_l$ and thus we have

$$u_l(r) = -2ikA_l j_l(kr) \quad (1.1.7)$$

The coefficients A_l are determined by normalizing the wave function $\Psi(\vec{r}, E)$ in Eq. (1.1.1) for free motion. Usually it is chosen in the form of plane wave in the direction of the initial beam $\exp(i\vec{k} \cdot \vec{r})$. Using the known expansion of the plane wave over spherical functions [11,12]

$$\exp(ikr \cos \theta) = \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} j_l(kr) [i^l Y_{l0}(\theta)]$$

the coefficient A_l in Eq. (1.1.7) can be determined as

$$A_l = (i/k) \sqrt{\pi(2l+1)} \quad (1.1.8)$$

b) For a non-zero scattering potential $V(r)$ with a finite radius (i.e., $V(r) = 0$ for $r > a$), the solution outside the potential (for $r > a$) has the same structure as that for free motion in Eq. (1.1.6). However, the coefficient of the scattered wave is different from A_l and thus it can be written as

$$u_l(kr) = (i/k) \sqrt{\pi(2l+1)} [I_l(kr) - U_l O_l(kr)] \quad (1.1.9)$$

where $U_l = B_l / A_l$ is the so-called collision function or scattering function which is independent of r . In the case when only the elastic scattering is possible, $U_l = \exp(-2i\varphi_l)$ with real “scattering phases” φ_l [1,9,10] determined by the solution of Eq. (1.1.2) for $r \leq a$. They can be considered as characteristics obtained from the experimental data, and by using them, the interaction potential $V(r)$ can in principle be unfolded (the reciprocal scattering problem [9,10]). The solution of Eq. (1.1.1) asymptotically as $r \rightarrow \infty$ can, for this case, be presented by a sum of plane and scattered waves:

$$\Psi_{as} = \exp(i\vec{k} \cdot \vec{r}) + r^{-1} f(\theta) \exp(ikr) \quad (1.1.10)$$

where $f(\theta)$ is the so-called scattering amplitude given by

$$f(\theta) = -(2\sqrt{\pi}/k) \sum_{l=0}^{\infty} \sqrt{2l+1} \exp(-i\varphi_l) \sin \varphi_l Y_{l0}(\theta)$$

The differential cross section is a ratio of the outgoing flux of particles, with velocity v through the surface element $dS = r^2 d\Omega$ at distance r in the direction $\vec{\Omega}$, to the incoming flux given by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = 4\pi k^{-2} \sum_{l'} \sqrt{(2l+1)(2l'+1)} \sin \varphi_l \sin \varphi_{l'} Y_{l0}(\theta) Y_{l'0}^*(\theta) \quad (1.1.11)$$

By integrating over all angles and taking into account the orthogonality of spherical functions, we obtain a total scattering cross section as

$$\sigma = 4\pi k^{-2} \sum_l (2l+1) \sin^2 \varphi_l \quad (1.1.12)$$

These are the simplest kinematic relations between cross sections and scattering phases that illustrate the idea of phase analysis – the determination of φ_l from scattering experiments [9,10,1,6].

c) For some forms of potential V , the scattering phases can be found simply. In the scattering by a hard sphere with radius a , the solutions in Eq. (1.1.9) must be zero at $r = a$, i.e.,

$$I_l(ka) = \exp(-2i\varphi_l) O_l(ka), \quad (1.1.13)$$

which corresponds to the phase:

$$\varphi_l = \arctan(F_l / G_l) = -\arctan[j_l(kr) / n_l(kr)]$$

Table I.1 shows these factors as a function of $\rho = kr$ for four l -states of practical interest.

Table I. 1 External functions and their factors on the boundary of nucleus

l	0	1	2	3
$O_l(\rho = kr)$	$e^{i\rho}$	$\rho^{-1}(1-i\rho)e^{i\rho}$	$\rho^{-2}(3-\rho^2-3i\rho)e^{i\rho}$	$\rho^{-3}[15-6\rho^2-i\rho(15-\rho^2)]e^{i\rho}$
$L_l(\rho = ka)$	$i\rho$	$\frac{-1+i\rho^3}{1+\rho^2}$	$\frac{-18-3\rho^2+i\rho^5}{9+3\rho^2+\rho^4}$	$\frac{-675-90\rho^2+6\rho^4+i\rho^7}{225+45\rho^2+6\rho^4+\rho^6}$
$\varphi_l(\rho = ka)$	ρ	$\rho - \arctan \rho$	$\rho - \arctan \frac{3\rho}{3-\rho^2}$	$\rho - \arctan \frac{\rho(15-\rho^2)}{15-6\rho^2}$

The factors characterizing the scattering by a hard sphere have an important meaning in **R**-matrix theory, which we use below. The free motion solutions determine the wave function structure in the region $r > a$ for a potential $V(r)$ limited over $r \leq a$. The most important factor is the logarithmic derivative at $r = a$, which is equal to the corresponding derivative for the solutions in the region of nuclear interaction ($r \leq a$). Denote the logarithmic derivative of the solution ru_l in Eq. (I.1.9) at $r = a$ by R_l^{-1} . It can be expressed as

$$R_l^{-1} = a \left[\frac{1}{ru_l} \frac{d}{dr} (ru_l) \right]_{r=a} = a \frac{I'_l - U_l O'_l}{I_l - U_l O_l} \Big|_{r=a}. \quad (\text{I.1.14})$$

This leads directly to the relation between collision function U_l and inverse logarithmic derivative R_l at $r = a$:

$$U_l = e^{-2i\varphi_l} (1 - R_l L_l)^{-1} (1 - R_l L_l^*), \quad (\text{I.1.15})$$

where φ_l is the hard sphere scattering phase in Eq. (I.1.13) and

$$L_l = \left[r O_l^{-1} \frac{dO_l}{dr} \right]_{r=a} = S_l + iP_l \quad (\text{I.1.16})$$

is the logarithmic derivative of the solution O_l at $r = a$ (given in Table I.1). The real part S_l is called the shift factor, and imaginary part P_l is the penetrability factor (Appendix I.A1).

d) The nuclear interaction effect at $r \leq a$ can be illustrated rather quantitatively using the example of the scattering by a spherical potential with finite depth (i.e., a rectangular well):

$$V(r) = \begin{cases} -V_0 & (r \leq a) \\ 0 & (r > a) \end{cases}$$

There are two typical space regions here: an external region ($r > a$) corresponding to the free motion of particles and an internal region ($0 < r \leq a$), where the solutions depend on the potential $V(r)$. A similar division in two regions takes place in both the continuous spectrum at $E > 0$ and the discrete spectrum at $E < 0$ [1,11]. When analyzing the scattering, we are interested only in the positive E values.

Let us turn now to Eq. (I.1.2) for $l = 0$. For the potential $V(r) = -V_0$, it has the following solution which is regular at $r = 0$:

$$u_0(r) = C \sin(\alpha r) / \alpha r, \quad (\text{I.1.17})$$

where $\alpha^2 = 2\mu(E + V_0)/\hbar^2$. This solution in the region $r \leq a$ permits us to determine directly the inverse logarithmic derivative at $r = a$:

$$R_0 = (a\alpha)^{-1} \tan(\alpha a), \quad \delta = R_0 P_0 = (k/\alpha) \tan(\alpha a) \quad (I.1.18)$$

Using $S_0 = 0$, $P_0 = ka$, and $\varphi_0 = ka$ given in Table I.1, the collision function in Eq. (I.1.15) can be written as

$$U_0 = e^{-2ia_0} = e^{-2ika} (1 - i\delta)^{-1} (1 + i\delta) \quad (I.1.19)$$

which corresponds to the scattering phase

$$\tan \omega_0 = [\tan(ka) - \delta] / [1 + \delta \tan(ka)] \quad (I.1.20)$$

The analysis of energy dependence of ω_0 based of these relations illustrates the peculiarities of the resonance type. The expansion of $\delta(E)$ over simple fractions gives [12]:

$$\delta(E) = (k/\alpha) \tan(\alpha a) = ka \sum_{\lambda=1}^{\infty} \frac{2}{\pi^2 (\lambda - 1/2)^2 - (a\alpha)^2} = \frac{1}{2} \sum_{\lambda} \frac{\Gamma}{E_{\lambda} - E}, \quad (I.1.21)$$

where

$$\Gamma = 2k\hbar^2 / \mu a, \quad E_{\lambda} = \pi^2 \hbar^2 (\lambda - 1/2)^2 / 2\mu a^2 - V_0. \quad (I.1.22)$$

The sum in Eq. (I.1.21) is an usual expansion of $\delta(E) = R_0 P_0$ in a series over the poles E_{λ} in $\mathbf{R}$ -matrix theory, situated both at positive and negative (for $\lambda < a\sqrt{2\mu V_0} / \pi\hbar$) energies. The latter ones are related to the bound states in the potential V . On the other hand, the resonances in the scattering cross section in Eq. (I.1.12) correspond to the energies, where the denominators in Eq. (I.1.20) equal to zero. It is possible to show directly that the number of positive roots of the equation $1 + \delta \tan(ka) = 0$ (with $ka > 0$) does not exceed the number of bound states in the potential V (Levinson's theorem [9,10]).

The example of scattering by a rectangular potential considered above illustrates a rather interesting problem for the practical use of pole expansion in real situations. When the number of observable resonances in the cross section is different from the number of poles in the sum of the kind in Eq. (I.1.21), the similar sums can correspond to the cross section depending smoothly on the energy [4,17].

e) The scattering of charged particles by Coulomb potential, which occurs at all r , is also one of the classical problems of quantum mechanics [11]. In this case, the solution of the radial equation has the same properties as Eq. (I.1.4) and Eq. (I.1.5) with the so-called Coulomb functions $I_{lq}(kr)$ and

$o_{lq}(kr)$ having the asymptote

$$\begin{aligned} I_{lq}(kr) &\rightarrow \exp[-\{kr - \pi l / 2 - \eta \ln(2kr) + \xi_l\}] \\ O_{lq}(kr) &\rightarrow \exp[kr - \pi l / 2 - \eta \ln(2kr) + \xi_l] \end{aligned} \quad (1.1.23)$$

where $\eta = z_1 z_2 e^2 \mu / \hbar^2 k$ and $\xi_l = \arg[\Gamma(l+1+i\eta)]$ [3,4,13]. Although the reactions with formation of charged particles are also considered, the specifics of Coulomb interaction does not influence practically the construction of the formulae for neutron resonance cross section parameterization in rather limited energy intervals. The energy dependence of the logarithmic derivative L_{lq} in Eq. (1.1.6) is determined by the penetrability of the corresponding Coulomb threshold – $L_{lq}(\sqrt{B_l - E})$ and at barrier height of $B_l > 5 \sim 10$ MeV the variation of $\sqrt{B_l - E}$ in the interval $0 < E < 10 \sim 100$ keV, which is typical for the region of resolved neutron resonances, could probably be neglected. We suppose in further considerations that L_{lq} is not dependent on energy, but regardless, the formalism of the resonance theory is universal and it is not connected with special restrictions concerning the reactions with charged particles. These problems are considered in details in some monographs [3,4,9] and the mathematical reference books about the Coulomb functions [13,14].

1.2 Reaction Channels and Cross Sections

- a) The joint description of different competitive reactions occurring simultaneously is given by the multichannel theory of nuclear interactions [1-8]. For the energy region of neutron resonances, these reactions are the radiative capture of neutrons (n, γ) , the elastic scattering (n, n) and the fission (n, f) for fissile nuclei. For some problems, the resonance reactions with emission of α -particles, $(n, \gamma f)$ -process and inelastic scattering are of practical interest too.

The multichannel theory suggests the availability of a complete system of interacting nucleons (a neutron plus A nucleons of the target nucleus) and different pairs of nuclei to which the given system of nucleons can be divided. Limiting the consideration to binary reactions only, we can avoid complications connected with multi-particle reaction kinematics. Radiative capture, followed by the release of a few gamma quanta, can be considered here as a sum of binary decays, supposing the emission of quanta to be successive [4].

The reaction channel for given pair of particles ($A_1 + A_2 = A + 1$) is characterized by a set of corresponding quantum numbers for $r > a$, where there is no nuclear interaction between particle, but where a Coulomb one is possible. The kinds of particles and their internal energy states are noted by index α , their spins $\vec{I}_1$ and $\vec{I}_2$ with the projections M_1 and M_2 , and the relative orbital angular momentum $\vec{l}$ with one of its projections m are included also. The total spin of the channel $j = |\vec{I}_1 + \vec{I}_2|$ with projection $m_j = M_1 + M_2$ is used, as a rule, in the case of un-polarized particles. Moreover, it is convenient to include in channel determination the total moment $J = |\vec{l} + \vec{j}|$ with the

projection $M = m_j + m$ and the common parity $\pi = (-1)^l \pi_1 \pi_2$, which are the integrals of the motion of the system in the region of nuclear interaction. So, we will consider below the index of reaction channel c as a set of quantum numbers $\{\alpha, l, j, J, M, \pi\}$.

Generally, the channel wave function is constructed by using the solutions about the relative motion of two particles both with and without interaction but with the same set c of quantum numbers. (In microscopic theory, this is the nucleon scattering by the shell model potential, but in **R**-matrix theory considered below, the channels are determined only in the external region where there is no nuclear interaction [1-4].) Let us write this solution in the form:

$$\Psi_c = v_c^{-1/2} r_c^{-1} [A_c I_c(r_c) - B_c O_c(r_c)] \psi_c, \quad (1.2.1)$$

where I_c and O_c are two independent solutions of the radial equation in Eq. (1.1.2) in the external region, corresponding at the asymptote to the incoming and outgoing waves in channel c . The multiplier $v_c^{-1/2}$ is connected with the normalization of Ψ_c on the flux density, and ψ_c is the so-called surface channel function, which is a product of eigenfunctions independent of r_c :

$$\psi_c = v_\alpha \chi_{jm_j} [i^l Y_{lm}(\theta, \phi)] , \quad (1.2.2)$$

where v_α characterizes the internal state of particles α , and χ is the spin function. These functions are orthogonal over their own variables and normalized.

The coefficients of incoming waves A_c for “entrance” (in our case the neutron) channels are $(i/k)\sqrt{\pi(2l+1)}$ in Eq. (1.1.8), and for the other ones they are zero. The coefficients B_c are expressed by A_c as

$$B_c = \sum_{c'} U_{c'c} A_{c'}, \quad (1.2.3)$$

which in general case is the definition of the collision matrix **U**. The basic properties of this matrix of being unitary and symmetric

$$\mathbf{U}\mathbf{U}^+ = \mathbf{I} \quad (\text{i.e., } \sum_{c'} |U_{c'c}|^2 = 1), \quad U_{c'c} = U_{cc'}, \quad (1.2.4)$$

follow from rather common physical principles - the balance of intensities over all reaction channels and the time invariance of the description [1-10]. The total solution in external region is

$$\Psi = \sum_c \Psi_c = \sum_{c'} A_{c'} [\delta_{c'c} I_{c'}(r_{c'}) - U_{c'c} O_{c'}(r_{c'})] r_{c'}^{-1} \psi_{c'} v_{c'}^{-1/2}. \quad (1.2.5)$$

Denoting the part corresponding to the incoming plane wave normalized to unit flux (formally Eq. (1.2.5) with $U_{c'c} = \delta_{c'c}$) by Ψ^0 and subtracting it from Ψ , we have

$$\Psi - \Psi^0 = \sum_{c'c} A_c [\delta_{c'c} - U_{c'c}] O_{c'}(r_{c'}) r_{c'}^{-1} \psi_{c'} v_{c'}^{-1/2} \quad (1.2.6)$$

This is the sum of outgoing waves in all the channels open at a given total energy of the system with amplitudes proportional to $\delta_{cc'} - U_{c'c}$.

- b) Let us consider the form of the expression in Eq. (1.2.6) for typical experimental situation, when the incoming beam of particles (neutrons) is a plane wave in direction z with given value of channel spin j , $m_j = M$ ($m = 0$), and the products of reaction are registered on the asymptote ($r_c > 0$):

$$\Psi_{jM} - \Psi_{jM}^0 = \sum_{\alpha j'm_j} F_{\alpha j'm_j, njM}(\theta, \phi) v_\alpha \chi_{j'm_j} r_\alpha^{-1} v_\alpha^{-1/2} e^{ik_\alpha r_\alpha} \quad (1.2.7)$$

The reaction amplitudes F are probabilities for transition of the system from the initial state (n, j, M) to different reaction channels with the formation of fragments pair α with given relative polarization ($\alpha, j', m_{j'}$). The expression for the amplitude taking into account the explicit form of the coefficients A_c and the conservation of the total moment (JM) and parity of the system can be written as [1-8]:

$$F_{\alpha j'm_j, njM}(\theta, \phi) = \frac{i\sqrt{\pi}}{k} \sum_{l'm'J} \left\{ \sqrt{2l+1} (l'j'm'm_{j'} | JM) \times Y_{l'm'}(\theta, \phi) (lj0M | JM) (\delta_{njl, \alpha j'l'} - U_{njl, \alpha j'l'}^{J\pi}) \right\} \quad (1.2.8)$$

where Clebsch-Gordan coefficients $(ljmm_j | JM)$ correspond to the summation of the moments $|\vec{j} + \vec{l}| = |\vec{j}' + \vec{l}'| = J$ [1,4,7,8]. It is noted that the elements of $\mathbf{U}^{J\pi}$ -matrix do not depend on the magnetic quantum number (if such a dependence exists, the intensity of reaction would change with a turn of the coordinate system).

- c) The differential cross section of the reaction $(njM) \rightarrow (\alpha j'm_{j'})$ is the ratio of the outgoing flux of particles α with given j' and $m_{j'}$ through the surface element $dS = r_\alpha^2 d\Omega$ in the direction (θ, ϕ) to the incoming flux, normalized to unity and it is equal to:

$$d\sigma_{\alpha j'm_j, njM} = |F_{\alpha j'm_j, njM}|^2 d\Omega \quad (1.2.9)$$

For non-polarized particles, differential cross section of the reaction (n, α) is found by summation of (1.2.9) over all possible values of jM and $j'm_{j'}$, taking into account that the incoming flux in this case

is the sum of incoherent components for $2(2I+1)$ relative orientations of spins of the neutron (1/2) and target nucleus (I) :

$$d\sigma_{\alpha n} = \frac{1}{2(2I+1)} \sum_{j'Mjm_j} |F_{\alpha j'm_j, njM}|^2 d\Omega \quad (1.2.10)$$

After substituting the expression for amplitude in Eq. (1.2.8), the summation of the moments can be performed. The most convenient representation of the final result is given by Blatt-Biedenharn formula [4,8]:

$$d\sigma_{\alpha n} = k^{-2} \sum_L B_L(\alpha, n) P_L(\cos \theta) d\Omega \quad (1.2.11)$$

where the coefficients of expansion B_L are independent of the angular variables and given by:

$$B_L(\alpha, n) = [8(2I+1)]^{-1} \sum \left\{ (-1)^{j-j'} Z(l_1 J_1 l_2 J_2 | jL) Z(l'_1 J'_1 l'_2 J'_2 | j'L) \right. \\ \left. \times (\delta_{\alpha j'l'_1, njl_1} - U_{\alpha j'l'_1, njl_1}^{J_1 \pi_1})^* (\delta_{\alpha j'l'_2, njl_2} - U_{\alpha j'l'_2, njl_2}^{J_2 \pi_2}) \right\} \quad (1.2.12)$$

with summation over all indexes except L . The coefficients of the vector summation $Z(l_1 J_1 l_2 J_2 | JL)$ are the corresponding combination of Clebsch-Gordan coefficients and these are tabulated and investigated in details [7,8]. We note here only one property of those coefficients

$$Z(l_1 J_1 l_2 J_2 | j0) = (2J_1 + 1)^{1/2} (-1)^{J_1 - j} \delta_{l_1 l_2} \delta_{J_1 J_2}, \quad (1.2.13)$$

which permits to obtain a simple expression for the cross section integrated over angles ($d\Omega$) determined by the coefficient $B_0(\alpha, n)$ [1-8]:

$$\sigma_{\alpha} \equiv \sigma_{\alpha n} = \pi k^{-2} \sum_{J\pi} g(J) \sum_{lj'l'j'} |U_{\alpha l'j', nlj}^{J\pi}|^2 \quad (\alpha \neq n) \quad (1.2.14)$$

where $g(J) = (2J+1)/2(2I+1)$ is the so-called spin factor. For neutron elastic scattering, we will have:

$$\sigma_n = \pi k^{-2} \sum_{J\pi} g(J) \left\{ \sum_{jl} |1 - U_{nlj, nlj}^{J\pi}|^2 + \sum_{j'l' \neq jl} |U_{nl'j', nlj}^{J\pi}|^2 \right\} \quad (1.2.15)$$

The last sum is referred to all possible neutron channels (j', l') different from (j, l) , but corresponding to the same values of the total moment and parity:

$$J = |\vec{j}' + \vec{l}'| = |\vec{j} + \vec{l}|, \quad \pi = \pi_0(-1)^l = \pi_0(-1)^{l'}$$

(π_0 is the parity of the target nucleus.) For even-even nuclei, $j = 1/2$ and only one neutron channel corresponds to the given sets of J and π . However, there exist multiple neutron channels for other nuclei. For example, for the nucleus ^{235}U with the spin and parity of the ground state of $(7/2)^-$, the following six (l, j) combinations are possible for the states of compound nucleus of 3^- : (0,3), (2,3), (2,4), (4,3), (4,4) and (6,3). However, in the region of resolved resonances, only the channels with minimal values of l are practically considered, and this is connected with the sharp decrease of penetrability factors $P_l \sim (ka)^{2l+1}$ with increasing l at $ka \approx 0.3 \times 10^{-3} A^{1/3} \sqrt{E} \ll 1$, where E is the neutron energy in eV (see Table I.1).

The total cross section is equal to the sum of cross sections for all channels, and using the unitary property of $\mathbf{U}^{J\pi}$ matrix, it can be written as

$$\sigma = 2\pi k^{-2} \sum_{J\pi} g(J) \sum_{lj} [1 - \text{Re}(U_{nlj, nlj}^{J\pi})] \quad (\text{I.2.16})$$

These are the most general kinematic relations between cross sections and collision matrix elements for unpolarized particles, which will be used further.

I.3 Resonance Collision Matrix

- a) The general approach to the theoretical description of the resonance cross sections is connected with the choice of some set of eigen-states for the system of $A+1$ interacting nucleons. The concept of a limited region of nuclear interactions or concepts of channel radii includes the assumption that the physical space for the nucleon system can be divided into two regions – the internal region, where nuclear forces act between all $A+1$ nucleons (compound nucleus), and the external region corresponding to reaction channels, for which the common solution structure in Eq. (I.2.5) is known. The idea of channel radius or the surface of channels $r_c = a_c$ dividing those two regions has a principle meaning in this concept.

The mathematical apparatus of the multichannel reaction theory is formulated for the so-called nuclear configuration space of $3(A+1)$ dimensions, where to each channel corresponds an own set of variables including the coordinates of relative motion $\vec{r}_c$, so that for the internal region $|\vec{r}_c| < a_c$ and for the external $|\vec{r}_c| > a_c$ [1-4]. The wave function of the internal region is presented as an expansion over some basic set of orthogonal states associated with the resonances of a compound nucleus. The condition for it to coincide with the first derivatives over $\vec{r}$ on the channel surface $r_c = a_c$ with the solution in the external region given by Eq. (I.2.5) ultimately determines the corresponding expansion of $\mathbf{U}$ -matrix. The successive consideration of a similar scheme for two different variants for choice of the basic set in the internal region has been given first by Kapur and Peierls [15] and Wigner [1,2,4] more

than 60 years ago and modified many times methodologically, guiding the final practical result to the same parameterization schemes for neutron resonance cross sections [4-6,16,17].

- b) Let us dwell briefly on the method of $\mathbf{U}$ -matrix construction by using the so-called boundary condition operator [16], also known as the block operator. This method is grounded in the comprehensive formalism of Lane and Robson [17] and appears to be the most well-founded one methodologically in the frame of channels radii concept.

We are considering the solution for the given value of the total angular momentum of the system J and parity π . In the external region, this solution is given by Eq. (I.2.1)

$$\Psi^{J\pi} = \sum_c \frac{1}{r_c v_c^{1/2}} [X_c I_c(r_c) - Y_c O_c(r_c)] |c\rangle, \quad (I.3.1)$$

where $|c\rangle$ are the surface functions in Eq. (1.2.2) of the corresponding channels in Dirac notation with $\langle c' | c \rangle = \delta_{c'c}$ and the coefficients X_c and Y_c are related through the collision matrix in Eq. (I.2.3)

$$Y_c = \sum_{c'} U_{c'c}^{J\pi} X_{c'}. \quad (I.3.2)$$

In the internal region, we use the expansion over some orthonormal set of eigenfunctions. Such a basic solution set can be introduced by different ways, and the Wigner method [4] is the simplest one from the methodological point of view. Let us note however that the exact Hamiltonian for the considered system of $A+1$ nucleons is not Hermitian in the bounded region $r_c < a_c$ (but only in the whole space $0 < r_c < \infty$). To have a Hermitian operator, which is necessary for the complete basis functions in the internal region, it is suggested instead of H to consider the Hamiltonian:

$$\tilde{H} = H + \mathcal{L}_w, \quad (I.3.3)$$

where

$$\mathcal{L}_w = \sum_c |c\rangle \frac{\hbar^2}{2\mu_c a_c} \delta(r_c - a_c) \left(\frac{d}{dr_c} r_c - B_c \right) \langle c| \quad (I.3.4)$$

is the operator of boundary conditions, and B_c is an arbitrary real number [16]. The operator $\tilde{H}$ in Eq. (I.3.3) is Hermitian in the region $r_c \leq a_c$, which can be proved directly (see [16,17]). For the exact equation written in the form,

$$(H + \mathcal{L}_w - E) |\Psi\rangle = \mathcal{L}_w |\Psi\rangle, \quad (I.3.5)$$

the complete eigenfunction set $|\lambda\rangle$ can be determined in the internal region by using the boundary

condition $\mathcal{L}_W |\lambda\rangle = 0$ or

$$(H - E_\lambda) |\lambda\rangle = 0 \quad \text{with} \quad \mathcal{L}_W |\lambda\rangle = 0, \quad (1.3.6)$$

where E_λ are the real eigen energies, which correspond to the Wigner basis [4].

The solution of Eq. (1.3.5) in the internal region and for an arbitrary energy E can be written formally through the reciprocal operator [16,17]:

$$|\Psi\rangle = (H + \mathcal{L}_W - E)^{-1} \mathcal{L}_W |\Psi\rangle. \quad (1.3.7)$$

By introducing the orthonormal basis

$$\sum_\lambda |\lambda\rangle \langle \lambda| = I \quad (\langle \lambda' | \lambda \rangle = \delta_{\lambda'\lambda})$$

we can present the expansion of $|\Psi\rangle$ in Eq. (1.3.7) over the states of $|\lambda\rangle$ as

$$|\Psi\rangle = \sum_\lambda |\lambda\rangle \frac{1}{E_\lambda - E} \langle \lambda | \mathcal{L}_W | \Psi \rangle. \quad (1.3.8)$$

Let us notice that in Dirac notations, the matrix elements $\langle \dots \rangle$ are determined over the whole configuration space and $(\dots)$ is related to the variables of the channel c surface function in Eq. (1.2.2).

This way, the elements $\langle c | \Psi \rangle$ and $\langle \lambda | c \rangle$ at $r_c = a_c$ are the values of radial solutions on this surface.

Now using the operator $\mathcal{L}_W$ in Eq. (1.3.4), we can find the matrix element in Eq. (1.3.8) as:

$$\langle \lambda | \mathcal{L}_W | \Psi \rangle = \sum_c u_\lambda(a_c) [a_c u'_E(a_c) - B_c u_E(a_c)] \quad (1.3.9)$$

where

$$\begin{aligned} u_E(a_c) &= \left(\frac{\hbar^2}{2\mu_c a_c} \right)^{1/2} a_c \langle c | \Psi \rangle, \\ u_\lambda(a_c) &= \left(\frac{\hbar^2}{2\mu_c a_c} \right)^{1/2} a_c \langle \lambda | c \rangle. \end{aligned} \quad (1.3.10)$$

Let us choose a certain channel c' and present the corresponding radial function $u(r_{c'})$ at $r_{c'} = a_{c'}$ as an expansion over λ by using the relation in Eq. (1.3.8):

$$u_E(a_{c'}) = \sum_c R_{c'c} [a_c u'_E(a_c) - B_c u_E(a_c)] \quad (I.3.11)$$

where

$$R_{c'c} = \sum_\lambda u_\lambda(a_{c'}) \frac{1}{E_\lambda - E} u_\lambda(a_c) = \sum_\lambda \frac{\gamma_{\lambda c'} \gamma_{\lambda c}}{E_\lambda - E} \quad (I.3.12)$$

with

$$\gamma_{\lambda c'} = u_\lambda(a_{c'}) = \left(\frac{\hbar^2}{2\mu_c a_{c'}} \right)^{1/2} a_{c'} < \lambda | c'), \quad \gamma_{\lambda c} = u_\lambda(a_c) \quad (I.3.13)$$

Let us notice that functions $|\lambda\rangle$ are normalized by the coefficient $(1/a_c)^{1/2}$, so $\gamma_{\lambda c}^2$ has the dimension of energy. By this way we have introduced **R**-matrix

$$R = \sum_\lambda (\gamma_\lambda \times \gamma_\lambda) \frac{1}{E_\lambda - E}, \quad (\gamma_\lambda \times \gamma_\lambda)_{c'c} = \gamma_{\lambda c'} \gamma_{\lambda c}, \quad (I.3.14)$$

where the parameters E_λ and $\gamma_{\lambda c}$ are real energy-independent numbers [4].

The sense of **R**-matrix is to relate the radial solutions at arbitrary energy E on the channel surface with its derivative at $r_c = a_c$ -- the values of these in the external and internal region must be the same. By using the external solution in Eq. (I.3.1) in the definition of $u_E(a_c)$ in Eq. (I.3.10), we have:

$$\begin{aligned} u_E(a_c) &= (\hbar/2)^{1/2} \rho_c^{-1/2} [X_c I_c(a_c) - Y_c O_c(a_c)] \\ u'_E(a_c) &= (\hbar/2)^{1/2} \rho_c^{-1/2} [X_c I'_c(a_c) - Y_c O'_c(a_c)] \end{aligned}$$

where $\rho_c = k_c a_c = (\mu_c v_c / \hbar) a_c$. By the substitution of these relations in Eq. (I.3.11) and using the corresponding matrix notations, we present the result in the following form:

$$\rho^{-1/2} (IX - OY) = R [a \rho^{-1/2} (I'X - O'Y) - \rho^{-1/2} B (IX - OY)],$$

or

$$[1 - R(aI' / I - B)] \rho^{-1/2} IX = [1 - R(aO' / O - B)] \rho^{-1/2} OY. \quad (I.3.15)$$

Then, introducing the collision matrix in Eq. (I.3.2) as

$$Y = UX, \quad (I.3.16)$$

we obtain the basic relation between **U** and **R** matrices [4]:

$$\begin{aligned} U &= \rho^{1/2} O^{-1} (1 - R\bar{L})^{-1} (1 - R\bar{L}^*) \rho^{-1/2} I \\ &= e^{-i\varphi} P^{1/2} (1 - R\bar{L})^{-1} (1 - R\bar{L}^*) P^{-1/2} e^{-i\varphi} \end{aligned} \quad (I.3.17)$$

where $\bar{L} = L - B$ ($\bar{L}_c = L_c - B_c$) is the diagonal matrix of logarithmic derivatives of O_c in Eq. (I.1.16), $e^{-i\varphi}$ is the diagonal matrix with the elements $\exp(-i\varphi_c) = (I_c / O_c)^{1/2}$ in Eq. (I.1.13), P is the diagonal matrix of penetrability factors $P_c = \rho_c / I_c O_c$ in Eq. (I.1.16) (Appendix I.A1).

c) The basic relation of **R**-matrix theory in Eq. (I.3.17) reflects the general symmetry and unitary properties of the collision matrix in Eq. (I.2.4); this is a consequence of the symmetry and reality of **R**-matrix. The various alternative representations of **U** follow from it too. Writing **U** in Eq. (I.3.17) in the form

$$U = e^{-i\varphi} W e^{-i\varphi}, \quad (I.3.18)$$

where

$$W = 1 + 2iP^{1/2} (1 - R\bar{L})^{-1} R P^{1/2} = 1 + 2iP^{1/2} G P^{1/2},$$

the collision matrix can be written in terms of the transformed matrix

$$G = (1 - R\bar{L})^{-1} R \quad (G = R + R\bar{L}G). \quad (I.3.19)$$

For this the **R**-matrix in Eq. (I.3.14) is presented into the form:

$$R = \gamma' (\varepsilon - E)^{-1} \gamma, \quad (I.3.20)$$

where γ ($\gamma_{\lambda c}$) is a $\lambda \times c$ rectangular matrix, γ' is the transposed matrix, and $\varepsilon - E$ is a diagonal matrix with the elements $E_\lambda - E$. Then writing G as

$$G = \gamma' A^{-1} \gamma \quad (I.3.21)$$

we will find according to the relation in Eq. (I.3.19) the matrix A^{-1} :

$$A^{-1} = (\varepsilon - E)^{-1} + (\varepsilon - E)^{-1} \gamma \bar{L} \gamma' A^{-1},$$

or

$$A = \varepsilon - E - \gamma \bar{L} \gamma', \quad (I.3.22)$$

with the rank equal to the number of terms in the sum over λ in Eq. (I.3.14) (“level matrix”). The elements of this matrix are

$$A_{\lambda\mu} = (E_\lambda - E) \delta_{\lambda\mu} - \sum_c \gamma_{\lambda c} \bar{L}_c \gamma_{\mu c} = (E_\lambda - E) \delta_{\lambda\mu} - \xi_{\lambda\mu}, \quad (I.3.23)$$

where

$$\xi_{\lambda\mu} = \sum_c \gamma_{\lambda c} (S_c - B_c) \gamma_{\mu c} + i \sum_c \gamma_{\lambda c} P_c \gamma_{\mu c} = \Delta_{\lambda\mu} + i \Gamma_{\lambda\mu} / 2. \quad (I.3.24)$$

The first term $\Delta_{\lambda\mu}$ are the elements of the “level-shift” matrix, and the second term $\Gamma_{\lambda\mu}$ corresponds to the total resonance widths:

$$\Gamma_{\lambda\mu} = \sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c}^{1/2}, \quad \Gamma_{\lambda c} = 2 P_c \gamma_{\lambda c}^2. \quad (I.3.25)$$

As a result we come to the **U**-matrix form with the level matrix:

$$W = 1 + 2i P^{1/2} \gamma' A^{-1} \gamma P^{1/2}, \quad (I.3.26)$$

or

$$W_{c'c} = \delta_{c'c} + 2i P_{c'}^{1/2} \left[\sum_{\lambda\mu} \gamma_{\lambda c'} (A^{-1})_{\lambda\mu} \gamma_{\mu c} \right] P_c^{1/2},$$

where $(A^{-1})_{\lambda\mu}$ are the elements of the matrix inverse to **A** in Eq. (I.3.22).

The relations for the collision matrix in Eq. (I.3.26) and Eq. (I.3.17) are generally identical and give a mathematically rigorous expansion for the **U**-matrix over the states of the basic set in the internal region. Traditionally, these are used for the determination of the approximate relations for the description of cross sections on the base of **R**-matrix formalism with the real and energy-independent parameters.

It is interesting to note that introducing the complete set of the states in the internal region for the exact Hamiltonian in Eq. (I.3.6) is not obligatory as it is in the theory of Wigner. It is possible to introduce the similar set for some model Hamiltonian $H_0 \neq H$ as well, but this one must correspond in the external region to the same reaction channels as the exact Hamiltonian [17].

The procedure of the expansion of **U**-matrix over a model basis is much similar to the above considered one [17,6], but the parameters here retrieve a physical interpretation corresponding to the model unlike the **R**-matrix approach, where those are rather phenomenological.

- d) Another variant of the **U**-matrix expansion, corresponding to the result of the Kapur-Peierls theory [15,4] can be obtained formally from the relation in Eq. (I.3.26) by diagonalizing the level matrix A in Eq. (I.3.22). This is a symmetric, non-degenerate matrix and it always can be reduced to the diagonal form by an orthogonal transformation [4,38].

$$T'AT = \tilde{\varepsilon} - E, \quad A^{-1} = T(\tilde{\varepsilon} - E)^{-1}T', \quad (I.3.27)$$

where T is the corresponding matrix of the orthogonal complex transformation ($TT' = 1$), and $\tilde{\varepsilon}$ is a diagonal matrix with the elements:

$$\tilde{E}_k = \sum_{\lambda} T_{\lambda k}^2 E_{\lambda} - \sum_{\lambda, \mu} T_{\lambda k} \xi_{\lambda \mu} T_{\mu k} \quad (I.3.28)$$

Substituting A^{-1} in Eq. (I.3.27) in Eq. (I.3.26) we obtain directly the result of Kapur-Peierls formalism [15,4]:

$$U_{c'c} = e^{-i\varphi_{c'}} \left\{ \delta_{c'c} + 2iP_{c'}^{1/2} \left[\sum_k \frac{\tilde{\gamma}_{kc'} \tilde{\gamma}_{kc}}{\tilde{E}_k - E} \right] P_c^{1/2} \right\} e^{-i\varphi_c}, \quad (I.3.29)$$

where

$$\tilde{\gamma}_{kc} = \sum_{\lambda} T_{k\lambda} \gamma_{\lambda c} \quad (I.3.30)$$

Although the representation of the resonance dependence in the **U**-matrix here seems more attractive than in **R**-matrix formalism in Eq. (I.3.17) and Eq. (I.3.26), the parameters $\tilde{E}_k$ and $\tilde{\gamma}_{kc}$ in Eq. (I.3.29) are complex and energy-dependent. Moreover, if the **U**-matrix in Eq. (I.3.17) is unitary for arbitrary values of parameters $\gamma_{\lambda c}$ and E_{λ} , then for the expansion in Eq. (I.3.29) the unitary condition leads to the specific relations between parameters $\tilde{E}_k$ and $\tilde{\gamma}_{kc}$ [18] (Appendix I.A3).

However the principle possibility exists for the pole representation of **U**-matrix via the variables $\sqrt{E}$ or momentum wave number k , in which the poles and residua are constants. The scheme of transition to the momentum domain in more general case is considered below (see Section I.7). Let us notice here only that the idea of pole formation via $\sqrt{E}$ (k) is in the base of so-called Humblet-Rosenfeld formalism [19] and reproduces evidently the analytical properties of the collision matrix and cross sections.

I.4 One-Level Approximation

- a) Let us consider the most common and simple approximations used in applications. First of all, this is one-level approach and it leads to the widely known Breit-Wigner formulae [1-6]. This is always evident at the energies $E \approx E_\lambda$ near the resonance maximum, where the sum in Eq. (I.3.14) may be limited to one term. The collision matrix $\mathbf{U}^{\pi}$ in Eq. (I.3.18) in one-level approximation also has only one term:

$$U_{cn}^{J\pi}(E) = e^{-i\varphi_c} \left[\delta_{cn} + i \frac{\Gamma_{\lambda c}^{1/2} \Gamma_{\lambda n}^{1/2}}{E_\lambda - E - i\Gamma_\lambda / 2} \right] e^{-i\varphi_n}, \quad (I.4.1)$$

where E_λ includes the level shift factor Δ_λ and

$$\Gamma_{\lambda c} = 2P_c \gamma_{\lambda c}^2, \quad \Gamma_\lambda = \sum_c \Gamma_{\lambda c} \quad (I.4.2)$$

are the resonance widths.

Substituting $U_{cn}^{J\pi}$ in Eq. (I.4.1) into the common cross section formula in Eq. (I.2.14) for some reaction (n, α) , we obtain:

$$\sigma_\alpha(E) = \frac{4\pi}{k^2} \sum_{J\pi} g(J) \frac{\Gamma_{\lambda n} \Gamma_{\lambda \alpha}}{4(E_\lambda - E)^2 + \Gamma_\lambda^2} = \frac{2\pi}{k^2} \sum_{J\pi} g(J) \frac{\Gamma_{\lambda n} \Gamma_{\lambda \alpha}}{\Gamma_\lambda} \operatorname{Re} \left(\frac{-i}{E_\lambda - E - i\Gamma_\lambda / 2} \right), \quad (I.4.3)$$

where

$$\Gamma_{\lambda n} = \sum_{jl} \Gamma_{\lambda n}^{jl}, \quad \Gamma_{\lambda \alpha} = \sum_{j'l'} \Gamma_{\lambda \alpha}^{j'l'} \quad (I.4.4)$$

are the neutron and (n, α) reaction widths and those are summated over all neutron and reaction $(n | \alpha)$ channels corresponding to given resonance spin value $J = |\vec{j} + \vec{l}| = |\vec{j}' + \vec{l}'|$ and parity π .

Analogously, for the total cross section in Eq. (I.2.17), we have

$$\begin{aligned} \sigma(E) &= \sigma_p + 4\pi k^{-2} \sum_{J\pi} g(J) \sum_{jl} \frac{\Gamma_{\lambda n}^{jl} [\Gamma_\lambda \cos(2\varphi_{jl}) - 2(E_\lambda - E) \sin(2\varphi_{jl})]}{4(E_\lambda - E)^2 + \Gamma_\lambda^2} \\ &= \sigma_p + 2\pi k^{-2} \sum_{J\pi} g(J) \sum_{jl} \Gamma_{\lambda n}^{jl} \operatorname{Re} \left[e^{-2\varphi_{jl}} \frac{(-i)}{E_\lambda - E - i\Gamma_\lambda / 2} \right] \end{aligned} \quad (I.4.5)$$

where

$$\sigma_p = 4\pi k^{-2} \sum_{J\pi} g(J) \sum_{jl} \sin^2 \varphi_{jl} \quad (1.4.6)$$

is the potential scattering cross section.

Although in the total cross section, the widths in neutron channels $\Gamma_{\lambda n}^{jl}$ are summed jointly with the corresponding phases φ_{jl} , in the most practical cases it is possible to keep only one channel with the minimum l value. For the even-even target nuclei with $I = 0$, only one reaction channel is possible with $j = 1/2$ and $l = J - 1/2$ or $l = J + 1/2$ depending on the resonance parity. In the case of $I \neq 0$, a few (jl) sets are possible for the given $(J\pi)$. However, for the resonances with relatively low energy, the penetration coefficients $P_n(E)$ for neutron channels decrease sharply with increasing l (in proportion to $(ka)^{2l+1}$, Table I.1), and for the given parity, l values must differ at least by 2. Thus, it is possible to consider only the channel with minimum $l = l_{\min}$ which gives the main contribution in the sum over (jl) in Eq. (1.4.4) and Eq. (1.4.5). Supposing also that the potential scattering phases do not depend on j , we can omit the summation over j in (1.4.5), using here the total neutron width $\Gamma_{\lambda n} = \sum_j \Gamma_{\lambda n}^{jl_{\min}}$. (Some resonances in light and medium nuclei with the energy of some hundreds keV are exceptions here; in such cases the channels with different (lj) must be taken into account jointly [20].)

b) We can present the one-level formulae in Eq. (1.4.3) and Eq. (1.4.5) in more compact form, useful in neutron physics applications:

$$\sigma_\alpha = \sigma_{0\lambda} \frac{\Gamma_{\lambda\alpha}}{\Gamma_\lambda} \frac{1}{1+x^2} = \sigma_{0\lambda} \frac{\Gamma_{\lambda\alpha}}{\Gamma_\lambda} \operatorname{Re} \left(\frac{-i}{x-i} \right), \quad (1.4.7)$$

$$\sigma = \sigma_p + \sigma_{0\lambda} \frac{\cos(2\varphi) - x \sin(2\varphi)}{1+x^2} = \sigma_p + \sigma_{0\lambda} \operatorname{Re} \left(e^{-2i\varphi} \frac{-i}{x-i} \right), \quad (1.4.8)$$

where $x = 2(E_\lambda - E) / \Gamma_\lambda$, $\sigma_{0\lambda} = 4\pi k^{-2} g(J) \Gamma_{\lambda n} / \Gamma_\lambda$ and φ_l is the potential scattering phase with $l = l_{\min}$.

For the relatively narrow resonances, excluding probably the lowest, the energy dependence of the parameters in these formulae in the interval of the considered resonance can be neglected. Then, for $\sigma_\alpha(x)$, we have the typical Lorentz curve symmetric on $x = 0$ ($E = E_\lambda$) with the half maximum width $\Delta x = 2\Delta E / \Gamma_\lambda$ (Fig. I.1). For the total cross section (and elastic scattering cross section), the resonance shape is in general non-symmetric because of the term proportional to x in Eq. (1.4.8), which characterizes the resonance and potential scattering interference (Fig. I.1). We can find the positions of the maximum and minimum total cross sections by analyzing the formula in Eq. (1.4.8) for extremes over

x :

$$x_{\min} = \cot \varphi, \quad x_{\max} = -\tan \varphi$$

or

$$E_{\min} = E_{\lambda} - \frac{\Gamma_{\lambda}}{2} \cot \varphi, \quad E_{\max} = E_{\lambda} + \frac{\Gamma_{\lambda}}{2} \tan \varphi \quad (1.4.9)$$

and the cross sections at these energies are

$$\sigma_{\min} = \sigma_p - \sigma_{0\lambda} \sin^2 \varphi, \quad \sigma_{\max} = \sigma_{\min} + \sigma_{0\lambda} \quad (1.4.10)$$

The least potential cross section value for $l = 0$ is equal to $4\pi k^{-2} \sin^2 \varphi_0$ and the greatest value for $\sigma_{0\lambda}$ is $4\pi k^{-2}$, so obviously $\sigma_{\min} > 0$ and only in the case of one-channel s -scattering, it can be rather close to zero. The observable deep interference minima in the total cross sections of ^{56}Fe , ^{26}Al , and ^{45}Sc can be taken as examples. Analogously, it is easy to see that $\sigma_{\max}$ does not exceed the unitary limit $4\pi k^{-2}$.

Figure I. 1 Symmetric and Anti-Symmetric Natural Line Shape Functions

The one-level formulae similar to Eq. (1.4.5) exist also for the differential cross sections and may be

obtained by the substitution of the corresponding elements of the $U_{c'c}^{J\pi}$ in the common relations in Eq. (I.2.11). These are adduced in many works [3-8] and are not given here because of unwieldy representations of them and the limited interest in the angular distribution features in resonances in the next parts. Let us notice only that the angular distributions of reaction products for single resonances are symmetric relatively to the angle $\theta = \pi/2$ (isotropic for all angles for $l = 0$), which is typical for the states with given parity. In the elastic scattering cross section, however, the asymmetry is possible because of the interference between the resonance scattering and the part of potential scattering whose parity is different [6].

- c) Traditionally, the one-level approach is a basis for the analysis of neutron cross section data in the region of experimentally resolved resonances and their parameters, E_λ , $\Gamma_{\lambda n}$, $\Gamma_{\lambda c}$ and Γ_λ , permit reproducing rather exactly the detailed energy structure of cross sections for most nuclei (maybe excepting the fissile ones) in this region, taking into account naturally the corrections of one-level formulae in respect to Doppler broadening (see Section I.5) and experimental resolution (Ch. 3). The large volume of data collected on the parameters of resolved neutron resonances (for some nuclei arrives up to hundreds of them), and the physical interpretation of the data in the frame of compound nucleus concept offer the possibility to reveal the main laws of parameter energy dependence and the character of fluctuations of those from level to level.

Let us notice first the energy dependence of neutron widths $\Gamma_{\lambda n} = 2P_l \gamma_{\lambda n}^2$, which is determined by the penetration factors P_l (Table I.1). For the s -wave resonances ($l = 0$), $\Gamma_{\lambda n} = \Gamma_{\lambda n}^0 \sqrt{E}$, where $\Gamma_{\lambda n}^0$ are so-called reduced neutron widths; for $l = 1$, $\Gamma_{\lambda n} \approx \Gamma_{\lambda n}^0 E^{3/2}$, and so on. The fluctuation in $\Gamma_{\lambda n}^0$ for different levels is rather significant, and for a large level set, it can be described satisfactorily by χ^2 distribution, named in application to the resonance widths Porter-Thomas distribution:

$$P(\zeta)d\zeta = \frac{1}{\sqrt{2\pi\zeta}} e^{-\zeta/2} d\zeta \quad (I.4.11)$$

where $\zeta = \Gamma_{\lambda n}^0 / \bar{\Gamma}_{\lambda n}^0$ and $\bar{\Gamma}_{\lambda n}^0$ is the averaged value over all analyzed levels.

The radiative widths $\Gamma_{\lambda \gamma}$ depend on the excitation energy of compound nucleus $U = E + B_n$, where B_n is the neutron binding energy (5~8 MeV), and in limited energy intervals of resolved levels it does not in practice depend on energy [5]. The fluctuations of radiative widths are non-significant and this is explained by the large number of different ways of compound nucleus decay. If these channels give nearly the same contributions in the radiative width $\Gamma_{\lambda \gamma} = \sum_{c(\gamma)} \Gamma_{\lambda c}$, their fluctuations obey the χ_ν^2 -distribution or the Porter-Thomas distribution for ν channels:

$$P_\nu(\zeta)d\zeta = \frac{\nu}{2\Gamma(\nu/2)} \left(\frac{\nu}{2} \zeta \right)^{\nu/2-1} e^{-\nu\zeta/2} d\zeta \quad (I.4.12)$$

with $\zeta = \Gamma_{\lambda\gamma} / \bar{\Gamma}_{\gamma}$. For a large ν , this distribution tends to δ -function at $\zeta = 1$ (Fig. I.2), which corresponds to $\Gamma_{\lambda\gamma} \approx \bar{\Gamma}_{\gamma}$.

Figure I. 2 Porter-Thomas Distributions for n Channels

The widths for fission and reactions producing charged particles in general depend on energy E through the corresponding penetration factors for the fission or coulomb barrier. We have noticed that the typical parameter is $B_f - E$, where B_f is the height of the barrier, and usually in the resonance analysis in relatively narrow intervals the barrier penetrations is supposed to be independent of neutron energy. It is true up to some degree for fissile nuclei resonances, observed up to 1 keV. For (n, p) and (n, α) reactions of light nuclei, the energy dependence of corresponding widths may be significant near the barrier [3,4].

The number of fission channels for different nuclei is estimated as in Eq. (I.4.12), but in the real situation the relative contributions of the channels are not the same and the $(n, \gamma f)$ -process (fission after preliminary release of γ -quanta) [21] is possible too. So, even in the frame of random number statistics, the distribution of $\Gamma_{\lambda f}$ -values may be more complicated than $P_\nu(\zeta)$ in Eq. (I.4.12) (see Chapter II).

- d) The dependence of the neutron widths of low-lying s -resonances on energy $\propto \sqrt{E}$ determines the known reaction cross section property $\sigma_\alpha(E) \propto 1/\sqrt{E}$ at $E \rightarrow 0$. This is true for most nuclei, although for quantitative estimation of neutron cross section value in this limit, it is necessary to account for not only the resonances nearest to zero, but sometimes also to include the negative

levels lying below the threshold of neutron emission. Such levels obviously exist and can be discovered experimentally in the stripping reaction (d, p) . The difference from $1/\sqrt{E}$ at low energy is observed in fissile nuclei and some non-fissile but strong neutron absorbing nuclei (Cd, Xe, Lu, etc.), where the lowest resonance is placed at $E_\lambda = 0.2 \div 0.5$ eV [22].

- e) The energy dependence of neutron widths for relatively broad resonances can deform noticeably the cross section profile, which is typical for the case of constant widths (Fig.1.1). So, even in the simplest one-level formula in Eq. (1.4.3) for the s -wave resonances, where $\Gamma_n = \Gamma_n^0 \sqrt{E}$ and the reaction width $\Gamma_\alpha = \text{const}$, the total width depends on E as $\Gamma = \Gamma_\alpha + \Gamma_n^0 \sqrt{E}$, the denominator may be presented as

$$E_\lambda - E - i(\Gamma_\alpha + \Gamma_n^0 \sqrt{E}) / 2 = (q_1 - \sqrt{E})(q_2 + \sqrt{E}), \quad (1.4.13)$$

where

$$q_{1,2} = [E_\lambda - i\Gamma_\alpha / 2 - (\Gamma_n^0 / 4)^2]^{1/2} \pm i\Gamma_n^0 / 4 = \sqrt{\varepsilon_\lambda} - i(\Gamma_\alpha \mp \Gamma_n^0 \sqrt{\varepsilon_\lambda}) / 4\sqrt{\varepsilon_\lambda} \\ (\sqrt{\varepsilon_\lambda} = \text{Re}\{[E_\lambda - i\Gamma_\alpha / 2 - (\Gamma_n^0 / 4)^2]^{1/2}\}) \quad (1.4.14)$$

are the roots of the equation. Taking into account that $k^2 = 2\mu E / \hbar^2$, we can write $\sigma_\alpha(E)$ in Eq. (1.4.3) in the form:

$$\sqrt{E}\sigma_\alpha(E) = \frac{\pi\hbar^2}{\mu} g(J)\Gamma_\alpha \text{Re} \left\{ (-i) \left[\frac{1}{(\gamma + \sqrt{E})(q_1 - \sqrt{E})(q_2 + \sqrt{E})} \right] \right\}, \quad (1.4.15)$$

where $\gamma = \Gamma_\alpha / \Gamma_n^0$. Let us present now the product of fractions in brackets as a sum:

$$\frac{1}{(q_1 + \gamma)(q_2 - \gamma)} \frac{1}{\gamma + \sqrt{E}} + \frac{1}{(q_1 + q_2)(q_1 + \gamma)} \frac{1}{q_1 - \sqrt{E}} + \frac{1}{(q_1 + q_2)(\gamma - q_2)} \frac{1}{q_2 + \sqrt{E}}. \quad (1.4.16)$$

It is easy to see that the first term here is real and the expression in Eq. (1.4.15) is the sum of the other two terms so that

$$\sqrt{E}\sigma_\alpha(E) = \text{Re} \left\{ (-i) \left[\frac{r_1^\alpha}{q_1 - \sqrt{E}} + \frac{r_2^\alpha}{(-q_2) - \sqrt{E}} \right] \right\}, \quad (1.4.17)$$

where

$$r_{1,2}^\alpha = \frac{\pi \hbar^2}{\mu} g(J) \Gamma_\alpha \frac{\Gamma_n^0}{\Gamma_n^0 q_{1,2} \pm \Gamma_\alpha} \frac{1}{q_1 + q_2} \quad (1.4.18)$$

and the sum $\gamma_1^\alpha + \gamma_2^\alpha$ is real. We obtain as a result the pole representation for $\sqrt{E}\sigma_\alpha(E)$ over the variable $\sqrt{E}$ (or k), where the poles q_1 , q_2 and the residua are the complex constants. The pole q_1 is associated, as a rule, with the resonance at $\sqrt{E} = \text{Re}(q_1) = \sqrt{\varepsilon_\lambda}$, and the pole $(-q_2)$ lying outside of the physical region ($\sqrt{E} > 0$) determines the background dependent smoothly on energy in the region of the resonance.

The expression for the cross section in Eq. (1.4.17) can be written also in the form:

$$\sqrt{E}\sigma_\alpha(E) = \text{Re} \left\{ (-i) \left[\frac{2q_1 r_1^\alpha}{q_1^2 - E} + \frac{r_1^\alpha}{(-q_1) - \sqrt{E}} + \frac{r_2^\alpha}{(-q_2) - \sqrt{E}} \right] \right\}, \quad (1.4.19)$$

where the first term corresponds to the traditional Breit-Wigner representation with energy-independent pole plus the smooth background. Let us notice that in the limit $\Gamma_\alpha \gg \Gamma_n^0 \sqrt{\varepsilon_\lambda}$, $q_1 \approx q_2$ and $r_1^\alpha \approx -r_2^\alpha$, and for $\Gamma_\alpha \ll \Gamma_n^0 \sqrt{\varepsilon_\lambda}$, $q_1 \approx q_2^*$ and $r_1^\alpha \approx r_2^\alpha$, so that the sum of the last two term in Eq. (1.4.19) is real and there is no more background. A similar representation can be obtained for the total cross section in Eq. (1.4.5) and also in the case of $l > 0$, where the number of background poles becomes larger (see Section 1.7).

1.5 Doppler Broadening of Resonances

- a) Accounting for thermal motion of nuclei of the media - resonance Doppler broadening - is very important in practical applications of resonance formulae. This is a rather difficult problem in general and it is connected with the analysis of atom energy bonds in molecules and crystals. However, in most cases, maybe with exception of the first resonance in fissile nuclei ($E_\lambda = 0.3 \sim 0.4$ eV), it can be approximated using the Maxwellian distribution of atom velocities ($\vec{u}$) for the gas:

$$P(\vec{u})d\vec{u} = \left(\frac{M}{2\pi kT} \right)^{3/2} \exp \left(-\frac{M}{2kT} u^2 \right) d\vec{u}, \quad (1.5.1)$$

where $k = 0.861 \times 10^{-4}$ eV/K is Boltzmann constant and T is temperature in $^\circ K$. The effective cross section at a given energy of relative motion E in the center of mass system (velocity v) with account of the thermal motion of atoms of the media in general is determined by the relation for a reaction rate

$$v\sigma_a(v, T) = \int |\vec{v} - \vec{u}| \sigma_a(|\vec{v} - \vec{u}|) P(\vec{u}) d\vec{u}, \quad (1.5.2)$$

where $\vec{v} - \vec{u}$ is the velocity of relative motion, and for the Maxwellian distribution in Eq. (I.5.1) we will have (Appendix I.A2):

$$\sqrt{E}\sigma_\alpha(E, T) = \int \sqrt{E'}\sigma_\alpha(E')S(E', E)dE', \quad (I.5.3)$$

where

$$S(E', E)dE' = \frac{1}{2\sqrt{\pi E}\delta} \left\{ \exp\left[-\frac{(\sqrt{E} - \sqrt{E'})^2}{\delta^2}\right] - \exp\left[-\frac{(\sqrt{E} + \sqrt{E'})^2}{\delta^2}\right] \right\} dE' \quad (I.5.4)$$

and $\delta = \sqrt{kT / (A+1)}$.

$S(E', E)$ is known as Solbrig's kernel [23]; its derivation is presented in Appendix I.A2.

b) The distribution function $S(E', E)$ is exact in the frame of "gas model," but practically in the resonance region the last term in Eq. (I.5.4) can be neglected for $\delta \leq 0.1$ eV. Usually the Gauss distribution is used

$$\tilde{S}(E', E)dE' = \frac{1}{\sqrt{\pi}\Delta} \exp\left[-\frac{(E - E')^2}{\Delta^2}\right] dE', \quad (I.5.5)$$

where $\Delta = 2\sqrt{E}\delta = 2\sqrt{kTE / (A+1)}$ is Doppler width and $-\infty < E - E' < \infty$. This follows from Eq. (I.5.4) at $E' \approx E$ ($\sqrt{E'} \approx \sqrt{E}[1 - (E - E') / 2E]$) and is practically suitable in the narrow interval of single resonance, where in averaging the energy dependence of kinematic factor and resonance parameters may be neglected in the one-level formulae in Eq. (I.4.3) and Eq. (I.4.5). Using the variable $x = 2(E_\lambda - E) / \Gamma_\lambda$, the Gauss distribution will take the form:

$$\tilde{S}(x', x)dx' = \frac{\xi}{\sqrt{\pi}} \exp[-\xi^2(x - x')^2] dx', \quad -\infty < x < \infty, \quad (I.5.6)$$

where $\xi = \Gamma / 2\Delta$ and the corresponding averaging of Eq. (I.4.7) and Eq. (I.4.8) leads directly to the expressions for Doppler broadened resonance cross sections:

$$\sigma_\alpha(x, \xi_\lambda) = \sigma_{0\lambda} \frac{\Gamma_{\lambda\alpha}}{\Gamma_\lambda} \Psi(x, \xi_\lambda), \quad (I.5.7)$$

and

$$\sigma(x, \xi_\lambda) = \sigma_p + \sigma_{0\lambda} [\cos(2\varphi)\Psi(x, \xi_\lambda) + \sin(2\varphi)X(x, \xi_\lambda)], \quad (I.5.8)$$

where

$$\Psi(x, \xi) = \frac{\xi}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp[-\xi^2(x-x')^2]}{1+x'^2} dx' , \quad (1.5.9)$$

and

$$X(x, \xi) = \frac{\xi}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{x' \exp[-\xi^2(x-x')^2]}{1+x'^2} dx' , \quad (1.5.10)$$

are so-called Doppler functions, or Voigt profiles (Fig. 1.3).

Figure 1.3 Symmetric and Anti-Symmetric Doppler-Broadened Line Shape Functions

The functions Ψ and X are the real and imaginary parts of the complex probability function $W(z)$, known as the Faddeeva function [24]:

$$W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2} dt}{z-t} = e^{-z^2} \operatorname{erfc}(-iz), \quad (\operatorname{Im} z \geq 0) \quad (1.5.11)$$

so that

$$\begin{aligned}\Psi(x, \xi) &= \sqrt{\pi} \xi \operatorname{Re}[W(\xi x + i\xi)] \\ X(x, \xi) &= \sqrt{\pi} \xi \operatorname{Im}[W(\xi x + i\xi)]\end{aligned}\quad (1.5.12)$$

The functions Ψ and X are tabulated functions some of whose mathematical properties we discuss here to illustrate the basic properties of Doppler broadening:

1. The total area under the resonance curve remains the same at temperature deformation of resonances (Fig. 1.3):

$$\int_{-\infty}^{\infty} \Psi(x, \xi) d\xi = \pi, \quad \int_{-\infty}^{\infty} X(x, \xi) d\xi = 0 \quad (1.5.13)$$

Moreover, we have the Parseval theorem [26]

$$\int_{-\infty}^{\infty} \Psi^2(x, \xi) d\xi = \int_{-\infty}^{\infty} X^2(x, \xi) d\xi = \frac{\pi}{2} \Psi(0, \sqrt{2}\xi) = \frac{\pi}{2} \sqrt{2\pi} \xi \exp(2\xi^2) \operatorname{erfc}(\sqrt{2}\xi) \quad (1.5.14)$$

and the asymmetry condition

$$\int_{-\infty}^{\infty} \Psi(x, \xi) X(x, \xi) d\xi = 0 \quad (1.5.15)$$

2. The asymptotic dependence for $\xi > 1$ ($\Gamma > 2\Delta$) can be found by expansion of the integrand in Eq. (1.5.9) and Eq. (1.5.10) in series at $x' \approx x$:

$$\begin{aligned}\Psi(x, \xi) &= \frac{1}{1+x^2} \left[1 + \frac{1}{2\xi^2} \frac{3x^2-1}{(1+x^2)^2} + \dots \right] \\ X(x, \xi) &= \frac{x}{1+x^2} \left[1 + \frac{1}{2\xi^2} \frac{x^2-3}{(1+x^2)^2} + \dots \right],\end{aligned}\quad (1.5.16)$$

and for $\xi > 3$ the Doppler broadening is not practically significant. It can be seen also from the expansion in Eq. (1.5.16) that on the wings of resonances at $x\xi > 5 \sim 10$, the Doppler functions coincide asymptotically with the originals $1/(1+x^2)$ and $x/(1+x^2)$.

3. By the Fourier transform method, the probability integral from complex argument $z = \xi x + i\xi$ in Eq. (1.5.11) may be reduced to the form [13,25]:

$$\xi \sqrt{\pi} W(z) = \int_0^{\infty} \exp\left[-(u/2\xi)^2 - u + i x u\right] du \quad (1.5.17)$$

and correspondingly:

$$\begin{aligned}\Psi(x, \xi) &= \int_0^\infty \exp\left[-(u/2\xi)^2 - u\right] \cos(xu) du \\ X(x, \xi) &= \int_0^\infty \exp\left[-(u/2\xi)^2 - u\right] \sin(xu) du\end{aligned}\quad (1.5.18)$$

The asymptotic relations for Doppler functions Ψ and X for $\xi \gg 1$ ($\Delta \ll \Gamma/2$) follow from here. In this case only one term $(u/2\xi)^2$ remains in the exponent and the integrals in Eq. (1.5.18) can be found as

$$\begin{aligned}\Psi(x, \xi) &\approx \sqrt{\pi} \xi \exp(-\xi^2 x^2) \\ X(x, \xi) &\approx 2\xi \exp(-\xi^2 x^2) \int_0^{\xi x} e^{t^2} dt = 2\xi D(\xi x)\end{aligned}\quad (1.5.19)$$

where $D(\xi x)$ is the Dawson integral, which is an asymmetric function with the maximum value $D(0.924) = 0.541$ [13].

4. The derivatives of the functions Ψ and X are:

$$\frac{\partial \Psi}{\partial x} = 2\xi^2 (X - x\Psi), \quad \frac{\partial X}{\partial x} = 2\xi^2 (1 - \Psi - xX), \quad (1.5.20)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -(2\xi^2)^2 \frac{\partial \Psi}{\partial (\xi^2)} = (2\xi^2)^2 \left[1 - \Psi \left(1 - x^2 + \frac{1}{2} \xi^2 \right) - 2xX \right], \quad (1.5.21)$$

$$\frac{\partial^2 X}{\partial x^2} = -(2\xi^2)^2 \frac{\partial X}{\partial (\xi^2)} = -(2\xi^2)^2 \left[X(1 - 2\Psi) + X \left(1 - x^2 + \frac{1}{2} \xi^2 \right) \right]. \quad (1.5.22)$$

Note that the derivatives on ξ^2 are practically the derivatives on the temperature ($\Delta^2 \propto T$):

$$-(2\xi^2)^2 \frac{\partial \Psi}{\partial (\xi^2)} = \Gamma^2 \frac{\partial \Psi}{\partial (\Delta^2)}, \quad (1.5.23)$$

which is of interest for the resonance self-shielding problem.

c) The use of the exact kernel (distribution function) $S(E', E)$ in Eq. (1.5.4) for analyzing the Doppler broadening of the lowest resonance in fissile nuclei ($E_0 \approx 0.3$ eV) also leads finally to the results, which may be presented by the $W(z)$ function with corresponding arguments. In fact, if in

estimating the Doppler broadening of the resonance E_0 the energy dependences of kinematic factor ($k^2 \propto E$) and $\Gamma_n = \Gamma_n^0 \sqrt{E}$ in the numerator of Eq. (I.4.3) are accounted for, but at the same time if it is proposed that $\Gamma = \text{const}$ ($\Gamma_\alpha \gg \Gamma_n$), the result of averaging by the common scheme in Eq. (I.5.3) may be found as [26,27]:

$$\begin{aligned} E\sigma_\alpha(E, T) &= \sigma_0(E_0) \frac{\Gamma_\alpha \sqrt{E_0}}{2\delta} \text{Re} \left\{ \frac{i}{\sqrt{\pi}} \int_0^\infty dq \frac{q}{d^2 - q^2} \left[e^{-(p-q)^2} - e^{-(p+q)^2} \right] \right\} \\ &= \sigma_0(E_0) \frac{\Gamma_\alpha \sqrt{E_0}}{4\delta} \sqrt{\pi} \text{Re}[W(d-p) - W(d+p)] \end{aligned} \quad (I.5.24)$$

where $p = \sqrt{E}/\delta$, $q = \sqrt{E'}/\delta$, and

$$d = \sqrt{E_0 + i\Gamma/2}/\delta = (\sqrt{E'_0} + i\Gamma/4\sqrt{E'_0})/\delta, \quad \sqrt{E'_0} = \text{Re} \sqrt{E_0 + i\Gamma/2}. \quad (I.5.25)$$

Note that we have chosen here the complex conjugate representation of the formula in Eq. (I.4.3). With notations $\Delta = 2\delta\sqrt{E'_0}$ and $\xi = \Gamma/2\Delta$, we obtain

$$\begin{aligned} E\sigma_\alpha(E, T) &= \sigma_0(E_0) \sqrt{E_0 E'_0} \frac{\Gamma_\alpha}{\Gamma} \\ &\quad \times \left\{ \Psi \left[\frac{4}{\Gamma} \sqrt{E'_0} (\sqrt{E'_0} - \sqrt{E}), \xi \right] - \Psi \left[\frac{4}{\Gamma} \sqrt{E'_0} (\sqrt{E'_0} + \sqrt{E}), \xi \right] \right\} \end{aligned} \quad (I.5.26)$$

For $E_0 \gg \Gamma$, $E'_0 \cong E_0$, and thus, by neglecting the second term in Eq. (I.5.26) and expanding $\sqrt{E}$ around E_0 ($\sqrt{E} = \sqrt{E_0} [1 - (E_0 - E)/2E_0]$), we come to the formula in Eq. (I.5.7). The expansion $W(d-p) - W(d+p) = -2W'(d)p \propto \sqrt{E}$ corresponds to the limit $E \rightarrow 0$ and this finally provides the dependence $\sigma_\alpha(E, T) \propto 1/\sqrt{E}$.

The more rigorous account of the energy dependence of total width $\Gamma = \Gamma_\alpha + \Gamma_n^0 \sqrt{E}$ in analyzing Doppler broadening of resonance leads finally to the averaging by the common scheme in Eq. (I.5.3) of the reaction cross section in the momentum ($\sqrt{E}$) representation in Eq. (I.4.17). Determining the resonance shape requires integrals like

$$\frac{i}{\delta\sqrt{\pi}} \int_0^\infty dq \frac{1}{d-q} \left[e^{-(p-q)^2} - e^{-(p+q)^2} \right] = \frac{\sqrt{\pi}}{\delta} [W(d-p) - c], \quad (I.5.27)$$

where

$$c = \frac{2id}{\pi} \int_0^\infty dq \frac{1}{d^2 - q^2} e^{-(p+q)^2} \quad (1.5.28)$$

is the correction term which is practically not significant for $p \ll 1$ ($E \ll kT / (A+1)$). An effective scheme for calculating c is elaborated also for the case $p \leq 1$ [27] (Appendix I.A2). Therefore, the account of Doppler broadening of Eq. (1.4.17) leads to the result close to (1.5.24):

$$E\sigma_\alpha(E, T) = (\sqrt{\pi} / \delta) [r_1^\alpha W(d_1 - p) - r_2^\alpha W(d_2 + p) - \Delta c] \quad (1.5.29)$$

where $d_1 = q_1 / \delta$, $d_2 = q_2 / \delta$, and Δc is the difference of correction terms. The passage to the ordinary formulae like Eq. (1.5.7) for $E_0 \gg \Gamma$ and to the limit $E \rightarrow 0$ is analogous to the previous case in Eq. (1.5.26).

- d) The variants for accounting the Doppler broadening of single resonances considered can be transferred in the most multilevel approaches (see Section I.7). It ought to be noted once more, however, that the Maxwellian distribution in Eq. (1.5.1) is a rather significant approximation from the point of view of condensed matter physics. The simplest crystal model of Debye takes into account the difference in the eigen-oscillation frequency of the atoms in lattice. The rigorous consideration of Doppler broadening of resonance in the frame of this model is performed in some works [28,29] where the results are compared with the gas approximation. The common approach is to use an effective temperature T_{eff} in the Maxwellian distribution instead of the thermodynamic temperature. Usually this temperature is estimated as:

$$T_{eff} = \frac{3}{2} T_D \int_0^1 x^3 \coth(xT_D / 2T) dx \quad (1.5.30)$$

where T_D is the Debye temperature ($T_D = 520K$ for uranium oxide and $T_D = 160K$ for uranium metal [30]).

- e) The detailed consideration of resonance deformation at Doppler broadening is necessary for both data analysis in neutron spectroscopy in the region of experimentally resolved levels and for reactor applications with respect to nuclear temperature effects in this region. However, at relatively wide resolution or in studying the averaged functionals over resonance cross section used in reactor physics, it is possible sometimes to limit oneself to approximate variants of Doppler line shape. The simplest way is the substitution for Gauss distribution in Eq. (1.5.5) in averaging one-level formulae in Eq. (1.4.7) and Eq. (1.4.8) by a suitable Cauchy distribution:

$$\tilde{S}(x, x') dx' = \frac{\delta}{\pi} \frac{dx'}{(x - x')^2 + \delta^2} \quad (-\infty < x' < \infty) \quad (1.5.31)$$

Then the corresponding Doppler functions in Eq. (1.5.9) and Eq. (1.5.10) are expressed as

$$\tilde{\Psi}(x, \delta) = \frac{1 + \delta}{x^2 + (1 + \delta)^2}, \quad \tilde{X}(x, \delta) = \frac{x}{x^2 + (1 + \delta)^2}, \quad (1.5.32)$$

which keeps the Breit-Wigner resonance shape in Eq. (1.4.3) and Eq. (1.4.5) with the modified, temperature-dependent total width in the denominator [$\Gamma \rightarrow \Gamma(1 + \delta)$]. The parameter δ can be found, for example, by comparing the integrals of the square of Doppler functions in Eq. (1.5.14), which gives

$$(1 + \delta)^{-1} = \Psi(0, \sqrt{2}\xi). \quad (1.5.33)$$

The solution of this transcendental equation is approximated well by the relation [31]:

$$\delta^{-1} = 2.5\xi[\sqrt{1 + 0.76\xi^2} + 0.87\xi]. \quad (1.5.34)$$

It is obvious that similar approximations for Doppler functions can be effective only in the case of relatively broad resonances with $\xi_\lambda \geq 1$ for structural material or fissile nuclei, for example. In the problem of resonance self-shielding, other variants of δ which give better agreement in data interpolation are also possible (see Chapter 4).

1.6 Resonance Interference

- a) The representation of resonance cross section as a sum of single Breit-Wigner terms in Eq. (1.5.7) and Eq. (1.5.8) is rather effective for many nuclei at energies where the distance between levels exceeds significantly their total width ($D \gg \Gamma_\lambda$). Therefore, for ^{238}U and ^{232}Th , all experimentally observed peculiarities of cross sections can be reproduced with good precision up to energy about 4 keV by the one-level resonance parameters (Fig. 1.4). However, for fissile nuclei, where $\Gamma_\lambda \approx D$ for lowest resonances, and many other nuclei of reactor materials, the one-level approach often turns out to be insufficient for the interpretation of the observed energy dependence of cross sections, particularly in the region between resonances (Fig. 1.5 and Fig. 1.6).

Figure I. 4 Total Cross Section of ^{238}U at 300K

Figure I. 5 Total Cross Section of ^{235}U at 300K

Figure I. 6 Total Cross Section of ^{239}Pu at 300K

Let us illustrate the effects of mutual influence (interference) of resonances by taking an example of the one-channel scattering of s -neutrons on even-even nuclei ($I = 0$). In such a case, the cross section is determined by the collision function in Eq. (I.3.17), which we write here in the form:

$$U = e^{-2i\varphi} \frac{1+iK}{1-iK} \quad (\text{I.6.1})$$

where $K = (1/2) \sum_{\lambda} \Gamma_{\lambda} / (E_{\lambda} - E)$. Then the cross section can be presented as

$$\frac{\sigma}{4\pi k^{-2}} = \frac{1}{2}(1 - \text{Re}U) = \sin^2 \varphi + \frac{K^2 \cos(2\varphi) - K \sin(2\varphi)}{1 + K^2} = \frac{(K \cos \varphi - \sin \varphi)^2}{1 + K^2} \quad (\text{I.6.2})$$

which reduces to Eq. (I.4.8) in one-level case with $K^{-1} = 2(E_{\lambda} - E) / \Gamma_{\lambda} = x$. However for two levels, where $2K = \Gamma_1 / (E_1 - E) + \Gamma_2 / (E_2 - E)$, the energy dependence of cross section in Eq. (I.6.2) becomes more complicated than the sum of two one-level formulae and depends on the relation between parameters $E_2 - E_1$, Γ_1 , Γ_2 , and φ (Fig. I.7). Let us note here that the interference minima (in our case up to zero) are kept at the levels that cannot be obtained by direct addition of two resonances of Eq. (I.4.8).

The following values correspond to the extremes of the cross section in Eq. (I.6.2):

$$K_{\max} = -\cot \varphi, \quad K_{\min} = \tan \varphi \quad (\text{I.6.3})$$

These values determine the positions of cross section minima and maxima on the energy E . In the case of two resonances we will have

$$E_{2\max} - E_{1\max} = \sqrt{[D - \tan \varphi(\Gamma_1 + \Gamma_2)/2]^2 + 2\Gamma_2 D \tan \varphi}, \quad (\text{I.6.4})$$

where $D = E_2 - E_1$. It is seen that as $D \rightarrow 0$ this difference tends to $\tan \varphi(\Gamma_1 + \Gamma_2)/2$, which illustrates the level “repulsion” effect due to the interference. The example of two interacting resonances in one-channel scattering gives equal cross section values in the minimum and maximum, changing only their positions. For close levels the width of interference gap between them ties so that in cross section measurement the both levels can be identified as one resonance. The existence of similar minima, however, can be discovered in the experiments of neutron transmission trough relatively thick target $[\exp(-n\sigma)]$ (see Chapter 3).

Figure I. 7 Illustration of Interference Effect of Two Interacting Resonances

- b) In the multichannel case, the interference effects are observed also in various reaction cross sections, and those lead to specific forms of energy dependence of cross sections, e.g. in fissile nuclei (Fig. I.5 and Fig. I.6). So, for two interacting resonances with equal J and π , the level matrix

$\mathbf{A}^{-1}$ in common expression for $\mathbf{U}$ -matrix in Eq. (I.3.26) is

$$A^{-1} = D^{-1} \begin{bmatrix} E_2 - E - \frac{i}{2}\Gamma_2 & i\frac{\Gamma_{12}}{2} \\ \frac{i}{2}\Gamma_{12} & E_1 - E - \frac{i}{2}\Gamma_1 \end{bmatrix}, \quad (I.6.5)$$

where $D = (E_1 - E - i\Gamma_1/2)(E_2 - E - i\Gamma_2/2) + \Gamma_{12}^2/4$ is the determinant of matrix A and $\Gamma_{12} = \sum_c \Gamma_{1c}^{1/2} \Gamma_{2c}^{1/2}$. (We included here the phase shift factors $\Delta_{1,2}$ in $E_{1,2}$.)

The corresponding $\mathbf{U}$ -matrix elements may be written as in [4]:

$$U_{cn} = e^{-i\varphi_c} \left(\delta_{cn} + i \frac{N_{cn} - iM_{cn}}{P - iQ} \right) e^{-i\varphi_n}, \quad (I.6.6)$$

where

$$\begin{aligned} N_{cn} &= \Gamma_{1c}^{1/2} \Gamma_{1n}^{1/2} (E_2 - E) + \Gamma_{2c}^{1/2} \Gamma_{2n}^{1/2} (E_1 - E), \\ M_{cn} &= \frac{1}{2} \sum_{c'} (\Gamma_{1c}^{1/2} \Gamma_{2c'}^{1/2} - \Gamma_{2c}^{1/2} \Gamma_{1c'}^{1/2}) (\Gamma_{1n}^{1/2} \Gamma_{2c'}^{1/2} - \Gamma_{2n}^{1/2} \Gamma_{1c'}^{1/2}), \\ P &= (E_1 - E)(E_2 - E) + (\Gamma_{12}^2 - \Gamma_1 \Gamma_2) / 4, \\ 2Q &= (E_1 - E)\Gamma_2 + (E_2 - E)\Gamma_1. \end{aligned}$$

Then the cross section of a reaction (n, x) with some number of channels $c(x)$ and one entrance channel n becomes

$$\sigma_x = \frac{\pi}{k^2} g(J) \sum_c (N_{cn}^2 + M_{cn}^2) / (P^2 + Q^2) \quad (I.6.7)$$

and the total cross section becomes

$$\sigma = \sigma_p + \frac{2\pi}{k^2} g(J) \frac{(N_{nn}Q - M_{nn}P) \cos(2\varphi_n) - (N_{nn}P + M_{nn}Q) \sin(2\varphi_n)}{P^2 + Q^2} \quad (I.6.8)$$

In the case of only two channels of c and n , $M_{cn} = 0$ and the reaction cross section in Eq. (I.6.7) may

turn to zero at the energy where $N_{cn} = 0$. However, in reality, there is always a multichannel radiative capture process and $M_{cn}^2 > 0$.

If the energy dependence of neutron widths in the denominator can be neglected, the cross section shape near the pair of resonances considered is described by the ratio of second degree polynomial to the polynomial of forth degree of E in Eq. (I.6.7) and correspondingly by the ratio of polynomials of 3rd and 4th degree for the total cross section in Eq. (I.6.8). In such a case the parameters are the coefficients of E^n , which are known combinations of the usual resonance parameters of the levels considered. Such structure of cross section expressions permits to present them as a sum of two Breit-Wigner terms (with a second order polynomial in the denominator). This procedure consists obviously of finding the roots of the equation $P - iQ = 0$ and the following expansion of resonance term on simple fractions (see Section I.8).

- c) Let us consider these transformations to the Kapur-Peierls formalism in Eq. (I.3.29) in the scheme of diagonalization of level matrix $\mathbf{A}$, which permits to determine clearly a number of rules for the parameters of similar expansion. For two levels, the matrix of orthogonal transformation is the rotation matrix

$$T = \begin{bmatrix} \cos \psi & \sin \psi \\ -\sin \psi & \cos \psi \end{bmatrix}, \quad (I.6.9)$$

which diagonalizes the level matrix $\mathbf{A}^{-1}$ in Eq. (I.6.5)

$$TA^{-1}T' = (\tilde{\epsilon} - E)^{-1}, \quad (I.6.10)$$

where the elements of diagonal matrix $\tilde{\epsilon}$ are the roots of the equation $D = P - iQ = 0$:

$$2\tilde{E}_{1,2} = E_1 + E_2 - \frac{i}{2}(\Gamma_1 + \Gamma_2) \pm \sqrt{(E_2 - i\Gamma_2/2 - E_1 + i\Gamma_1/2)^2 - \Gamma_{12}^2} \quad (I.6.11)$$

and

$$\sin(2\psi) = \frac{i\Gamma_{12}}{\sqrt{(E_2 - i\Gamma_2/2 - E_1 + i\Gamma_1/2)^2 - \Gamma_{12}^2}}. \quad (I.6.12)$$

The expression for the U_{cn} elements, corresponding to the diagonal level matrix or to the “ $\mathbf{U}$ -matrix formalism” in our case of two resonances is

$$U_{cn} = e^{-i\varphi_c} \left(\delta_{cn} + i \frac{\tilde{\Gamma}_{1c}^{1/2} \tilde{\Gamma}_{1n}^{1/2}}{\mu_1 - E - i\nu_1} + i \frac{\tilde{\Gamma}_{2c}^{1/2} \tilde{\Gamma}_{2n}^{1/2}}{\mu_2 - E - i\nu_2} \right) e^{-i\varphi_n}, \quad (I.6.13)$$

where

$$\begin{aligned}\mu_1 - i\nu_1 &= \tilde{E}_1, \quad \mu_2 - i\nu_2 = \tilde{E}_2, \\ \tilde{\Gamma}_{kc}^{1/2} &= \Gamma_{1c}^{1/2} T_{1k} + \Gamma_{2c}^{1/2} T_{2k} \quad (k=1,2).\end{aligned}\tag{I.6.14}$$

These parameters, as it is easy to be convinced, satisfy the summation rules

$$\mu_1 + \mu_2 = E_1 + E_2, \quad \nu_1 + \nu_2 = (\Gamma_1 + \Gamma_2) / 2,$$

$$\tilde{\Gamma}_{1c}^{1/2} \tilde{\Gamma}_{1n}^{1/2} + \tilde{\Gamma}_{2c}^{1/2} \tilde{\Gamma}_{2n}^{1/2} = \Gamma_{1c}^{1/2} \Gamma_{1n}^{1/2} + \Gamma_{2c}^{1/2} \Gamma_{2n}^{1/2},$$

$$\text{Im}(\tilde{\Gamma}_{1c}^{1/2} \tilde{\Gamma}_{1n}^{1/2} + \tilde{\Gamma}_{2c}^{1/2} \tilde{\Gamma}_{2n}^{1/2}) = 0,$$

which provides the equivalence of the **U**-matrix in Eq. (I.6.13) and the **R**-matrix representation. Let us notice that similar summation rules have a place also in the case of multilevel interference (see Section I.8).

The total cross section in Eq. (I.2.16) can be expressed as a sum of one level terms:

$$\begin{aligned}\sigma &= \sigma_p + \frac{2\pi}{k^2} g(J) \text{Re} \left[-ie^{-2i\varphi} \left(\frac{\tilde{\Gamma}_{1n}}{\mu_1 - E - i\nu_1} + \frac{\tilde{\Gamma}_{2n}}{\mu_2 - E - i\nu_2} \right) \right] \\ &= \sigma_p + \frac{\pi g(J)}{k^2} \sum_{\lambda=1,2} \frac{\nu_\lambda [g_\lambda \cos(2\varphi) + h_\lambda \sin(2\varphi)] + (\mu_\lambda - E)[h_\lambda \cos(2\varphi) - g_\lambda \sin(2\varphi)]}{(\mu_\lambda - E)^2 + \nu_\lambda^2}\end{aligned}\tag{I.6.15}$$

where

$$g_1 + ih_1 = 2\tilde{\Gamma}_{1n}, \quad g_2 + ih_2 = 2\tilde{\Gamma}_{2n},\tag{I.6.16}$$

$$g_1 + g_2 = 2(\Gamma_{1n} + \Gamma_{2n}), \quad h_1 + h_2 = 0.\tag{I.6.17}$$

The (n, c) reaction cross section in **U**-matrix representation in Eq. (I.6.13) is brought to the similar form [18]:

$$\begin{aligned}\sigma_c &= \frac{\pi}{k^2} g(J) \left[\frac{g_1^c \nu_1 + h_1^c (\mu_1 - E)}{(\mu_1 - E)^2 + \nu_1^2} + \frac{g_2^c \nu_2 + h_2^c (\mu_2 - E)}{(\mu_2 - E)^2 + \nu_2^2} \right] \\ &= \frac{\pi}{k^2} g(J) \text{Re} \left[-i \left(\frac{g_1^c + ih_1^c}{\mu_1 - E - i\nu_1} + \frac{g_2^c + ih_2^c}{\mu_2 - E - i\nu_2} \right) \right]\end{aligned}\tag{I.6.18}$$

where

$$h_1^c = 2 \frac{(\nu_1 + \nu_2) \xi_{12}^c + (\mu_2 - \mu_1) \xi_{12}^c}{(\mu_2 - \mu_1)^2 + (\nu_1 + \nu_2)^2} = -h_2^c,$$

$$g_1^c - \xi_{11}^c / \nu_1 = g_2^c - \xi_{22}^c / \nu_2 = 2 \frac{(\nu_1 + \nu_2) \xi_{12}^c - (\mu_2 - \mu_1) \xi_{12}^c}{(\mu_2 - \mu_1)^2 + (\nu_1 + \nu_2)^2}, \quad (I.6.19)$$

$$\xi_{11}^c = |\tilde{\Gamma}_{1c} \parallel \tilde{\Gamma}_{1n}|, \quad \xi_{22}^c = |\tilde{\Gamma}_{2c} \parallel \tilde{\Gamma}_{2n}|, \quad \xi_{12}^c + i \zeta_{12}^c = \tilde{\Gamma}_{1c}^{1/2} \tilde{\Gamma}_{1n}^{1/2} \tilde{\Gamma}_{2c}^{*1/2} \tilde{\Gamma}_{2n}^{*1/2}. \quad (I.6.20)$$

Both variants of cross section representation in **R**-matrix formalism in Eq. (I.6.7) and Eq. (I.6.8) and in **U**-matrix formalism in Eq. (I.6.15) and Eq. (I.6.18) are mathematically identical. For practical analysis near a closely-placed pair of interfering resonances, however, the **U**-matrix representation appears to be clearer so that the resonance energy dependence is described by the sum of two Breit-Wigner terms, and Doppler broadening is taken into account by linear combination of the functions Ψ and X . The parameters g , μ , and ν are determined to first approximation by the shape of resonance line near the maximum or by the area under the resonances. The interference parameter h characterizes the cross section value between resonances and the degree of asymmetry of those on the half-maximum width. For example, as in the case of two interfering resonances $h_1^c = -h_2^c$, if $h_1^c < 0$, the cross section between resonances will be smaller than that without interference $h_1^c = 0$ (destructive interference), and an increase of cross section is observed for $h_1^c > 0$ (constructive interference) (Fig. I.8).

Figure I. 8 Illustrative Example of Constructive and Destructive Interferences

- d) The case of weak interference corresponds to the small ψ approximation of Eq. (I.6.10). In this case, $\mu_1 - i\nu_1 = E_1 - \Gamma_1 / 2$, $\mu_2 - i\nu_2 = E_2 - \Gamma_2 / 2$, $\tilde{\Gamma}_{1c}^{1/2} \tilde{\Gamma}_{1n}^{1/2} = \Gamma_{1c}^{1/2} \Gamma_{1n}^{1/2}$, $\tilde{\Gamma}_{2c}^{1/2} \tilde{\Gamma}_{2n}^{1/2} = \Gamma_{2c}^{1/2} \Gamma_{2n}^{1/2}$ and U_{cn} in Eq. (I.6.13) has the form:

$$U_{cn} = e^{-i\varphi_c} \left(\delta_{cn} + i \frac{\Gamma_{1c}^{1/2} \Gamma_{1n}^{1/2}}{E_1 - E - i\Gamma_1 / 2} + i \frac{\Gamma_{2c}^{1/2} \Gamma_{2n}^{1/2}}{E_2 - E - i\Gamma_2 / 2} \right) e^{-i\varphi_n}. \quad (\text{I.6.21})$$

Then, the parameters in the reaction cross section formula in Eq. (I.6.15) become

$$g_1^c - 2 \frac{\Gamma_{1c} \Gamma_{1n}}{\Gamma_1} = g_2^c - 2 \frac{\Gamma_{2c} \Gamma_{2n}}{\Gamma_2} = \Gamma_{12c} \Gamma_{12n} \frac{\Gamma_1 + \Gamma_2}{(E_2 - E_1)^2 + (\Gamma_1 + \Gamma_2)^2 / 4},$$

$$h_1^c = -2 \Gamma_{12c} \Gamma_{12n} \frac{E_2 - E_1}{(E_2 - E_1)^2 + (\Gamma_1 + \Gamma_2)^2 / 4} = -h_2^c.$$

The use of approximate formula for collision matrix in Eq. (I.6.21), which corresponds to the so-called multilevel Breit-Wigner (MLBW) representation (see Section I.8), is rather convenient for the estimation of values and signs of **R**-matrix parameter products $\Gamma_{12c} \Gamma_{12n}$ directly from the analysis of reaction cross section between resonances. However, the total cross section here is the sum of one-level expressions in Eq. (I.4.5) with $g - ih \approx 2\Gamma_n e^{-2i\phi_n}$ in Eq. (I.6.18) and does not depend on the interference between resonances. This restricts evidently the possibility for joint description of the energy dependence of different cross sections for given pair of interacting resonances by a unique set of **R**-matrix parameters. The reason for such restriction is mainly that the matrix in Eq. (I.6.20) is not unitary, which leads to a non-balanced sum of the cross sections of all reactions and the total cross section at independent choice of **R**-matrix resonance parameters of the levels.

- e) The transition to the pole representation of the collision matrix elements in the momentum domain (on the variable $\sqrt{E}$) permits accounting for the energy dependence of the neutron widths of two interfering resonances in a form convenient for practical use. Similarly to the one-level example (see Section I.4), we represent the widths in A in Eq. (I.6.5) as $\Gamma_{\lambda\mu} = \Gamma_{\lambda\mu}^\alpha + \Gamma_{\lambda\mu}^n \sqrt{E}$. Then the determinant D is a polynomial of forth degree on $\sqrt{E}$:

$$D = (q_1 - \sqrt{E})(q_2 - \sqrt{E})(q_3 - \sqrt{E})(q_4 - \sqrt{E}), \quad (\text{I.6.22})$$

where q_k ($k=1,2,3,4$) are the roots of the equation $D=0$, two of which have a positive real part and the other two a negative real part. For the level matrix elements $(A^{-1})_{\lambda\mu}$ in Eq. (I.6.5), which in our case are the ratios of the first and second order polynomials of $\sqrt{E}$ to D in Eq. (I.6.22), the expansion to the simple fraction is determined:

$$(A^{-1})_{\lambda\mu} = \sum_{k=1}^4 \frac{a_{\lambda\mu}^{(k)}}{q_k - \sqrt{E}} \quad (1.6.23)$$

where $a_{\lambda\mu}^{(k)}$ ($\lambda, \mu = 1, 2$) are the energy independent complex values and moreover $a_{12}^{(k)} = a_{21}^{(k)}$. Though the analytical representation of the results of such an expansion is rather bulky even in the case of two levels, the computer realization of it at given **R**-matrix parameters is not complicated and is reduced at the end to the finding of the complex roots of the equation $D = 0$ (q_k).

The corresponding pole representation of the elements of G -matrix in Eq. (1.3.21) in the momentum domain is

$$G_{cn} = \sum_{\lambda, \mu=1}^2 \gamma_{\lambda c} (A^{-1})_{\lambda\mu} \gamma_{\mu n} = \sum_{k=1}^4 \frac{\rho_k^{cn}}{q_k - \sqrt{E}}, \quad (1.6.24)$$

where

$$\rho_k^{cn} = \sum_{\lambda, \mu=1}^2 \gamma_{\lambda c} a_{\lambda\mu}^{(k)} \gamma_{\mu n} \quad (1.6.25)$$

are the energy-independent complex values. Let us choose here two poles with the positive real parts (e.g., q_1 and q_2) and write G_{cn} in Eq. (1.6.24) in the form

$$G_{cn} = \frac{\rho_1^{cn} 2q_1}{q_1^2 - E} + \frac{\rho_2^{cn} 2q_2}{q_2^2 - E} + G_{cn}^0 \quad (1.6.26)$$

with

$$G_{cn}^0 = \frac{\rho_3^{cn}}{q_3 - \sqrt{E}} + \frac{\rho_4^{cn}}{q_4 - \sqrt{E}} + \frac{\rho_1^{cn}}{(-q_1) - \sqrt{E}} + \frac{\rho_2^{cn}}{(-q_2) - \sqrt{E}}. \quad (1.6.27)$$

So, we divided G_{cn} into two parts: the resonant part with the energy independent complex poles

$$q_1^2 = \mu_1 - i\nu_1, \quad q_2^2 = \mu_2 - i\nu_2$$

and the non-resonant “background” part formed by the sum in Eq. (1.6.27), where the poles have a negative real part ($\text{Re}(q_{3,4}) < 0$). A similar division into two components occurs for the **U**-matrix elements in Eq. (1.3.18) and Eq. (1.3.26) and in the cross sections formulae. Therefore, the cross section for a reaction (n, x) can be written in the following form:

$$\begin{aligned}
\sqrt{E}\sigma_x(E) &= \frac{\pi}{k^2} g(J) \sqrt{E} 4 \sum_{c(x)} P_c |G_{cn}|^2 P_n \\
&= \text{Re} \left(-i \left[\sum_{k=1}^2 \frac{2q_k r_k^x}{q_k^2 - E} + \sum_{k=3}^4 \frac{r_k^x}{q_k - \sqrt{E}} + \sum_{k=1}^2 \frac{r_k^x}{(-q_k) - \sqrt{E}} \right] \right),
\end{aligned} \tag{I.6.28}$$

where

$$r_k^x = 4i \frac{\pi \hbar^2}{\mu} g(J) \sum_{c(x)} P_c \sum_{k'=1}^4 \frac{\rho_k^{cn} (\rho_{k'}^{cn})^*}{q_{k'}^* - q_k} \frac{P_n}{\sqrt{E}} \tag{I.6.29}$$

are energy independent complex values. The first sum in Eq. (I.6.28) agrees with the Kapur-Peierls formalism result in Eq. (I.6.18) but the parameters are energy independent while $g_k^c - i\hbar_k^c \propto \sqrt{E}$, which corresponds to the Adler's scheme [18] (see Section I.8), popular in the resonance cross section parameterization. The effect of energy dependence of neutron widths gives the “background” cross section, determined by two last sums in Eq. (I.6.28) with the poles in the negative region of momentum domain. In limiting cases for relatively small ($\Gamma_{\lambda n} \ll \Gamma_{\lambda \alpha}$) and relatively large ($\Gamma_{\lambda n} \gg \Gamma_{\lambda \alpha}$) neutron widths, the background cross section is negligibly small -- this follows from the fact that the equation $D = 0$ in Eq. (I.6.22), the roots of which correspond to the resonant denominators in the cross sections, do not contain in these cases the terms with odd degrees of $\sqrt{E}$ (these are forth degree polynomials of $\sqrt{E}$).

The possibility of using the standard functions of the one-level approach, which account the resonance Doppler broadening $W(z)$ (see Section I.5), and the convenience in comparing the results of one-level approach with those of two-level approach in the practical resonance self-shielding problems is a definite advantage of our representation of the collision matrix as a sum of the pole terms on the variable $\sqrt{E}$ with energy independent values of the poles.

The example of two-resonance interference reflects to a high degree both the merits and the inadequacies of various representations of the cross section's energy structure. We noticed the clarity of the **U**-matrix description in the interpretation of the energy structure in Eq. (I.6.15) and Eq. (I.6.18) because the cross sections here are the sum of Breit-Wigner terms (with account of the interference). However, the independent searching of parameters can lead to the paradox of “negative cross sections” at energies far from resonances. The correct analysis needs to account for all correlations between parameters in Eq. (I.6.17), Eq. (I.6.19), and Eq. (I.6.20) while keeping the unitary condition of **U**-matrix, which leads finally to **R**-matrix variant in Eq. (I.6.5) and Eq. (I.6.6), where the parameters are, in general, independent. Moreover, if the transformation scheme of **R**-matrix parameters into **U**-matrix parameters is rather consistent and unique, the inverse transformation leads to the lack of uniqueness of the results.

I.7 Some Transformations of Collision Matrix

The common results of formal theory seem fascinating for the multilevel parameterization of neutron cross sections in the resolved resonance range with accounting for the interference effects. However,

the direct use of those for resonance cross section analysis encounters some major difficulties because of the limited number of observable levels associated with the terms in the sum over λ in Eq. (I.3.14) and the lack of the experimental information about all the individual channels c . Certain approximations and corresponding transformations appropriate to the practical situation are necessary.

- a) The problem of limiting the basis or the number of **R**-matrix terms in Eq. (I.3.21) that are accounted for explicitly in the multilevel analysis of resonance cross sections has an important meaning for construction of the corresponding calculating schemes and their physical interpretations. It depends mainly on the degree of completeness and precision of the experimental information and the same on the results of its physical interpretation. Let us present the **R**-matrix as a sum of two parts:

$$R = R^0 + R^1 = R^0 + \sum_{\lambda=1}^N (\gamma_{\lambda} \times \gamma_{\lambda}) / (E_{\lambda} - E) , \quad (I.7.1)$$

where R^1 contains some limited set of states and the contribution of the rest is included in R^0 . The latter may be interpreted as a non-resonant part of the interaction on the base, e.g., the known suggestions about the direct and intermediate processes [4-6,17]. Formally, the collision matrix or W -matrix in Eq. (I.3.18) in such a division of R is transformed as [4]:

$$W = W_0 + 2iP^{1/2}(1 - R^0\bar{L})^{-1}(1 - R^1\bar{L}^1)R^1(1 - \bar{L}R^0)P^{1/2} , \quad (I.7.2)$$

where

$$W_0 = P^{1/2}(1 - R^0\bar{L})^{-1}(1 - R^0\bar{L}^*)P^{1/2} \quad (I.7.3)$$

is a symmetric unitary matrix and

$$L^1 = \bar{L}(1 - R^0\bar{L})^{-1} . \quad (I.7.4)$$

Various approximations of this expression are known in applications to the specific problems [4,17]. In the resonance analysis, the suggestion about the diagonal R^0 -matrix is normally used and

$$U = e^{-i\varphi}P^{1/2}(1 - R^1\bar{L}^1)^{-1}(1 - R^1\bar{L}^*)P^{1/2}e^{-i\varphi} . \quad (I.7.5)$$

with

$$e^{-2i\varphi_l} = (-1)^l e^{-2i\rho} \frac{\phi_l^*(\rho)}{\phi_l(\rho)} \quad (I.7.6)$$

The over-determination of the scattering phases explains the difference between the observed values of the potential scattering cross sections from the hard sphere values in Eq. (I.1.13), which is practically

equivalent to the over-determination of the channel radius $a_c \rightarrow a_c(1 - R_{cc}^0)$ in the phases φ_c . This effect is interpreted quantitatively in the model of the complex potential [4-6]. After the determination of R_0 and using the potential scattering, the energy-dependence of the logarithmic derivative for neutron channels $L^1(E)$ in Eq. (I.7.4) may be found.

However, in our applications to the relatively low energy neutron resonances, as a rule the expected value of non-resonant processes contribution is negligibly small in comparison with the contribution of the tails of the wide resonances lying off the analyzed energy interval. Here the idea for R^0 matrix parameterization in Eq. (I.7.1) by using some limited set of resonance terms with energies off the interval considered in the positive as well as in the negative region is more attractive. Including formally those terms in R^1 , it is possible to extend this matrix to reduce the residual of R^0 to the minimum. In addition, if the separation of non-resonant processes in explicit form is not posed as the aim of the analysis, it is possible to consider this residual zero. So, the background problem in the resonance cross sections may be solved by the expansion of R^1 -matrix in comparison with the real number of the observed resonances in the analyzed interval by adding certain finite pole terms outside of this interval. In the following representation, using the general results of formal theory, we will suppose $R = R^1$ in Eq. (I.3.12) and Eq. (I.7.1) with arbitrary finite number of terms in the sum over λ .

- b) The problem of the limited number of channels accounted explicitly in the parameterization of the observed resonance cross sections is solved rather effectively by the method of reaction channels exclusion, which permits to reduce significantly the rank of collision matrix. The procedure of the channel exclusion was proposed by Teichmann and Wigner [4] and it consists of the transition to the cell form of G -matrix representation in Eq. (I.3.19) as

$$G = (1 - R\bar{L})^{-1}R = \begin{bmatrix} G^{++} & G^{+-} \\ G^{-+} & G^{--} \end{bmatrix}, \quad (I.7.7)$$

where + and - characterize two arbitrary groups of channels, to which we have divided their full set. With the corresponding representation

$$1 - R\bar{L} = \begin{bmatrix} 1 - R^{++}\bar{L}^+ & -R^{+-}\bar{L}^- \\ -R^{-+}\bar{L}^+ & 1 - R^{--}\bar{L}^- \end{bmatrix} \quad (I.7.8)$$

the inverse matrix is [32]

$$(1 - R\bar{L})^{-1} = \begin{bmatrix} (1 - \Re^{++}\bar{L}^+)^{-1} & (1 - \Re^{++}\bar{L}^+)^{-1}\Re^{+-}\bar{L}^- \\ \Re^{-+}(1 - \bar{L}^+\Re^{++})^{-1}\bar{L}^+ & (1 - \Re^{--}\bar{L}^-)^{-1} \end{bmatrix} \quad (I.7.9)$$

where

$$\begin{aligned}
\mathfrak{R}^{++} &= R^{++} + R^{+-} \bar{L}^- (1 - R^{--} \bar{L}^-)^{-1} R^{-+} \\
\mathfrak{R}^{-+} &= (1 - R^{--} \bar{L}^-)^{-1} R^{-+} = (\mathfrak{R}^{++})' \\
\mathfrak{R}^{--} &= R^{--} + R^{-+} \bar{L}^+ (1 - R^{++} \bar{L}^+)^{-1} R^{+-}
\end{aligned}$$

are the so-called reduced $\mathfrak{R}$ -matrices [4]. It is possible to present the cells of matrix G in Eq. (I.7.7) by using these matrices as

$$\begin{aligned}
G^{++} &= (1 - \mathfrak{R}^{++} \bar{L}^+)^{-1} \mathfrak{R}^{++} = \mathfrak{R}^{++} (1 - \bar{L}^+ \mathfrak{R}^{++})^{-1}, \\
G^{-+} &= \mathfrak{R}^{-+} (1 - \bar{L}^+ \mathfrak{R}^{++})^{-1}, \quad \dots
\end{aligned} \tag{I.7.10}$$

In turn, the reduced $\mathfrak{R}$ -matrices may be expressed through the corresponding level matrix following the general scheme of transformation in Eq. (I.3.22) [4]:

$$\mathfrak{R}^{++} = \sum_{\lambda\mu} (\gamma_\lambda^+ \times \gamma_\mu^+) (B^{-1})_{\lambda\mu}, \quad \mathfrak{R}^{-+} = \sum_{\lambda\mu} (\gamma_\lambda^- \times \gamma_\mu^+) (B^{-1})_{\lambda\mu}, \tag{I.7.11}$$

where

$$B = \varepsilon - E - \xi' \quad [B_{\lambda\mu} = (E_\lambda - E) \delta_{\lambda\mu} - \xi'_{\lambda\mu}] \tag{I.7.12}$$

is the level matrix and, moreover, the elements of the symmetric matrix ξ' are determined by the sum only over the channels included in the group (—)

$$\xi'_{\lambda\mu} = \sum_{(c^-)} \gamma_{\lambda c} \bar{L}_c \gamma_{\mu c} \tag{I.7.13}$$

Realizing now the division of the complete set of reaction channels so that the radiative capture channels are included in the group (—) and supposing that the number of these channels is big and their amplitudes $\gamma_{\lambda c}$ are distributed randomly, the corresponding matrix ξ in Eq. (I.7.13) may be considered as a diagonal one

$$\xi'_{\lambda\mu} = \sum_{c(\gamma)} \gamma_{\lambda c} \bar{L}_c \gamma_{\mu c} \approx \frac{i}{2} \Gamma_{\lambda\mu} \delta_{\lambda\mu} \tag{I.7.14}$$

Then the reduced matrix $\mathfrak{R}^{++}$ in Eq. (I.7.11), having in this case the rank equal to the number of neutron channels (one or two for the system with given J and π (see Section I.4)) plus a few fission channels for fissile nuclei, is

$$\mathfrak{R}^{++} = \sum_{\lambda} (\gamma_\lambda^+ \times \gamma_\lambda^+) / (E_\lambda - E - i\Gamma_{\lambda\gamma} / 2) \tag{I.7.15}$$

and the corresponding reduced collision matrix has the form

$$U^{++} = e^{-i\varphi} [1 + 2iP^{1/2} (1 - \Re^{++} \bar{L}^+)^{-1} \Re^{++} P^{1/2}] e^{-i\varphi} \quad (1.7.16)$$

with the same rank as the matrix $\Re^{++}$. In the following, the reduced matrix with radiative channels excluded will be used by omitting the upper indexes **(++)**.

The reduced collision matrix in Eq. (1.7.16) is no longer unitary, as it does not contain the radiative channels, and if the total cross section $\sigma \propto (1 - \text{Re} U_{nn})$ and e.g., the fission cross section $\sigma_f \propto \sum_{c(f)} |U_{cn}|^2$ are expressed through the elements of this matrix in the usual way, the radiative cross section is determined here as a difference

$$\sigma_\gamma \propto 1 - \sum_c |U_{cn}|^2, \quad (1.7.17)$$

where the sum over c is related to the channels of the reduced matrix (see Section 1.8).

The representation of the reduced collision matrix U^{++} in Eq. (1.7.16) through the level matrix is analogous by the form to the general relation in Eq. (1.3.26) with the elements

$$A_{\lambda\mu} = (E_\lambda - E - i\Gamma_{\gamma\lambda} / 2) \delta_{\lambda\mu} - \xi'_{\lambda\mu}, \quad (1.7.18)$$

where $\xi'_{\lambda\mu} = \sum_c \gamma_{c\lambda} L_c \gamma_{c\mu} = \Delta'_{\lambda\mu} + i\Gamma'_{\lambda\mu} / 2$ are the sums over the channels remaining after the exclusion

of the radiative channels. In our applications, $\Gamma'_{\lambda\mu} = \Gamma_{\lambda\mu n} + \Gamma_{\lambda\mu f}$ and $\Delta'_{\lambda\mu} = \sum_n \gamma_{\lambda n} \bar{S}_n \gamma_{\mu n}$. This

representation of the A -matrix in the common expression for reduced collision matrix in Eq. (1.3.26) was used by Reich and Moore in 1958 for the analysis of ^{235}U resonance fission cross section in the region of low resonances [36], and the procedure of channels-exclusion in resonance cross section parameterization is usually referred to as the Reich-Moore (RM) approximation. The precision of the Reich-Moore approximation is determined by the smallness of the ratio $(\Gamma_\gamma / D) \ll 1$, which practically is always fulfilled for neutron resonances. The specific problems arise only in account of the possibility for $(n, \gamma f)$ reaction, which in this approximation is included formally in the radiative capture, so the corresponding corrections are necessary in multilevel analysis of the fission cross section [20,31,34,37].

- c) In principle, all reaction channels ($c \neq n$) can be excluded and fission channels for fissile nuclei are among them. In such a case the rank of the reduced matrix $\Re^{++}$ (the number of columns in the rectangular matrix $\Re^{++}$) is minimal and equal to the number of neutron channels of the considered level system with fixed total momentum J and parity π . There are one or two channels in our applications. The G -matrix elements in Eq. (1.7.10) are expressed as ratios of the meromorphic functions of energy (momentum) and illustrate the possibility of transformation of our matrix elements to similar meromorphic (pole) form of representation with account of energy dependence

of the neutron logarithmic derivatives $\bar{L}_l(\rho)$, where $\rho = (a\sqrt{2\mu}/\hbar)\sqrt{E}$ (Appendix I.A1).

Let us consider the case of one neutron channel and an arbitrary number of reaction channels. Then, from Eq. (I.7.10), we have

$$G_{cn} = \Re_{cn} (1 - \bar{L}_l \Re_{nn})^{-1}. \quad (I.7.19)$$

For the reduced matrix elements in non-fissile nuclei, the RM-approximation in Eq. (I.7.18) is always used. In the general case, it is possible, e.g., to pass to the representation $\Re_{cn}$ in Eq. (I.7.11) with a diagonalized level matrix B by using the method of orthogonal transformation in Eq. (I.3.27), for example:

$$\Re_{cn} = \sum_{k=1}^N \tilde{\gamma}_{kc} \tilde{\gamma}_{kn} / (\tilde{\varepsilon}_k - E), \quad (I.7.20)$$

where

$$\tilde{\varepsilon}_k = \sum_{\lambda, \mu=1}^N T_{k\lambda} (E'_\lambda \delta_{\lambda\mu} - i\Gamma_{\lambda\mu}^\alpha / 2) T_{k\mu}, \quad (I.7.21)$$

$$\tilde{\gamma}_{kc} = \sum_{\lambda} T_{k\lambda} \gamma_{\lambda c}. \quad (I.7.22)$$

By our assumption $\Gamma_{\lambda\mu}^\alpha$ does not depend on energy, so the elements of the matrix of orthogonal transformation $T_{k\lambda}$ ($TT^T = 1$), and the parameters of representation in Eq. (I.7.20) are energy independent too. Therefore, in our case, the expression in Eq. (I.7.20) is the rigorous pole form for $\Re_{cn}(E)$.

In practice, the complicated procedure for finding the transformation matrix T can generally be avoided by transforming $\Re_{cn}(E)$ in Eq. (I.7.11) to the form in Eq. (I.7.20) following the usual scheme of inverting matrix B :

$$\Re_{cn}(E) = \sum_{\lambda\mu} \gamma_{\lambda c} \gamma_{\lambda n} M_{\lambda\mu}(E) / D(E), \quad (I.7.23)$$

where $D(E)$ is the determinant of the matrix B in Eq. (I.7.12) and $M_{\lambda\mu}(E)$ is the corresponding cofactor. The roots of the equation $D(E) = 0$ coincide with $\tilde{\varepsilon}_k$ in Eq. (I.7.21) and

$$D(E) = \prod_{k=1}^N (\tilde{\varepsilon}_k - E)$$

Using the expansion in Eq. (I.7.23) into the simple fractions, we pass directly to the representation in Eq. (I.7.20) with

$$\tilde{\gamma}_{kc} \tilde{\gamma}_{kn} = \sum_{\lambda\mu} \gamma_{\lambda c} \gamma_{\lambda n} M_{\lambda\mu}(\tilde{\varepsilon}_k) / \left[\frac{d}{dE} D(E) \right]_{E=\tilde{\varepsilon}_k}$$

In the following applications, using $\mathfrak{R}_{cn}(E)$ with the diagonalized level matrix, the amplitudes $\tilde{\gamma}_{kc}$ enter always as a quadratic combination of a kind in Eq. (I.7.23).

The logarithmic derivatives $\bar{L}_l$ in Eq. (I.7.19) are the meromorphic functions of $\rho = (a\sqrt{2\mu}/\hbar)\sqrt{E}$ and it can be chosen for example in the form (Appendix 1):

$$\bar{L}_l(\sqrt{E}) = (\phi_l \phi_l^*)^{-1} \left[\frac{\rho}{2} \frac{d}{d\rho} (\phi_l \phi_l^*) + i\rho^{2l+1} \right], \quad (I.7.24)$$

where $\phi_l(\rho) = \phi_l(\sqrt{E})$ are the known l -th order polynomials of ρ (Appendix I.A1). Substituting Eq. (I.7.20) and Eq. (I.7.24) in our expression for G_{cn} in Eq. (I.7.19), we can present the result as a ratio of the polynomials of $\sqrt{E}$:

$$G_{cn}(\sqrt{E}) = \wp_{2N-2+2l}^{cn}(\sqrt{E}) / Q_{2N+2l}(\sqrt{E}), \quad (I.7.25)$$

where

$$\wp_{2N-2+2l}^{cn}(\sqrt{E}) = (\phi_l \phi_l^*) \sum_{\lambda=1}^N \tilde{\gamma}_{\lambda c} \tilde{\gamma}_{\lambda n} \prod_{\lambda' \neq \lambda} (\varepsilon_{\lambda'} - E), \quad (I.7.26)$$

$$Q_{2N+2l}^{cn}(\sqrt{E}) = (\phi_l \phi_l^*) \prod_{\lambda=1}^N (\varepsilon_{\lambda} - E) - \rho \left[\frac{1}{2} \frac{d}{d\rho} (\phi_l \phi_l^*) + i\rho^{2l} \right] \sum_{\lambda=1}^N \tilde{\gamma}_{\lambda n}^2 \prod_{\lambda' \neq \lambda} (\varepsilon_{\lambda'} - E). \quad (I.7.27)$$

The transition to the pole representation for the meromorphic function $G_{cn}(\sqrt{E})$ in Eq. (I.7.25) is in finding the roots of the equation $Q_{2N+2l}(\sqrt{E}) = 0$. Denoting them as q_k , we have

$$Q_{2N+2l}(\sqrt{E}) = (a\sqrt{2\mu/\hbar})^l \prod_{k=1}^{2N+2l} (q_k - \sqrt{E}) , \quad (1.7.28)$$

and the following expansion of Eq. (1.7.25) over simple fractions

$$G_{cn}(\sqrt{E}) = \sum_{k=1}^{2N+2l} \frac{\rho_k^{cn}}{q_k - \sqrt{E}} , \quad (1.7.29)$$

where

$$\rho_k^{cn} = \wp_{2N-2+2l}^{cn}(q_k) / \left[\frac{d}{d\sqrt{E}} Q_{2N+2l}(\sqrt{E}) \right]_{\sqrt{E}=q_k} . \quad (1.7.30)$$

Since the functions ϕ_l satisfy the relation $\phi_l' \phi_l^* - \phi_l \phi_l'^* = 2i(\rho^{2l} - \phi_l \phi_l^*)$ (Appendix I.A1), the terms inside the bracket of $Q_{2N+2l}(\sqrt{E})$ in Eq. (1.7.27) can be written as

$$\frac{1}{2} \frac{d}{d\rho} (\phi_l \phi_l^*) + i\rho^{2l} = \phi_l' \phi_l^* + i\phi_l \phi_l'^* \quad (1.7.31)$$

Therefore, the common multiplier ϕ_l^* can be omitted from the numerator and the denominator of Eq. (1.7.25). As a result, the pole expansion in Eq. (1.7.29) contains only $2N + l$ terms. The form $G_{cn}(\sqrt{E})$ in Eq. (1.7.29) is useful, however, for making the similar scheme of the corresponding pole expansion of different partial cross sections (see Section I.8).

d) The expressions for the elements G^{--} and G^{++} , in the case of two neutron channels n and n' with identical l , can also be brought to a similar form:

$$G_{cn} = \frac{1}{\Delta} [\Re_{cn} - \bar{L}_l (\Re_{cn} \Re_{n'n'} - \Re_{cn'} \Re_{n'n})] \\ \Delta = 1 - \bar{L}_l (\Re_{nn} + \Re_{n'n'}) + \bar{L}_l^2 (\Re_{nn} \Re_{n'n'} - \Re_{n'n}^2) \quad (1.7.32)$$

In fact, the quadratic combinations of the elements entering in the numerator and denominator can be transformed as

$$\Re_{cn} \Re_{n'n'} - \Re_{cn'} \Re_{n'n} = \sum_{\lambda} \frac{1}{\tilde{\epsilon}_{\lambda} - E} \sum_{\lambda' \neq \lambda} \frac{(\tilde{\gamma}_{\lambda n'} \tilde{\gamma}_{\lambda' n} - \tilde{\gamma}_{\lambda n} \tilde{\gamma}_{\lambda' n'}) (\tilde{\gamma}_{\lambda c} \tilde{\gamma}_{\lambda' n'} - \tilde{\gamma}_{\lambda n'} \tilde{\gamma}_{\lambda' c})}{\tilde{\epsilon}_{\lambda} - \tilde{\epsilon}_{\lambda'}} , \quad (1.7.33)$$

where the sum over λ' does not depend on energy. Then, similarly to the previous case of one neutron channel, Eq. (1.7.32) can be presented as a ratio of polynomials of the form

$$G_{cn}(\sqrt{E}) = \wp_{2N-2+4l}^{cn}(\sqrt{E}) / Q_{2N+4l}(\sqrt{E}), \quad (1.7.34)$$

the order of which is greater by $2l$, which is connected with the last summand $\propto \bar{L}_l^2$ in the determinant Δ in Eq. (1.7.32). Correspondingly, the expansion over the simple fractions will contain $2N + 4l$ summands in Eq. (1.7.29) (or $2N + 2l$ in consideration that is more precise).

- e) The examples of one level (see Section 1.4) and two level (1.6) approximations, and the quantitative analysis of the solutions q_k have shown that these compose the pair for each level E_λ with the generally opposite sign of $\text{Re } q_k$. This indicates that in the sum in Eq. (1.7.29), we can isolate a certain set of N_1 terms with $\text{Re } q_k > 0$, which are directly associated with observed resonances in the energy interval in question, or near it. The expansion in Eq. (1.7.29) can be transformed into the form:

$$G_{cn} = \sum_{k=1}^{N_1} \frac{2\rho_k^{cn} q_k}{q_k^2 - E} + G_{cn}^0 = G_{cn}^1 + G_{cn}^0, \quad (1.7.35)$$

where

$$G_{cn}^0 = \sum_{k=N_1+1}^{2N+1} \frac{\rho_k^{cn}}{q_k - \sqrt{E}} + \sum_{k=1}^{N_1} \frac{\rho_k^{cn}}{(-q_k) - \sqrt{E}} \quad (1.7.36)$$

includes the terms with the poles at negative $\sqrt{E}$, and probably with $\text{Re } q_k > 0$ but positioned rather distantly from the considered energies. Therefore, we divided G_{cn} to properly resonant part with energy independent parameters of denominators $q_k^2 = \mu_k - i\nu_k$ and smoothly dependent at our energies “background” part. Practically this is a correct transition from **R**-matrix parameterization to Adler scheme with determined background part of the collision matrix [18].

1.8 Multilevel Formulae for Resonance Cross Sections

- a) For the problem of multilevel parameterization of resonance cross sections and particularly for the fissile nuclei cross sections in the resolved resonance region, the effective mathematical methods using directly the results of **R**-matrix theory [33] have been developed. In the reduced **R**-matrix scheme, where the radiative capture channels are excluded, the collision matrix in Eq. (1.7.16) has the rank equal to the number of neutron channels plus fission channels, in the case of fissile nuclei, for the considered system with given total momentum J and parity π . Writing the matrix in the form [33,35]:

$$e^{i\varphi} U^J e^{i\varphi} = 1 + 2iP^{1/2} G^J P^{1/2} = (1 - iK^J)^{-1} (1 + iK^J), \quad (1.8.1)$$

or

$$iP^{1/2}G^JP^{1/2} = (1 - iK^J)^{-1} - 1,$$

we determine K^J as a matrix with the elements

$$K_{c'c}^J = P_c^{1/2}[(1 - \Re S)^{-1}\Re]_{c'c}P_{c'}^{1/2} = \frac{1}{2} \sum_{\lambda\mu} \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c'}^{1/2} (C^{-1})_{\lambda\mu} \quad (1.8.2)$$

where

$$C_{\lambda\mu} = (E_\lambda - E - i\Gamma_{\lambda\gamma}/2)\delta_{\lambda\mu} - \sum_n \gamma_{\lambda n} S_n \gamma_{\mu n} \quad (1.8.3)$$

is the corresponding level matrix. As the level shift factors for the reaction channels are supposed to be zero, the non-diagonal part C is connected only with neutron channels. Obviously it is equal to zero for s -neutrons and $K = P^{1/2}\Re P^{1/2}$. The expression in Eq. (1.8.2) is brought to a diagonal form with slightly modified parameters by using linear approximation $S_n(E) = a + b(E)$, which is valid for $\rho^2 < 1$ and all l [4]. Another variant providing the exact passage to the limit to the one level approximation is connected with the neglect of the non-diagonal terms in matrix C in Eq. (1.8.3). Then

$$K_{c'c}^J(E) = \frac{1}{2} \sum_{\lambda} \Gamma_{\lambda c}^{1/2} \Gamma_{\lambda c'}^{1/2} / (E'_\lambda - E - i\Gamma_{\lambda\gamma}/2), \quad (1.8.4)$$

where

$$E'_\lambda = E_\lambda - \Gamma_{\lambda n}(E_\lambda)S_n(E)/2P_n(E_\lambda) \quad (1.8.5)$$

generally depend on energy. Finally, using the fact that S_n is a rational function of $\rho^2(E)$, K^J in Eq. (1.8.2) can be transformed to the pole representation in the energy space. This leads at the end to the expression of the kind in Eq. (1.8.4) with energy-independent poles, but with additional l terms in the sum over λ , and some of those poles are lying outside of the resonance energy interval (see Section 1.7).

In practice, however, even in the most complicated problem here - the fissile nuclei resonance cross section parameterization in the resolved region - apparently the matrix K^J can be used always in the form in Eq. (1.8.4) with $E'_\lambda = E_\lambda$ [33]. For non-fissile nuclei under the energy of inelastic scattering threshold, the rank of the reduced U^J -matrix is substantively no more than two and the use of the common expression of RM-approximation in Eq. (1.7.16) does not lead to the complications of the mathematical scheme of the resonance cross section analysis [19,34] (see below).

The multilevel formulae for cross sections can be expressed through the elements of the matrix $P^{1/2}G^JP^{1/2}$, which is determined in the RM-approximation by the relation in Eq. (1.8.1). So, the total

cross section is

$$\sigma(E) = \sigma_p + \frac{4\pi}{k^2} \sum_J g(J) \sum_n \operatorname{Re}[-ie^{-2i\varphi_n} G_{nn}^J(E) P_n(E)] \quad (1.8.6)$$

and the fission cross section is

$$\sigma_f(E) = \frac{4\pi}{k^2} \sum_J g(J) \sum_{c(f)} P_c |G_{cn}^J(E)|^2 P_n(E) \quad (1.8.7)$$

where the sum over $c(f)$ is related to the fission channels of the given system $J(\pi)$, and for the neutrons there is only one channel as a rule. The neutron absorption cross section σ_a and radiative capture cross section, which for the fissile nuclei is equal to the difference $\sigma_\gamma = \sigma_a - \sigma_f$, are determined as

$$\sigma_a(E) = \frac{4\pi}{k^2} \sum_J g(J) \sum_n \left\{ \operatorname{Re}[-iG_{nn}^J(E)] - \sum_{n'} |G_{n'n}^J(E)|^2 P_{n'}(E) \right\} P_n(E) \quad (1.8.8)$$

$$\sigma_\gamma(E) = \frac{4\pi}{k^2} \sum_J g(J) \sum_n \left\{ \operatorname{Re}[-iG_{nn}^J(E)] - \sum_c |G_{cn}^J(E)|^2 P_c \right\} P_n(E) \quad (1.8.9)$$

where the last sum over c is related to all channels of the reduced matrix U^J in Eq. (1.8.1). The scattering cross section is a difference

$$\sigma_n(E) = \sigma(E) - \sigma_a(E) \quad (1.8.10)$$

The certain advantage of the **R**-matrix description of the resonance cross sections is above all the energy-independence of the real parameters of various levels grouped into $K^J(E)$ in Eq. (1.8.4). For each set of those parameters, the complete (non-reduced) $U^{J\pi}$ -matrix is always unitary, which leads at the end to the balance of the widths (Appendix I.A3):

$$\Gamma_{\lambda\mu} = \sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c}^{1/2} = \Gamma_{\lambda\gamma} \delta_{\lambda\mu} + \sum_n \Gamma_{\lambda n}^{1/2} \Gamma_{\mu n}^{1/2} + \sum_{c(f)} \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c}^{1/2} \quad (1.8.11)$$

This provide the positiveness of the cross sections, which are determined formally as differences in Eq. (1.8.8) and Eq. (1.8.9) and the limitations from above (the unitary limit) without introducing any additional conditions. The parameters of the formalism - the width amplitudes $\Gamma_{\lambda c}^{1/2}$ and the energies E_λ have some physical meaning and find their theoretical interpretation in the compound nucleus

model [1-6]. For non-fissile nuclei, e.g., in the case of one neutron channel, we will have the reduced $U^{J\pi}$ -function in Eq. (I.7.16) and Eq. (I.8.1) with

$$K^J = K_{nn}^J = \frac{1}{2} \sum_{\lambda} \Gamma_{\lambda n} / (E_{\lambda} - E - i\Gamma_{\lambda\gamma} / 2) \quad (I.8.12)$$

Here the parameters are the same as in the one level analysis - resonance widths and E_{λ} . There are no new parameters in the multilevel case. For two neutron channels, and the same in the general case taking account of the fission channels, except the same widths in the separate channels, the multilevel analysis gives the signs of the products $\Gamma_{\lambda c}^{1/2} \Gamma_{n'c}^{1/2}$ too.

- b) However, the practical use of **R**-matrix parameterization results is not trivial, mainly due to with the complicated energy dependence of cross sections, which are reproduced by the multilevel formulae in Eq. (I.8.6) to Eq. (1.8.9) in the present approach. It is essential that the form of energy dependence is different at different level numbers and ranks of the reduced matrix $K^J(E)$ in Eq. (I.8.4). The account of resonance Doppler broadening, the investigation of cross section functionals, which characterize the resonance self-shielding effects, and the analysis of neutron transmission for thick samples, all need direct numerical calculations and make the qualitative analysis of the observed dependencies difficult.

It is more convenient from this point of view, as we have mentioned already, to use in applications the resonance cross section representation in the Adler scheme (AA), where in the general case the energy dependence is reproduced by the sum of one-channel (Breit-Wigner) terms plus background. Traditionally this scheme is considered as a result of Kapur-Peierls parameterization of the collision matrix $U^J(E)$ in Eq. (I.3.29) or

$$G_{cn}^J(E) = \sum_{k=1}^{N(J)} \tilde{\gamma}_{kc} \tilde{\gamma}_{kn} / (\tilde{E}_k - E) + G_{cn}^{0J} = G_{cn}^{1J} + G_{cn}^{0J} \quad (I.8.13)$$

assuming the complex parameters $\tilde{\gamma}_{kc}$ and $\tilde{E}_k = \mu_k - i\nu_k$ are not dependent on energy. This means actually that the energy dependence of the total widths ($\Gamma_{\lambda\mu}(E) \approx \sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c}^{1/2}(E_{\mu})$) is not taken into

account in the transformation of **R**-matrix form A to Kapur-Peierls variant in Eq. (I.3.7). The practical application of the Adler scheme was limited until now to fissile nuclei, where such an approximation is justified somehow by the smallness of energy dependent neutron widths of resonances. In a general case, the problem of the transition from **R**-matrix formalism to the Adler scheme is solved by the pole expansion of G^J -matrix in Eq. (I.7.32) in momentum domain (see Section I.9).

Substituting G_{cn}^J in Eq. (I.8.13) in Eq. (I.8.6) and assuming $l = 0$, we obtain the total cross section formula in the AA approximation [18,34,39]:

$$\begin{aligned}
\sigma(E) &= \sigma'_p + \frac{\pi\sqrt{E}}{k^2} \sum_J g(J) \sum_{k=1}^N \operatorname{Re} \left[-ie^{-2i\varphi_0} \frac{g_k + ih_k}{\mu_k - E - i\nu_k} \right] \\
&= \sigma'_p + \frac{\pi\sqrt{E}}{k^2} \sum_J g(J) \\
&\quad \times \sum_{k=1}^{N(J)} \frac{\nu_k (g_k \cos 2\varphi_0 + h_k \sin 2\varphi_0) + (\mu_k - E)(h_k \cos 2\varphi_0 - g_k \sin 2\varphi_0)}{(\mu_k - E)^2 + \nu_k^2}
\end{aligned} \tag{I.8.14}$$

where

$$\sigma'_p = \sigma_p + \frac{4\pi}{k^2} \sum_J g(J) \operatorname{Re}[-ie^{-2i\varphi_0} G_{nn}^{0J} P_n(E)] \tag{I.8.15}$$

is the potential cross section with account of the non-resonant background G_{nn}^{0J} for all neutron channels in principle, while the resonant part, which is written here formally for the two systems with $J_1 = I + 1/2$ and $J_2 = I - 1/2$ for $l = 0$, is the sum of $N(J_1)$ and $N(J_2)$ one-type resonant terms. Here the resonance parameters μ_k , ν_k and

$$g_k + ih_k = 4\tilde{\gamma}_{kn}^2 P_0(E) / \sqrt{E} = 2\tilde{\Gamma}_{kn}(\mu_k) / \sqrt{\mu_k} \tag{I.8.16}$$

do not depend on energy.

A similar form of cross section representation for reaction cross sections follows from the transformation in Eq. (I.8.13):

$$\begin{aligned}
4P_c P_n |G_{cn}|^2 &= 4P_c P_n \left[|G_{cn}^1|^2 + |G_{cn}^0|^2 + 2\operatorname{Re}(G_{cn}^{0*} G_{cn}^1) \right] \\
&= |\tilde{G}_{cn}^0|^2 + \sum_{k=1}^N \operatorname{Re} \left[-i \frac{g_k^c + ih_k^c}{\mu_k - E - i\nu_k} \sqrt{E} \right], \quad (c \neq n)
\end{aligned} \tag{I.8.17}$$

where $\tilde{G}_{cn}^0 = 2\sqrt{P_c P_n} G_{cn}^0$ and

$$g_k^c + ih_k^c = 2i\tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{kn}^{1/2} \mu_k^{-1/4} \left[\tilde{G}_{cn}^{0*} + \sum_{k'=1}^N \frac{\tilde{\Gamma}_{k'c}^{1/2} \tilde{\Gamma}_{k'n}^{1/2} \mu_{k'}^{-1/4}}{(\mu_{k'} - \mu_k) + i(\nu_k + \nu_{k'})} \right]. \tag{I.8.18}$$

Here $\tilde{\Gamma}_{kn} = \tilde{\Gamma}_{kn}(\mu_k)$ and assuming the background part $\tilde{G}_{cn}^0$ is constant in the analyzed region of resolved resonances, the values $g_k^c + ih_k^c$ can be considered as energy independent. The fission cross section can be written in the form [18,31]:

$$\begin{aligned}
\sigma_f(E) &= \sigma_f^0 + \frac{\pi\sqrt{E}}{k^2} \sum_J g(J) \sum_{k=1}^{N(J)} \operatorname{Re} \left[-i \frac{g_k^f + ih_k^f}{\mu_k - E - i\nu_k} \right] \\
&= \sigma_f^0 + \frac{\pi\sqrt{E}}{k^2} \sum_J g(J) \sum_{k=1}^{N(J)} \frac{\nu_k g_k^f + (\mu_k - E)h_k^f}{(\mu_k - E)^2 + \nu_k^2},
\end{aligned} \tag{I.8.19}$$

where the first term is determined by the background and the resonant part is the sum of Breit-Wigner terms with energy independent parameters μ_k , ν_k and

$$g_k^f + ih_k^f = \sum_{c(f)} (g_k^c + ih_k^c). \tag{I.8.20}$$

Let us notice that if the set of parameters of the Adler scheme μ_k , ν_k , G_{nn}^{0J} , and $g_k + ih_k$ are obtained by analyzing the total cross section, which is usually measured with the highest precision, and if the spin of resonances is known, it is possible, generally speaking, to construct it by using these parameters of the summarized reaction cross section $\sigma_a(E)$ in Eq. (I.8.8). In our case it is

$$\sigma_a(E) = \sigma_a^0 + \frac{\pi\sqrt{E}}{k^2} \sum_J g(J) \sum_{k=1}^{N(J)} \operatorname{Re} \left[-i \frac{g_k^a + ih_k^a}{\mu_k - E - i\nu_k} \right], \tag{I.8.21}$$

where

$$\sigma_a^0 = \pi k^{-2} \sum_J g(J) \left[2 \operatorname{Re}(-i\tilde{G}_{nn}^{0J}) - |\tilde{G}_{nn}^{0J}|^2 \right], \quad \tilde{G}_{nn}^{0J} = 2P_n G_{nn}^{0J}, \tag{I.8.22}$$

and

$$g_k^a + ih_k^a = (g_k + ih_k) \left[1 - i \left(\tilde{G}_{nn}^{0*} + \frac{\sqrt{E}}{2} \sum_{k'} \frac{g_{k'} + ih_{k'}}{(\mu_{k'} - \mu_k) + i(\nu_k + \nu_{k'})} \right) \right] \tag{I.8.23}$$

are determined by the parameters of the total cross section. Let us notice that $g_k^a + ih_k^a$ formally depend on energy because of the penetrability factor in the neutron widths. Usually, in the AA schemes in Eq. (I.8.19), it is supposed $\sqrt{E} \approx \sqrt{E_k}$. In cross section analysis however, in relatively wide intervals containing the resonances with large widths, the influence of energy dependence can be significant [36]. The radiative capture cross section can be found here as a difference

$$\sigma_\gamma(E) = \sigma_a(E) - \sigma_f(E) = \sigma_\gamma^0 + \frac{\pi\sqrt{E}}{k^2} \sum_J g(J) \sum_{k=1}^{N(J)} \operatorname{Re} \left[-i \frac{g_k^\gamma + ih_k^\gamma}{\mu_k - E - i\nu_k} \right] \tag{I.8.24}$$

with parameters formally dependent on energy

$$g_k^\gamma + ih_k^\gamma = g_k^a - g_k^f + i(h_k^a - h_k^f).$$

The background part of the cross section in the Adler approach is approximated usually by limited series on the degrees of $\sqrt{E}$ with constant coefficients [18,34]. If G^{0J} in Eq. (I.8.13) is a diagonal matrix, the background cross section is accounted for only in the total cross section (and scattering cross section) and $\sigma_a^0 = 0$ ($\sigma_c^0 = 0$). In general, however, considering the system of resonances in an energy interval, the fission cross section, e.g., can be parameterized in principle without subtraction of the background part and relating it to the wings of resonances, which are lying outside of the interval. The sum in Eq. (I.8.19) is alternating, so it is impossible to guarantee that in the free parameter search the cross section would not become negative somewhere outside of the interval. The correct account of Adler's parameter correlation, which follows from the unitary and symmetry conditions of U^J -matrix (Appendix I.A3), of energy dependence of the penetrability factors in neutron channels, and of the background matrix structure reduces at the end the problem for determination of the self-consistent Adler scheme parameter set to finding of the equivalent set of **R**-matrix formalism in Eq. (I.8.4) parameters (see Section I.9).

Although the formulae of AA approach are obtained here for the case of one neutron channel with $l = 0$, those are keeping the similar form in the case $l \geq 1$. In fact, using for $P_l(E)$ the following representation (Appendix I.A1):

$$P_l(E) = c\sqrt{E} \left(1 + \sum_{p=1}^l \frac{c_p}{E_p - E} \right),$$

where $\text{Re}(E_p) < 0$, the product $G_{nn}P_l(E)$ e.g. can be transformed into the form:

$$\begin{aligned} G_{nn}P_l(E) &= \left(\sum_{k=1}^N \frac{\tilde{\gamma}_{kn}^2}{\tilde{E}_k - E} + G_{nn}^0 \right) \left(1 + \sum_{p=1}^l \frac{c_p}{E_p - E} \right) c\sqrt{E} \\ &= \sqrt{E} \sum_{k=1}^N \frac{\tilde{\gamma}_{kn}^2 P_l(\tilde{E}_k)}{\tilde{E}_k - E} \frac{1}{\sqrt{\tilde{E}_k}} + c\sqrt{E} \sum_{p=1}^l \frac{c_p}{E_p - E} G_{nn}^1(E_p) + G_{nn}^0 P_l(E) \end{aligned}$$

By joining the last two terms, which do not contain the poles in the physical region $E > 0$, to the common background part $\tilde{G}_{nn}^0$, we come again to the formulae for the total cross section in Eq. (I.8.14) and the neutron absorption cross section in Eq. (I.8.21) with an over-determined background part and parameters $g_k + ih_k = 4\tilde{\gamma}_{kn}^2 P_l(\tilde{E}_k) / \sqrt{\tilde{E}_k}$. The similar transformation occurs for the fission cross section in Eq. (I.8.19).

- c) For many nuclei, e.g., ^{238}U and ^{232}Th , the cross sections in the resolved resonance region are described satisfactorily by the usual sum of one-level terms (see Section I.4). The multilevel Breit-

Wigner Approximation (MLBW) can be useful sometimes as some generalization of **R**-matrix formalism, where the non-diagonal terms of the level matrix A in Eq. (I.3.23) are supposed negligible. In this approach

$$U_{cn}^J = e^{-i\varphi_c} \left[\delta_{cn} + i \sum_{\lambda} \frac{\Gamma_{\lambda c}^{1/2} \Gamma_{\lambda n}^{1/2}}{E'_{\lambda} - E - i\Gamma_{\lambda} / 2} \right] e^{-i\varphi_n} \quad (I.8.25)$$

with E'_{λ} in Eq. (I.8.5), $\Gamma_{\lambda n} = 2P_n(E)\gamma_{\lambda n}^2$, and $\Gamma_{\lambda} = \sum_c \Gamma_{\lambda c}$, which are dependent on energy. (We

assume here the background is diagonal and take it into account in the phases φ_n in Eq. (I.7.6)). The total cross section in Eq. (I.2.16) here evidently is the sum of independent Breit-Wigner terms in Eq. (I.4.5):

$$\sigma(E) = \sigma_p + 2\pi k^{-2} \sum_J g(J) \sum_{\lambda=1}^{N(J)} \operatorname{Re} \left[-ie^{-2\varphi_n} \frac{\Gamma_{\lambda n}}{E'_{\lambda} - E - i\Gamma_{\lambda} / 2} \right] \quad (I.8.26)$$

But in this approach the elastic scattering cross section in Eq. (I.2.15) with one neutron channel for each system (J, π) already contains the interference part σ_n^I , except the sum of one-level terms, as:

$$\sigma_n(E) = \sigma(E) - 2\pi k^{-2} \sum_J g(J) \sum_{\lambda=1}^{N(J)} \operatorname{Re} \left[-i \frac{\Gamma_{\lambda n} \Gamma_{\lambda a} / \Gamma_{\lambda}}{E'_{\lambda} - E - i\Gamma_{\lambda} / 2} \right] + \sigma_n^I, \quad (I.8.27)$$

where

$$\sigma_n^I = \pi k^{-2} \sum_J g(J) \sum_{\lambda=1}^{N(J)} \operatorname{Re} \left[-i \frac{\tilde{g}_{\lambda}^n + i\tilde{h}_{\lambda}^n}{E'_{\lambda} - E - i\Gamma_{\lambda} / 2} \right], \quad (I.8.28)$$

and

$$\tilde{g}_{\lambda}^n + i\tilde{h}_{\lambda}^n = 2i \sum_{\mu \neq \lambda} \frac{\Gamma_{\lambda n} \Gamma_{\mu n}}{(E'_{\mu} - E'_{\lambda}) + i(\Gamma_{\mu} + \Gamma_{\lambda}) / 2}. \quad (I.8.29)$$

The same interference term must be correspondingly in the neutron absorption cross section too:

$$\sigma_a(E) = \sigma(E) - \sigma_n(E).$$

Moreover, by determining the radiation capture cross section, which for the non-fissile nuclei coincides with σ_a in Eq. (I.2.3):

$$\begin{aligned}
\sigma_\gamma(E) &= \pi k^{-2} \sum_J g(J) \sum_{c(\gamma)} |U_{cn}^J|^2 \\
&\approx \pi k^{-2} \sum_J g(J) \sum_{c(\gamma)} \sum_{\lambda\mu} \frac{\Gamma_{\lambda c}^{1/2} \Gamma_{\lambda n}^{1/2} \Gamma_{\mu c}^{1/2} \Gamma_{\mu n}^{1/2}}{(E'_\lambda - E - i\Gamma_\lambda / 2)(E'_\mu - E + i\Gamma_\lambda / 2)}
\end{aligned} \tag{I.8.30}$$

We see that with the assumption of a large number of radiation channels (RM-approximation)

$$\sum_{c(\gamma)} \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c}^{1/2} \approx \Gamma_{\lambda\gamma} \delta_{\lambda\mu}$$

and $\sigma_\gamma(E)$ is the sum of non-interfering one-level terms. Here the evident contradiction of MLBW approximation arises; it, accounts practically for only the interference in the neutron channel and with the precision up to the terms of prime order of smallness of the ratio Γ / D , which corresponds to the neglect of the off-diagonal terms of the level matrix A in Eq. (I.8.25). So, the analysis with the use of MLBW scheme can be considered only as an approximation of more general schemes of multilevel description.

- d) The volume of the available experimental information about the resonance structure of fissile and non-fissile nuclei cross sections is enormous and growing, so its analysis is being continuously enhanced by means of more exact parameterization methods, accounting for the mutual influence of resonances in broad energy intervals of the resolved levels region. The absolute advantage of **R**-matrix schemes is due to the real and energy independent resonance parameters and the possibility of effective accounting for non-resonant background by the corresponding widening of **R**-matrix. However, the mathematical difficulties in searching these parameters even at the reduced number of **K**-matrix channels in Eq. (I.8.1), related to the inversion of complex and energy dependent matrices, are obvious too. The use of Kapur-Peierls formalism and its practical scheme of the Adler approximation, although giving the simple forms for cross section relations, in the simultaneous analysis of a large number of resonances in a relatively wide energy interval leads to the uncertainties in the reconciliation of the formalism parameters, their energy dependence, and the background determination.

The “combined” method, operating with the reduced matrices, where are excluded all reaction channels $c \neq n$ (see Section I.7), can be considered as a synthesis of the characteristic (for these two schemes) mathematical techniques. In fact, the neutron cross sections are determined only by the elements $U_{cn}^{J\pi}$ in the complete collision matrix $U^{J\pi}$, and moreover for all even-even nuclei and s -wave resonances in other nuclei, there is only one neutron (entrance) channel at given J and π . These are fissile nuclei, fertile isotopes ^{238}U and ^{232}Th , the majority of design elements and so on. For the nuclei with spin $I \neq 0$ and $l \geq 1$, some entrance neutron channels are possible in the resonance region, but practically no more than 2 and then only in special cases of the resonances in certain light nuclei at MeV energies, accounting for a bigger channel number n is necessary [19]. Excluding all the reaction channels $c \neq n$, we minimize the rank of the reduced matrix $\Re^{++}(G^{++})$ in Eq. (I.7.10) for one (or two) neutron channels and obtain, instead of a matrix, a simple functional relation between $U_{cn}(E)$ and the elements of $\Re_{cn}(E)$ in Eq. (I.7.11).

In the case of one neutron channel, e.g. the diagonal element of the collision matrix in Eq. (I.7.26) can be written in the form in Eq. (I.8.1):

$$U_{nn}^J = e^{-2i\varphi} (1 - \Re_{nn}^J \bar{L}_{nn})^{-1} (1 - \Re_{nn}^J \bar{L}_{nn}^*) = e^{-2i\varphi} (1 - iK_{nn}^J)^{-1} (1 + iK_{nn}^J) \quad (I.8.31)$$

where

$$K_{nn}^J = (1 - \Re_{nn}^J \bar{S})^{-1} \Re_{nn}^J P = \frac{1}{2} \sum_{\lambda\mu} \Gamma_{\lambda n}^{1/2} \Gamma_{\mu n}^{1/2} (\bar{C}^{-1})_{\lambda\mu} \quad (I.8.32)$$

and

$$\bar{C}_{\lambda\mu} = (E_\lambda - E) \delta_{\lambda\mu} - i\Gamma_{\lambda\mu}^a / 2 - \gamma_{\lambda n}^a \bar{S}_n \gamma_{\mu n} \quad (\Gamma_{\lambda\mu}^a = \sum_{c \neq n} \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c}^{1/2}) \quad (I.8.33)$$

is the level matrix coinciding with $C_{\lambda\mu}$ in Eq. (I.8.3) for non-fissile nuclei. In such a form of representation of U_{nn}^J the total cross section in Eq. (I.2.16) is expressed by K_{nn}^J as

$$\sigma = \sigma_p + \frac{4\pi}{k^2} \sum_J g(J) \frac{[\text{Im}(K_{nn}^J) + |K_{nn}^J|^2] \cos(2\varphi_n) - \text{Re}(K_{nn}^J) \sin(2\varphi_n)}{|1 - iK_{nn}^J|^2} \quad (I.8.34)$$

and the summarized cross section of neutron absorption is

$$\sigma_a = \frac{4\pi}{k^2} \sum_J g(J) \frac{\text{Im}(K_{nn}^J)}{|1 - iK_{nn}^J|^2} \quad (I.8.35)$$

Apparently, for non-fissile nuclei we can use the RM-approximation, where $K_{nn}^J(E)$ in Eq. (I.8.32) is chosen in the form in Eq. (I.8.4), $K_{nn}^J(E) = (1/2) \sum_{\lambda} \Gamma_{\lambda n} / (E'_\lambda - E - i\Gamma_{\lambda\gamma}/2)$, and moreover the parameters determined in the multilevel analysis $\Gamma_{\lambda n}$, $\Gamma_{\lambda c}$ and E'_λ are the same as in the one-level analysis by their physical meaning (see Section I.4). A similar scheme for resonance cross section parameterization, however, can be applied in the case of fissile nuclei. By neglecting the phase shift factor $\bar{S}_n \approx 0$, the fission cross section in Eq. (I.8.7) with account of the relation in Eq. (I.7.10) can be written in the form:

$$\sigma_f = \frac{4\pi}{k^2} \sum_J g(J) \sum_{c(f)} \frac{|K_{cn}^J|^2}{|1 - iK_{nn}^J|^2}, \quad (I.8.36)$$

where

$$K_{cn}^J = \frac{1}{2} \sum_{\lambda\mu} \Gamma_{\lambda c}^{1/2} \Gamma_{\lambda n}^{1/2} (B^{-1})_{\lambda\mu} \quad (1.8.37)$$

with

$$B_{\lambda\mu} = (E_\lambda - E) \delta_{\lambda\mu} - i \Gamma_{\lambda\mu}^a / 2$$

(The element K_{nn}^J has a similar form as for $\bar{S} = 0$; the matrices C and B in Eq. (1.7.12) coincide.) The parameters E_λ and $\Gamma_{\lambda\mu}^a$ in the level matrix do not depend on energy, therefore in diagonalizing this matrix by transformation in Eq. (1.8.37) to the simple sum in Eq. (1.7.20)

$$K_{cn}^J = \frac{1}{2} \sum_k \tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{kn}^{1/2} / (\tilde{\varepsilon}_k - E), \quad (1.8.38)$$

the new complex parameters $\tilde{\Gamma}_{kc}^{1/2}$, $\tilde{\Gamma}_{kn}^{1/2} / P_n(E)$ and $\tilde{\varepsilon}_k = \mu_k - i\nu_k$ are also energy-independent.

The parameterization of fissile nuclei resonance cross section by using the relations in Eq. (1.8.34), Eq. (1.8.35), and Eq. (1.8.36), where the elements $K_{cn}^J(E)$ and $K_{nn}^J(E)$ are chosen into the form in Eq. (1.8.37), is at the base of the idea of combined method of analysis, corresponding to the RM-approximation for non-fissile nuclei. The relatively non-complicated algorithm for parameters search for the latter in the case of one (or two) neutron channels can be used in the combined method too. The problem of transformation of the obtained parameters to the **R**-matrix parameters is solved by the comparison of two identical forms of representation the elements $K_{cn}^J(E)$ in Eq. (1.8.38) and Eq. (1.8.37). Let us notice that unlike the Kapur-Peierls scheme (or Adler scheme) here, no complications arise due to the determination of the energy dependence of diagonalized level matrix parameters, and all cross sections are rigorously “positive” by definition in Eq. (1.8.34), Eq. (1.8.35), and Eq. (1.8.36) with an arbitrary choice of $K_{cn}^J(E)$ parameters. Therefore, from the unitary condition of the collision matrix, it follows (Appendix I.A3):

$$\text{Im}(K_{nn}^J) = \sum_{c \neq n} |K_{cn}^J|^2 \quad (1.8.39)$$

Evidently, the radiative capture cross section $\sigma_\gamma = \sigma_a - \sigma_f$ here is a positively determined function too.

The similar functional dependence between cross sections and the elements $K_{cn}^J(E)$ also occur in the case of two neutron channels n and n' , and it is seen from the representation in Eq. (1.7.10):

$$(P^{1/2} G^J P^{1/2})_{cn} = [K_{cn}^J (1 - iK_{n'n'}^J) + iK_{cn'}^J K_{n'n}^J] / [(1 - iK_{nn}^J)(1 - iK_{n'n'}^J) + (K_{n'n}^J)^2] \quad (1.8.40)$$

This determines the correspondent dependence of the collision matrix elements in Eq. (I.8.1) and cross sections in Eq. (I.8.6) to Eq. (I.8.9). The two-channel variant is realized practically for $l \geq l$ in non-fissile nuclei, so here for the function $K_{cn}^J(E)$, the RM-approximation in Eq. (I.8.4) can be applied and, for construction of the cross sections only, the elements U_{nn}^J , $U_{n'n'}^J$ and $U_{n'n}^J$ are necessary.

I.9 Pole representation of Cross Sections

The task of the resonance cross sections analysis is obviously finding the resonance parameters of one or another formalism of the reaction theory, and the results must in principle obtain a self-consistent set of **R**-matrix parameters. These parameters characterize directly the compound nucleus states, the probabilities of the decay of those on different channels, and have their own quantitative physical interpretation on the base of nuclear models [1-6,42]. It is important that these parameters are mutually independent real constants and that their transformation to the parameters of other formalisms used in applications is in general unique. The **R**-matrix formalism parameter sets for the major part of reactor elements, which reproduce the detailed energy dependence of cross sections in the whole interval of resolved resonances and presented in nuclear data libraries, are the basic information for the input of the cross sections in the codes for reactor calculations [31,33,35,37].

- a) The rather high requirements to the precision of reactor calculations on the base of recent computer codes undoubtedly inspire the tendency to the most effective use of the information about the evaluated cross sections of reactor elements. The direct input of resonance cross sections in **R**-matrix representation with the evaluated parameters turns out to be practically rather troublesome because of the necessity of the numerical account of Doppler broadening of the resonances and the improbability, in general, of the use in the self-shielding problems of the analytical results obtained for the Breit-Wigner shape of resonances (Ch. IV). Therefore, the formal transformation of the **R**-matrix representation of elements of the collision matrix $U_{cn}(E)$ to the pole form, leading at the end to cross sections in the form of the sum of resonances with energy-independent parameters, is, by our opinion, rather useful in application procedure for correct input of the evaluated data for resonances.

The transformation scheme for the resonance part of the collision matrix elements G_{cn}^J to the meromorphic function in the momentum domain $\sqrt{E}$ has been considered earlier (see Section I.7), and formally this is solving the problem of pole representation. The fact that the external penetrability factors $P_n(E)$ in cross section formulae in Eq. (I.8.6) to Eq. (I.8.9) (and the factors of potential scattering $\exp(-\varphi_l + \rho)$ too) are meromorphic functions of $\rho = (a\sqrt{2\mu}/\hbar)\sqrt{E}$, gives the possibility of cross section transformation to the simplest forms of the resonance dependence, universal for different l [35]. In fact, the product $G_{nn}P_n$ in the expression for the total cross section in Eq. (I.8.6) can obviously be presented into the form similar to Eq. (I.7.29):

$$G_{nn}P_n = \rho \sum_{k=1}^{2N+2l} \frac{\tilde{\rho}_k^{nn}}{q_k - \sqrt{E}}, \quad (I.9.1)$$

where the factors $\tilde{\rho}_k^{nn}$ are determined by the same way as ρ_k^{nn} in Eq. (I.7.30), but for the polynomial

$$\tilde{\rho}_{2N-2+2l}^{nn}(E) = \rho^{2l} \sum_{\lambda=1}^N \tilde{\gamma}_{\lambda n}^2 \prod_{\lambda' \neq \lambda} (\tilde{\epsilon}_{\lambda'} - E), \quad \rho = (a\sqrt{2\mu} / \hbar) \sqrt{E} \quad (I.9.2)$$

Then the total cross section can be written in the form:

$$\sigma(E) = \sigma_p + \frac{1}{\sqrt{E}} \sum_J \sum_{k=1}^{2N_J+2l} \operatorname{Re} \left[-ie^{-2i\varphi_n} \frac{r_k^n}{q_k - \sqrt{E}} \right], \quad (I.9.3)$$

where

$$r_k^n = \frac{4\pi a \hbar}{\sqrt{2\mu}} g(J) \tilde{\rho}_k^{nn} \quad (I.9.4)$$

The pole representation for reaction (n, x) - fission and radiative capture cross sections in Eq. (I.8.7) follows from the corresponding representation for the product

$$G_{cn} P_n^{1/2} = G_{cn} \rho^{(2l+1)/2-1} \phi_l \left(\frac{\phi_l}{\phi_l^*} \right)^{1/2} = \rho^{1/2} \sum_{k=1}^{2N+2l} \frac{\tilde{\rho}_k^{cn}}{q_k - \sqrt{E}} \left(\frac{\phi_l}{\phi_l^*} \right)^{1/2}, \quad (I.9.5)$$

where the factors $\tilde{\rho}_k^{cn}$ are determined according to Eq. (I.7.30) for the polynomial

$$\tilde{\rho}_{2N-2+2l}^{cn}(E) = \rho^l \phi_l^* \sum_{\lambda=1}^N \tilde{\gamma}_{\lambda n}^2 \prod_{\lambda' \neq \lambda} (\tilde{\epsilon}_{\lambda'} - E), \quad (I.9.6)$$

and the ratio ϕ_l / ϕ_l^* is the phase multiplier and it is not important in finding the module square in Eq. (I.8.7). Then

$$\begin{aligned} \sigma_x(E) &= \frac{4\pi}{k^2} \rho \sum_J g(J) \sum_{c(x)} P_c \left| \sum_{k=1}^{2N_J+2l} \frac{\tilde{\rho}_k^{cn}}{q_k - \sqrt{E}} \right|^2 \\ &= \frac{1}{\sqrt{E}} \sum_J g(J) \sum_{k=1}^{2N_J+2l} \operatorname{Re} \left[-i \frac{r_k^x}{q_k - \sqrt{E}} \right] \end{aligned} \quad (I.9.7)$$

where

$$r_k^x = \frac{8\pi a\hbar}{\sqrt{2\mu}} g(J) \sum_{c(x)} P_c \tilde{\rho}_k^{cn} \sum_{k'} \frac{i\tilde{\rho}_k^{cn*}}{q_{k'}^* - q_k} . \quad (I.9.8)$$

The sum over J is related here to the different independent systems of the states $(J\pi)$, and practically Eq. (I.9.7) is one common sum of all polynomials in the momentum domain.

The multilevel representation of the cross sections in the pole form in Eq. (I.9.3) and Eq. (I.9.7) corresponds to the sum of one-level terms with energy independent parameters - the poles q_k and residues r_k^n and r_k^x (see Section I.4). Let us notice that the number of poles for the separate system $(J\pi)$ with $l \geq 0$ in reality is smaller by l (i.e., $2N_J + l$), which is obvious for the reaction cross section in Eq. (I.9.7), where the polynomial $\tilde{\rho}_{2N-2+2l}^{cn}$ in Eq. (I.9.6) and the denominator Q_{2N+2l} in Eq. (I.7.27) contain a common multiplier ϕ_l^* . We have chosen here methodically the variant enlarged on k for the formal equality of the pole number in the reaction cross section and the total cross section in Eq. (I.9.3). However, taking into consideration that:

$$e^{-2i\phi_l} = e^{-2i\rho} (-1)^l \phi_l^* / \phi_l \quad (\rho = ka) \quad (I.9.9)$$

(Appendix I.A1), the expression for the diagonal element of the collision matrix in Eq. (I.8.31) for $l \geq 1$ can be transformed into the form:

$$U_{nn}^J = e^{-2i\rho} (-1)^l \frac{\phi_l^*(\rho) - i\rho^2 \phi_{l-1}^*(\rho) \Re_{nn}^J}{\phi_l(\rho) + i\rho^2 \phi_{l-1}(\rho) \Re_{nn}^J} = e^{-2i\rho} \frac{\tilde{Q}_{2N+l}(-\rho)}{\tilde{Q}_{2N+l}(\rho)} , \quad (I.9.10)$$

where

$$\tilde{Q}_{2N+l} = (\phi_l^*)^{-1} Q_{2N+2l} = (a\sqrt{2\mu} / \hbar) \prod_{k=1}^{2N_J+l} (q_k - \sqrt{E}) \quad (I.9.11)$$

does not contain (unlike Eq. I.7.28) the cofactors determined by the roots of polynomial $\phi_l^*(\sqrt{E}) = 0$. We will have as a result an expression of the kind:

$$U_{nn}^J = e^{-2i\rho} \prod_{k=1}^{2N_J+l} \frac{q_k + \sqrt{E}}{q_k - \sqrt{E}} , \quad (I.9.12)$$

where the product can be presented as a sum of $2N_J + l$ pole terms.

- b) This expression in the form of Eq. (I.9.12) is interesting for the following procedure of separation of the complete set of the poles to the “physical” ones - corresponding to the observed resonances and the remaining, which are forming the background dependent smoothly on the energy -

potential scattering, in our case. In fact, let us select N_1 resonant terms in the product in Eq. (I.9.12) ($1 < k < N_1$), then

$$U_{nn}^J = e^{-2i\varphi_n} \prod_{k=1}^{N_1} \frac{q_k + \sqrt{E}}{q_k - \sqrt{E}} = e^{-2i\varphi_n} \left[\prod_{k=1}^{N_1} \frac{q_k - \sqrt{E}}{q_k + \sqrt{E}} + \frac{\prod_{k=1}^{N_1} (q_k + \sqrt{E})^2 - \prod_{k=1}^{N_1} (q_k - \sqrt{E})^2}{\prod_{k=1}^{N_1} (q_k^2 - E)} \right], \quad (\text{I.9.13})$$

where

$$e^{-2i\varphi_n} = e^{-2i\rho} \prod_{k=N_1+1}^{2N_1+1} \frac{q_k + \sqrt{E}}{q_k - \sqrt{E}} \quad (\text{I.9.14})$$

does not contain the poles in the resonance region and the determined phases φ_n are the smooth functions of energy, although possibly complex. In our representation of the sum over k in Eq. (I.9.13), where are included the terms with $\text{Re}(q_k) > 0$, the first term in the parenthesis is not resonant and the second corresponds to the poles in the energy space at $q_k^2 = \mu_k - i\nu_k$. Let us notice that the numerator here is the polynomial with odd degrees on $\sqrt{E}$ so that

$$\prod_{k=1}^{N_1} (q_k + \sqrt{E})^2 - \prod_{k=1}^{N_1} (q_k - \sqrt{E})^2 = 2\sqrt{E}\wp(E), \quad (\text{I.9.15})$$

where $\wp(E)$ is a polynomial on the degrees of E . The following expansion of the last term to the simple fractions offers the possibility to present U_{nn}^J in the usual form:

$$U_{nn}^J = U_{nn}^{J0} + i\sqrt{E}e^{-2i\varphi_n} \sum_{k=1}^{N_1} \frac{\bar{\rho}_k^n}{q_k^2 - E}, \quad (\text{I.9.16})$$

where

$$U_{nn}^{J0} = e^{-2i\varphi_n} \prod_{k=1}^{N_1} \frac{q_k - \sqrt{E}}{q_k + \sqrt{E}} \quad (\text{I.9.16})$$

is the non-resonant background part of the diagonal element and

$$\bar{\rho}_k^n = \wp(q_k^2) / \left[\frac{d}{dE} \prod_{k'=1}^{N_1} (q_{k'}^2 - E) \right]_{E=q_k^2}. \quad (\text{I.9.17})$$

Finally, we come to the total cross section formula as a superposition of the pole terms in the energy space and similar to Eq. (I.8.14):

$$\sigma(E) = \sigma'_p + \frac{1}{\sqrt{E}} \sum_J \sum_{k=1}^{N_{IJ}} \operatorname{Re} \left[-ie^{-2i\varphi_0} \frac{g_k + ih_k}{\mu_k - E - i\nu_k} \right] \quad (I.9.18)$$

where

$$\sigma'_p = \frac{2\pi}{k^2} \sum_J g(J) [1 - \operatorname{Re}(U_{nn}^{J0})] \quad (I.9.19)$$

and

$$g_k + ih_k = (\pi\hbar^2 / \mu) \bar{\rho}_n^n g(J), \quad \mu_k - i\nu_k = q_k^2. \quad (I.9.20)$$

Although this expression coincides with the AA approximation results in Eq. (I.8.14), here the parameters do not depend rigorously on energy, and their mutual consistency is established by our scheme of transformation from **R**-matrix formalism to the pole (in momentum domain) expansion.

The separation of N_{IJ} physical resonances in the reaction σ_x cross section in Eq. (I.9.7) leads to the formula of the kind in Eq. (I.8.16):

$$\sigma_x(E) = \sigma_x^0 + \frac{1}{\sqrt{E}} \sum_J \sum_{k=1}^{N_{IJ}} \operatorname{Re} \left[-i \frac{g_k^x + ih_k^x}{\mu_k - E - i\nu_k} \right] \quad (I.9.21)$$

with the background part

$$\sigma_x^0 = \frac{1}{\sqrt{E}} \sum_J \operatorname{Re} \left[-i \left(\sum_{k=1}^{N_{IJ}} \frac{r_k^x}{(-q_k) - \sqrt{E}} + \sum_{k=N_{IJ}+1}^{2N_J+1} \frac{r_k^x}{q_k - \sqrt{E}} \right) \right] \quad (I.9.22)$$

determined by the “external” poles and

$$g_k^x + ih_k^x = 2q_k r_k^x. \quad (I.9.23)$$

By self-consistent choice of the background and resonant parts of the cross section and with the requirement of unitary property for collision matrix (Appendix I.A3), the expression in Eq. (I.9.21) is mathematically identical to the **R**-matrix one in Eq. (I.8.36). Both expressions keep the properties of positiveness and boundedness by the unitary condition.

More cumbersome, but similar in principle, is the scheme of transformation of **R**-matrix expressions for the cross sections in Eq. (I.8.6) and Eq. (I.8.7) to the pole form in Eq. (I.9.18) and Eq. (I.9.21) in the case

of two neutron channels for level systems ($J\pi$) with $l \geq 1$ (see Section I.7.d).

I.9.1 Appendix I.A1 Outgoing Wave Functions and Their Boundary Factors

The outgoing wave functions O_l are defined in Eq. (I.1.4) as linear combinations of the spherical Bessel functions $j_l(\rho)$ and $n_l(\rho)$,

$$O_l(\rho) = -\rho[n_l(\rho) - ij_l(\rho)] \quad (\rho = kr) \quad (\text{I.A1.1})$$

These correspond to the outgoing waves in neutron channels and determine both the logarithmic derivatives for these channels at the nuclear radius $r = a$ in Eq. (I.1.16):

$$L_l = [\rho O'_l(\rho) / O_l(\rho)]_{\rho=ka},$$

and the phases of neutron scattering by hard sphere in Eq. (I.1.13):

$$\exp(-2i\phi_l) = (I_l / O_l)_{r=a} = (O_l^* / O_l)_{r=a}.$$

For $l = 0$, using the spherical Bessel functions, the wave function and the factors at the boundary of nucleus can be obtained as

$$O_0(\rho) = e^{i\rho}, \quad L_0 = (i\rho)_{r=a} = ika, \quad \phi_0 = (\rho)_{r=a} = ka. \quad (\text{I.A1.2})$$

The functions for higher moments $l \geq 1$ can be obtained using the recurrent relations [13]

$$O_l = (l / \rho) O_{l-1} - O'_{l-1}, \quad l O_l + \rho O'_l = \rho O_{l-1}, \quad (\text{I.A1.3})$$

and the corresponding relation for logarithmic derivatives

$$L_l + l = \rho^2 / (l - L_{l-1}), \quad (\rho = ka). \quad (\text{I.A1.4})$$

The wave function $O_l(\rho)$ in Eq. (I.A1.1) can be written in the form

$$O_l(\rho) = e^{i\rho} (i / \rho)^l \phi_l(\rho), \quad (\text{I.A1.5})$$

where ϕ_l is a l -th order polynomial of ρ given by

$$\begin{aligned}\phi_0 &= 1, \quad \phi_1 = -i - \rho, \quad \phi_2 = -3 + 3i\rho + \rho^2, \\ \phi_3 &= 15i + 15\rho - 6i\rho^2 - \rho^3, \quad \phi_l + i(2l-1)\phi_{l-1} = \rho^2\phi_{l-2} \quad (l \geq 2)\end{aligned}\tag{I.A1.6}$$

Correspondingly, the relation for logarithmic derivatives is given by

$$L_l + l = [i\rho + \rho\phi'_l / \phi_l]_{r=a} = [-i\rho^2\phi_{l-1} / \phi_l]_{r=a},\tag{I.A1.7}$$

which is the ratio of two polynomials in $\rho = ka$ ($\sim \sqrt{E}$) of degree $l+1$ to l with complex coefficients. The polynomials $\phi_l(\rho)$ in Eq. (I.A1.6) can be written in terms of its roots as

$$\phi_l(\rho) = \prod_{p=1}^l (\rho_p^{(l)} - \rho)\tag{I.A1.8}$$

with

$$\rho^{(1)} = -i, \quad \rho_{1,2}^{(2)} = -\frac{3}{2}i \pm \frac{\sqrt{3}}{2}, \quad \rho_1^{(3)} = -2.3222i, \quad \rho_{2,3}^{(3)} = \pm 1.7544 - 1.8389i$$

The logarithmic derivative in Eq. (I.A1.7) can be represented as a partial fraction expansion in $\rho = ka$ ($\propto \sqrt{E}$) as

$$L_l + l = i\rho \left[1 + i \sum_{p=1}^l \frac{1}{\rho_p^{(l)} - \rho} \right]\tag{I.A1.9}$$

or

$$L_l = i\rho - \sum_{p=1}^l \frac{\rho_p^{(l)}}{\rho_p^{(l)} - \rho}\tag{I.A1.10}$$

Therefore, the logarithmic derivatives for $l = 1, 2, 3$ can be obtained as

$$\begin{aligned}
L_1 + 1 &= \frac{\rho^2 + i\rho^3}{1 + \rho^2} = i\rho \left[1 + i \frac{1}{(-i) - \rho} \right], \\
L_2 + 2 &= \frac{\rho^2(3 + 2\rho^2 + i\rho^3)}{9 + 3\rho^2 + \rho^4} = i\rho \left[1 - i \frac{2\rho + 3i}{\rho^2 + 3i\rho - 3} \right] = i\rho \left[1 + i \sum_{p=1}^2 \frac{1}{\rho_p^{(2)} - \rho} \right], \\
L_3 + 3 &= \frac{\rho^2(45 + 12\rho^2 + 3\rho^4 + i\rho^5)}{225i + 45\rho^2 + 6\rho^4 + \rho^6} = i\rho \left[1 + i \frac{3\rho^2 + 12i\rho - 15}{15i + 15\rho - 6i\rho^2 - \rho^3} \right] \\
&= i\rho \left[1 + i \sum_{p=1}^3 \frac{1}{\rho_p^{(3)} - \rho} \right]
\end{aligned}$$

Substituting $\rho = ka = c\sqrt{E}$ and $\rho_p^{(l)} = c\sqrt{\varepsilon_p^{(l)}}$, where E is the laboratory energy of neutron in eV and $c = 2.2 \times 10^{-4} aA / (A+1)$ with the mass ratio A of target nucleus and neutron and the radius of nucleus a in units of 10^{-13} cm, we obtain the corresponding expansion over the variable $\sqrt{E}$ in the form:

$$L_l(\sqrt{E}) + l = ic\sqrt{E} \left[1 + ic^{-1} \sum_{p=1}^l \frac{1}{\sqrt{\varepsilon_p^{(l)}} - \sqrt{E}} \right], \quad (\text{I.A1.11})$$

and the relation in Eq. (I.A1.7) can be written as

$$L_l(\sqrt{E}) + l = \left[ic\sqrt{E} + \frac{\sqrt{E}}{\phi_l(\sqrt{E})} \frac{d}{d\sqrt{E}} \phi_l(\sqrt{E}) \right] = -ic^2 E \phi_{l-1}(\sqrt{E}) / \phi_l(\sqrt{E}). \quad (\text{I.A1.12})$$

The Wronskian of the pair of complex conjugate solutions $O_l(\rho)$ and $I_l(\rho) = O_l^*(\rho)$ is

$$I_l(\rho)O_l'(\rho) - I_l'(\rho)O_l(\rho) = 2i, \quad (\text{I.A1.13})$$

which follows from the Wronskian of the spherical Bessel functions [13]

$$j_l(\rho)n_l'(\rho) - n_l(\rho)j_l'(\rho) = \rho^{-2}. \quad (\text{I.A1.14})$$

By using (I.A1.13), we have for the penetrability factors:

$$P_l = \text{Im} \left(\rho \frac{O_l'}{O_l} \right)_{\rho=ka} = \frac{\rho}{I_l O_l} \bigg|_{\rho=ka} = \frac{\rho^{2l+1}}{\phi_l(\rho)\phi_l^*(\rho)} \bigg|_{\rho=ka}, \quad (\text{I.A1.15})$$

The level shift factors are expressed through the functions $\phi_l(\rho)$ as

$$S_l + l = \text{Re} \left(\rho \frac{O'_l}{O_l} \right) = \frac{1}{2} \rho \left(\frac{\phi'_l}{\phi_l} + \frac{\phi_l^{*'}}{\phi_l^*} \right) \quad (\text{I.A1.16})$$

and using the definition $L_l = S_l + iP_l$ and Eq. (I.A1.7), another relation between the functions $\phi_l(\rho)$ can be obtained as

$$\phi'_l \phi_l^* - \phi_l \phi_l^{*'} = 2i(\rho^{2l} - \phi_l \phi_l^*) \quad (\text{I.A1.17})$$

which corresponds to the Wronskian in Eq. (I.A1.13).

The scattering phases can also be written in terms of $\phi_l(\rho)$ functions as

$$e^{-2i\varphi_l} = \left(\frac{I_l}{O_l} \right) = (-1)^l e^{-2i\rho} \frac{\phi_l^*(\rho)}{\phi_l(\rho)} \quad (\text{I.A1.18})$$

or

$$\tan(\varphi_l - \rho + \pi l / 2) = \text{Im}(\phi_l) / \text{Re}(\phi_l) \quad (\text{I.A1.19})$$

which leads to the known phase relations (Table I.1):

$$\begin{aligned} \tan(\rho - \varphi_1) &= \rho, \quad \tan(\rho - \varphi_2) = 3\rho / (3 - \rho^2), \\ \tan(\rho - \varphi_3) &= \rho(15 - \rho^2) / (15 - 6\rho^2). \end{aligned} \quad (\text{I.A1.20})$$

I.9.2 Appendix I.A2 Doppler Functions

Let us find the energy distribution function for the relative motion of neutrons $S(E', E)$ in the relation in Eq. (I.5.4) for the Maxwellian distribution of the atomic thermal motion velocities in the medium from the common scheme of averaging the reaction rates in Eq. (I.5.3):

$$v\sigma_x(v, T) = 2\pi \int_0^\infty du u^2 \int_{-1}^1 d(\cos \theta) W \sigma_x(W) \left(\frac{M}{2\pi kT} \right)^{3/2} \exp \left(-\frac{M}{2kT} u^2 \right) \quad (\text{I.A2.1})$$

where

$$W^2 = |\vec{v} - \vec{u}|^2 = v^2 - 2uv \cos \theta + u^2. \quad (\text{I.A2.2})$$

Transforming the integration from the cosine of polar angle to the variable W yields

$$v\sigma_x(v, T) = \frac{2\pi}{v} \int_0^\infty du u \int_{|v-u|}^{v+u} dW W^2 \sigma_x(W) \left(\frac{M}{2\pi kT} \right)^{3/2} \exp\left(-\frac{M}{2kT} u^2 \right)$$

By changing the order of integration, we obtain

$$\begin{aligned} v\sigma_x(v, T) &= \frac{2\pi}{v} \left(\frac{M}{2\pi kT} \right)^{3/2} \int_0^\infty dW W^2 \sigma_x(W) \int_{|W-v|}^{W+v} du u \exp\left(-\frac{M}{2kT} u^2 \right) \\ &= \int_0^\infty dW \sigma_x(W) S(W, v) \end{aligned} \quad (\text{I.A2.3})$$

where

$$S(W, v) = \left(\frac{M}{2\pi kT} \right)^{1/2} \frac{W^2}{v} \left\{ \exp\left[-\frac{M}{2kT} (W-v)^2 \right] - \exp\left[-\frac{M}{2kT} (W+v)^2 \right] \right\} \quad (\text{I.A2.4})$$

is the distribution function of the relative motion velocities W at the neutron velocity v in the Lab system. We will have for the corresponding energies in the center of mass system:

$$\sqrt{E} \sigma_x(E, T) = \int_0^\infty dE' \sqrt{E'} \sigma_x(E') S(E', E) \quad (\text{I.A2.5})$$

where

$$S(E', E) = \frac{1}{2\sqrt{\pi E} \delta} \left\{ \exp\left[-\frac{(\sqrt{E} - \sqrt{E'})^2}{\delta^2} \right] - \exp\left[-\frac{(\sqrt{E} + \sqrt{E'})^2}{\delta^2} \right] \right\}$$

and $\delta^2 = \mu kT / M = kT / (A+1)$. This function is normalized to unity, and in the limit of low energies, where $\sqrt{E} \sigma_x(E) = \text{const}$, it preserves the reaction rate and the cross section does not depend on the temperature.

I.9.3 Appendix I.A3 Unitary Property of U-Matrix

The basic relation for **U**-matrix is unitary and symmetric by definition due to the symmetry and reality of the **R**-matrix in Eq. (I.3.14). In the representation using the level matrix A in Eq. (I.3.22), these properties must be fulfilled for the matrix [38]

$$W = 1 + i(\Gamma^{1/2})' A^{-1} \Gamma^{1/2}, \quad (\text{I.A3.1})$$

where $\Gamma^{1/2}$ is a $\lambda \times c$ rectangular matrix with the elements $\Gamma_{\lambda c}^{1/2} = \sqrt{2P_c} \gamma_{\lambda c}$ and $(\Gamma^{1/2})'$ is the transposed matrix in Eq. (I.3.26). The condition $WW^+ = 1$ gives

$$(\Gamma^{1/2})' [A^{-1} - (A^*)^{-1}] \Gamma^{1/2} = i(\Gamma^{1/2})' A^{-1} \Gamma^{1/2} (\Gamma^{1/2})' (A^*)^{-1} \Gamma^{1/2} \quad (\text{I.A3.2})$$

Using the identity

$$A^{-1} - (A^*)^{-1} = A^{-1} (A^* - A) (A^*)^{-1}$$

we will have

$$A^* - A = i\Gamma^{1/2} (\Gamma^{1/2})', \quad \left[A_{\lambda\mu}^* - A_{\lambda\mu} = i \sum_c \Gamma_{\lambda c}^{1/2} \Gamma_{\mu c}^{1/2} \right], \quad (\text{I.A3.3})$$

which corresponds to the A -matrix definition in Eq. (I.3.22).

In the formalism of Kapur-Peierls, is used the diagonalized level matrix in Eq. (I.3.27)

$$\tilde{\varepsilon} - E = T' A T, \quad [A = T(\tilde{\varepsilon} - E) T'] \quad (\text{I.A3.4})$$

where T is the matrix of the orthogonal complex transformation $T T' = 1$. Let us write the relation in Eq. (I.A3.3) as

$$T' A^* T^* - T' A T^* = iT' \Gamma^{1/2} (\Gamma^{1/2})' T^*.$$

Then, from the definition in Eq. (I.3.30), $\tilde{\Gamma}^{1/2} = T' \Gamma^{1/2}$, we will have

$$T' T^* \tilde{\varepsilon}^* - \tilde{\varepsilon} T' T^* = i \tilde{\Gamma}^{1/2} (\tilde{\Gamma}^{1/2})' \quad (\text{I.A3.5})$$

or

$$(T' T^*)_{kk'} = i \sum_c \tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{k'c}^{1/2*} / (\tilde{\varepsilon}_{k'}^* - \tilde{\varepsilon}_k)$$

Let us multiply then the both parts of this equation by $\tilde{\Gamma}_{k'n}^{1/2*}$ and summarize over k' . Then we obtain the relation between the parameters of the formalism [18,38]:

$$\tilde{\Gamma}_{kn}^{1/2} = i \sum_{k'} \sum_c \tilde{\Gamma}_{k'n}^{1/2*} \tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{k'c}^{1/2*} / (\tilde{\varepsilon}_{k'}^* - \varepsilon_k) , \quad (\text{I.A3.6})$$

which corresponds to the U -matrix unitary property. In the Reich-Moore approximation in Eq. (I.7.18), the reduced U^{++} matrix is no longer unitary, but the identity in Eq. (I.A3.4) is kept. In the special case of equal radiative widths of the levels, $\Gamma_{\lambda\gamma} = \Gamma_{\gamma}$, the relation in Eq. (I.A3.6) comes to the form:

$$\tilde{\Gamma}_{kn}^{1/2} = i \sum_{k'} \sum_c \tilde{\Gamma}_{k'n}^{1/2*} \tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{k'c}^{1/2*} / (\tilde{\varepsilon}_{k'}^* - \varepsilon_k - i\Gamma_{\gamma}) , \quad (\text{I.A3.7})$$

where the summation over c includes here only the channels remaining after the exclusion of radiative channels. In the general case, however, the transformation matrix and the relations in Eq. (I.A3.6) and Eq. (I.A3.7) depend on energy. These are relations between energy independent parameters only in Adler approximation, where $\tilde{\Gamma}_{kn} = 2P_n \tilde{\gamma}_{kn}^2$ and $\varepsilon_k = \mu_k - i\nu_k = \text{const}$ [18,36].

Let us consider the consequences of the unitary property of collision matrix in the scheme with excluded reaction channels (see Section I.7). With the most general representation in Eq. (I.3.18), we have

$$W^{++} = 1 + 2i(P^+)^{1/2} G^{++} (P^+)^{1/2}, \quad W^{+-} = 2i(P^+)^{1/2} G^{+-} (P^-)^{1/2} = (W^{-+})' \quad (\text{I.A3.8})$$

Then, from the unitary condition $|W^{++}|^2 + |W^{+-}|^2 = 1$, the equivalent relation between the cells of $\mathbf{G}$ -matrix in Eq. (I.7.7) can be found:

$$G^{++} - (G^{++})^* = 2i[G^{++} P^+ (G^{++})^* + G^{+-} P^- (G^{++})^*] . \quad (\text{I.A3.9})$$

Using the expressions in Eq. (I.7.10) for G^{++} and G^{+-} , we obtain the relation between the cells of the reduced $\mathfrak{R}$ -matrix:

$$\mathfrak{R}^{++} - (\mathfrak{R}^{++})^* = 2i\mathfrak{R}^{+-} P^- (\mathfrak{R}^{-+})^*, \quad \text{Im } \mathfrak{R}_{nn} = \sum_{c \neq n} P_c |\mathfrak{R}_{cn}|^2 \quad (\text{I.A3.10})$$

to the corresponding definition in $\mathbf{R}$ -matrix form in Eq. (I.7.11):

$$\begin{aligned} \mathfrak{R}^{++} &= (\gamma^+)' B^{-1} \gamma^+, \quad \mathfrak{R}^{+-} = (\gamma^+)' B^{-1} \gamma^-, \\ B &= \varepsilon - E - \frac{i}{2} (\Gamma^-)^{1/2}, \quad (\Gamma^-)^{1/2} = \gamma^- \sqrt{2P^{-1}} \end{aligned} \quad (\text{I.A3.11})$$

In the RM-approximation, where the group of channels $(-)$ is related to the radiation capture, and the remaining channels $(+)$ are neutron and fission ones, so this relation is reduced to the identity similar to Eq. (I.A3.3)

$$B_{\lambda\mu}^* - B_{\lambda\mu} = i\Gamma_{\lambda\gamma}\delta_{\lambda\mu}, \quad [(\Gamma^-)^{1/2}\{(\Gamma^-)^{1/2}\}']_{\lambda\mu} = \Gamma_{\lambda\gamma}\delta_{\lambda\mu}. \quad (\text{I.A3.12})$$

For the version with exclusion of all reaction channels $c \neq n$ (see Section 1.7.c), using in the case of fissile nuclei the representation with diagonalized level matrix in Eq. (1.7.20):

$$\bar{T}'B\bar{T} = \bar{\varepsilon} - E, \quad \Re_{cn} = \sum_{k=1}^N \tilde{\gamma}_{kc}\tilde{\gamma}_{kn} / (\bar{\varepsilon}_k - E), \quad \tilde{\gamma}_{kc} = (\bar{T}'\gamma)_{kc}$$

the condition in Eq. (I.A3.10) leads to the relation between the parameters similar to Eq. (I.A3.6):

$$\tilde{\gamma}_{kn} = i \sum_{k'} \sum_c \tilde{\gamma}_{k'n}^* \tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{k'c}^{1/2*} / (\tilde{\varepsilon}_{k'}^* - \varepsilon_k) , \quad (\text{I.A3.13})$$

or with the supposition of equal radiative widths $\Gamma_{\lambda\gamma} = \Gamma_{\gamma}$

$$\tilde{\gamma}_{kn} = i \sum_{k'} \sum_{c(f)} \tilde{\gamma}_{k'n}^* \tilde{\Gamma}_{kc}^{1/2} \tilde{\Gamma}_{k'c}^{1/2*} / (\tilde{\varepsilon}_{k'}^* - \varepsilon_k - i\Gamma_{\gamma}) \quad (\text{I.A3.14})$$

with the summation only over the fission channels $c(f)$. However, unlike Kapur-Peierls scheme in Eq. (I.A3.6), the relations in Eq. (I.A3.13) and Eq. (I.A3.14) do not depend on energy and have the role of sum rules for the resonance parameters determined directly in the combined method (see Section 1.8.d).

For the pole representation in momentum domain, the unitary condition in the form in Eq. (I.A3.9) permits also to establish the similar summation rules for parameters. This condition can be rewritten as

$$G_{nn} - G_{nn}^* = 2i \left[G_{nn} P_n G_{nn}^* + \sum_{c \neq n} G_{cn} P_c G_{cn}^* \right] \quad (\text{I.A3.15})$$

Using the definition in Eq. (1.7.29)

$$G_{cn} = \sum_k \frac{\rho_k^{cn}}{q_k - \sqrt{E}}, \quad (\text{I.A3.16})$$

the summand in the last term in Eq. (I.A3.15) can be presented as

$$G_{nc} P_c G_{cn}^* = \sum_k \frac{\rho_k^{cn}}{q_k - \sqrt{E}} \sum_{k'} \frac{(\bar{\rho}_{k'}^{cn})^*}{q_{k'}^* - q_k} + conj, \quad (\text{I.A3.17})$$

where $\bar{\rho}_{cn}^k = \rho_{cn}^k P_c$ do not depend on energy. The first term in the right part of Eq. (I.A3.15), containing $P_n(E)$, can be transformed into the form:

$$G_{nn} P_n G_{cn}^* = \sum_k \frac{\bar{\rho}_k^{nn}}{q_k - \sqrt{E}} \sum_{k'} \frac{(\bar{\rho}_{k'}^{nn})^*}{q_{k'} - q_k} + conj, \quad (I.A3.18)$$

where $\bar{\rho}_k^{nn} = \rho_k^{nn} \sqrt{P_n(q_k)} [\phi_l^*(q_k) / \phi_l(q_k)]^{1/2}$. Here we used the scheme of determination of ρ_k^{nn} in Eq. (I.7.26) and Eq. (I.7.30) and $P_n(E)$ in Eq. (I.A1.15). This way to our unitary condition in Eq. (I.A3.15) corresponds to the following summation rule:

$$\rho_k^{nn} = 2i \sum_c \bar{\rho}_k^{cn} \sum_{k'} (\bar{\rho}_{k'}^{cn})^* / (q_{k'}^* - q_k) \quad (I.A3.19)$$

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Chapter II UNRESOLVED RESONANCES

In the time-of-flight measurements for the energies higher than ~ 1 KeV for heavy nuclei and ~ 100 KeV for medium mass nuclei, the resolution function ($\sim E^{3/2}$) becomes so wide that it exceeds the spacing between the compound resonances and the identification of the single resonances is no longer possible. Despite the lack of direct information about the resonance structure of cross sections, it evidently exists and appears indirectly, e.g., in the data of transmission measurements through the relatively thick samples (see Chapter III).

The unresolved resonance region amasses the essential part of the neutron spectrum in the reactors, especially in the fast neutron reactors. Therefore the investigations of the resonance self-shielding effects in this region is of practical interest and a number of calculating schemes and methods are developed here, using the model presentation for the resonance structure of cross sections.

Unlike the resolved range, we cannot determine the parameters of single resonances, using the common results of the formal theory of resonance reactions for description of the cross sections in the unresolved region, and the only possible variant for this is passing to statistical interpretation. The statistical theory of compound processes forms a rather wide and developing part of nuclear reaction physics in low and intermediate energies. Unlike the resolved resonances, where the parameters have in general the phenomenological sense, the average cross sections in the statistical theory are interpreted on the base of the particular nuclear models and serve for the physical justification of those [4-6,7]. Evidently, the consideration of the average cross sections is touching rather a large volume of nuclear physics problems and fall outside the limits of our practical applications. Therefore, we will present here only the results, referring directly to the self-shielding problems in the unresolved region, not turning our attention explicitly to the methods of obtaining those in the statistical reaction theory.

For our applications are necessary not only the average cross sections, but mainly different averages of the resonance cross sectional functionals, such as the transmission $\langle \exp(-n\sigma) \rangle$, the effective resonance integral $\langle \sigma_a / \sigma \rangle$ and so on. The consecutive solution in the frame of the common schemes of the statistical theory is rather cumbersome and it is hardly necessary for the practical purposes. Finally, it is sufficient for us to model the resonance structure of cross sections in the averaging interval (resonance ladder) reproducing the necessary average cross sectional functional with required accuracy, including the average cross sections themselves. Therefore, the model must reflect the main peculiarities of the resonance dependence, the interference ones in particular, to which our functionals are rather sensitive, beginning with averaging from the known statistical theory, to average

cross sections formulae with corresponding parameters. Let us note, however, that the self-shielding is significant only for relatively low energies up to ~ 100 KeV in heavy nuclei and ~ 1 MeV in medium, and moreover below the threshold of inelastic scattering as a rule. Therefore, practical interest focuses on the results of average cross sections theory in the region of weakly overlapping resonances $\bar{\Gamma} \ll D$ at small number of reaction channels of the reduced collision matrix (RM-approximation with a constant radiative width).

II.1 Average Cross Sections

- a) The experimentally determined average cross section $\langle \sigma_\alpha(E) \rangle$ of some reaction α in the energy interval $[E - I/2, E + I/2]$ is the ratio of the area under the cross section curve $\sigma_\alpha(E)$ to the width of the interval:

$$\langle \sigma_\alpha(E) \rangle = \frac{1}{I} \int_{E-I/2}^{E+I/2} \sigma_\alpha(E') dE', \quad (\text{II.1.1})$$

and for a sufficiently large I it does not depend on the resolution function and Doppler broadening. In the average cross sections theory, the averaging over the Cauchy distribution is frequently used:

$$\langle \sigma_\alpha(E) \rangle = \frac{I}{\pi} \int \sigma_\alpha(E') \frac{dE'}{(E' - E)^2 + I^2} \quad (\text{II.1.2})$$

with the integration limits significantly exceeding I . It is possible to choose the Gauss distribution too, which formally is equivalent to the Doppler broadening in multilevel cross section formulae in the asymptotical form of those (as $\Gamma / \Delta \rightarrow 0$).

The application of the statistical methods to the construction of average cross sections implies that the averaging interval contains a sufficiently large number of resonances, i.e. $I \gg D$ (the average resonance spacing). At the same time, this interval must be limited so that the energy dependence of the logarithmic derivatives can be neglected or to use their values averaged over the interval ($I \ll E$). For the medium nuclei this interval can be ~ 100 - 200 KeV and for the heavy ones ~ 100 - 200 eV.

The simplest averaging is performed in the region of single levels, where $\Gamma \ll D$. So, the area under a separate resonance in the cross section $\sigma_\alpha(E)$ in Eq. (I.5.7) is

$$S_\alpha^\lambda = \int_{E_\lambda - D/2}^{E_\lambda + D/2} \sigma_\alpha(E) dE = \frac{\Gamma_{\lambda\alpha}}{2} \sigma_{0\lambda} \int_{-\infty}^{\infty} \Psi(x, \xi_\lambda) dx = \frac{2\pi^2}{k^2} g(J) \sum_n \sum_{c(\alpha)} \frac{\Gamma_{\lambda n} \Gamma_{\lambda c}}{\Gamma_\lambda}, \quad (\text{II.1.3})$$

where the sums over n and $c(\alpha)$ are related to the possible neutron and α -reaction channels that have the total moment J and the parity π of the resonance. Let us next present the cross section in some interval I as a sum of N Breit-Wigner resonances for some possible systems $(J\pi)$. Then the average cross section in Eq. (II.1.2) is

$$\langle \sigma_\alpha(E) \rangle = \frac{1}{I} \sum_{\lambda=1}^N S_\alpha^\lambda \approx \frac{2\pi^2}{k^2} \sum_J g(J) \frac{1}{N(J)} \sum_{\lambda(J)=1}^{N(J)} \sum_n \sum_{c(\alpha)} \frac{\Gamma_{\lambda n} \Gamma_{\lambda c}}{\Gamma_\lambda D_J} \quad (\text{II.1.4})$$

where $D_J = I / N(J)$ is the average spacing between the levels of the given system. The resonance widths (penetrability factors) and kinematical multiplier k^2 are chosen here at the energy E in the center of the averaging interval, which in general is some approximation, and the precision of this is determined by the degree of the smallness of the ratio I / E . Our presentation of the one-level formula in Eq. (I.4.7) with the energy independent parameters shows that this approximation is equivalent to

$$\langle \sqrt{E} \sigma_\alpha(E) \rangle \approx \sqrt{E} \langle \sigma_\alpha(E) \rangle. \quad (\text{II.1.5})$$

Let us pass now to the average resonance parameters in the interval I :

$$\bar{\Gamma}_n^J(E) = \frac{1}{N(J)} \sum_{\lambda(J)=1}^{N(J)} \Gamma_{\lambda n}, \quad \bar{\Gamma}_c^J(E) = \frac{1}{N(J)} \sum_{\lambda(J)=1}^{N(J)} \Gamma_{\lambda c}, \quad \bar{\Gamma}^J = \sum_c \bar{\Gamma}_c^J. \quad (\text{II.1.6})$$

The energy dependence of the average widths is determined by the corresponding factors $P_c(E)$, so the expression for the average cross section in Eq. (II.1.4) can be presented in the form:

$$\langle \sigma_\alpha(E) \rangle = \frac{2\pi^2}{k^2} \sum_J \frac{g(J)}{D_J} \sum_n \sum_{c(\alpha)} \frac{\bar{\Gamma}_n^J(E) \bar{\Gamma}_c^J(E)}{\bar{\Gamma}^J(E)} F_{nc}(E) \quad (\text{II.1.7})$$

where the function

$$F_{nc}(E) = \frac{1}{N(J)} \sum_{\lambda(J)=1}^{N(J)} \frac{\Gamma_{\lambda n} \Gamma_{\lambda c}}{\Gamma_\lambda} / \frac{\bar{\Gamma}_n^J \bar{\Gamma}_c^J}{\bar{\Gamma}^J} \quad (\text{II.1.8})$$

accounts for the effect of the fluctuation of resonance widths in the averaging interval. In statistical consideration of these effects (at $N(J) \geq 10$ in practice), this function is estimated as the integral [8]:

$$F_{nc}(E) = \int_0^\infty \dots \int_0^\infty \frac{x_1 x_2 P_1(x_1) P_2(x_2) \dots}{x_1 b_1 + x_2 b_2 + x_3 b_3 + \dots} dx_1 dx_2 \dots, \quad (\text{II.1.9})$$

where $x_1 = \Gamma_{\lambda n} / \bar{\Gamma}_n^J$, $x_2 = \Gamma_{\lambda c} / \bar{\Gamma}_c^J$, and $x_3 = \Gamma_{\lambda 3} / \bar{\Gamma}_3^J$, $\dots$ are other possible reaction channels, and $b_i = \bar{\Gamma}_i^J / \bar{\Gamma}^J$ is the relative contribution of the i -th channel in the average total width, and $P_i(x_i)$ is the function of Porter-Thomas statistical distribution in Eq. (I.4.11). In our presentation of average cross section in Eq. (II.1.7), where all possible statistically independent reaction channels are selected separately, all functions $P_i(x_i)$ are chosen for $\nu_i = 1$. If widths of various processes, summed over some channels, are considered, then in the corresponding integrals in Eq. (II.1.9) the distributions $P_\nu(x)$ with $\nu > 1$ are used as a rule [9,10]. However, it must be taken into consideration that the distribution

$P_\nu(x)$ corresponds to ν independent channels with an equal relative contribution to the average width. However, for fission, e.g., different average widths are possible in the individual channels, and that changes the corresponding functions of distribution of the summed fission width (see Section II.2). Our averaging method with selection of all possible individual channels accounts for this effect and seems to be adequate.

The manifold integral in Eq. (II.1.9) can be reduced to the one-fold integral for arbitrary ν_i in the channels [9-11]. For our variant with $\nu_i = 1$, we will have:

$$F_{nc}(E) = (1 + 2\delta_{nc}) \int_0^\infty dz \prod_i (1 + 2zb_i)^{-(\delta_m + \delta_{ic} + 1/2)} , \quad (II.1.10)$$

where the product includes all the accounted channels. The part of this product related to the multichannel radiative capture with $b_i \approx \bar{\Gamma}_\gamma / \nu_\gamma \bar{\Gamma} \ll 1$ can be substituted as [10]:

$$\lim_{\nu_\gamma \rightarrow \infty} \prod_{i(\gamma)=1}^{\nu_\gamma} (1 + 2zb_i)^{-1/2} \approx \lim_{\nu_\gamma \rightarrow \infty} (1 + 2z\bar{\Gamma}_\gamma / \nu_\gamma \bar{\Gamma})^{-\nu_\gamma/2} = e^{-z\bar{\Gamma}_\gamma / \bar{\Gamma}} . \quad (II.1.11)$$

Therefore, in a typical example for non-fissile nuclei with one neutron channel and multichannel radiative capture, the corresponding function $F_{nc} = F_\gamma$ in the average cross section $\langle \sigma_\gamma(E) \rangle$ is [8]:

$$F_\gamma = \int_0^\infty dz e^{-z\bar{\Gamma}_\gamma / \bar{\Gamma}} (1 + 2z\bar{\Gamma}_n / \bar{\Gamma})^{-3/2} = (1 + \eta) [1 - (\pi\eta / 2)^{1/2} \exp(\eta/2) \operatorname{erfc}(\sqrt{\eta/2})] \quad (II.1.12)$$

where $\eta = \bar{\Gamma}_\gamma / \bar{\Gamma}_n$ (Fig. II.1). With a precision of ~1%, this function is approximated by the relation [6]:

$$F_\gamma(\eta) \approx \frac{1 + \eta^{1/2} + 0.625\eta^{3/2}}{1 + 2.25\eta^{1/2} + 0.625\eta^{3/2}} . \quad (II.1.13)$$

Figure II. 1 Fluctuation Factor for Multi-Channel Radioactive Capture

The fluctuation effect in the radiative capture cross section for this case:

$$\langle \sigma_\gamma(E) \rangle = \frac{2\pi^2}{k^2} \sum_J \frac{g(J)}{D_J} \frac{\bar{\Gamma}_n^J(E) \bar{\Gamma}_\gamma^J}{\bar{\Gamma}^J(E)} F_\gamma(\bar{\Gamma}_\gamma^J / \bar{\Gamma}_n^J) \quad (\text{II.1.14})$$

leads to a decrease of the capture cross section value in comparison with the variant of identical resonances by 20-30% and is maximal at $\bar{\Gamma}_\gamma^J \approx \bar{\Gamma}_n^J$. For the elastic scattering and fission cross section, similar fluctuation functions can exceed the unit (see Section II.2). The expression for the average total cross section is determined analogically [1-6]:

$$\langle \sigma(E) \rangle = \sigma_p + \frac{2\pi^2}{k^2} \sum_J g(J) \sum_n \frac{\bar{\Gamma}_n^J}{D_J} \cos(2\varphi_n), \quad (\text{II.1.15})$$

where the summation over n refers to different neutron channels (jl) for a given level system ($J\pi$).

The average of cross sections presented as a sum of Breit-Wigner resonances over the Cauchy distribution in Eq. (II.1.2) leads formally to the result in Eq. (I.5.32):

$$\langle \sigma_\alpha(E) \rangle = \sum_{\lambda=1}^N \sigma_{0\lambda} \Gamma_{\lambda\alpha} \frac{\Gamma_{\lambda\alpha} + 2I}{4(E - E_\lambda)^2 + (\Gamma_{\lambda\alpha} + 2I)^2}, \quad (\text{II.1.16})$$

and in the limit $I \gg \bar{D} > \Gamma_\lambda$, i.e., for a statistically large number of terms in the sum over λ , by passing from summation to the integration on dE_λ / D [4], we come finally to the expressions in Eq. (II.1.7) and Eq. (II.1.15). This presentation, however, can turn out to be more convenient in analysis of cross section data in the unresolved region, if we choose I as the width of the experimental function of resolution. Then the observed energy structures in the experimental cross sections can be identified as the effect of anomalously broad resonances in the sum in Eq. (II.1.16) or as statistical fluctuations connected with the irregularity of the level distribution in the interval [12,13,,5,6,7,9]. However, the average cross sections in Eq. (II.1.7) and Eq. (II.1.15) do not depend in fact on the resonance energy distribution and give the values averaged over the experimentally observed energy irregularities. For more exact agreement of the experimental and calculated cross sections here, we introduce the corresponding corrections for energy dependence of the average resonance widths $\bar{\Gamma}_c(E)$ and the physical explanation for this is found in [5,6,9,14] (II.4). For this reason, even in the frame of one-level presentation, the average resonance parameters in Eq. (II.1.6) can differ from the corresponding values, determined from the data in the resolved region and extrapolated proportionally to $P_c(E)$ into the considered energies.

- b) The one-level model of the resonance cross sections in the unresolved region is most interesting for the self-shielding problems in the nuclei ^{238}U , ^{232}Th and many design elements. Practically, in the whole energy interval where this effect is considerable, the one level approximation satisfies the requirements of the reactor calculations. This is more complicated somewhat with the nuclei of fissile elements, where the resonance interference is significant at all energies. However, as a first approximation, taking into account that the self-shielding of fissile nuclei in the unresolved region in the real systems is not practically very significant, so the one-level model with determined correction can be useful here (Ch. IV).

The region of unresolved compound resonances itself has no upper boundary in energy. In the limit of overlapping resonances $\bar{\Gamma} \approx \bar{D}$, or $\langle \sigma_\alpha(E) \rangle \approx \sigma_\alpha(E)$, the statistical interpretation of cross sections does not produce problems of exactly modelling the resonance structure since different variants can lead at the end to equal average cross sections [9]. The main attention is paid to the choice of more physically justified forms of parameterization and methods of deriving parameters. The results obtained by direct averaging of the common multilevel expressions for the cross sections containing the sequential transition from the region of isolated ($\bar{\Gamma} \ll D$) to overlapping resonances [9,10,15] are most interesting for us. Finally, the use for self-shielding analysis of the unresolved region resonance cross section models through picket fence resonance ladders must lead to the same average cross sections, as in the statistical reaction theory.

The procedure of averaging the diagonal element of collision matrix using Eq. (I.2.16) is in principle quite justified in determining the average total cross section. In fact, the averaging (II.1.2) yields:

$$\langle U_{cc}(E) \rangle = \frac{I}{\pi} \int U_{cc}(E') \frac{dE'}{(E - E')^2 + I^2} \approx U_{cc}(E + iI) \quad (\text{II.1.17})$$

This result is obtained by the contour integration method with spreading of the limits on $(E' - E) / I$ from $-\infty$ to ∞ , accounting that $U_{cc}(E')$ has no pole in the upper semicircle [4]. By choosing here the reduced form of the collision matrix (function) with the exclusion of all $c' \neq c$ channels as in Eq. (I.8.1)

and neglecting the energy dependence of logarithmic derivatives $L_c = iP_c (S_c = B_c)$, we will have in the averaging interval:

$$\langle U_{cc}(E) \rangle = e^{-2i\varphi_c} [1 - i \langle \wp_{cc}(E) \rangle P_c(E)]^{-1} [1 + i \langle \wp_{cc}(E) \rangle P_c(E)], \quad (\text{II.1.18})$$

where the average values $\langle \wp_{cc}(E) \rangle$ for the reduced and non-reduced matrices coincide

$$\langle \wp_{cc}(E) \rangle = \langle R_{cc} \rangle = R(E + iI) \approx \sum_{\lambda} \frac{\gamma_{\lambda c}^2}{E_{\lambda} - E - iI}. \quad (\text{II.1.19})$$

In the limit of a large number of terms, the sum can be replaced with the integral on dE_{λ} / D

$$\langle R_{cc}(E) \rangle \approx \int \frac{\tilde{S}_c(E_{\lambda})}{E_{\lambda} - E - iI} dE_{\lambda} = R_c^{\infty}(E) + i\pi \tilde{S}_c(E), \quad (\text{II.1.20})$$

where R_c^{∞} is the real part (main value) of the integral and

$$\tilde{S}_c(E) = \overline{(\gamma_{\lambda c}^2 / D)} \quad (\text{II.1.21})$$

is the imaginary part called the “strength function” in channel c [4]. As has been noticed, the strength functions $\tilde{S}_c(E)$ in the unresolved region can differ from the values determined by the parameters of resolved resonances. An effective method for determination of those gives the complex potential model, the results of which play a fundamental role in the average cross sections theory [15,16,5,7].

Let us write the expression for $\langle U_{cc}(E) \rangle$ in Eq. (II.1.18) with account of Eq. (II.1.20) as

$$\langle U_{cc}(E) \rangle = e^{-2i\varphi_c} \frac{1 + iR_c^{\infty} P_c - \pi \tilde{S}_c P_c}{1 - iR_c^{\infty} P_c + \pi \tilde{S}_c P_c} = e^{-2i(\varphi'_c - i\eta_c)} \quad (\text{II.1.22})$$

where φ'_c is the shape elastic phase shift.

$$\varphi'_c = \varphi_c - \xi_c, \quad \tan(\xi_c + i\eta_c) = R_c^{\infty} P_c + i\pi \tilde{S}_c P_c \quad (\text{II.1.23})$$

or

$$\tan(2\xi_c) = \frac{2P_c R_c^{\infty}}{1 - P_c^2 (R_c^{\infty})^2 - P_c^2 (\pi \tilde{S}_c)^2}, \quad \tanh(2\eta_c) = \frac{2\pi \tilde{S}_c P_c}{1 + P_c^2 (R_c^{\infty})^2 + P_c^2 (\pi \tilde{S}_c)^2}$$

However, the solution of the scattering of neutrons (or other nuclear particles) by a complex potential well is determined in the same form with complex scattering phase. In the example of rectangular well

considered in (I.1.d), this is obvious with $V = U(1 + i\xi)$, and moreover

$$R_c^\infty + i\pi\tilde{S}_c = \frac{\hbar}{\mu a^2} \left[\sum_{n=1}^{\infty} \frac{E_n - E}{(E_n - E)^2 + (\xi U)^2} + i \sum_{n=1}^{\infty} \frac{\xi U}{(E_n - E)^2 + (\xi U)^2} \right]. \quad (\text{II.1.24})$$

If a potential qualitatively close to the shell model is chosen as U , then E_n are the energies of single particle states. The relation in Eq. (II.1.24) reflects the single particle character of the energy dependence of both the effective scattering radius determined by R_c^∞ and the strength function. This is generally confirmed by the analysis of the data for total cross section in the whole region of unresolved levels and scattering cross sections (integral, differential, and polarized) in the region of overlapping resonances. The example of rectangular well is certainly the first approximation of the model only. Rather complicated forms of potentials are used in practice, and the phase calculations for them are performed now by using the special codes (see Ref. 17 e.g.). The principle means for constructing the average reaction cross sections include, as well, so-called penetrability factors T_c (these should not be confused with the P_c factors):

$$T_c(E) = 1 - |\langle U_{cc}(E) \rangle|^2 = 1 - e^{-4\eta_c} = \frac{4\pi\tilde{S}_c P_c}{(1 + \pi\tilde{S}_c P_c)^2 + (PR_c^\infty)^2}, \quad (\text{II.1.25})$$

and moreover $0 < T_c(E) < 1$. In the region of weekly interfering resonances, the presentation $S_{cc}(E)$ in the MLBW approximation in (I.8.c) can be used and

$$|\langle U_{cc}(E) \rangle| \approx 1 - \pi\bar{\Gamma}_n / D \quad (\text{II.1.26})$$

so that

$$T_c(E) = 2\pi\bar{\Gamma}_n / D - (\pi\bar{\Gamma}_n / D)^2 \approx 2\pi\bar{\Gamma}_n / D. \quad (\text{II.1.27})$$

This is one of the conditions for the agreement of strength function (the imaginary part of complex potential) with the resonance data in resolved region [9].

The problem of averaging the diagonal elements of collision matrix over the compound resonances is also resolved for more common cases in the microscopic theory of nuclear reactions [7,5,6] by separation of the doorway states of the single particle and here apparently there are no principal complications from both the methodological and calculating points of view, at least in the energy region of interest to us. In the limit of a large number of levels, the resonance part of the average non-diagonal element, $\langle U_{c'c}(E) \rangle$ ($c' \neq c$), is usually assumed to be zero in averaging interval because of the random values and signs of the products $\gamma_{\lambda c'} \gamma_{\lambda c}$ [4]. The non-zero values of $\langle U_{c'c} \rangle$ are connected with direct processes and the methods of determination of those follow from the corresponding models of interaction. In our applications, we neglect the contributions of direct processes in reaction cross sections.

- c) The traditional approach to the determination of average reaction cross sections in the unresolved region is based on the method of Hauser-Feshbach [18]. The fluctuation cross section concept is introduced:

$$\sigma_{c'c}^{fl} = \pi k^{-2} g \left(\langle |U_{c'c}|^2 \rangle - |\langle U_{c'c} \rangle|^2 \right) \quad (\text{II.1.28})$$

so that the average cross section of the corresponding reaction (for one level system) is presented as

$$\langle \sigma_{c'c} \rangle = \pi k^{-2} g |\langle U_{c'c} \rangle|^2 + \sigma_{c'c}^{fl}, \quad (\text{II.1.29})$$

where the first term characterizes the direct process. The average elastic scattering cross section can be written in the same form:

$$\langle \sigma_{cc} \rangle = \pi k^{-2} g \langle |1 - U_{cc}|^2 \rangle = \pi k^{-2} g |1 - \langle U_{cc} \rangle|^2 + \sigma_{cc}^{fl}. \quad (\text{II.1.30})$$

The sum of the fluctuation cross sections over all channels c' is:

$$\sigma_c^{fl} = \pi k^{-2} g \left(\langle \sum_{c'} |U_{c'c}|^2 \rangle - \sum_{c'} |\langle U_{c'c} \rangle|^2 \right) \approx \pi k^{-2} g \left(1 - |\langle U_{cc} \rangle|^2 \right) = \pi k^{-2} g T_c \quad (\text{II.1.31})$$

if we assume the non-diagonal elements $\langle U_{c'c} \rangle = 0$ ($c' \neq c$).

The structure of the partial fluctuation cross sections, which in our case are the average cross sections of corresponding reactions, is established in first approximation on the base of Bohr hypothesis for independence of the processes of compound nucleus formation and decay

$$\sigma_{c'c}^{fl} = \pi k^{-2} g \xi_{c'} \xi_c.$$

Comparing the sum of similar expressions with Eq. (II.1.30), we come directly to the Hauser-Feshbach formula for the average reaction cross section:

$$\sigma_{c'c}^{fl} \approx \pi k^{-2} g \frac{T_{c'} T_c}{T}, \quad (\text{II.1.32})$$

where $T = \sum_c T_c$ [18]. However, as it is seen, even averaging over the single resonances in Eq. (II.1.7), the determined correlation of the channels is possible because of the fluctuation factor $F_{c'c}$ in Eq. (II.1.8). The Hauser-Feshbach formula and the Bohr concept itself for compound reaction can be justified by statistical averaging $\langle |U_{c'c}|^2 \rangle$, and this is quite useful from the both theoretical and practical points of view in applications to the cross sections analysis part of the physics of nuclear reactions at low and medium energies. Studies on this topic closest to our problems are the results of Moldauer [9] and Weidenmuller with collaborators [14], where the factorization of the average cross sections in the spirit of the independence concept was justified for the random matrix models to the extent that their results became in a sense standard for parameterization of average reaction cross sections.

Let us mention here one of those, based on the analysis and systematization of the wide set of calculations of the average cross sections in **R**-matrix theory by the method of random sampling of parameters (Monte-Carlo) [14]. For the reaction channels $c' \neq c$, the fluctuation cross section is chosen in the form of Eq. (II.1.32):

$$\sigma_{c'c}^{fl} = \pi k^{-2} g V_{c'} V_c / V, \quad (V = \sum_v V_c), \quad (\text{II.1.33})$$

and the elastic scattering contains the so-called enhancement factor ω_n , accounting the correlation in the entrance channel

$$\sigma_{cc}^{fl} = \pi k^{-2} g (V_c^2 / V) \omega_c. \quad (\text{II.1.34})$$

Then the unitary condition in Eq. (II.1.31) determines the system of equations for V_c of the kind

$$V_c = T_c / [1 + (V_c / V)(\omega_c - 1)], \quad (\text{II.1.35})$$

and the solution of this can be found by successive approximations, if the factor ω_c is known. For the last one, the authors [14] recommend the relation

$$\omega_c = 1 + 2 \left(1 + T_c^{0.3} + 1.5 \frac{T_c}{T} \right)^{-1} + 2 \left(\frac{T_c}{T} - \frac{1}{\nu} \right)^2, \quad (\text{II.1.36})$$

where ν is the total number of open channels, giving the best agreement with the results of cross section calculation by the random sampling method.

The successive works of this group [14,18] contain the convincing theoretical justification of the concept of independence of the compound nucleus formation and decay on the base of statistical **R**-matrix theory and analytical solutions for average fluctuation cross sections similar to Eq. (II.1.7):

$$\sigma_{c'c}^{fl} = \pi k^{-2} g \frac{T_{c'} T_c}{T} F_{c'c}, \quad (\text{II.1.37})$$

where the factors $F_{c'c}$ are calculated in general case as threefold integrals [18]. This factorization of the cross sections is rather important in both the regions of isolated and overlapping resonances and is obviously useful for our applications in constructing the models of resonance dependence in unresolved region. On the base of this fluctuation cross section form in Eq. (II.1.37) and the relation in Eqs. (II.1.29-30), we have:

$$\sum_{c'} T_{c'} F_{c'c} = \sum_{c'} T_{c'}. \quad (\text{II.1.38})$$

By re-determining the penetrability factors for any channel c' as

$$\bar{T}_{c'} = T_{c'} F_{c'c} / F_{cc}, \quad (II.1.39)$$

we come to the Hauser-Feshbach formulae in Eq. (II.1.32) of the kind

$$\sigma_{c'c}^{fl} = \pi k^{-2} g \frac{\bar{T}_{c'} \bar{T}_c}{\bar{T}}, \quad \bar{T} = \sum_{c'} \bar{T}_{c'}, \quad (II.1.40)$$

which fully correspond to the Bohr concept and accounts the statistical fluctuations of **R**-matrix parameters (II.2).

This way, for the average cross sections of neutron reactions in the energy region in question, the formulae of the kind in Eq. (II.1.7) are valid

$$\langle \sigma_{\alpha}(E) \rangle = \pi k^{-2} \sum_J g(J) \sum_{c(\alpha)} \sum_n \frac{T_n^J(E) T_c^J(E)}{T^J(E)} F_{nc} \quad (II.1.41)$$

with

$$T_c(E) \approx 2\pi \bar{\Gamma}_c(E) / D(E) \quad (c \neq n)$$

$$T_n(E) = \frac{4S_n}{(1+S_n)^2 + (P_n R_n^{\infty})^2} \approx \frac{4S_n}{(1+S_n)^2}, \quad S_n = \pi P_n \tilde{S}_n.$$

The total cross section (assuming $P_n R_n^{\infty} \ll 1$) is presented as Eq. (II.1.15):

$$\langle \sigma(E) \rangle = \sigma_p + 4\pi k^{-2} \sum_J g(J) \sum_n \frac{S_n}{1+S_n} \cos(2\varphi'_n) \quad (II.1.42)$$

with the strength functions ($S_n = \pi P_n \tilde{S}_n$) and phases of the potential scattering φ'_n determined in the general case with the complex potential model in Eq. (II.1.22).

II.2 Statistical Distributions of Resonance Parameters

- a) The hypothesis of the random (Gaussian) distribution of the resonance reduced width amplitudes $\overline{\gamma_{\lambda c}}$ with $\overline{\gamma_{\lambda c}} = 0$ follows from the common dynamic structural formation of the complicated compound nucleus states [20,21,4-6,7]. The character of the excitation of two neighboring levels can be entirely different, which is traced schematically in the microscopic models of interaction as a different way of the successive formation of particle-hole configurations [7]. The methodological justification for this can be found in the statistical central limit theorem, according to which the linear combination of many independent random variables distributed according to some law, in the limit, must obey the Gauss distribution. The physical confirmations of this hypothesis are the

observations of real distributions of the reduced resolved resonance widths and the necessity for justifying the independence of compound nucleus formation and decay in the region of overlapping resonances [20,19].

In this way, considering statistically the resonance width fluctuations, it is supposed that the signs and values of the amplitudes $\gamma_{\lambda c}$ are distributed randomly in each channel c with the density:

$$F(\xi_c)d\xi_c = \frac{1}{\sqrt{2\pi}} \exp(-\xi_c^2 / 2) d\xi_c \quad (-\infty < \xi_c < \infty), \quad (II.2.1)$$

where $\xi_c = \gamma_{\lambda c} / \sqrt{\overline{\gamma_{\lambda c}^2}}$. (For resolved resonances $\overline{\gamma_{\lambda c}^2} = \overline{\Gamma_{\lambda c}} / 2P(E_\lambda)$.) For the reduced resonance widths in channel c , $\gamma_{\lambda c}^2 = \Gamma_{\lambda c} / 2P_c(E)$, the variable $x_c = \xi_c^2$ follows the $\chi^2(1)$ or Porter-Thomas distribution for one channel [5]:

$$P_1(x_c)dx_c = \frac{1}{\sqrt{2\pi x_c}} \exp(-x_c / 2) dx_c \quad (0 < x_c < \infty). \quad (II.2.2)$$

As has been noted, this distribution corresponds entirely to the observed fluctuations of the reduced neutron widths of resolved levels. For a reaction with ν independent channels, $\Gamma_{\lambda\alpha} = \sum_{c(\alpha)=1}^{\nu_\alpha} \Gamma_{\lambda c}$ and

$$x_\alpha = \Gamma_{\lambda\alpha} / \overline{\Gamma}_\alpha = \sum_{c(\alpha)=1}^{\nu_\alpha} (\Gamma_{\lambda c} / \overline{\Gamma}_c) (\overline{\Gamma}_c / \overline{\Gamma}_\alpha) = \sum_{c(\alpha)=1}^{\nu_\alpha} \beta_c x_c.$$

The distribution function $F(x_\alpha)$ in general case must depend on the number of channels ν_α of the considered reaction and on their relative contribution β_c in the summarized average width. The characteristic function of this distribution is found relatively simply [22]:

$$X(t) = \prod_{c(\alpha)} \int_{-\infty}^{\infty} e^{it\beta_c \xi_c^2} F(\xi_c) d\xi_c = \prod_{c(\alpha)=1}^{\nu_\alpha} (1 - 2it\beta_c)^{-1/2}. \quad (II.2.3)$$

When $\beta_c = 1 / \nu_\alpha$,

$$X(t) = \tilde{X}(t) = (1 - 2it / \nu_\alpha)^{-\nu_\alpha/2}. \quad (II.2.4)$$

The inverse Fourier transformation of $\tilde{X}(t)$ leads directly to $\chi^2(\nu)$ distribution or Porter-Thomas distribution with ν degrees of freedom [21]:

$$P_\nu(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{X}(t) e^{-itx} dt = \frac{\nu}{2\Gamma(\nu/2)} \left(\frac{\nu x}{2} \right)^{\nu/2-1} e^{-\nu x/2} \quad (0 < x < \infty) \quad (II.2.5)$$

So, for $\nu = 2$,

$$P_2(x)dx = e^{-x}dx. \quad (II.2.6)$$

In the limiting case of a large reaction channel number $\nu_\alpha \gg 1$, and in particular for radiative neutron capture,

$$\tilde{X}(t) \approx \lim_{\nu_\alpha \rightarrow \infty} (1 - 2it / \nu_\alpha)^{-\nu_\alpha/2} = e^{it}, \quad (II.2.7)$$

and correspondingly

$$P_\infty(x)dx = \delta(x-1), \quad (II.2.8)$$

that is, all $\Gamma_{\lambda\gamma} = \bar{\Gamma}_\gamma$ (Fig. I.2).

The moments of the function $P_\nu(x)$ in Eq. (II.2.5) are

$$\overline{x^n} = \int_0^\infty x^n P_\nu(x)dx = \left(\frac{2}{\nu}\right)^n \left[\frac{\nu}{2} \left(\frac{\nu}{2} + 1 \right) \cdots \left(\frac{\nu}{2} + n - 1 \right) \right], \quad (II.2.9)$$

and the second moment, e.g., offers the possibility to determine the number of reaction channels for the resolved resonances widths:

$$\overline{x^2} - 1 = \frac{\overline{\Gamma_{\lambda\alpha}^2} - (\overline{\Gamma_{\lambda\alpha}})^2}{(\overline{\Gamma_{\lambda\alpha}})^2} = \frac{2}{\nu_\alpha}. \quad (II.2.10)$$

The obtained ν_α values are often non-integer and it is explained by different relative contribution of the channels β_c in Eq. (II.2.3).

b) Let us consider different variants of the inverse Fourier transformation of the characteristic function $X(t)$ in Eq. (II.2.3) for unequal β_c . Therefore, for two channels, we will have [11,22]:

$$\wp(x, \beta_1, \beta_2) = \frac{1}{2\sqrt{\beta_1\beta_2}} \exp(-x / 4\beta_1\beta_2) I_0 \left(\frac{\beta_1 - \beta_2}{4\beta_1\beta_2} x \right), \quad (II.2.11)$$

and $\beta_1 + \beta_2 = 1$. For $\beta_1 = \beta_2$, this is reduced to $P_2(x)$ distribution in Eq. (II.2.6), and for $\beta_2 = 0$ it coincides with P_1 in Eq. (II.2.2) (Fig. I.2). For three channels, two of which are identical, $\beta_2 = \beta_3 = \beta$, $\beta_1 = 1 - 2\beta$, we will have [11]:

$$\wp(x, \beta_1, \beta, \beta) = \left(\frac{x}{2\pi\beta_1\beta^2} \right)^{1/2} e^{-x/2\beta} \int_0^1 dt \exp\left(-\frac{\beta - \beta_1}{2\beta\beta_1} xt^2 \right) \quad (\text{II.2.12})$$

(Fig. II.2). In the limiting case of $\beta_1 \rightarrow 0$, or $\beta \rightarrow 1/2$, (II.2.12) is again reduced as expected to $P_2(x)$ distribution. In a general case for an arbitrary channel number with unequal β_c , the probability density function can be found by the inverse transformation of the convolution of Eq. (II.2.3) or by more simple method of manifold integral transformation [22]:

$$\begin{aligned} \wp(x, \beta_1, \beta_2, \dots, \beta_v) = & (\beta_1\beta_2 \dots \beta_v)^{-1} x^{v-1} \int_0^1 dz_1 P_1\left(\frac{xz_1}{\beta_1}\right) \int_0^{1-z_1} dz_2 P_1\left(\frac{xz_2}{\beta_2}\right) \dots \\ & \times \int_0^{1-z_1-\dots-z_{v-2}} dz_{v-1} P_1\left(\frac{xz_{v-1}}{\beta_{v-1}}\right) P_1\left[(1-z_1-\dots-z_{v-1})\frac{x}{\beta_v}\right] \end{aligned} \quad (\text{II.2.13})$$

Figure II. 2 Three Channel Probability Distribution Function ($\beta_1 = 1 - \beta$, $\beta_2 = \beta_3 = \beta$)

Let us consider a variant with 1 to 3 dominant channels and a set of weak channels of which the summed relative contribution in the average width is ε . A practical example is the reaction $(n, \gamma f)$, i.e., the fission after the emission of different cascades of photons [5,23]. Assuming the number of channels of this process is extremely large, as in the case of neutron radiative capture in Eq. (II.2.7), the characteristic function of the resonance fission widths distribution in Eq. (II.2.3) can be presented

approximately as

$$X(t) \approx \prod_{c=1}^n (1 - 2it\beta_c)^{-1/2} e^{it\varepsilon}, \quad (\text{II.2.14})$$

where the product is referred only to the direct fission. Then the inverse Fourier transformation of $X(t)$ in Eq. (II.2.14) gives the function

$$\wp(x - \varepsilon, \beta_1, \dots, \beta_n) \quad \left(\sum_{c=1}^n \beta_c = 1 - \varepsilon \right) \quad (\text{II.2.15})$$

for $x > \varepsilon$ and zero for $x < \varepsilon$, i.e., the fission widths of resonances cannot be less than a constant component related to the $(n, \gamma f)$ process.

The characteristic function $X(t)$ in Eq. (II.2.4) determines the moments of the distribution function in Eq. (II.2.13):

$$\overline{x^n} = (-i)^n \frac{d^n}{dt^n} X(t) \big|_{t=0} \quad (\text{II.2.16})$$

so that

$$\overline{x} = \sum_{c=1}^{\nu} \beta_c = 1; \quad \overline{(x-1)^2} = 2 \sum_{c=1}^{\nu} \beta_c^2; \quad \overline{(x-1)^3} = 8 \sum_{c=1}^{\nu} \beta_c^3 \quad (\text{II.2.17})$$

This is a practical system of equations for determination of the relative contribution of different reaction channels to the average widths of the resolved resonances, where the values of moments are known:

$$\overline{(x-1)^n} = \overline{[(\Gamma_{\lambda\alpha} - \bar{\Gamma}_{\alpha}) / \bar{\Gamma}_{\alpha}]^n}. \quad (\text{II.2.18})$$

The examples considered in the framework of random number statistics of resonance width distributions illustrate the variety of their dependence on the relative contributions β_c . These are obviously useful for the corresponding analysis of the fluctuations of the resolved resonance widths. However, in the problem of cross section averaging and just for determination of the factors F_{nc} in Eq. (II.1.8) and Eq. (II.1.37), it is more convenient, as noted above, to separate different reaction channels, except non-fluctuating width of the radiative capture (and probably that of $(n, \gamma f)$ process). Then, in each of the remaining channels, we will have the one-channel distribution density in Eq. (II.2.1) and Eq. (II.2.2); this offers the possibility to standardize the F_{nc} factor presentation preserving the applicability of the mathematical schemes, and without using special distribution functions for different reactions.

For the case of one-channel scattering and multi-channel radiative capture, only the factor F_{ny} / F_{γ} is determined as if the corresponding fluctuation factor of the elastic scattering cross section is expressed

through F_γ , by the summation rule in Eq. (II.1.38). For example, by using the approximate form in Eq. (II.1.13) for F_γ , we find the corresponding expression for $F_{nn} = F_n$ as

$$F_n = 1 + \eta(1 - F_\gamma) \approx 1 + \frac{1.25\eta^{3/2}}{1 + 2.25\eta^{1/2} + 0.625\eta^{3/2}}, \quad (\text{II.2.19})$$

where $\eta = \Gamma_\gamma / \bar{\Gamma}_n$ or $\eta \approx T_\gamma / T_n$ (see Section II.3).

In the two-channel problem, e.g., one neutron (n) and one fission (c) channels plus multi-cascade radiative capture (or two neutron channels), the fluctuation factors $F_{n\gamma}$ and F_{nc} required for average cross sections are determined in the SLBW approximation with Eq. (II.1.10) and Eq. (II.1.11) as the integrals:

$$F_{n\gamma} = \int_0^\infty dz \left(1 + 2z \frac{\bar{\Gamma}_n}{\bar{\Gamma}}\right)^{-3/2} \left(1 + 2z \frac{\bar{\Gamma}_c}{\bar{\Gamma}}\right)^{-1/2} e^{-z\bar{\Gamma}_\gamma/\bar{\Gamma}} \quad (\text{II.2.20})$$

$$F_{nc} = \int_0^\infty dz \left(1 + 2z \frac{\bar{\Gamma}_n}{\bar{\Gamma}}\right)^{-3/2} \left(1 + 2z \frac{\bar{\Gamma}_c}{\bar{\Gamma}}\right)^{-3/2} e^{-z\bar{\Gamma}_\gamma/\bar{\Gamma}} \quad (\text{II.2.21})$$

(Fig. II.3). However, in a three-channel case (two fission channels c and c'), two equivalent variants are possible for determining fluctuation factors: 1) as a twofold integral in Eq. (II.1.9) with a two-channel distribution function for the fission width in Eq. (II.2.11) - F_{nf} and 2) in the form of Eq. (II.1.10) for each of the channels c and c' separately - F_{nc} and $F_{nc'}$. Then the average fission cross section for one system is

$$\langle \sigma_f^J \rangle = \frac{2\pi^2}{D_j k^2} g \frac{\bar{\Gamma}_n \bar{\Gamma}_f}{\bar{\Gamma}} F_{nf} = \frac{2\pi^2}{D_j k^2} g \frac{\bar{\Gamma}_n}{\bar{\Gamma}} (\bar{\Gamma}_c F_{nc} + \bar{\Gamma}_{c'} F_{nc'}) \quad (\text{II.2.22})$$

The advantage of channel-by-channel accounting of the fluctuation factors in calculating the average cross sections is seen from the point of view of the uniform algorithm of those in the form of Eq. (II.1.10) or practically as

$$F_{nc} \left(\frac{\bar{\Gamma}_c}{\bar{\Gamma}} \right) = (1 + 2\delta_{nc}) \int_0^\infty dz \prod_i \left(1 + 2z \frac{\bar{\Gamma}_i}{\bar{\Gamma}}\right)^{-(\delta_{in} + \delta_{ic} + 1/2)} e^{-z\bar{\Gamma}_\gamma/\bar{\Gamma}} \quad (\text{II.2.23})$$

where the product does not contain the radiation channels. Apparently these functions obtained in one-level approximations are close to the corresponding functions for partially overlapping resonances, in the unresolved resonance region of interest, where the resonance self-shielding occurs, if the width ratio in Eq. (II.2.20) is substituted formally by the ratio of penetrability factors T_i / T (see Section II.3).

Figure II. 3 Fluctuation Factor for Two-Channel Problem

- c) Although the effect of resonance spacing fluctuations is not as significant for the average cross sections as is the fluctuation effect of one-channel neutron widths and two- or three-channel fission ones, the analysis of this is much more complicated both methodologically and in practical calculations. The reason for this is the correlation of the probability of appearance in the given value of the spacing between neighboring levels $E_\lambda - E_{\lambda-1}$ with the similar probability for other resonances, whereas the distributions of the resonance width amplitudes are independent. On the other hand, as it is illustrated by the example of single resonances, the average cross sections at $\Gamma_\lambda \ll D$ generally do not depend on level spacing fluctuations. The situation apparently is the same for fully overlapping resonances. Therefore, the fluctuation effect for the values $\varepsilon_\lambda = (E_\lambda - E_{\lambda-1}) / D$ can be observable in the region of partial overlapping resonances. This can be interesting for the applications requiring estimation the influence of tight grouping of some resonances on the average cross sections.

II.3 Resonance Ladder Method

- a) The use of resonance cross section modeling in the unresolved resonance region (resonance ladder) for the analysis of cross sections and the average cross sectional functionals over given energy intervals (groups) is a direct and widely distributed approach in applications [9,14,24]. This is evidently simpler than statistical averaging over “Gaussian orthogonal ensemble (GOE)” for the physical interpretation of resonance self-shielding features in the unresolved region via many methods and for the results obtained for the resolved levels.

In general, the resonance ladder method is usually reduced to statistical modeling of K -matrix elements in Eq. (I.8.4):

$$K_{c'c} = \frac{1}{2} \sum_{\lambda} \frac{\Gamma_{\lambda c'}^{1/2} \Gamma_{\lambda c}^{1/2}}{E_{\lambda} - E - i\Gamma_{\lambda\gamma} / 2} = (S_{c'} S_c)^{1/2} \sum_{\lambda} \frac{\xi_{\lambda c'} \xi_{\lambda c}}{\delta_{\lambda} + z - iy}, \quad (\text{II.3.1})$$

where $S_c = \pi \bar{\Gamma}_c / 2D = \pi P_c \tilde{S}_c$, $y = \pi \Gamma_{\gamma} / 2D$ ($\Gamma_{\lambda\gamma} \approx \Gamma_{\gamma}$), $\delta_{\lambda} = \pi(E_{\lambda} - E_0) / D$, $z = \pi(E_0 - E) / D$. The values $\xi_{\lambda c} = \Gamma_{\lambda c}^{1/2} / \bar{\Gamma}_c^{1/2}$ are chosen as independent random numbers following the scheme [14]:

$$\xi_{c'} = (-2 \ln \beta_1)^{1/2} \cos(2\pi\beta_2), \quad \xi_c = (-2 \ln \beta_1)^{1/2} \sin(2\pi\beta_2), \quad (\text{II.3.2})$$

where β_1 and β_2 are given by the random number generator in the interval [0,1]. The energy levels $\delta_{\lambda} = \pi(E_{\lambda} - E_0) / D$ are situated on the both sides of the center of averaging interval E_0 and, moreover, the spaces between the neighboring pairs of levels are generated as

$$\delta_{\lambda} - \delta_{\lambda-1} = 2\sqrt{\pi} \sqrt{-\ln(1 - \beta_3)}, \quad (\text{II.3.3})$$

which corresponds to the Wigner distribution [25]. For each sample (i) of random numbers are found the functions $K_{c'c}^{(i)}(z)$, $U_{c'c}^{(i)}(z)$ and cross sections $\sigma^{(i)}(z)$, $\sigma_a^{(i)}(z)$, where generally the Doppler broadening is taken into account. The necessary cross sectional functional $F(\sigma^{(i)}, \sigma_a^{(i)})$ is determined

for the i -th sample by using these model cross sections and the subsequent averaging over energy, and a wide set of different statistical samples (m) gives at the end the average over the energy group (Δz) value of this functional

$$\langle F \rangle = \frac{1}{m} \sum_{i=1}^m \frac{1}{\Delta z} \int dz F[\sigma^{(i)}(z), \sigma_a^{(i)}(z)]. \quad (II.3.4)$$

In realization, such an approach uses the Monte Carlo technique with the specific features in various known codes [14,25-27]. The physical grounds of the method are modeling the multilevel resonance cross sections for each sample (history), and as in the resolved region, the various presentations of energy dependence are possible for these.

In the limiting case of a large number of λ -levels in K -matrix in Eq. (II.3.1), the results of calculating $\langle F \rangle$ by Monte Carlo technique must be the same as the average of the corresponding functional over GOE with some statistical uncertainty, typical for the method. However, as we have seen in the average cross section example, the systematics of these results is usually reduced to the construction of the empirical dependence on penetrability factors, and generally, those can hardly be interpreted from the physical point of view. In applications to the analysis of data for the transmission and self-shielding cross sections in the unresolved region, the Monte Carlo calculations are reduced mainly to confirmation or more accurate determination of the average resonance parameters used in the limited thickness interval of measured targets. The extrapolation of calculations to a thick region can be rather dubious in some cases of non-statistical features in the resonance cross section structure. Even a single interference minimum in the considered energy group can determine all the transmission on the asymptote, for example.

b) The available set of data about average cross sections and some average cross sectional functionals in separate energy groups evidently does not give the possibility of unfolding the precise resonance dependence of cross sections in the unresolved region. However, the task of creating some picket-fence model of such cross section and giving the correct results on average can, in principle, be done. However, in this case, it is necessary to limit the number of level parameters in the corresponding K -matrix in Eq. (II.3.1) because of the lack of the data for determination of the parameters. It is possible for this to propose the model of periodical ladder from N -levels, where

$$\delta_{\lambda+N} = \delta_{\lambda} + \pi N, \quad \delta_{\lambda+2N} = \delta_{\lambda} + 2\pi N, \quad \dots, \quad \Gamma_{\lambda+N,c}^{1/2} = \Gamma_{\lambda,c}^{1/2}, \quad \dots. \quad (II.3.5)$$

Then, spreading the summation over λ in Eq. (II.3.1) up to infinity ($-\infty < \lambda < \infty$), we obtain the periodical functions with a limited number of free parameters [26]:

$$K_{c'c}(z) = (S_{c'} S_c)^{1/2} \frac{1}{N} \sum_{\lambda=1}^N \xi_{\lambda c'} \xi_{\lambda c} \cot[(\delta_{\lambda} + z - iy) / N]. \quad (II.3.6)$$

The model of identical equidistant resonances ($N = 1$) in the problem with one neutron channel and excluded radiative channels (RM-approximation with $\Gamma_{\lambda\gamma} = \bar{\Gamma}_{\gamma}$) is the simplest one here. Then the corresponding function K in Eq. (I.8.12) is [4,9,6]:

$$K(z) = S \cot(z - iy)$$

with $S = \pi P_n \tilde{S}_n$. It is supposed that the non-resonant part of K is accounted in the potential scattering phase as in Eq. (I.8.15). In this case, the collision function in Eq. (I.8.1) can be written as

$$\begin{aligned} U &= e^{-2i\varphi} \frac{1 + iS \cot(z - iy)}{1 - iS \cot(z - iy)} = e^{-2i\varphi} [\cosh(2\eta) + i \sinh \eta \cot(z - iy - i\eta)] \\ &= e^{-2i\varphi} \left[\cosh(2\eta) + i \sinh \eta \sum_{\lambda=-\infty}^{\infty} \frac{1}{\pi\lambda + z - i(y + \eta)} \right] \end{aligned} \quad (II.3.7)$$

where $\tanh \eta = S$ [see Eq. (II.1.23)]. The last presentation corresponds to the E -pole form (Kapur-Peierls scheme) similar to the results of MLBW approach. The determined U model cross sections (for one system $J\pi$) are periodical functions [25]:

$$\sigma_{\gamma}^J = \frac{\pi}{k^2} g_J [1 - |U|^2] = \sigma_{0\gamma}^J \frac{1 + \tan^2 z}{1 + P^{-2} \tan^2 z}, \quad (II.3.8)$$

where

$$P = \tanh(\eta + y), \quad \sigma_{0\gamma}^J = \frac{4\pi}{k^2} g_J \frac{S \tanh y}{P^2 (1 + S \tanh y)^2} = \frac{4\pi}{k^2} g_J \frac{S \tanh y}{(S + \tanh y)^2}, \quad (II.3.9)$$

and

$$\sigma^J = \sigma_{\min}^J + \sigma_0^J \frac{(\cos \varphi - P^{-1} \tan z \sin \varphi)^2}{1 + P^{-2} \tan^2 z} \quad (II.3.10)$$

with

$$\sigma_0^J = \frac{4\pi}{k^2} g_J \frac{S(1 - \tanh^2 y)}{P(1 + S \tanh y)}, \quad \sigma_{\min}^J = \frac{4\pi}{k^2} g_J \frac{\tanh y}{P(1 + S \tanh y)} (\sin^2 \varphi + SP \cos^2 \varphi). \quad (II.3.11)$$

It is not hard to see that in the case of isolated resonances ($S \ll 1$, $y \ll 1$), these formulae coincide with the one-level ones in Eq. (I.4.3) and Eq. (I.4.5).

The averaging on energy in the model of identical resonances is reduced to finding the corresponding functions averaged over the period $0 \leq z \leq \pi$. So,

$$\langle K \rangle = S \frac{1}{\pi} \int_0^{\pi} \cot(z - iy) dz = iS, \quad \langle K^m \rangle = (iS)^m, \quad (II.3.12)$$

which at our choice $S = \pi P_n \tilde{S}_n$ corresponds to the common definition in Eq. (II.1.20) (with $R_n^\infty = 0$). A similar agreement with Eq. (II.1.22) is obtained by averaging over the period of the model U-function in Eq. (II.3.7):

$$\langle U \rangle = e^{-2i\varphi} \frac{1}{\pi} \int_0^\pi \frac{1 + iS \cot(z - iy)}{1 - iS \cot(z - iy)} dz = e^{-2i\varphi} \frac{1 - S}{1 + S}, \quad (\text{II.3.13})$$

so that the average total cross section in Eq. (II.3.10) is similar to the one in Eq. (II.1.42):

$$\langle \sigma \rangle = \frac{4\pi}{k^2} g_J \left[\sin^2 \varphi + \frac{S}{1 + S} \cos(2\varphi) \right]. \quad (\text{II.3.14})$$

The result of average radiative capture cross section in Eq. (II.3.8) leads directly to Hauser-Feshbach formula in Eq. (II.1.32):

$$\langle \sigma_\gamma \rangle = \sigma_{0\gamma} P = \frac{2\pi}{k^2} g_J \frac{\sinh(2\eta) \sinh(2y)}{\sinh[2(\eta + y)]} = \frac{\pi}{k^2} g_J \frac{T_n T_\gamma}{T_{n+\gamma}} \quad (\text{II.3.15})$$

with the penetrability coefficients $T_n = 1 - e^{-4\eta}$ in Eq. (II.1.25), $T_\gamma = 1 - e^{-4y} = 1 - e^{-2\pi\Gamma_\gamma/D}$, and $T_{n+\gamma} = 1 - e^{-4(\eta+y)}$. Let us note once more, that the condition $\Gamma_\gamma / D \ll 1$ in our model is common for RM-approximation in Eq. (II.3.1).

The formulation of resonance cross sections as periodical functions permits us, in most cases, to obtain the relatively simple analytical expressions for different average cross sectional functionals of practical interest. For example, the average cross section dispersions (Ch. III), which are determined from the data of neutron transmission experiments in the unresolved region and the measurements of reaction cross sections by the self-shielding method in our model, are found as:

$$\langle \sigma^2 \rangle - (\langle \sigma \rangle)^2 = 2 \left(\frac{\pi}{k^2} g_J \right)^2 \frac{T_n^2}{T_{n+\gamma}}, \quad (\text{II.3.16})$$

$$\langle \sigma_\gamma \sigma \rangle - \langle \sigma_\gamma \rangle \langle \sigma \rangle = 2 \left(\frac{\pi}{k^2} g_J \right)^2 \text{Re}(\langle U \rangle) \frac{T_n^2 T_\gamma}{T_{n+\gamma}^2}, \quad (\text{II.3.17})$$

$$(\text{Re}(\langle U \rangle) = \cos 2\varphi \sqrt{1 - T_n}).$$

The capture cross-section on the filtered beam (self-indication) is determined in our model as [25]:

$$\langle \sigma_{\gamma} e^{-n\sigma} \rangle = \langle \sigma_{\gamma} \rangle \exp\left(-\frac{n\sigma_0}{2} - n\sigma_{\min}\right) I_0\left(\frac{n\sigma_0}{2}\right), \quad (\text{II.3.18})$$

where n corresponds to the filter thickness, and the effective resonance integral in the group related to the unresolved region (Ch. IV), becomes in the form

$$\left\langle \frac{\sigma_{\gamma}}{\sigma} \right\rangle = \frac{\langle \sigma_{\gamma} \rangle}{(\sigma_{\min} \sigma_{\max})^{1/2}}, \quad (\text{II.3.19})$$

where $\sigma_{\max} = \sigma_{\min} + \sigma_0$. The function of neutron transmission in general case is expressed as an integral or an infinite sum with the asymptote at $n\sigma_0 \gg 1$ of the kind

$$\langle e^{-n\sigma} \rangle \rightarrow \frac{P}{\sin^2 \varphi + P \cos^2 \varphi} \frac{1}{(\pi n \sigma_0)^{1/2}} \exp(-n\sigma_{\min}). \quad (\text{II.3.20})$$

Evidently, all these results of the identical resonance model used are qualitative because the important effects as resonance parameter fluctuations and Doppler broadening are not accounted for here.. The accounting of the latter in our formulae does not present principal complications. This is clear in general from the pole presentation of U in Eq. (II.3.7), similar in form to the MLBW approximation in (I.8.c) (Appendix I.A2). However, according to the model of rather qualitative character, the approximate Doppler function form can also be obtained by substituting the Gaussian distribution for nuclear velocities by the equivalent Cauchy distribution in Eq. (I.5.31). Moreover, the total cross section expression in Eq. (II.3.10) is kept with redetermination $y \rightarrow y' = y + \tilde{\delta}$, where $\tilde{\delta} = \pi\Delta/D$ depends on the temperature (see Section I.5). In the radiative capture cross section expression (II.3.8), the coefficient P in the denominator is only changed as $P \rightarrow P' = \tan(y + \eta + \delta)$ whereas in σ_{0r} the multiplier P/P' appears, which ensures the correct transition to the average cross section in Eq. (II.3.15).

Therefore, our model of identical resonances for the one-channel case is in agreement with one-level description at $S \ll 1$ and gives the correct average cross sections at arbitrary values of S (the effect of parameters fluctuations in $\langle \sigma_r \rangle$ can be accounted for formally with corresponding redetermination of T_{γ} in Eq. (II.1.25)). The simple analytical expressions for average cross sectional functionals in Eq. (II.3.17) to Eq. (II.3.19) are certainly rather approximate and only qualitatively reflect their dependence on average resonance parameters. But these can be grounds for the analysis and systematization of the data for neutron transmission and capture cross sections in the groups measured by self-shielding method varying the complementary and arbitrary (up to some degree) parameter $\sigma_{\min}$, which is temperature-dependent.

Obviously, other variants of picket-fence models, giving correct values for $\langle K \rangle$, $\langle U \rangle$, and average cross sections [9] can be proposed too. Practically, such an approach is justified in the one-channel case. For the two-channel problem, even in the identical resonance approximation, an uncertainty arises

related to the choice of the products $\xi_{\lambda c'} \xi_{\lambda c}$ in Eq. (II.3.6). The assumption about determined correlation of these signs seems to be rather artificial and only a random distribution of those arises as a somehow justified supposition [4]. In fact, however, this leads to the necessity of a reversion to the statistical modelling of level parameters in K -matrix.

- c) For constructing some determined mathematically picket-fence model that reproduces the full set of group averaged cross sectional functionals with the necessary precision, it is possible to employ the integral transformation method or the method of characteristic function. This method is formally equivalent to a transition to averaging over the distribution function of K -matrix elements in Eq. (II.3.1). For the small number of reduced K -matrix channels, this function related to the mutual distribution of the real and imaginary parts of $K_{c'c}$ elements depends on the limited number of $n(n+1)/2$ parameters, where n is the matrix rank. We determine the characteristic function of such a distribution in our method.

The most simple method here is the variant of one-channel problem (RM-approximation), where an arbitrary cross sectional functional can be cast as a function of the real and imaginary parts of $(1-iK)^{-1}$ or equivalently as a function of $(1-iK)^{-1}$ and its complex conjugate

$$F(\sigma, \sigma_\gamma) = F\left(\frac{1}{1-iK}, \frac{1}{1+iK^*}\right). \quad (\text{II.3.21})$$

Let us suppose now that the integral transformation of following kind exists:

$$F\left(\frac{1}{1-iK}, \frac{1}{1+iK^*}\right) = \int_0^\infty dt \int_0^\infty dt' f(t, t') \exp[-t(1-iK)] \exp[-t'(1+iK^*)] \quad (\text{II.3.22})$$

This is actually a two-dimensional Laplace transformation employed to determine the original $f(t, t')$ of the functional $F[1/(1-iK), 1/(1+iK^*)]$. Thus the problem of averaging an arbitrary cross sectional functional

$$\langle F \rangle = \int_0^\infty dt \int_0^\infty dt' f(t, t') e^{-(t+t')} \langle e^{iKt-iK^*t'} \rangle \quad (\text{II.3.23})$$

is reduced formally to finding the average over resonance function

$$X = \langle e^{iKt-iK^*t'} \rangle = \frac{1}{\Delta z} \int dz \prod_\lambda \int d\xi_\lambda^2 d\delta_\lambda P(\xi_\lambda^2) Q(\delta_\lambda) \exp\left[iS\xi_\lambda^2 \left(\frac{t}{z+\delta_\lambda-iy} - \frac{t'}{z+\delta_\lambda+iy}\right)\right] \quad (\text{II.3.24})$$

where $K = K_m$ in Eq. (II.3.6), $P(\xi_\lambda^2)$ is the Porter-Thomas distribution in Eq. (I.4.11) and $Q(\delta_\lambda)$ is the distribution of level spacing. The meaning of X is the characteristic function of the distribution of the real and imaginary parts of $K = K_1 + iK_2$:

$$X = \langle e^{iKt - iK^*t'} \rangle = \int_{-\infty}^{\infty} dK_1 \int_{-\infty}^{\infty} dK_2 e^{iK_1 v - K_2 u} \wp(K_1, K_2) \quad (\text{II.3.25})$$

with $v = t - t'$ and $u = t + t'$.

This way, the idea of the characteristic function method consists first in the determination of the averaged over resonances combination of K_1 and K_2 , universal for all physical cross sectional functionals. The integration over independent variables $\xi_{\lambda c}$ that obey the distribution $P(\xi_{\lambda c})$ gives directly:

$$X = \frac{1}{\Delta z} \int dz \prod_{\lambda} \int d\delta_{\lambda} Q(\delta_{\lambda}) \left[\frac{(z + \delta_{\lambda})^2 + y^2}{(z + \delta_{\lambda} - ip)(z + \delta_{\lambda} + iq)} \right]^{1/2}, \quad (\text{II.3.26})$$

where $p = f + \beta$, $q = f - \beta$, $f^2 = \beta^2 + 2\gamma y + y^2$ with $\beta = Sv$, $\gamma = Su$. So, the problem of determination of the characteristic function is reduced at the end to the choice of a model for relative distribution of the level energies $Q(\delta_{\lambda})$ satisfactory for our purposes.

Let us notice first that at $y = 0$ (and $\beta = \gamma$, too) the characteristic function is

$$X_0 = e^{-Su} \quad (\text{II.3.27})$$

which corresponds to the distribution function in Eq. (II.1.2) and Eq. (II.1.16):

$$\wp(K) = \frac{1}{\pi} \frac{S}{S^2 + K^2}. \quad (\text{II.3.28})$$

The model of identical resonances leads to the same result in Eq. in Eq. (II.3.12). It is possible to conclude from here that for determination of cross sectional functionals at negligible radiative capture the identical resonances model can be treated as "exact".

In the problem with radiative capture, the analytical presentation for the characteristic function in Eq. (II.3.25) can be obtained for equidistant levels $\delta_{\lambda} = \pi\lambda$. Spreading the product over λ up to infinity ($-\infty < \lambda < \infty$) and using the known relation:

$$\sin x = x \prod_{\lambda=1}^{\infty} [1 - (x / \pi\lambda)^2] \quad (\text{II.3.29})$$

we will have:

$$X = \frac{1}{\pi} \int_0^{\pi} dz \left[\frac{\sin(z - iy) \sin(z + iy)}{\sin(z - ip) \sin(z + iq)} \right]^{1/2}.$$

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Chapter III RESONANCE SELF-SHIELDING EFFECTS

This chapter deals with the conceptual as well as the practical aspects of the problems associated with the treatment of resonance absorption in the macroscopic reactor cells [1,2]. The purpose here is to present a comprehensive description of this extremely complex subject along with the state-of-art methodologies in practical applications.

Like other subjects in reactor theory, the treatment of resonance absorption in a reactor under steady state condition requires the knowledge of neutron distribution in energy and space. With no loss of generality, the Boltzmann's transport equation defined as follows is a convenient starting point from which many simplified versions can be derived for practical purposes [3,4,5].

$$[\Omega \cdot \nabla + \Sigma_t(r, E)]\phi(r, \Omega, E) = s(r, \Omega, E) \quad (\text{III.1})$$

where

$$s(r, \Omega, E) = \int \int dE' d\Omega' \Sigma_s(r, E') f(r, E' \rightarrow E, \Omega' \rightarrow \Omega) \phi(r, \Omega, E') + Q(r, \Omega, E) \quad (\text{III.2})$$

is the source term due to elastic scattering as denoted by the term with double integrals, and due to inelastic scattering and fission processes as denoted by $Q(r, \Omega, E)$. $\Sigma_t(r, E)$ and $\Sigma_s(r, E)$ are the macroscopic total cross section and total elastic scattering cross section, respectively. The elastic scattering kernel $f(r, E' \rightarrow E, \Omega' \rightarrow \Omega)$ physically represents the probability that a neutron at its initial energy E' and in the direction of Ω' will emerge in the direction of $\Omega + d\Omega$ with energy $E + dE$ upon collision.

Eq. (III.1), in principle, specifies the neutron distribution required in a reactor, and given the necessary cross section data, various quantities of interest to reactor applications can be determined. With the exception of perhaps the Monte Carlo approaches, however, such a description involving the extremely complex dependence on phase space is obviously not suitable for routine applications especially when resonances are considered. Simplifications are apparently necessary before its deployment. Four assumptions are commonly used in conjunction with the resonance theory. First, the elastic scattering is assumed to be isotropic in the center of the mass system. This implies that only s-wave scattering needs be considered. Since the p-wave will play a role only if the DeBroglie wavelength of the neutron becomes comparable to the nuclear dimension, its contribution is not expected to be significant especially in the low keV region and below where resonance absorptions are important. Secondly, the

crystalline binding effects are neglected. This implies that the neutron energy is large compared to the vibrational energy associated with the chemical binding of the target nucleus. It is clearly true in the resonance regions for most of the nuclide of interest. Thirdly, the inelastic scattering and fission sources are assumed absent. For most of cases considered, the crucial energy region of interest is well below the first excited state and the tail end of the fission spectrum so that these sources are not important to the self-shielding effects to be discussed. However, it should be noted that for the more advanced computer codes such as the MC²-2/RABANL [6], these sources need not be precluded. Fourthly, the spatial treatment of a reactor cell is restricted to simple one-dimensional convex geometries. To our knowledge, the multi-dimensional cell treatments at this time are only feasible at the multigroup level where the energy meshes are substantially greater than the extent of the resonances of actinides.

III.1 General Remarks on the Physical Meaning of Self-Shielding Effect

One unique feature of the reaction processes in the presence of resonances is the accompanying self-shielding effect, which has played a significant role since the conception of the fission reactors. Such a phenomenon is directly attributed to the localized fluctuations in neutron cross sections on the averaged reaction rates over energy and space in a reactor lattice. For our purposes here, it is perhaps more illustrating to define the physical meaning of the effect in question first before going into the detailed discussions that follows. To put the question in perspective, it is necessary to describe briefly the concept based on historical development as well as that based on current thinking.

From the earlier days of reactor development that focused on thermal reactors with low enrichment fuel, a reactor lattice is usually assumed to be composed of a handful of light nuclide with relatively constant cross sections serving as coolant and/or moderator and cladding along with fuel element dominated by U^{238} [7]. A few low-lying resonances of the latter are essentially responsible for the absorption rates over the resonance energy range that in turn, determines the fraction of neutrons that can reach the thermal energy via the elastic scattering. Qualitatively, the presence of the resonances will give rise to the localized depression of neutron flux in energy and in space, and the degree of the impact is obviously dependent upon the relative concentration of the resonant nuclide with respect to other background material in the system. In the limit of infinitely dilute concentration of resonant absorber, the neutron flux is constant in energy and in space. Since the flux and the resonance are generally anti-correlated, the magnitude of the absorption rate per atom for the system with finite dilution must be smaller than that for the infinitely dilute system. The reduction in the absorption rate per atom with respect to the infinitely dilute limit is generally referred to as the self-shielding effect and the degree of this effect is measured by their ratio known as the self-shielding factor defined as:

$$f_x = \frac{\langle \sigma_x(E) \phi(E, r) \rangle_{E,r}}{\langle \sigma_x(E) \rangle_{E,r} \phi_{asymp}} \quad (\text{III.1.1})$$

where x and ϕ_{asymp} denote the reaction type in question and the asymptotic flux at the infinitely dilute limit, respectively.

Two commonly considered scenarios in reactor applications were usually restricted to either the infinite homogeneous medium or infinite lattice consisting of repeated cells with fuel lumps surrounded by cladding and moderator. The resonance effect in the former attributed to the flux depression in energy alone is generally referred to as the energy self-shielding effect whereas the energy and spatial self-

shielding effects are inseparable in the latter. For a system with high U^{238} concentration, the self-shielding factor can be substantially smaller than unity especially in the low energy region where resonances are extremely sharp. Thus, one consequence of practical interest is that more high-energy neutrons can escape the resonance absorption and reach the thermal energy via elastic scattering than what would have been otherwise without the self-shielding effects. In addition, for the heterogeneous reactor cells in which the effects are localized to the fuel lumps, the over-all resonance absorption rate is generally smaller than that of the homogeneous system with the same composition as discovered by Fermi 50 years ago. It is, in effect, one of the key factors leading to the successful development of thermal reactors with low enrichment fuel. One other important characteristics of the self-shielding effect are that it gives rise to the temperature dependence of the reaction rate, i.e.

$$\frac{\partial f_x}{\partial T} = \frac{\left\langle \frac{\partial \sigma_x(E)}{\partial T} \phi(E, r) \right\rangle_{E,r} + \left\langle \sigma_x(E) \frac{\partial \phi(E, r)}{\partial T} \right\rangle_{E,r}}{\left\langle \sigma_x(E) \right\rangle_{E,r} \phi_{asym}} \quad (\text{III.1.2})$$

which vanishes if and only if $\phi(E, r) = \phi_{asym}$ under the infinitely dilute limit as $\langle \partial \sigma_x(E) / \partial T \rangle_E = 0$ resulting from the fundamental properties of the Doppler-broadened line shape functions described in Chapter I. The temperature dependence of f_x is directly responsible for the instantaneous reactivity feedback in a reactor in the event of power excursion. From the point of view of reactor safety, the criterion of having a negative temperature coefficient is one of the most important considerations in the design of new generation reactors.

Since the early 1960s, advances in three major areas have significant impact on our perceptions as well as the methodologies for treating the self-shielding effects. First, the emergence of the liquid metal fast breeder reactor development cast the traditional resonance treatment into different light. Here, the focus is no longer on the question of how many high neutrons can survive resonance absorption to reach the thermal energy. Instead, it is the intricate neutronic balance over an extremely large energy span ranging from high keV region down to thermal energy with numerous number of nuclide that exhibit resonant behavior. Thus, unlike the oversimplified model adopted earlier, one must also deal with resonances of many other actinides, structural isotopes, as well as coolant in addition to those of U^{238} in both the resolved and the unresolved energy regions. Of particular concern are the estimation of the Doppler coefficient and the sodium void coefficient crucial to reactor safety. Both these quantities require accurate resonance treatment. Consequently, our perception of self-shielding effects must be modified accordingly in order to accommodate the situation involving the mutual self-shielding effect of all resonances. Secondly, there have been continuous and relentless efforts in the international nuclear data communities in recent years to improve the required database systematically. The improvements in resonance data through dramatic extension of the resolved resonance range and the introduction of the R-matrix parameters described in Chapter I are particularly remarkable. Although the long-standing difficulty of applying the Breit-Wigner to the closely spaced resonances has been eliminated, the traditional concept of resonance integral based on isolated resonances must also be modified. Thirdly, the amazing progress in our computational capabilities provides strong motivations for reactor physicists to venture into previously unimaginably rigorous treatments of the resonance effects in reactor lattices. One notable consequence is the availability of both the deterministic and Monte Carlo codes for treating the lattice physics problems on a continuous energy basis whereby the continuous nature of neutron flux in energy is preserved. It is important to realize, however, that the former is

generally not free from simplifying assumptions while the latter is only useful as a benchmark tool but still too costly for routine applications in spite of the high-speed computing facilities now in existence. The most commonly used method for reactor neutronic calculations today are still based on the multigroup concept. It is, therefore, useful to cast the self-shielding concept within the context of the multigroup approach.

One essential principle of the multigroup approach is the separation of the fine structure effect treatment from the global neutronic calculations of the entire reactor[5]. This can be best accomplished by first computing a set of effective group cross-sections for each nuclide and reaction type at a given location of the reactor lattice, i.e.

$$\tilde{\sigma}_x = \frac{\langle \sigma_x(E) \phi(E, r) \rangle_{E, r}}{\langle \phi(E, r) \rangle_{E, r}} \quad (\text{III.1.3})$$

where the actual flux $\phi(E, r)$ is usually replaced by $\tilde{\phi}(E, r)$ with close resemblance in shape, typically taken as that of the repeated cell in an infinite lattice. It is worth noting that $\tilde{\sigma}_x$, unlike the reaction rate, is more susceptible to the multigroup approach without the recourse of the potentially troublesome renormalization of neutron source. These effective cross sections are also readily amenable to various diffusion or S_N codes whereby a great reduction in labor required solving the neutronic problems could be achieved.

Within the context of the effective cross section concept, the self-shielding effect can be viewed as a measure of correlation between the microscopic cross section and the neutron flux in energy and in space at a given temperature. With no loss of generality, the self-shielding effect can be defined as:

$$f_x = \frac{\tilde{\sigma}_x}{\langle \sigma_x(E) \rangle_E} = 1 + \frac{\text{COV}[\sigma_x(E), \phi(E, r)]}{\langle \sigma_x(E) \rangle_E \langle \phi(E, r) \rangle_{E, r}} \quad (\text{III.1.4})$$

where the covariance (COV) signifies the degree of correlation between σ_x and ϕ . All averages here also implicitly include those over statistical properties of cross sections if resonances are unresolved, and can be cast either into the form of the usual Riemann integrals or Lebesgue integrals.

Conceptually, such a description provides a plausible basis for much of the discussions that follow. The main difference among various methods in practical applications is the rigor by which such a correlation is treated. For the resolved resonance energy range, the degree of correlation is clearly deterministic and multi-variant in nature. Many existing methodologies are implicitly built around the premise that the correlation defined in Eq. (III.1.4) is short range in nature with respect to space and/or energy. For instance, in a highly heterogeneous cell with well-separated fuel regions sandwiched between substantial amounts of moderators, the spatial correlation is obviously localized and thus the use of $\tilde{\phi}(E, r)$ for the infinitely repeated lattice in Eq. (III.1.3) and Eq. (III.1.4) is warranted. On the other hand, in a closely spaced lattice consisting of fuel lumps with different composition, such an assumption may not be justified. The preservation of the rigor in energy correlation is also a primary concern. As described in Chapter I, the energy dependence of resonance cross sections can always be specified concisely by a linear combination of the Doppler-broadened line shape functions characterized by the

relatively short range of fluctuations with respect to their peaks. Hence, many methods based on the traditional resonance integral approach, in effect, took advantage of such behavior as one shall see. For the unresolved resonance energy range, the statistical properties of the widths and level spacing of resonances must also be considered in the determination of the self-shielding effect. It is quite natural that the mutual self-shielding effects of neighboring resonances exhibit strikingly different characteristics depending on whether they belong to the same or different spin sequences. More discussions will be given in the later sections.

It is interesting to note that the self-shielding factor described here is identifiable with the physically measurable quantities discussed in Chapter II. The cumulative self-indication ratio over samples with various thicknesses is simply:

$$[\text{SIR}]_{\text{cum.}} = \frac{\left\langle \int_0^\infty dt \sigma_x(E) e^{-\Sigma_t(E)t} \right\rangle}{\left\langle \sigma_x(E) \right\rangle \left\langle \int_0^\infty dt e^{-\Sigma_t(E)t} \right\rangle} = \frac{\left\langle \frac{\sigma_x(E)}{\Sigma_t(E)} \right\rangle}{\left\langle \sigma_x(E) \right\rangle \left\langle \frac{1}{\Sigma_t(E)} \right\rangle} \quad (\text{III.1.5})$$

which is equivalent to the self-shielding factor defined in Eq. (III.1.4) under the narrow resonance approximation, i.e. $\phi = 1/\Sigma_t(E)$, that will be discussed. Hence, the self-indication measurements are valuable means to verify the viability of resonance data and calculational methods outside of the more complex environment of reactors.

III.2 Slowing-Down Theory for Infinite Homogeneous Media

The simplest scenario for the neutron distribution of practical interest is the case involving the infinite homogeneous medium. In lieu of the spatial dependence and with the assumption of isotropic scattering in the center of the mass system, Eq. (III.1) reduces to the following form generally referred to as the slowing-down equation.

$$\phi(E)\Sigma_t(E) = \sum_i \int dE' \phi(E') \Sigma_{si}(E') f_i(E' \rightarrow E) + Q(E) \quad (\text{III.2.1})$$

where $\Sigma_{si}(E)$ and $f_i(E' \rightarrow E)$ are the macroscopic elastic scattering cross section and scattering kernel for a given nuclide i , respectively. Note that the quantity $\Omega' \rightarrow \Omega$ in Eq. (III.2) is defined in the laboratory system where the target nucleus is assumed at rest and the scattered neutron depends exclusively on the cosine of the angle between two unit vectors, i.e. $\mu_0 = \Omega' \cdot \Omega$. Physically, the scattering kernel $f_i(E' \rightarrow E)$ is

$$f_i(E' \rightarrow E) = \frac{1}{4\pi} \int d\Omega' f_i(\mu_0, E' \rightarrow E) \quad (\text{III.2.2})$$

which is the average of that defined in Eq. (III.2) over all solid angle. The energy/angle correlation is determined by the kinematics of elastic collision under the assumption of isotropic scattering in the center of the mass system.

III.2.1 Kinematics of Elastic Scattering and Scattering Kernel

The kinematics of elastic scattering can be best illustrated via the use of simple vector algebra. Let $\vec{v}'$ (in the direction of Ω') and $\vec{w}'$ be the initial velocities of the neutron and the nucleus respectively in the laboratory system. The conservation of momentum requires that the center-of-mass moves with velocity

$$\vec{v}_0 = \frac{\vec{v}' + A_i \vec{w}'}{1 + A_i} \quad (\text{III.2.3})$$

where A_i is the atomic mass of the target nucleus i .

On the other hand, in the C-system where the center of mass is assumed to be stationary, the initial neutron and nucleus velocities are

$$\vec{v}'_c = \vec{v}' - \vec{v}_0 = \frac{(\vec{v}' - \vec{w}')A_i}{1 + A_i} \quad (\text{III.2.4})$$

$$\vec{w}'_c = \vec{w}' - \vec{v}_0 \quad (\text{III.2.5})$$

respectively. One unique feature of the scattering in the C-system is that the absolute velocity of the neutron remains unchanged when a collision occurs, i.e. $|\vec{v}'_c| = |\vec{v}_c|$ where $\vec{v}_c$ is the final neutron velocity. Let θ_c denote the angle between these two vectors in the C-system so that

$$\mu_c = \cos \theta_c = \frac{\vec{v}'_c \cdot \vec{v}_c}{|\vec{v}'_c| |\vec{v}_c|} \quad (\text{III.2.6})$$

The invariance of the absolute magnitude makes possible the derivation of the relationship between energy and angle via the identity $|\vec{v}' - \vec{v}_0|^2 = |\vec{v} - \vec{v}_0|^2$. It follows that

$$v^2 = v'^2 - \frac{2A_i(1-\mu_c)v'^2}{(1+A_i)^2} \left[1 - \frac{A_i w'^2}{v'^2} + (A_i - 1)\mu_A \frac{|\vec{w}'|}{|\vec{v}'|} \right] \quad (\text{III.2.7})$$

and

$$E' - E = 2(1 - \mu_c) \frac{A_i E'}{(1 + A_i)^2} \left[1 - \frac{E'_A}{E'} + \frac{A_i - 1}{\sqrt{A_i}} \sqrt{E'_A / E'} \mu_A \right] \quad (\text{III.2.8})$$

where $\mu_A = \vec{w}' \cdot \vec{v}' / [|\vec{w}'| |\vec{v}'|]$ and $E'_A = m_n A w'^2 / 2$, and m_n is the mass of neutron, respectively. Since E' is generally much greater than E'_A and $(A-1)^2 E'_A / A$ in the resonance region of practical interest,

the impact of thermal excitation on the scattering kernel, unlike its impact on the resonance cross section described previously, is not of practical interest. Thus, Eq. (III.2.8) can be simplified significantly by neglecting all terms attributed to the thermal motions of the nucleus (i.e. by setting $\vec{w}' = 0$).

$$E' - E = \frac{2A}{(1+A)^2} E' (1 - \mu_c) \quad (\text{III.2.9})$$

Eq. (III.2.9) defines the minimum and maximum allowable fractional losses in neutron energy due to elastic collision corresponding to θ_c equal to 0 and π , respectively. The maximum fractional neutron energy loss per collision with a given nucleus i is customarily written as

$$1 - \alpha_i = \left(\frac{E' - E}{E'} \right)_{\max} = \frac{4A_i}{(1 + A_i)^2} \quad (\text{III.2.10})$$

or the maximum energy loss per collision is simply $\alpha_i E'$ for a neutron with initial energy E' .

Fig. III.1 illustrates the geometric relationship between various quantities in the C-system and those in the L-system that leads immediately to the following identity:

$$\frac{A_i \vec{v}'}{A_i + 1} \mu_c + \frac{\vec{v}'}{A_i + 1} = \mu_0 \vec{v} \quad (\text{III.2.11})$$

Combining Eq. (III.2.11) and Eq. (III.2.9), one obtains the relationship between μ_0 and E/E' as well as μ_c , i.e.

$$\mu_0 = \frac{A_i + 1}{2} \sqrt{\frac{E}{E'}} - \frac{A_i - 1}{2} \sqrt{\frac{E'}{E}} = \frac{1 + A_i \mu_c}{(1 + 2A_i \mu_c + A_i^2)^{1/2}} \quad (\text{III.2.12})$$

Figure III. 1 Velocities and Scattering Angles in C- and L-Systems

The isotropic scattering in the center of the mass system implies that

$$d\Omega_c = 2\pi \sin \theta_c d\theta_c = -2\pi d\mu_c. \quad (\text{III.2.13})$$

From Eq. (III.16), it is clear that $f_i(\mu_c, E' \rightarrow E)$ can be defined in terms of a Dirac δ - function of the form

$$f_i(\mu_c, E' \rightarrow E) = \delta \left[E - E' + \frac{2A_i E'}{(1 + A_i)^2} (1 - \mu_c) \right] \quad (\text{III.2.14})$$

where the range of E is subject to the constraint defined by Eq. (III.2.10). Using Eq. (III.2.10), Eq. (III.2.13) and Eq. (III.2.14), one obtains

$$f_i(E' \rightarrow E) dE = \begin{cases} \frac{1}{1 - \alpha_i} \frac{dE}{E'}, & \alpha_i E' \leq E \leq E' \\ 0, & \text{elsewhere} \end{cases} \quad (\text{III.2.15})$$

Physically, the above equation is equivalent to the statement that the neutron energy distribution after collision is equally probable within the maximum allowable interval $E'(1 - \alpha_i)$. The same result can also be obtained via $f_i(\mu_0, E' \rightarrow E)$ using Eq. (III.2.2) and Eq. (III.2.12).

From practical point of view, the treatment of the slowing-down problems over a large interval along the energy axis is rather inconvenient [8,9,10]. A more attractive approach widely used is to examine the problem on the basis of the logarithmic scale of energy. This is accomplished by defining a new variable u known as 'lethargy', $u = \ln(E_0 / E)$ where E_0 is an arbitrary initial energy that the calculation is to begin. In the u -domain, the scattering kernel defined by the condition,

$$K_i(u - u') du = f_i(E' \rightarrow E) dE \quad (\text{III.2.16})$$

is of the following form:

$$K_i(u - u') = \begin{cases} \frac{e^{-(u-u')}}{1 - \alpha_i} du, & 0 \leq u - u' \leq \varepsilon_i \\ 0, & \text{elsewhere} \end{cases} \quad (\text{III.2.17})$$

where $\varepsilon_i = \ln(1/\alpha_i)$ is the maximum lethargy increment per collision. Two quantities of particular interest in the slowing-down theory are the first two moments defined by:

$$\xi_i = \frac{1}{1 - \alpha_i} \int_0^{\varepsilon_i} u e^{-u} du = 1 - \frac{\alpha_i \varepsilon_i}{1 - \alpha_i} \quad (\text{III.2.18})$$

and

$$\chi_{2i} = \frac{1}{1 - \alpha_i} \int_0^{\varepsilon_i} u^2 e^{-u} du = 2\xi_i - \frac{\varepsilon_i(1 - \xi_i)}{1 - \alpha_i} = 2\xi_i \gamma_i \quad (\text{III.2.19})$$

respectively. Physically, ξ_i represents the average lethargy increment per collision with nuclide i . Its importance will be further discussed.

III.2.2 Characteristics of Slowing-Down Equation

In the presence of resonances, the neutron flux can fluctuate significantly as a function of energy or lethargy [11]. One quantity that is relatively well behaved in the lethargy domain during the slowing-down process is the collision density defined as

$$F(u) = \Sigma_t(u) \phi(u) \quad (\text{III.2.20})$$

where $\Sigma_t(u)$ is the total macroscopic cross section of all nuclide present. Physically, it signifies the total collision rate per volume by those neutrons within the element du . By utilizing the scattering kernel derived previously, the slowing-down equation defined by Eq. (III.2.1) can be cast into the following form [12,13,14]:

$$F(u) = \sum_{i=1}^I \int_{u-\epsilon_i}^u du' F(u') h_i(u) K_i(u-u') + Q(u) \quad (\text{III.2.21})$$

where $h_i(u) = \Sigma_{si}(u) / \Sigma_i(u)$ and I is total number of nuclide in the system. Another quantity of practical interest is the slowing-down density, which is a measure of the total number of neutrons slowed down past a given energy E (or 'above' the corresponding lethargy u), defined as:

$$\begin{aligned} q(u) &= \sum_{i=1}^I \int_{u-\epsilon_i}^u du' F(u') h_i(u') \int_{u'}^{u'+\epsilon_i} du'' K_i(u''-u') \\ &= \sum_{i=1}^I \int_{u-\epsilon_i}^u du' F(u') h_i(u') \left[\frac{e^{-(u-u')}}{1-\alpha_i} - \frac{\alpha_i}{1-\alpha_i} \right] \end{aligned} \quad (\text{III.2.22})$$

The differentiation of Eq. (III.29) leads to the following identity:

$$\frac{dq(u)}{du} = Q(u) - \phi(u) \Sigma_a(u) \quad (\text{III.2.23})$$

and it follows that

$$q(u) = \int_{-\infty}^u du' Q(u') - \int_{-\infty}^u du' \phi(u') \Sigma_a(u') \quad (\text{III.2.24})$$

where $\Sigma_a(u) = \Sigma_i(u) - \Sigma_s(u)$ is the total absorption of the system not precluding the inelastic scattering cross section. These equations provide the theoretical basis for many useful methods in reactor applications. The former, though not suitable for treatment of the detailed resonance structures, provides the foundation for the widely used continuous slowing-down approach via the attenuation of $q(u)$ once the absorption probabilities for each resonance are known. The latter, under the assumption of a mono-energetic source, is physically equivalent to the resonance escape probability for neutrons that reach u without being absorbed. In the following discussions, the treatment of resonance effects will be addressed first.

For detailed investigations of resonance effects, it suffices to focus on the Green's function solution of Eq. (III.2.21) equivalent to the case of mono-energetic source whereby,

$$F_0(u) = \sum_{i=1}^I \int_{u-\epsilon_i}^u du' F_0(u') h_i(u') K_i(u-u') + \delta(u) \quad (\text{III.2.25})$$

so that

$$F(u) = \int_{-\infty}^u Q(u') F_0(u-u') du' \quad (\text{III.2.26})$$

The solution to Eq. (III.2.25), in turn, can be pictured as a linear combination of a δ -function and a

function $F_s(u)$, i.e. $F_0(u) = \delta(u) + F_s(u)$. Thus,

$$F_s(u) = \sum_{i=1}^I \int_{u-\varepsilon_i}^u du F_s(u') h_i(u') K_i(u-u') + \sum_{i=1}^I h_i(0) K_i(u) \quad (\text{III.2.27})$$

represents the collision density away from the mono-energetic source. Here, $h_i(0) = \text{constant}$ will henceforth be assumed. One unique characteristics of $F_s(u)$ is generally referred to as the Placzek oscillations[2]. Such a phenomenon can be best illustrated by casting Eq. (III.2.27) into an alternative form as proposed by Corngold[10]. This can be accomplished readily by using the Laplace transform approach.

Let $\tilde{y}(p)$ be the Laplace transform of a function $y(u)$, i.e.,

$$\tilde{y}(p) = \mathcal{L}\{y(u)\} = \int_0^\infty du e^{-pu} y(u) \quad (\text{III.2.28})$$

and, conversely, its inverse be

$$\mathcal{L}^{-1}\{\tilde{y}(p)\} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dp e^{pu} \tilde{y}(p) \quad (\text{III.2.29})$$

where $c > 0$. Upon Laplace transform, Eq. (III.2.27) becomes

$$\tilde{F}_s(p) = \frac{\sum_{i=1}^I h_i(0) \tilde{K}_i(p)}{1 - \sum_{i=1}^I h_i(0) \tilde{K}_i(p)} - \frac{\sum_{i=1}^I \tilde{K}_i(p) \mathcal{L}\{g_i(u) F_s(u)\}}{1 - \sum_{i=1}^I h_i(0) \tilde{K}_i(p)} \quad (\text{III.2.30})$$

where $g_i(u) = h_i(0) - h_i(u)$. The inversion of the above equation yields an alternative form of the slow-down equation for the Placzek function explicitly:

$$F_s(u) = P(u) - \sum_{i=1}^I \int_0^u du' G_i(u-u') g_i(u') F_s(u') \quad (\text{III.2.31})$$

where the kernel $G_i(u-u')$ and the Placzek function are defined as :

$$G_i(u) = \mathcal{L}^{-1} \left\{ \frac{\tilde{K}_i(p)}{1 - \sum_{i=1}^I h_i(0) \tilde{K}_i(p)} \right\} \quad (\text{III.2.32})$$

$$P(u) = \sum_{i=1}^I h_i(0) G_i(u) \quad (\text{III.2.33})$$

respectively. Physically, $P(u)$ is equivalent to the collision density $F_s(u)$ as if the resonances were absent. $G_i(u)$ signifies a special case of the Placzek function in which the source term (second term on the RHS of Eq. (III.2.30) is attributed to the nuclide i alone.

Although Eq. (III.2.31) does not appear to offer any advantage over the traditional slowing-down equation specified by Eq. (III.2.21) in so far as the complexity of the solution is concerned, nevertheless, it provides a much clearer picture of the basic phenomenon associated with elastic scattering process in the presence of resonances via the explicit entry of the Placzek function.

III.2.3 Concept of Placzek Oscillations

The alternative form of the slowing-down equation defined by Eq. (III.2.31) is seldom used in practical applications due to the obvious complexities involved in computing the Placzek function [2] and the related kernel. On theoretical grounds, however, it does provide the invaluable analytical insight required for our understanding of the fundamental phenomenon associated with the neutron moderation process. Conceptually, Eq. (III.2.31) explicitly relates the collision density to the Placzek function characteristic of the elastic collision process. Thus, the collision density can be viewed as a superposition of two terms, of which the first corresponds to that in absence of resonances as denoted by $P(u)$ while the second represents the interaction between the Placzek function and the resonance cross sections manifested through the quantity $g_i(u)$. It is quite apparent that the understanding of such a function is essential if one wishes to study the detailed behavior of neutron spectrum in the presence of resonances.

The most crucial quantity that dictates the outcome of the Placzek function is the scattering kernel $K_i(u)$. Its discontinuous nature in the energy lethargy domain for all nuclides with the exception of hydrogen is directly responsible for the subsequent oscillations in collision density. The Laplace transform of $K_i(u)$ assumes the form,

$$\tilde{K}_i(p) = \frac{1}{1 - \alpha_i} \frac{1 - e^{-\varepsilon_i(1+p)}}{(1+p)} \quad (\text{III.2.34})$$

Hence, from Eq. (III.2.32) and Eq. (III.2.33), one obtains,

$$\mathcal{L}\{P(u)\} = \frac{\sum_{i=1}^I \frac{h_i(0)}{1 - \alpha_i} [1 - e^{-\varepsilon_i(1+p)}]}{(p+1) - \sum_{i=1}^I \frac{h_i(0)}{1 - \alpha_i} [1 - e^{-\varepsilon_i(1+p)}]} \quad (\text{III.2.35})$$

The inversion of the above equation is obviously not so simple if many nuclides are present. For illustrative purposes, the simplest case with one nuclide will be examined first.

For a single nuclide, the kernel $G_i(u)$ is the same as $P(u)$ and Eq. (III.2.35) becomes,

$$\mathcal{L}\{P(u)\} = \left(\frac{1}{1-\alpha} \right) \frac{1 - \alpha e^{-\varepsilon p}}{\left(p - \frac{\alpha}{1-\alpha} \right) + \frac{\alpha}{1-\alpha} e^{-\varepsilon p}} \quad (\text{III.2.36})$$

where the subscript i is dropped for convenience. The simplest possible case is obviously that of the hydrogen for which α is equal to zero. Thus, Eq. (III.2.36) leads immediately to $P(u)=1$ upon inversion. For all $A > 1$, the solution of the inverse is by no means simple. Of particular theoretical interest is the inversion of the above equation under two physical conditions: (1) near the source or small value of u ; (2) asymptotic condition as u becomes large. In the p -domain, the former is equivalent to the situation where $|p|$ becomes very large whereas the latter is associated with the case of p approaching zero.

Hence, for large p , Eq. (III.2.36) can be expressed in terms of a power series:

$$\mathcal{L}\{P(u)\} = \left(\frac{1}{1-\alpha} \right) \frac{1 - \alpha e^{-\varepsilon p}}{\left(p - \frac{\alpha}{1-\alpha} \right)} \sum_{n=0}^{\infty} \frac{(-1)^n \left(\frac{\alpha}{1-\alpha} \right)^n e^{-n\varepsilon p}}{\left(p - \frac{\alpha}{1-\alpha} \right)^n} \quad (\text{III.2.37})$$

Note that the presence of the exponential term $\exp(n\varepsilon p)$ indicates its inverse consists of unit step functions for each interval $n\varepsilon$. The inversion of Eq. (III.2.37) can be carried out readily term-by-term and, upon rearrangement, one obtains

$$P(u) = \frac{e^{\frac{\alpha}{1-\alpha}u}}{1-\alpha} + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \left(\frac{\alpha}{1-\alpha} \right)^n e^{\frac{\alpha}{1-\alpha}(u-n\varepsilon)} \left(n + \frac{u-n\varepsilon}{1-\alpha} \right) (u-n\varepsilon)^{n-1} H(u-n\varepsilon) \quad (\text{III.2.38})$$

where the Heaviside function (or unit step function) is defined as:

$$H(u) = \begin{cases} 1 & \text{for } u > 0 \\ 0 & \text{elsewhere} \end{cases} \quad (\text{III.2.39})$$

Thus, the analytical behavior of the Placzek function is explicitly defined in the subsequent lethargy intervals 'above' the initial source lethargy. In particular, its values at the first few intervals of practical interest are presented as follows:

(1) First interval ($0 \leq u \leq \varepsilon$):

$$P(u) = \frac{1}{1-\alpha} e^{\frac{\alpha}{1-\alpha}u} \quad (\text{III.2.40})$$

(2) Second interval ($\varepsilon \leq u \leq 2\varepsilon$):

$$P(u) = \frac{1}{1-\alpha} e^{\frac{\alpha}{1-\alpha}u} \left[1 - e^{\frac{-\alpha\varepsilon}{1-\alpha}} \left(1 + \frac{u-\varepsilon}{1-\alpha} \right) \right] \quad (\text{III.2.41})$$

(3) Third interval ($2\varepsilon \leq u \leq 3\varepsilon$):

$$P(u) = \frac{1}{1-\alpha} e^{\frac{\alpha}{1-\alpha}u} \left[1 - e^{\frac{-\alpha\varepsilon}{1-\alpha}} \left(1 + \frac{u-\varepsilon}{1-\alpha} \right) + \alpha(u-2\varepsilon) e^{\frac{-2\alpha\varepsilon}{1-\alpha}} \left(1 + \frac{1}{2} \frac{u-2\varepsilon}{1-\alpha} \right) \right] \quad (\text{III.2.42})$$

Fig. III.2 illustrates the behavior of the Placzek function as a function of u for nuclide of various mass within first few scattering intervals. These plots clearly exhibit the same distinct properties of fluctuations. Such fluctuations are at its greatest amplitudes in the first scattering interval and damp out rapidly as u increases. Since the amplitude of fluctuations is inversely propositional to $1/(1-\alpha)$ the fluctuations are much more severe as A increases. Furthermore, a discontinuity occurs at the junction of the first and the second scattering intervals as the natural consequence of the finite range of the permissible energy loss per collision for all $A > 1$. The asymptotic property can be shown analytically by letting p in Eq. (III.2.37) approach zero, i.e.

$$\lim_{p \rightarrow 0} \mathcal{L}\{p(u)\} = \frac{1}{p \left[1 - \frac{\alpha\varepsilon}{1-\alpha} \right]} \quad (\text{III.2.43})$$

and from Eq. (III.2.43) and the basic property of Laplace transform it follows

$$\lim_{p \rightarrow 0} P(u) = \frac{1}{\xi} \quad (\text{III.2.44})$$

where ξ is the average lethargy increment per collision previously described. The rapidity by which $P(u)$ can reach its asymptotic value is clearly illustrated in Fig. III.2. The short-range nature of the Placzek oscillations makes possible the derivation of many simplified methods for treating the resonance absorption.

Figure III. 2 Placzek Function in a Mixture of Fast Reactor Composition

For practical applications, however, the reactor compositions usually consist of multiple nuclides with a wide range of atomic masses. The amplitudes of fluctuation for the heavy nuclides can be significantly reduced when mixed with lighter ones. Furthermore, the knowledge of the individual components specified by the kernel $G_i(u)$ is conceptually essential in order to understand this rather intricate phenomenon of oscillation in the presence of resonances. To put the theoretical aspects of the issue in perspective, the Placzek oscillations for the mixture will be briefly described.

Like the case of a single nuclide, similar expressions for a mixture containing I nuclides under two limiting conditions can be derived. For large $|p|$, the power series expansion yields

$$\mathcal{L}\{p(u)\} = \left[\sum_{i=1}^I h_i(0) \frac{1}{p-k} \frac{1}{1-\alpha_i} (1-\alpha_i e^{-\varepsilon_i p}) \right] \sum_{n=0}^{\infty} (-1)^n \left[\frac{\sum_{i=1}^I k_i e^{-\varepsilon_i p}}{p-k} \right]^n \quad (\text{III.2.45})$$

where $k = \sum_{i=1}^I k_i$ and $k_i = h_i(0) \alpha_i / (1 - \alpha_i)$. The inversion of the above equation requires the explicit knowledge of ε_i and $h_i(0)$. The presence of overlapping intervals can make the inversion extremely difficult. For illustrative purposes here, a simple case in which all heavy nuclides are assumed to have the same mass in the mixture with lighter nuclides of arbitrary masses will be considered. Under such a condition, the Placzek function and $G_i(u)$ for the first few intervals of the heavy nuclide can be carried out explicitly. In particular, if subscript h denotes any heavy nuclide in the mixture, $P(u)$ and the

corresponding $G_h(u)$ for the first two intervals are given as follows.

(1) First interval ($0 \leq u \leq \varepsilon_h$):

$$P(u) = \sum_{i=1}^I h_i(0) G_i(u) = \sum_{i=1}^I \frac{h_i(0)}{1 - \alpha_i} e^{ku} \quad (\text{III.2.46})$$

where k is defined by Eq. (III.2.45).

(2) Second interval ($\varepsilon_h \leq u \leq 2\varepsilon_h$):

$$P(u) = \sum_{i=1}^I h_i(0) G_i(u) = \sum_{i=1}^I h_i(0) \frac{e^{ku}}{1 - \alpha_i} \left\{ 1 - e^{-k\varepsilon_i} \left[\alpha_i + \sum_{i=1}^I \frac{\alpha_i h_i(0)}{1 - \alpha_i} (u - \varepsilon_i) \right] \right\} \quad (\text{III.2.47})$$

The derivation of $P(u)$ in all subsequent intervals can be obtained by the same procedure and will not be presented here. Fig. III.2 illustrates the behavior of $P(u)$ and $G_h(u)$ for a typical mixture of fast reactor composition with oxide fuel as compared to that of the case of 'pure' U^{238} . It is seen that the amplitude of fluctuations in $P(u)$ for the mixture is substantially reduced by the presence of diluents. Nevertheless, the fluctuations in $G_h(u)$ for the heavy isotopes like U^{238} are still considerable. The latter is directly responsible for the fluctuations in collision density in the presence of resonances, as one shall see shortly. Like the case of the single nuclide, such fluctuations damp out rapidly as $P(u)$ approaches its asymptotic value $1/\bar{\xi}$, where $\bar{\xi}$ is the average increment in lethargy per collision for the mixture. This can be shown readily by setting $p \rightarrow 0$ in Eq. (III.2.35)

$$\lim_{p \rightarrow 0} \mathcal{L}\{p(u)\} = \frac{1}{p \left[1 - \sum_{i=1}^I \frac{h_i(0) \alpha_i \beta_i}{1 - \alpha_i} \right]} = \frac{1}{p \bar{\xi}} \quad (\text{III.2.48})$$

It follows that

$$\lim_{p \rightarrow 0} P(u) = \frac{1}{\bar{\xi}} \quad (\text{III.2.49})$$

where $\bar{\xi}$ is related to the individual ξ_i defined by Eq. (III.2.18) via $\bar{\xi} = \sum_{i=1}^I h_i(0) \xi_i$. By utilizing the short-range nature of fluctuations in $P(u)$ and by rearranging the integrand of Eq. (III.2.31), one has

$$F_s(u) = \frac{1}{\bar{\xi}} - \int_0^\infty du' \Xi(u - u') F_s(u') \quad \text{for all } u > 0 \quad (\text{III.2.50})$$

where

$$\Xi(u-u') = P(u-u') \frac{\Sigma_R(u')}{\Sigma_t(u')} - \sum_{h=1}^M G_h(u-u') \frac{\Sigma_{si}(u')}{\Sigma_t(u')} \quad (\text{III.2.51})$$

with $\Sigma_R(u)$, total macroscopic resonance cross section of all resonance isotopes, $\Sigma_{si}(u)$, macroscopic resonance scattering cross section for isotope i , and M , total number of resonance isotopes respectively. Since the value of $\Xi(u-u')$ can be either negative or positive, the corresponding collision density must vary above or below the asymptotic limit accordingly in the presence of resonances. The obvious factor beside the relative amplitudes of $G_h(u-u')$ and $P(u-u')$ that determines the nature of the oscillations is the relative importance of the resonance scattering cross section with respect to the absorption cross section. For a Breit-Wigner resonance, for instance, the collision density is expected to rise above its asymptotic value starting near the resonance energy before the oscillations if the neutron width constitutes a significant portion to the total width as is the case for many s-wave resonances of U^{238} . The opposite is true if the neutron width is small compared to other partial widths as expected for many resonances of fissile isotopes. Fig. III.3 shows a typical example of the Placzek oscillations in the presence of a Breit-Wigner resonance in a typical sodium-cooled fast reactor with oxide fuel and stainless steel cladding. Two contrasting behaviors of U^{238} and Pu^{239} are given. Again, the oscillations damp out rapidly within first few intervals of the resonance isotopes. It should be noted, however, that, unlike the case without a resonance, the collision density could no longer recover to its original asymptotic value due to the resonance absorption. For a single resonance given in Fig. III.3, the constant value $\lim_{p \rightarrow 0} [\bar{\xi} F(u)]$ is commonly referred to as resonance escape probability for an isolated resonance. Also shown in Fig. III.3 are points obtained analytically by an approximate method to be described.

Figure III. 3 Placzek Oscillations in the Presence of a Breit-Wigner Resonance

From the foregoing discussions, it is quite apparent that the oscillations in collision density when neutrons suffer collisions near a resonance reflect the fundamental mechanism of the elastic scattering process. For a mixture with many nuclides with $A > 1$, the Placzek function and its related kernel consist of a superposition of Heaviside functions and become hopelessly intertwined when more than one nuclide are present. Consequently, no analytical solution of the closed form is feasible without simplified assumptions as long as the mixture contains non-hydrogenous material. In the following section, various practical methods for dealing with the slowing-down problems will be considered.

III.2.4 Traditional Treatment of Neutron Slowing-Down Problems in Presence of Resonances

With exception of the rigorous numerical treatment to be described later, existing methods for treating the slowing-down problems in the presence of resonances are based on approximations of various degrees of sophistication in order to circumvent the difficulties directly or indirectly attributed to the Placzek oscillations. In this section, the fundamental aspects of the traditional resonance treatment that eventually lead to the continuous slowing-down theory and the effective resonance concept will be

addressed.

Perhaps the most logical starting point for our discussions here is the simplest possible case in which the neutron moderation is due entirely to hydrogen alone while other heavier isotopes in the mixture provide absorption only. In lieu of the Placzek oscillations, Eq. (III.2.31) becomes a simple first order differential equation upon differentiation and one obtains

$$F_s(u) = \frac{\Sigma_s(0)}{\Sigma_t(0)} \exp \left[- \int_0^u du' \frac{\Sigma_a(u')}{\Sigma_t(u')} \right] = q(u) \quad (\text{III.2.52})$$

where the exponential term signifies the probability that neutrons escape absorption in the span from the source lethargy to u . From Eq. (III.2.52), it is obvious that the slowing-down density $q(u)$ becomes equal to $F_s(u)$ as ε_i becomes infinity. Conceptually, two scenarios are of particular interest here. First, if $\Sigma_a \sim 1/\sqrt{E}$ and $\Sigma_s(u)$ is dominated by its potential scattering component, the integral in the exponent can be evaluated analytically so that

$$q(u) = \frac{\Sigma_s^2(0)}{\Sigma_t^2(u)}, \quad \phi(u) = \frac{\Sigma_s^2(0)}{\Sigma_t^3(u)} \quad (\text{III.2.53})$$

Secondly, if, in addition to the $1/v$ absorption, an ensemble of 'narrow' resonances of Breit-Wigner type is also present, Eq. (III.2.52) can be cast into the following form

$$q(u) \approx q_{as}(u) \prod_{u_r < u} (1 - p_r) \quad (\text{III.2.54})$$

where $q_{as}(u)$ can be identified with that defined by Eq. (III.2.53) and

$$p_r = \int_0^\infty \frac{\Sigma_{ar}(u)}{\Sigma_t(u)} du \quad (\text{III.2.55})$$

is the absorption probability due to the 'narrow' resonance r with its peak $u_r < u$.

Although the hypothetical case described above has little resemblance to the problems of practical interest, it does provide some analytical insight to the role of the resonance integral in the slowing-down problems. Physically, it clearly illustrates the theoretical basis of the continuous slowing-down approach. The rationale of such an approach is to treat the effects attributed to the relatively smoothly varying cross sections and those attributed to the sharp resonances separately thereby better computing efficiencies can be achieved. However, the mixtures considered in reactor applications inevitably involve non-hydrogen constituents with energy dependent cross sections of various types, which give rise to the Placzek oscillations discussed in the foregoing section. By and large, the cross sections in the resonance range can be divided into two general categories as specified by the existing nuclear data files, namely, the 'smooth' and the resonance cross sections. For the continuous slowing-down approach, the 'narrow' resonances are considered separately in the context of Eq. (III.2.54) when

the spectrum is treated. Resonances of which the extent is small compared to the energy meshes for the spectrum calculations are taken to be 'narrow'. These include practically all resonances of actinides and some of the $l > 0$ resonances of the intermediate weight nuclides. Much of the efforts in the earlier development of the slowing-down theory are focused on various means to achieve the similar solution under the more general environment pertinent to reactor applications. To achieve such a goal, it is quite apparent that either the integrand of Eq. (III.2.21) or the Placzek function of Eq. (III.2.33) must be simplified. One best-known approximation of this kind is that proposed by Greuling and Goertzel[15]. There are many ways to solve the Greuling-Goertzel form. For our discussions here, it suffices to begin with what is most obvious on theoretical grounds.

Many earlier methods for treating the slowing-down problems in the absorbing media can be construed as the natural consequence of applying the Taylor's expansion to the quantity $\Sigma_{si}(u)\phi(u)$ in the integrand of the slowing-down equation whereby

$$\Sigma_{si}(u')\phi(u') = \sum_{n=0}^{\infty} (-1)^n \frac{(u-u')^n}{n!} \frac{d^n}{du^n} [\Sigma_{si}(u)\phi(u)] \quad (\text{III.2.56})$$

Physically, the validity of using the low order terms in such an expansion requires that $\Sigma_{si}(u')\phi(u')$ must vary slowly as a function of u' . If one retains only the zeroth and first order terms, Eq. (III.2.21)

becomes a first order differential equation of the form

$$\frac{d}{du} [\bar{\xi}(u) \Sigma_s(u) \phi(u)] = Q(u) - \Sigma_a(u) \phi(u) \quad (\text{III.2.57})$$

where $\Sigma_x(u)$ will, henceforth, be referred to as $\sum_{i=1}^I \Sigma_{xi}(u)$ for any reaction process x and $\bar{\xi}(u)$, analogous to the lethargy-independent $\bar{\xi}$ defined previously in Eq. (III.2.48), is denoted by $\bar{\xi}(u) = \sum_{i=1}^I \xi_i \Sigma_{si}(u) / \Sigma_s(u)$. On the other hand, by substituting only the zeroth order term of the series into Eq. (III.29), one obtains

$$q(u) = \bar{\xi}(u) \Sigma_s(u) \phi(u) \quad (\text{III.2.58})$$

Thus, the combination of Eq. (III.2.57) and Eq. (III.2.58) immediately yields the well-known age approximation

$$\phi(u) = \frac{Q_0}{\bar{\xi}(u) \Sigma_s(u)} \exp \left[- \int_0^u \frac{\Sigma_a(u')}{\bar{\xi}(u') \Sigma_s(u')} du' \right] \quad (\text{III.2.59})$$

at the energy far below the source energy.

Similarly, if one retains up to second order term in Eq. (III.2.56), the substitution into Eq. (III.2.21) gives

$$\frac{d}{du} \left\{ \left[\bar{\xi}(u) \Sigma_s(u) \phi(u) \right] (1 - \bar{\gamma}'(u)) - \bar{\gamma}(u) \frac{d}{du} \left[\bar{\xi}(u) \Sigma_s(u) \phi(u) \right] \right\} = Q(u) - \Sigma_a(u) \phi(u) \quad (\text{III.2.60})$$

where the additional parameter $\bar{\gamma}(u)$, analogous to isotopic γ_i defined by Eq. (III.2.19), is related to the second order moment χ_{2i} as

$$\bar{\gamma}(u) = \frac{\sum_{i=1}^I \chi_{2i} \Sigma_{si}(u)}{2 \bar{\xi}(u) \Sigma_s(u)} \quad (\text{III.2.61})$$

and $\bar{\gamma}'(u) = d\bar{\gamma}/du$. If one assumes the validity of Eq. (III.2.57), Eq. (III.2.60) is reduced to the generalized form of the Greuling-Goertzel approximation

$$\frac{dq(u)}{du} = [1 + \bar{\gamma}'(u)] N(u) Q(u) - \frac{\Sigma_a(u)}{M(u)} q(u) \quad (\text{III.2.62})$$

where

$$M(u) = \bar{\xi}(u) \Sigma_s(u) [1 - \bar{\gamma}'(u)] + \bar{\gamma}(u) \Sigma_a(u) \quad (\text{III.2.63})$$

$$q(u) = M(u) \phi(u) \quad (\text{III.2.64})$$

and $N(u) = [\bar{\xi}(u) \Sigma_s(u)] / M(u)$ is a normalization factor. Hence, the solution to the first order differential equation is simply

$$q(u) = [q(0) + q^{(1)}(u)] \exp \left[- \int_0^u du' \frac{\Sigma_a(u')}{M(u')} \right] \quad (\text{III.2.65})$$

where

$$q^{(1)}(u) = \int_0^u du' \frac{\bar{\xi}(u') [1 + \bar{\gamma}'(u')] \Sigma_s(u') Q(u')}{M(u')} \exp \left[- \int_0^{u'} du'' \frac{\Sigma_a(u'')}{M(u'')} \right] \quad (\text{III.2.66})$$

Equations (III.2.65) and (III.2.66) provide a simplified means of estimating the neutron spectrum for the infinite homogeneous media and the theoretical basis for the continuous slowing-down approaches. For the resonance treatment, sometimes it suffices to examine the case in absence of the non-elastic scattering sources, i.e., $q^{(1)}(u) = 0$, and negligible $\bar{\gamma}'(u)$. Physically, the Greuling-Goertzel approximation exhibits the general feature of the exact solution for the case of the hydrogen given by Eq. (III.2.52) with exception of the presence of the average scattering parameters $\bar{\xi}(u)$ and $\bar{\gamma}(u)$. For reactor applications, $q(u)$ defined in Eq. (III.2.65) is taken to be equal to $q_{as}(u)$ excluding the contributions from 'narrow' resonances and the actual spectrum is obtained by the attenuation scheme

defined by Eq. (III.2.54) once the absorption probability p_r in the context of Eq. (III.2.55) is known.

There are other ways by which Eq. (III.2.65) can be derived. As a matter of fact, the original derivation by Goertzel and Greuling was based on the assumption that the discontinuous scattering kernel $K_i(u - u')$ given in Eq. (III.2.17) by a synthetic kernel $K_i^*(u - u')$ analogous to that of the hydrogen where

$$K_i^*(u - u') = \frac{\xi_i}{\gamma_i} \exp\left[-\frac{(u - u')}{\gamma_i}\right] \quad \text{for } u \geq u' \quad (\text{III.2.67})$$

The requirement that the zeroth and the first order moments of $K_i(u - u')$ and $K_i^*(u - u')$ be equal leads directly to Eq. (III.2.65). The well-known Wigner approximation can be pictured as a special case that γ_i is equal to ξ_i . Similar results can also be obtained by making a two term Taylor's expansion of $\Sigma_{si}(u')\phi(u')[\exp(u' - u) - \alpha_i]/[1 - \alpha_i]$ as shown by Segev[16].

The question arises, however, as to the validity of the low order expansion that obviously requires the smooth variation of $\Sigma_{si}(u')\phi(u')$ as a function of u' in deriving Eq. (III.2.65). In view of the Placzek oscillation characteristics described by Eq. (III.2.27), such a condition may become questionable in the presence of a relatively 'narrow' resonance with sizable Γ_n especially for the s-wave resonances of structural material in the high energy region important to fast reactor applications. One remedy suggested by Stacey is to make the Taylor's expansion on the total collision density $F(u')$ instead, because it is obviously a more slowly varying quantity than the corresponding isotopic scattering collision densities especially for the relatively heavy elements in the mixture. By so doing, one can still retain the general features of the Greuling-Goertzel approximation except that the scattering parameters must be redefined, i.e.

$$\hat{\xi}(u) = \tilde{\xi}(u) + \frac{\bar{a}(u)\bar{c}(u)}{\bar{e}(u)} \quad (\text{III.2.68})$$

$$\hat{\gamma}(u) = \tilde{\gamma}(u) + \frac{\bar{a}(u)}{\bar{e}(u)}[1 + \bar{c}(u)] \quad (\text{III.2.69})$$

where the pertinent parameters are given by

$$\tilde{\xi}(u) = \sum_{i=1}^I \int_{u-\varepsilon_i}^u du' \frac{\Sigma_{si}(u')}{\Sigma_t(u')} \frac{e^{u'-u} - \alpha_i}{1 - \alpha_i} \quad (\text{III.2.70})$$

$$\bar{a}(u) = \sum_{i=1}^I \int_{u-\varepsilon_i}^u du' \frac{\Sigma_{si}(u')}{\Sigma_t(u')} \frac{e^{u'-u} - \alpha_i}{1 - \alpha_i} (u' - u) \quad (\text{III.2.71})$$

$$\bar{c}(u) = \sum_{i=1}^I \left[\frac{\Sigma_{si}(u)}{\Sigma_t(u)} - \int_{u-\varepsilon_i}^u du' \frac{\Sigma_{si}(u')}{\Sigma_t(u')} \frac{e^{u'-u}}{1-\alpha_i} \right] \quad (\text{III.2.72})$$

$$\bar{e}(u) = \sum_{i=1}^I \int_{u-\varepsilon_i}^u du' \frac{\Sigma_{si}(u')}{\Sigma_t(u')} \frac{e^{u'-u}}{1-\alpha_i} (u' - u) \quad (\text{III.2.73})$$

Thus, the general form of the Greuling-Goertzel approximation remains intact at the expense of the need to evaluate additional set of parameters. This improved version has been successfully demonstrated when used in conjunction with the MC²-2 code using the ultra-fine group structure designed for fast reactor applications and the highly efficient resonance integral algorithms to be discussed.

III.3 Resonance Integrals and Their Applications

The continuous slowing-down approach discussed in the foregoing section provides the rationale whereby the treatment of the resonance absorption attributed to the relatively ‘narrow’ resonances can be treated separately from the global spectrum calculations at much coarser energy meshes. One widely used tool for treating the resonance absorption is via the use of the resonance integral concept. In this section, both the conceptual and practical aspects of the problems associated with the resonance integrals will be examined.

III.3.1 Traditional Resonance Integral Concept

In the earlier days of the reactor development with focus on the light water reactor with low enrichment fuel, the treatment of the resonance absorption is centered on a handful of low-lying resonances of U²³⁸. All methodologies were based exclusively on the premise that resonances were well isolated. Under such a condition, one only needs to deal with a single resonance at a time. Thus, within the extent of the resonance in question, the neutron slowing-down problem becomes significantly simplified because the resonance alone is responsible for the energy-dependence in cross sections for practical purposes. The problem was still insurmountable without additional assumptions in lieu of the modern computing tools. Three main assumptions that eventually led to four widely used approximations are: (1) flux recovery between resonances; (2) $\phi(0) \approx 1$ (or $F(0) = \Sigma_p$) above each resonance; (3) $\Sigma_{si}(u')\phi(u')$ in the integrand of the slowing-down equation is taken to be constant for all nuclides in the mixture except for the resonant isotope in question. This assumption is equivalent to the use of the ‘narrow’ resonance approximation in the integrands of all non-resonant constituents in the mixture. Hence, the slowing-down equation at the energy far below the source becomes

$$\Sigma_t(u)\phi(u) = \Sigma_m + \int_{u-\varepsilon}^u du' \frac{e^{-(u-u')}}{1-\alpha} \Sigma_{sr}(u')\phi(u') \quad (\text{III.3.1})$$

where Σ_m is the energy-independent macroscopic scattering cross section of non-resonance nuclides and the subscripts for various parameters of the resonant isotope will, henceforth, be dropped for convenience. The simplified equation above also implies that the absorption of the medium is due entirely to the resonance under consideration. For some more recent work, the assumption (3) can be somewhat relaxed.

Physically, these assumptions lead immediately to the direct relationship between the absorption rate and the absorption probability of the isolated resonance in question, i.e.

$$p_r = \int_0^\infty \Sigma_{ar}(u) \phi(u) du \quad (\text{III.3.2})$$

where the integral, when divided by the concentration of the resonance absorber, is generally referred to as the resonance integral. Therefore, the spectrum of the mixture is defined via the attenuation of the 'asymptotic' flux (or $q(u)$) defined by Eq. (III.2.65) using the factor $\prod_{u_r < u} (1 - p_r)$. It will be shown that

(with the attenuation factors) the effective group cross-section given by Eq. (III.1.3) can be readily obtained. In the following discussions, we shall focus on the derivations of the four widely used approximations for resonance integrals first.

(1) Narrow Resonance Approximation (NR)

If the extent of the resonance is small compared to the maximum energy loss per collision, the resonance contribution to the integral term in Eq. (III.3.1) becomes negligible and consequently, $\Sigma_{sr}(u') \phi(u')$ is approximately equal to Σ_{pr} for practical purposes in so far as the evaluation of the integral is concerned. Thus, Eq. (III.3.1) is reduced to

$$\phi(u) = \frac{\Sigma_p}{\Sigma_t(u)} \quad (\text{III.3.3})$$

where $\Sigma_p = \Sigma_m + \Sigma_{pr}$ is the total macroscopic potential scattering cross section. Similar conclusion can also be reached directly from the alternative form of slowing-down equation given by Eq. (III.2.21). The fact is that $\phi(u) \sim 1/\Sigma_t(u)$ is equivalent to the zeroth's order term of the Neumann series solution to the integral equation in absence of contribution from the Placzek oscillations. Therefore, the corresponding resonance integral becomes

$$(RI)_{NR} = \sigma_p \int_0^\infty \frac{\Sigma_{ar}(u)}{\Sigma_t(u)} du \quad (\text{III.3.4})$$

where $\sigma_p = \Sigma_p / N_r$ in unit of barns per atom and N_r is the concentration of the absorber in question. Since the majority of resonances of heavy nuclides within the resolved as well as unresolved regions fits into this category, the NR-approximation is extremely important especially in the fast reactor applications. For a Breit-Wigner resonance, the substitution of the Doppler-broadened line shape function yields the traditional $J(\theta_r, \beta_r, a_r)$ integral

$$(RI)_{NR} = \frac{\sigma_p \Gamma_{ar}}{E_r} J(\theta_r, \beta_r, a_r) = \frac{\sigma_p \Gamma_{ar}}{E_r} \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\theta_r, x)}{\beta_r + \psi(\theta_r, x) + a_r \chi(\theta_r, x)} dx \quad (\text{III.3.5})$$

where $\Gamma_{ar} = \Gamma_{\gamma r} + \Gamma_{fr}$, $\beta_r = \Sigma_p / \Sigma_{0r}$ and $a_r = 2 \tan \phi_l$. Here, Σ_{0r} is the total macroscopic peak

resonance cross section of the level r . It is worth noting that the hard sphere phase shift factor is accounted for rigorously whereas $\sin 2\varphi_0 \approx 2\varphi_0$ and $\varphi_l \approx 0$ for $l > 0$ are usually assumed in the traditional expression. In fact, the asymmetric Doppler-broadened line shape function is often ignored for the sake of expediency in many earlier works. Since $J(\theta_r, \beta_r)$, in absence of a_r , is readily amenable to the utilization of a pre-computed table in two-dimensional array, it is most widely used in the Western countries.

Alternatively, the resonance integral can also be expressed in a different form

$$(RI)_{NR} = I_r^{(\infty)} \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\theta_r, x)}{1 + h_r \psi(\theta_r, x) + \iota_r \chi(\theta_r, x)} dx = I_r^{(\infty)} K(h_r, \theta_r, \iota_r) \quad (\text{III.3.6})$$

where $h_r = 1/\beta_r$, $\iota_r = a_r/\beta_r$ and $I_r^{(\infty)} = \pi\sigma_{0r}\Gamma_{ar}/(2E_0)$ is the resonance integral at infinite dilution respectively. The K-integral here represents the self-shielding factor for the resonance integral in question directly. Such a representation is widely used in Russia and Eastern Europe.

The question arises as to the justification of neglecting the effect of the Placzek oscillations. As illustrated in Fig. III.3, such an effect on the collision density can be significant for resonances with relatively significant Γ_n with respect to Γ_t even if the extent of the resonance is small compared to the maximum energy loss per collision. One remedy is to solve Eq. (III.2.50) directly within the constraints of the criteria assumed. Since the resonance is narrow and the ψ -function dies out rapidly away from the peak, it suffices to assume that the kernel $\Xi(u-u')$ is essentially representable by its value in the first collision interval defined by Eq. (III.2.46) so far as the evaluation of the resonance integral is concerned. Under such a condition, the integral equation is solvable by using the method of the resolvent kernel. Furthermore, if one further assumes that $G_h(u)$ defined in Eq. (III.2.32) can be approximated by [17]

$$G_i(u-u') = \frac{1}{1-\alpha_i} \quad \text{for } u'-u > 0 \quad (\text{III.3.7})$$

the solution becomes

$$F(u) = \frac{1}{\xi} \exp \left\{ - \int_0^u \left[\kappa_1 \frac{\Sigma_{Rh}(u')}{\Sigma_t(u')} - \frac{1}{1-\alpha_h} \frac{\Sigma_{Rsh}(u')}{\Sigma_t(u')} \right] du' \right\} \quad (\text{III.3.8})$$

where $\kappa_1 = \kappa + 1 = \sum_{i=1}^I h_i(0)/(1-\alpha_i)$, and $\Sigma_{Rh}(u)$ and $\Sigma_{Rsh}(u)$ are the total resonance cross section and resonance scattering cross sections, respectively. The above equation can be considered as the generalized form of Spinney's approximation obtained by entirely different approach. In absence of moderator effect, it becomes identical with that derived by Spinney.

Equation (III.3.8) immediately leads to the improved version of the NR-approximation of the following form for an isolated resonance including the effects of Placzek oscillations,

$$RI = (RI)_{NR} \left\{ 1 + \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{(m+1)!} \left[\left(\frac{\Gamma_n / \Gamma_t}{1 - \alpha_h} - \kappa_1 \right) \frac{\Gamma_t}{\sigma_p \Gamma_x} (RI)_{NR} \right]^m \right\} \quad (\text{III.3.9})$$

where Γ_x denotes the partial width x with $x \in \gamma$ or $x \in f$. For most of applications, one term correction in the sum is usually sufficient. Physically, Eq. (III.3.9) provides a vivid illustration of the effects of the Placzek oscillations on the resonance integral. For a resonance with relatively large neutron width, the correction term tends to contribute positively corresponding to the effect of a sudden rise in the collision density as illustrated in Fig. III.3 whereas the opposite is expected when an absorption-dominated resonance is considered.

(2) Infinite Mass Approximation (NRIM or WR)

In the limit of infinite mass, i.e., $\varepsilon \rightarrow 0$ in Eq. (III.3.1), the flux is also reduced to a simple form

$$\phi(u) = \frac{\Sigma_m}{\Sigma_m + \Sigma_a(u)} \quad (\text{III.3.10})$$

This approach is sometimes referred to as the NRIM-approximation in the sense that the resonance is considered as ‘narrow’ compared to the scattering intervals of the diluents (assumption (3)) in addition to the infinite mass assumption. It is also known as the ‘wide’ resonance approximation (WR) because the extent of the resonance obviously has to be wide compared to the scattering interval if $\varepsilon \rightarrow 0$. Note that, unlike the case of the NR-approximation, the only energy-dependent quantity at the resonance is the absorption cross section. The substitution of the Doppler-broadened line shape function leads to the resonance integral of the same functional form

$$(RI)_{NRIM} = \frac{\sigma_m \Gamma_t}{E_r} J(\theta_r, \beta_r) = I_r^{(\infty)} K(h_r, \theta_r) \quad (\text{III.3.11})$$

except $\beta_r = \Sigma_m / (\Sigma_{0r} \Gamma_a / \Gamma_t)$ and σ_m is the diluent cross section per absorber atom. For some low-lying resonances of fissionable isotopes where Γ_n is small, Eq. (III.3.5) and Eq. (III.3.11) are almost the same for practical purposes. On the other hand, for sharp resonances with relatively large neutron width, the resonance integrals based on these two approximations can be significantly different. Only a handful of low-lying actinide resonances can be considered as candidates for the NRIM-approximation.

(3) Intermediate Resonance Approximation (IR)

Two approximations described above provide efficient means for treating two classes of resonances according to whether their extent are small or large compared to the maximum neutron energy loss per collision. It is apparent that some means to bridge the gap between these two extremes are needed.

One widely used approximation that serves this purpose is the ‘intermediate resonance’ (IR) approximation originally proposed by Goldstein and Cohen[18,19]. The rationale is to utilize a parameterization scheme to unify the strikingly similar flux shapes exhibited within the narrow and wide resonance. From the foregoing discussions, it is reasonable to conjecture that the neutron flux across a resonance generally resemble the following approximate form

$$\phi(u) = \frac{\Sigma_m + \lambda \Sigma_{pr}}{\Sigma_m + \Sigma_a(u) + \lambda \Sigma_{sr}} \quad (\text{III.3.12})$$

where λ is a parameter characteristic of the resonance to be determined. The expression obviously leads to the NR- and WR-approximations as λ approaches 1 and 0 respectively. Furthermore, the corresponding resonance integral based on such a flux shape must retain the same general forms defined by Eq. (III.3.5) and Eq. (III.3.11) provided that λ is insensitive to energy [9]. By substituting the Doppler-broadened line shape into Eq. (III.3.2), one obtains

$$(RI)_{IR} = \frac{\sigma_p^{(\lambda)} \Gamma_{xr}^{(\lambda)}}{E_r} J(\theta_r, \beta_r^{(\lambda)}) \quad (\text{III.3.13})$$

where

$$\sigma_p^{(\lambda)} = \frac{\Sigma_m + \lambda \Sigma_{pr}}{N_r} \quad (\text{III.3.14})$$

$$\Gamma_{xr}^{(\lambda)} = \left[\frac{\Gamma_{ar} + \lambda \Gamma_{nr}}{\Gamma_t} \right] \Gamma_{xr} \quad (\text{III.3.15})$$

$$\beta_r^{(\lambda)} = \frac{\sigma_p^{(\lambda)}}{\sigma_{0r} (\Gamma_{ar} + \lambda \Gamma_{nr}) / \Gamma_t} \quad (\text{III.3.16})$$

which amounts to redefining the parameters in (III.3.5) and Eq. (III.3.11). Of course, the key question here is how to define λ in order to reflect the characteristics of the resonance. Goldstein and Cohen argued that Eq. (III.3.12) could be viewed as the first order iterant of the solution to the integral equation of the Fredholm type defined by Eq. (III.3.11). If one assumes $\phi^{(1)}(u) = \phi(u)$ given by Eq. (III.3.12), the substitution of it into Eq. (III.3.1) yields the second order iterant of the form

$$\Sigma_t(u) \phi^{(2)}(u) \approx \Sigma_m + \frac{1}{\delta} \int_{x_r}^{x_r + \delta} \Sigma_{si}(x') \phi^{(1)}(x') dx' \quad (\text{III.3.17})$$

where $\delta = 2E_r(1 - \alpha) / \Gamma_t$. If the iterative process converges rapidly, $\phi^{(1)}(u)$ and $\phi^{(2)}(u)$ must not be significantly different. The criterion for determining λ , therefore, was defined by setting

$$\int_0^\infty \Sigma_{ar}(u) \phi^{(1)}(u) du = \int_0^\infty \Sigma_{ar}(u) \phi^{(2)}(u) du \quad (\text{III.3.18})$$

From this transcendental equation, one may deduce the value of λ provided that the integration on the right hand side can be carried out analytically into a manageable form. One obvious problem that hinders such procedure is the complexity of the Doppler-broadened line shape function. By ignoring the temperature effect and using the Lorentzian shape for the resonance, they were able to obtain a simple expression for λ given as follows.

$$\lambda = 1 - \frac{\arctan x_{1\lambda}}{x_{1\lambda}} \quad (\text{III.3.19})$$

where

$$x_{k\lambda} = \frac{2E_r(1-\alpha)}{\Gamma_t(B_k + B_\lambda)} \quad (\text{III.3.20})$$

$$B_\lambda = \sqrt{1 + \frac{\Sigma_{0r}}{\Sigma_m + \lambda \Sigma_p} \left(\frac{\Gamma_a + \lambda \Gamma_n}{\Gamma_t} \right)} \quad (\text{III.3.21})$$

The relatively simple expression for the parameter λ makes the IR-approximation attractive in thermal reactor applications especially in the early days when modern computing facilities were not available. The evaluation of λ can become extremely complicated if the rigor in the temperature dependence is required. One special case of some theoretical interest is when δ is large compared to the extent of the resonance similar to the condition leading to the improved NR-approximation given by Eq. (III.3.9). By setting $\delta \approx \infty$, Eq. (III.3.17) reduces to a transcendental equation involving the linear combination of the usual J -integral and J^2 , and from which the temperature-dependent λ can be deduced. This case is, of course, not of practical interest because Eq. (III.3.18) provides much more rigor as well as simplicity under the same criterion.

Because of its importance to the thermal reactor applications, a great deal of work on the generalization of the IR-approximation can be found in the literature. Much of the efforts were focused on three general areas; namely, inclusion of the contribution from the asymmetric line-shape function attributed to the interference between the potential scattering and resonance scattering, elimination of the NR-approximation for the diluents in the mixture, and the means to account for the temperature-dependence of the IR-parameters. With no loss of generality, the IR-approximation can be represented in the generalized form as follows.

$$\int_{u-\varepsilon}^u \phi(u') \Sigma_{si}(u') K_i(u-u') du' = \eta_i \Sigma_{pi} + (1-\eta_i) \phi(u) \Sigma_{si}(u) \quad (\text{III.3.22})$$

so that

$$\phi(u) = \frac{\sum_i \eta_i \Sigma_{pi}}{\Sigma_a(u) + \sum_i \eta_i \Sigma_{si}(u)} \quad (\text{III.3.23})$$

The above equation retains the general features of the original form defined by Eq. (III.3.12). It reduces to the NR and WR limits as η_i approaches unity and zero respectively. Like the IR parameter described previously, η_i must also be determined by the similar iterative scheme. The parameter η_i is, strictly speaking, dependent not only on the composition and the characteristics of individual resonances but also on the temperature. The obvious question may arise as to whether the IR approximation is actually competitive in comparison with the direct numerical method to be described. One alternative to alleviate the problem is to define an average IR parameter $\bar{\eta}_i$ for a group of resonances within an energy interval along with the use of an approximate method to incorporate the temperature effect. A practical scheme for such a purpose is given in Appendix I.A1.

(4) Direct Numerical Approach (Nordheim's Method)

The availability of modern computers made it possible an alternative of the rigorous treatment of the isolated resonance integral without resulting to approximations and complications illustrated by the IR approximation [20,21]. One such method widely used in the thermal reactor applications, especially in the United States, is that pioneered Nordheim[22]. Nordheim's method was intended for the treatment of resonance integrals in the two-region repeated cells imbedded in an infinite reactor lattice via the collision probability method. For our purpose here, it suffices to focus only on its basic algorithms of treating the slowing-down equation and resonance integral for the limiting case of the infinite homogeneous medium. The subject of collision probabilities will be addressed separately in the next chapter.

In the Nordheim's method, two key assumptions are necessary to circumvent the problems associated with the cumbersome calculations in conjunction with the evaluation of integrals involved.

(a) Finite Interval of Integration

A finite energy interval large enough to cover the substantial portion of the resonance is chosen as the interval of integration while simple analytical approximations are used as corrections to the tails outside of the predetermined range. This amount to break up the resonance integral into the following form:

$$(RI)_{Nordheim} = \int_{u_1}^{u_2} \sigma_x(u') \phi(u') du' + \Delta I \quad (III.3.24)$$

and

$$\Delta I = \int_{u_2}^{\infty} \sigma_x(u') \hat{\phi}(u') du' + \int_0^{u_1} \sigma_x(u') \hat{\phi}(u') du' \quad (III.3.25)$$

where $\phi(u)$ is the rigorous flux defined by Eq. (III.2.1) or Eq. (III.3.1), $\hat{\phi}(u)$ the NR or WR flux where appropriate, and the lethargies u_1 and u_2 correspond to the predetermined energy boundaries E_1 and E_2 with

$$E_j = E_0 \pm m \left(\frac{\Gamma_p}{2} \right), \quad j \in 1, 2 \quad (\text{III.3.26})$$

Physically, the interval is taken to be 'm' multiple of the 'practical' width $\Gamma_p = \Gamma_t / \beta^{1/2}$ approximately equivalent to the 'half' width of the integrand based on the NR or WR approximations at zero temperature. If $m \cdot \Gamma_p$ is taken to be much greater than the Doppler width, ΔI becomes analytically integrable upon substitution of the Lorentzian line shape functions for the Breit-Wigner resonance. For instance, $(\Delta I)_{NR}$ based on the NR flux becomes

$$(\Delta I)_{NR} = \frac{\Gamma_x \sigma_p}{E_0 \sqrt{\beta(\beta+1) - (a/2)^2}} \frac{1}{2} \left[\pi - \arctan \frac{a}{\sqrt{\beta(\beta+1) - a^2/2 + (\beta x_1)^2}} \right] \quad (\text{III.3.27})$$

where $x_1 = m / \sqrt{\beta}$ is the predetermined interval according to Eq. (III.3.26) in x-domain and the condition $\beta(\beta+1) > (a/2)^2$ corresponding to the physically meaningful criterion of $\Sigma_t > 0$ is implicitly assumed. Otherwise, a singularity in the neutron flux results from the theory. A similar expression can also be obtained for $(\Delta I)_{WR}$ for the low-lying resonances in which the $1/v$ dependence of the absorption cross section may also be included.

(b) Simpson's Rule for Integration

To evaluate the integral defined in Eq. (III.3.24) requires the solution of the slowing-down equation at each mesh point u_j between u_1 and u_2 . Thus, it amounts to the evaluation of a double integral, which can be extremely costly if the NR-approximation is not used for all diluents with light atomic mass. The original Nordheim's method was intended for only a handful of integrals in the slowing-down equation. For our illustrative purpose here, Eq. (III.3.1) is assumed. If the Simpson's rule with equally spaced mesh is assumed, one obtains

$$\int_{u_{j-n\varpi}}^{u_j} f(u') du' = \frac{\varpi}{3} \left[f_{j-n} + 4 \sum_{l=0}^{(n-2)/2} f_{j-n+1+2l} + 2 \sum_{m=0}^{(n-4)/2} f_{j-n+2+2m} + f_j \right] \quad (\text{III.3.28})$$

where $n\varpi = \varepsilon$ and n is taken to be an even integer. The substitution of the above equation into Eq. (III.3.1) yields the following recurrence relation, which permits a step-by-step evaluation of F_j .

$$F_j \left[1 - \frac{\varpi}{3} R_j \right] = \frac{\varpi}{3} \left[f_{j-n} + 4 \sum_{l=0}^{(n-2)/2} f_{j-n+1+2l} + 2 \sum_{m=0}^{(n-4)/2} f_{j-n+2+2m} \right] + \Sigma_m \quad (\text{III.3.29})$$

where $R_l = \frac{\exp[-(u_j - u_l)] \Sigma_{sr}(u_l)}{1 - \alpha} \frac{\Sigma_t(u_l)}{\Sigma_t(u_l)}$ and $f_j = F_j \cdot R_j$. If there is more than one integral in the slowing-down equation, similar procedure can be used. As a general rule, the NR-approximation is used for light

nuclides in the mixture [20].

III.3.2 Fast Reactor Considerations

The emergence of the fast reactor development and modern computing facilities has significant impact on our philosophies for treating the resonance phenomena in practical applications. The former casts the role of resonance cross sections into a somewhat different light while the latter makes possible the development of many rigorous methods for the routine applications unimaginable in the earlier days. In contrast to the traditional concept focused on a handful of low-lying, isolated resonances of U^{238} and Th^{232} , not only the resonances of all actinides but also those of structural material and coolant over a much larger energy span must also be seriously considered. This requirement provided strong motivations for improvement in methodologies as well as nuclear data. From the perspective of method development, a great deal of work has been carried out to improve our capability of resonance treatment in both the resolved and the unresolved regions with particular emphasis on the treatment of the Doppler effect essential to the fast reactor safety. Again, our discussions here will concentrate on the resolved resonances only while the treatment of the unresolved resonances will be addressed later.

One important consideration from the perspectives of fast reactor applications is the presence of large quantities of nuclides of intermediate atomic weight. The s-wave resonances of these nuclides are characterized by the extremely large natural widths dominated by the neutron width with magnitude of several keV while their resonances of the higher angular momentum states are relatively narrow. Thus, the presence of these extremely large resonances will undoubtedly have significant impact on the neutronic balance of a fast reactor system via the elastic scattering process. In the earlier work pioneered by Hummel[23], it was found that the accurate treatment of these scattering resonances is essential because of their impact on the estimation of the neutron spectrum in general and the neutron leakage in particular over the large energy span, which, in turn, will significantly affect the reactivity coefficients of the system that are extremely important for reactor safety. Such a problem clearly requires a more detailed treatment of the localized spectrum within the extent of each wide resonance not achievable via the usual resonance integral concept intended for the relatively low-lying resonances of the actinides on the basis of the simplified slowing-down equation given by Eq. (III.3.1). One well-known method originally suggested by Hummel[24] and subsequently incorporated into the MC²-2 code is the ultra-fine group approach. The idea is to compute the fundamental mode spectrum using the usual P_N or B_N approximations based on a 2000 equal lethargy group structure covering the effective energy region from 14 MeV to 0.4 eV of practical interest to fast reactor applications. The group width of $\Delta u = 1/120$ is approximately equivalent to 1/2 of the maximum increment in lethargy per collision with an actinide nucleus which is generally small compared to the extent of the s-wave scattering resonances of the intermediate weight nuclide but still far wider than that for most of the resonances of the actinides. Such an approach makes possible not only a more realistic estimation of the slowing-down problem taking into account the anisotropic scattering effect attributed to the relatively light nuclides and the leakage effect in great detail. It also permits the treatment of the inelastic scattering process and the fission spectrum with greater rigor while the traditional resonance integral concept remains intact when applied to the relatively narrow resonances within each ultra-fine group. The most commonly used methods are the consistent P_1 and B_1 approximations which amount to the solution of the coupled equations of the fundamental mode flux and current. The resulting spectrum so obtained is then used as the tool to collapse the ultra-fine group constants into the broad group constants more amenable to the diffusion theory codes or the S_N transport theory codes for routine applications.

The development of the fast critical assemblies[25] (such as ZPR's, ZEBRA, and ZPPR) as the experimental tools to verify various fast reactor parameters of practical interest also broadened our perceptions of the fast reactor physics problems at hand. The complexities of the geometric configurations of these assemblies and their intricate experiments provided further motivation to improve our capabilities of treating the resonance phenomena in order to analyze various experiments. One consequence is the rise of the effective cross section concept described earlier as a convenient means of treating the resonance effects in the multi-region system without ambiguity. Another spin-off is the development of the integral transport theory codes whereby the extremely complex intra and inter cell effects in the presence of resonances can be treated accurately. More details will be discussed later.

From the perspectives of the resonance theory, one immediate consequence on the traditional resonance integral concept is the inevitable occurrence of the mutual self-shielding effect due to the neighboring resonances commonly known as the resonance overlap effect. Such an effect generally manifests itself through the localized flux depression and must not be confused with the 'intrinsic' overlap of resonances inherently present in the R-matrix representation of cross sections. Two types of overlap effects are usually encountered independent of the cross section formalisms used. The first type is referred as 'in sequence' overlaps effect attributed to the neighboring resonances belonging to the same J-state. Although resonances of the same J-state of a given I are subject to the Wigner's repulsion, the mutual self-shielding effect for the closely spaced resonances notably in fissionable isotopes still can impact the Doppler effect calculations. The second type is referred as 'accidental' overlap effect attributed to neighboring resonances belonging to either a different state or a different isotope. The presence of overlapping resonances and the continuity requirement of neutron flux are the principal reasons that the traditional Breit-Wigner approximation must be used within the context of the ENDF/B description discussed in Chapter I instead of being treated as discontinuous entities envisioned in the earlier days.

The significant improvement in our knowledge of nuclear data in the past three decades also has considerable impact on the resonance treatment in reactor applications. Two most notable areas that constitute the major accomplishment are the dramatic extension of the resolved energy regions for all major actinides and the structural isotopes, and the use of the Reich-Moore parameters to preserve the rigor of these cross sections. The former makes possible the realistic estimation of self-shielding effects in the presence of overlapping resonances, while the latter represents a major departure from the traditional concept based on the isolated resonances. Fortunately, the problems associated with the other cross section representations can be readily resolved via the use of the pole representation whereby all cross sections are viewed as a linear combination of the Breit-Wigner-like terms.

From the foregoing background discussions, it is quite obvious that our perception of the resonance theory must be put in the context including various considerations not addressed in the earlier development. As described earlier, the traditional resonance integral concept is premised on the basic assumption that the resonances are well isolated. The presence of overlapping resonances raises serious questions about the justification of adopting the traditional methodologies to the fast reactor applications without considering overlap. There are two ways that the neighboring resonances can affect a resonance integral in question. First, the effect can manifest through the collision density by altering the characteristics of the Placzek oscillations. Secondly, the magnitude of the macroscopic cross section can be affected significantly even under the limiting conditions of the NR- or WR-approximations. Furthermore, the intrinsic multilevel nature reflected by the newly released resonance data was not accounted for in the earlier development. The former can be fatal to all four

approximations discussed previously, should it become an issue.

Conceptually, there is no simple fix possible in lieu of the ‘flux recovery’ assumption common to all four approximations if the rigor is required. Strictly speaking, the entire resonance integral concept breaks down if resonances become intertwined. On the other hand, the remedy for the latter is relatively simple if one neglects the effect of the Placzek oscillations and uses the pole representation of cross sections whenever the multilevel representation is considered. From a practical point of view, there are two options open. One is to extend the existing resonance integral concept at the expense of the rigor in collision density and the other is the rigorous continuous energy approach in which the rigors of both the slowing-down equation and the cross sections are preserved. Since the impact of the Placzek oscillations plays somewhat less important role in the high-energy region with exception of a handful of large scattering resonances, one simple option is the extension of the NR-approximation to include the neighboring levels or poles where appropriate. The resulting resonance integrals are then applied in the context of the ultra-fine group approach so that the effect of the Placzek oscillations attributed to the s-wave resonances of the structural isotopes can be accounted for. On the other hand, it is certainly not satisfying if rigor is required. Thus, it provides the motivation for the subsequent development of the continuous energy approach whereby the slowing-down equation, in the presence of many resonant nuclides, is treated rigorously starting from the highest upper bound of the resolved energy boundary. This can be accomplished via either the deterministic method or the Monte Carlo method. For our purposes here, we shall focus on the deterministic approach only. The rigorous methods are made possible via an exceedingly efficient numerical algorithms and the availability of the modern computing facilities. The latter are usually accompanied by the capabilities of treating the lattice effects via the collision probability method. The coexistence of both types of approaches provides the tools for the routine calculations as well as the benchmark-quality calculations of interest in fast reactor applications.

In the following discussions, a generalized representation of the traditional J-integral and its applications in the fast reactor calculations will be presented first while the rigorous approach will be given in section III.4.

III.3.3 Generalization of Resonance Integrals

With no loss of generality, the resonance integral can always be cast into a form consisting of superposition of two terms as long as the cross sections are expressible as a linear combination of the Breit-Wigner terms. For the sake of simplicity, let $\Sigma_t = \Sigma_p + \sum_k \Sigma_{rk}$ be the macroscopic cross section. The resonance integral can be cast into the following form via partial fraction:

$$(RI)_k = \frac{1}{\Phi_{asym}} \left[\int_0^\infty \frac{\sigma_{ak}(u)}{\Sigma_p + \Sigma_{rk}(u)} F(u) du - \int_0^\infty \frac{\sigma_{ak}(u)}{\Sigma_p + \Sigma_{rk}(u)} \frac{\sum_{k' \neq k} \Sigma_{rk'}}{\sum_{all k} \Sigma_{rk}} F(u) du \right] \quad (III.3.30)$$

where the first term signifies the contribution attributed to the resonance (or pole) in question, and the second term denotes that attributed to the overlapping of the neighboring resonances. If one neglects the overlapping effect, the above equation becomes identical to the traditional resonance integral and all four commonly used approximations remain valid where appropriate. The presence of the overlapping resonances changes the complexion of the traditional concept perceived in the earlier days

if the rigor in $F(u)$ is required. The natural consequence is the development of the continuous energy approach used in conjunction with the effective cross section concept. On the other hand, the practical value of the NR-approximation in routine fast reactor applications provides a strong incentive to retain the resonance integral approach to supplement the more costly alternative based on the continuous energy approach.

(1) J^* Integral Representation

In lieu of the Placzek oscillation (i.e., $F(u) = \text{constant}$), the traditional J-integral can be readily generalized in the context of Eq. (III.3.30). By substituting the Doppler-broadened functions into Eq. (III.3.30), one obtains

$$J_k^* = J_k(\beta_k, \theta_k, a_k, b_k) - \sum_{k' \neq k} O_{kk'} \quad (\text{III.3.31})$$

where

$$J_k(\beta_k, \theta_k, a_k, b_k) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\theta_k, x_k) + b_k \chi(\theta_k, x_k)}{\beta_k + \psi(\theta_k, x_k) + a_k \chi(\theta_k, x_k)} dx_k \quad (\text{III.3.32})$$

$$O_{kk'} = \frac{A_{k'}}{2} \int_{-\infty}^{\infty} \frac{\psi(\theta_k, x_k) + b_k \chi(\theta_k, x_k)}{\beta_k + \psi(\theta_k, x_k) + a_k \chi(\theta_k, x_k)} r_{k'} dx_k \quad (\text{III.3.33})$$

$$r_{k'} = \frac{\psi(\theta_{k'}, x_{k'}) + a_{k'} \chi(\theta_{k'}, x_{k'})}{\beta_k + \psi(\theta_k, x_k) + a_k \chi(\theta_k, x_k) + \sum_{k' \neq k} A_{k'} [\psi(\theta_{k'}, x_{k'}) + a_{k'} \chi(\theta_{k'}, x_{k'})]} \quad (\text{III.3.34})$$

Here, $A_{k'}$ denotes the ratio of the peak macroscopic resonance cross section of the k' -th level to that of the k -th, and b_k , the ratio of the real part of the k -th residue for the absorption cross section to that of the imaginary part if the pole representation or the Adler-Adler approximation are used, is zero otherwise. All parameters retain the same physical meaning described in the previous section according to the type of representation used. One possible exception should be noted when the pole representation or the Adler-Adler approximation are used. The peak value (or real component of the residue) of the total resonance cross-section for a given pole k may assume negative sign, although such an occurrence is extremely rare. If one wishes to maintain the positive nature of β_k by taking it as the ratio of the macroscopic total potential scattering cross section (plus background), the sign of $\psi(\theta_k, x_k)$ in the denominators of all integrals above must be taken to be the sign of its peak value accordingly. Thus, the traditional resonance integral expression defined by Eq. (III.3.32) remains intact if one replaces the J -integral by the J_k^* -integral and introduces a quantity ζ_k equivalent to the usual partial width thereby,

$$\zeta_k = \begin{cases} 2 \operatorname{Im}(p_k) \frac{\sigma_{x0k}}{\sigma_{r0k}}, & \text{for multilevel} \\ \Gamma_x, & \text{for single level} \end{cases} \quad (\text{III.3.35})$$

where σ_{x0k} and σ_{r0k} are the peak partial cross section of the process x and total resonance cross section for the k -th pole p_k respectively.

Physically, the generalized J^* -integral consists of an 'isolated' resonance term signified by $J_k(\beta_k, \theta_k, a_k, b_k)$ resulting from the contribution of an individual pole k (or resonance where appropriate) in question, and an overlap term $\sum_{k' \neq k} O_{kk'}$ to account for the mutual self-shielding effect due to the neighboring poles. The representation is not only applicable to all practical cross section formalisms described in Chapter I but also amenable to all traditional resonance integral approximations in absence of the overlap contributions.

The principal term of the generalized integral can be expressed in a more convenient form directly in terms of the traditional J -integral widely used. Note that the quantity $\beta_k + \psi(\theta_k, x_k) + a_k \chi(\theta_k, x_k)$ has the physical meaning of the macroscopic total cross section for a given mixture which must be positive everywhere at least for the case of a Breit-Wigner resonance. If so, the condition $\beta_k + \psi(\theta_k, x_k) > a_k \chi(\theta_k, x_k)$ must also be true. Under such a condition, $J_k(\beta_k, \theta_k, a_k, b_k)$ can be written in terms of the usual $J_k(\beta_k, \theta_k)$ and two uniformly convergent geometric series of integrals with even integrands only which, in turn, can be recombined into the following closed forms:

$$J(\beta_k, \theta_k, a_k, b_k) = J(\beta_k, \theta_k) + I(\beta_k, \theta_k, a_k) - b_k M(\beta_k, \theta_k, a_k) \quad (\text{III.3.36})$$

where

$$I(\beta_k, \theta_k, a_k) = a_k^2 \int_{-\infty}^{\infty} \frac{\chi^2(\theta_k, x_k)}{[\beta_k + \psi(\theta_k, x_k)]^2 - [a_k \chi(\theta_k, x_k)]^2} \frac{\psi(\theta_k, x_k)}{\beta_k + \psi(\theta_k, x_k)} dx_k \quad (\text{III.3.37})$$

$$M(\beta_k, \theta_k, a_k) = a_k \int_0^{\infty} \frac{\chi^2(\theta_k, x_k)}{[\beta_k + \psi(\theta_k, x_k)]^2 - [a_k \chi(\theta_k, x_k)]^2} dx_k \quad (\text{III.3.38})$$

Physically, Eq. (III.3.36) unambiguously defines the concise role of the interference terms for each individual pole or resonance where appropriate. The I -integral signifies the interference effect between the hard-sphere potential scattering and resonance scattering while the M -integral reflects the inherent tilt in the multilevel description of cross sections. All integrands in the integrals above are even functions in the x_k -domain and all integrals that exhibit asymmetry are removed analytically. The elimination of the asymmetric terms characterized by $1/x_k$ tails, which constitute the most difficult problem in the evaluation, makes possible the development of an exceedingly efficient numerical quadrature to be described later.

As mentioned earlier, the validity of Eq. (III.3.36) is contingent upon the condition that the denominator of the integrand in Eq. (III.3.32) must be greater than zero at any temperature. For any viable set of Breit-Wigner parameters supplemented by the ‘smooth’ data such as the ENDF/B V5, the condition is mandatory. For the pole representations, this condition may become questionable especially for the case in which β_k becomes very small. It is, therefore, useful to define a criterion by which such a condition can be assured.

A practical criterion for the condition $\beta_k + \psi(\theta_k, x_k) + a_k \chi(\theta_k, x_k) > 0$ at any temperature can be readily achieved by taking advantage of the fact that the minimum of the asymmetric function is at its lowest value in absence of Doppler-broadening. Thus, the necessary and sufficient condition can be premised on the basis that the following quadratic equation corresponding to the case of zero temperature must not have any real root for $J(\beta_k, \theta_k, a_k, b_k)$ to be meaningful, i.e.

$$\beta_k x_k^2 + a_k x_k + (\beta_k + 1) = 0 \quad (\text{III.3.39})$$

It follows that the condition

$$\beta_k > \frac{\sqrt{1 + a_k^2} - 1}{2} = c_k \quad (\text{III.3.40})$$

is required for Eq. (III.3.36) to be valid.

It is noteworthy that Eq. (III.3.40) also provides a convenient means to extend the range of validity of Eq. (III.3.36) to all β_k and a_k of interest. In the event of $\beta_k < c_k$, the validity of Eq. (III.3.36) can be maintained by replacing β_k and r_k by β'_k and r'_k respectively, where

$$\beta'_k = \beta_k + c_k \quad (\text{III.3.41})$$

$$r'_k = \frac{\psi(\theta_{k'}, x_{k'}) + a_{k'} \chi(\theta_{k'}, x_{k'}) - c_k / A_{k'}}{\beta_k + \psi(\theta_k, x_k) + a_k \chi(\theta_k, x_k) + \sum_{k' \neq k} A_{k'} [\psi(\theta_{k'}, x_{k'}) + a_{k'} \chi(\theta_{k'}, x_{k'})]} \quad (\text{III.3.42})$$

This amounts to the reassignment of the ‘isolated’ resonance term and the overlap term so that the general forms of Eq. (III.3.32) through Eq. (III.3.34) remain intact without ambiguity.

(2) Considerations Pertinent to the Evaluations of Various Integrals

For fast reactor applications [26,27,28], both accuracy and efficiency are essential in the evaluation of various integrals resulting from the J_k^* - representation. The former stems from the needs of the Doppler effect calculations crucial to reactor safety while the latter is required because one must deal with numerous resonances over an exceedingly large energy span. To evaluate various integrals rigorously without introducing approximations to the Doppler-broadened line shape functions can be an insurmountable numerical task unless their analytical properties are fully utilized. In the following

discussions, one attractive method that can meet both of these requirements without compromising the rigor is presented. The emphasis will focus on the aspects of theoretical interest only. For the details, the readers are referred to Ref. 29.

For the integrals associated with the principal term $J(\beta_k, \theta_k, a_k, b_k)$, one unique common to all integrands is that their asymptotic limits are rational functions of even order as the ψ and χ functions approach their Lorentzian limits when x_k increases [30]. Such behavior immediately suggests that a change of this variable via the rational transformation can lead to integrands more susceptible to the Gauss quadrature in the domain of the new variable. This can be accomplished by letting

$$u_k^2 = \frac{C^2 x_k^2}{1 + C^2 x_k^2} \quad (\text{III.3.43})$$

and it follows that the Jacobian of the transformation is defined by

$$|j| = \frac{1}{C} \frac{1}{(1 - u_k^2)^{3/2}} \quad (\text{III.3.44})$$

where C is a constant for a given β_k and θ_k to be defined. Thus, if $f(x_k)$ is the integrand under consideration, one obtains

$$\int_0^\infty f(x_k) dx_k = \frac{1}{C} \int_0^1 \frac{du_k}{\sqrt{1 - u_k^2}} \frac{f(u_k)}{1 - u_k^2} \quad (\text{III.3.45})$$

Mathematically, the procedure amounts to the transformation of the pertinent integrals in question into those of the Euler type. The quantity $f(x_k) / [1 - u_k^2]$ must be a smooth function of u_k especially when the Doppler-broadened line shape functions approach their Lorentzian limits. Numerically, it is quite obvious that this type of integral is particularly amenable to the Gauss-Jacobi quadrature where $1 / \sqrt{1 - u_k^2}$ is taken to be the weight. Hence, if the total number of quadrature points N is taken to be an odd number, one obtains

$$\int_0^1 \frac{dx_k}{\sqrt{1 - u_k^2}} \frac{f(x_k)}{1 - u_k^2} = \frac{\pi}{N} \left\{ \frac{1}{2} f(0) + \sum_{n=1}^{[N/2]} \frac{f(u_{kn})}{1 - u_{kn}^2} \right\} + R_N \quad (\text{III.3.46})$$

where the quadrature point u_{kn} is given by

$$u_{kn} = \cos \frac{(2n-1)\pi}{2N} \quad (\text{III.3.47})$$

and π / N and R_N are the constant weight and the remainder, respectively.

In Ref. 29, it was shown that such a procedure can be optimized by the appropriate choice of C as a function of β_k and θ_k . As a general rule, the value of C is chosen so that the integrand must approach the rational function form before u_{kn} becomes too close to unity. This ensures the inclusion of ample number of mesh points prior to the expected Lorentzian limits. One way to accomplish this is to define C in three distinct regions in the domain of β_k and θ_k of practical interest. For our purpose here, it suffices to present a brief discussion on the basis used.

(a) Typical Region for Fast Reactor Calculations

A significant portion of the resolved resonances in the energy region of interest to fast reactor calculations belongs to the category in which θ_k is smaller than unity and, at the same time, the corresponding β_k is greater than or comparable to the peak value $\psi(\theta_k, 0)$ [31]. Thus, under this condition, the behavior of the integrand as a function of x_k is mainly determined by that of the Doppler-broadened line shape functions but less sensitive to the values of β_k . From numerical experimentation, it was found that

$$C = \frac{\theta_k}{5} \quad (\text{III.3.48})$$

will yield the most accurate results.

(b) Semi-Lorentzian Region

One obvious situation in which the integrand will exhibit the behavior closely resembling that of rational function is when θ_k is comparable to or greater than unity, or when $\beta_k / \psi(\theta_k, 0)$ becomes exceedingly small. Under such condition, best results can be achieved by setting

$$C = \sqrt{3\beta / (\beta + 1)} \quad (\text{III.3.49})$$

Physically, it means that $u_k^2 = 1/2$ at the location in the x_k domain corresponding to the point of inflection for the quantity $\psi(\theta_k, x_k) / [\beta_k + \psi(\theta_k, x_k)]$ under the Lorentzian limit.

(c) Remaining Region

The choice of C in the remaining domain of β_k and θ_k is less obvious. However, since we are dealing with resonances with relatively small β_k and θ_k , it is reasonable to assume that the behavior of the quantity $\psi(\theta_k, x_k) / [\beta_k + \psi(\theta_k, x_k)]$ resulting from the Gaussian nature of $\psi(\theta_k, x_k)$ must diminish substantially when u_k^2 becomes equal to or greater than 1/2. A reference point x_{k1} is chosen such that the quantity mentioned above becomes approximately 1/6 of its value at the peak, i.e.

$$x_{k1} = \frac{2}{\theta_k} \left[1.8971 + \ln \left(1 + 0.85 \frac{\sqrt{\pi} \theta_k}{2\beta_k} \right) \right]^{1/2} \quad (\text{III.3.50})$$

By numerical experimentation, it was found that best results can be achieved by setting

$$\frac{1}{C} = 0.8292 x_{k1} \rho \quad (\text{III.3.51})$$

where

$$\rho = 1 + \frac{0.018(\beta_k - 0.00128)(1 + 11.291 \theta_k^2)}{\beta_k + 0.00128} + \frac{0.08 \beta_k}{\psi(\theta_k, 0)} \quad (\text{III.3.52})$$

for $\beta_k \leq 0.00128$, and

$$\rho = 1 + \frac{0.018(\beta_k - 0.00128)[1 + 10.892(\theta_k + \beta_k / \psi(\theta_k, 0))]}{\beta_k + 0.00128} \quad (\text{III.3.53})$$

for $\beta_k > 0.00128$.

Since the asymptotic properties of ψ and χ^2 are strikingly similar, all three integrals can be evaluated simultaneously using the same set of mesh points based on the same C value. Thus, the computational efficiency can be significantly enhanced. Based on this procedure, the total number of entries to the computation of the broadened line-shape functions can be minimized to as few as seven (or $N=13$). It ensures the accuracy for the principal integral to better than $|\varepsilon| \leq 0.1\%$ and yields less accurate yet tolerable results for the second-order integrals ($|\varepsilon| \sim 1\%$). The integration scheme becomes practically exact if one doubles the total number of mesh points even for the worst possible situation where the asymmetric component dominates.

The same procedure is also applicable to the evaluation of the overlap integrals. Because the integrand is no longer symmetric, the quadrature points must cover the entire domain of $-1 < u_k < 1$ and the total number is far greater than that required for the principle term. It is quite obvious that the problem can become unmanageable if too many overlapping resonances are included. Fortunately, the overlap effect in the context of Eq. (III.3.33) implicitly premised on the validity of the narrow resonance assumption is generally short range in nature in lieu of the extremely wide, s-wave scattering resonances of structural isotopes. The effect becomes unimportant as the separation between the k' -th and the k -th resonance in question becomes much greater than the Doppler width (or natural width whichever is greater). Thus, the total number required for a typical fast reactor system seldom exceeds ten on either side of a given resonance and the use of a total of no more than 61 points was found to be satisfactory. Besides, for the well-separated resonances, the overlap integrals can also be estimated analytically as described in Ref. 29.

(3) Analytical Approach under Limiting Conditions (Large/Small β Approximations)

Under two limiting conditions, the generalized J^* - integral can be evaluated analytically. One case is the zero temperature limit whereby the integration can be carried out via the usual method of finding the poles and residues of a rational function. This case, however, is of little interest from the perspective of the Doppler effect in the fast reactor calculations. Another extreme of more theoretical and practical importance is the situation when β_k becomes large compared to other terms in the denominators of the J_k^* . Many resonances of interest to the fast reactor calculations fall into this category. By the appropriate use of the large β_k approximation to supplement the quadrature scheme, the computation efficiency can be improved significantly.

The large β_k approximation can be readily established via the Fourier transform identities described in Chapter I based on the Parseval theorem and the convolution theorem. By utilizing Eq. (III.112) through Eq. (III.118), one obtains

$$J(\beta_k, \theta_k) \approx \frac{\pi}{2\beta_k} - \frac{\pi}{4\beta_k^2} \psi(\sqrt{2}\theta_k, 0) \quad (\text{III.3.54})$$

$$I(\beta_k, \theta_k, a_k) \approx \frac{\pi^{3/2} \theta_k^2}{4\sqrt{3}\beta_k^3} \int_{\theta_k/\sqrt{6}}^{\infty} \exp(-t^2) \text{erfc}(\sqrt{3}t) dt \quad (\text{III.3.55})$$

$$M(\beta_k, \theta_k, a_k) \approx \frac{a_k}{4\beta_k^2} \psi(\sqrt{2}\theta_k, 0) \quad (\text{III.3.56})$$

$$O_{kk'} \approx \frac{\pi}{2} \frac{A_{k'}}{\beta_k^2} \frac{\Gamma_{k'}}{\Gamma_k + \Gamma_{k'}} [(1 + b_k a_k) \psi(\theta_{kk'}, x_{kk'}) + (-b_k + a_k) \chi(\theta_{kk'}, x_{kk'})] \quad (\text{III.3.57})$$

where

$$\theta_{kk'} = \frac{\Gamma_k + \Gamma_{k'}}{\sqrt{\Delta_k^2 + \Delta_{k'}^2}}, \quad x_{kk'} = \frac{2(E_{0k} - E_{0k'})}{\Gamma_k + \Gamma_{k'}} \quad (\text{III.3.58})$$

With no loss of generality, it is understood that all parameters should correspond to appropriate pole and residue parameters if any form of pole representation is used. Physically, these equations specify the high-energy limit of the self-shielding effect. With exception of the I - integral, the degree of the self-shielding effect and mutual self-shielding effects are expressible in terms of the usual ψ and χ function in the limit. This helps to minimize the need to perform the numerical integration for many relatively weak resonances over the large energy span of interest in reactor applications.

The analytical behavior here, in effect, defines the high-energy limit for the temperature derivative of the resonance integral as a function of temperature. Since the ψ -function approaches its Gaussian limit

when θ_k becomes small, it is quite obvious that

$$\frac{\partial J_k^*}{\partial T} \sim \frac{\text{constant}}{T^{3/2}} \quad (\text{III.3.59})$$

This implies that the Doppler coefficient also exhibits such a behavior in the high-energy region.

In contrast, another extreme case is when both β and θ become very small. If the $\psi(\theta_k, x_k)$ reaches its Gaussian limit and the condition $\sqrt{\pi}\theta_k / (2\beta_k) \gg 1$ also exists, the integrand of the J -integral will become nearly unity until $x_k = (2 / \theta_k) \sqrt{\ln[\sqrt{\pi}\theta_k / (2\beta_k)]}$ and then falls rapidly to zero as observed by Wigner et al. The J -integral under such a condition can be approximated by

$$J_k(\theta_k, \beta_k) \approx \frac{2}{\theta_k} \sqrt{\ln\left(\frac{\sqrt{\pi}\theta_k}{2\beta_k}\right)} \quad (\text{III.3.60})$$

The corresponding can be approximated by

$$\frac{\partial J_k}{\partial T} \sim \frac{\text{constant}}{T^{1/2}} \quad (\text{III.3.61})$$

which describes the temperature behavior of the Doppler effect in the low energy region under the extremely broadened condition.

Thus, these two limiting conditions provide useful basis for studying the temperature behavior of the Doppler coefficient for fast reactors. It is reasonable to assume that the Doppler coefficient of a fast reactor system may be predicted by a simple form of $1/T^x$ dependence within certain temperature range where the exponent x has a value between 3/2 and 1/2 depending on the spectrum of the system. This simple temperature dependence provides a simple means to compute the Doppler coefficient $\partial k / \partial T$ from δk , the change in the criticality factor due to the change in temperature.

III.3.4 Applications in Conjunction to Effective Cross Section Approach

As discussed in Section III.1, the effective cross section approach provides one of the most useful tools for treating the resonance effects in conjunction to the most widely used multigroup method in reactor applications. It is especially true for problems in which both the energy and the spatial effects must be treated. The methodologies for computing the multigroup constants via the modern computers are usually based on the three-step approach. In the first step, the effective resonance cross sections are calculated at the fine (or ultra-fine) group level. The short-range nature of the correlations between the highly fluctuating cross section and neutron flux makes plausible the use of the relatively simple models for treating the slowing-down and transport of neutrons as to account for the self-shielding effects. These effective cross sections along with the relatively smoothly-varying cross sections permits the computation of the fine (or ultra-fine) group spectrum in the second step that includes the effects resulting from the global variations of the reactor lattice and the intricate anisotropic scattering

attributed to the lighter nuclides. Finally, the fine (or ultra-fine) group spectrum so obtained can be used to collapse the corresponding effective cross sections into the group constants for the broad energy group structures more amenable to various neutronic codes. For our purpose here, a brief discussion will be given on how the resonance integral concept can fit into this procedure for the case of the homogeneous medium. The questions concerning the heterogeneous lattice will be further addressed in the next chapter.

In terms of the resonance integral concept, the effective cross section for a given ultra -fine group g in the context described in Section III.I can be expressed as

$$\tilde{\sigma}_x^{(g)} = \frac{\sigma_p^{(g)} \sum_{k \in g} \zeta_k J_{xk}^* F_k / E_{0k}}{\Delta u_g f_g} \quad (\text{III.3.62})$$

where f_g , sometimes referred to as the flux correction factor, is defined as

$$f_g = \langle F_k \rangle - \frac{1}{\Delta u_g E_{0k}} \sum_{k \in g} \zeta_k J_{xk}^* F_k \quad (\text{III.3.63})$$

and F_k is the collision density at the peak energy of the k -th resonance. One inherent assumption is that all resonances (or poles) with peaks falling into the group boundaries are assigned to the group because of the infinite integral nature of the resonance integrals. This introduces a certain degree of arbitrariness in the localized reaction rate because the tail of resonances can obviously extend beyond the group boundaries especially if the group width is small. The cumulative effects on the overall reaction rate, however, are not expected to be important over a large energy span.

There are two ways to approximate the collision density F_k . One obvious alternative is to set it to unity if the absorption probability is small within the group g . The assumption of constant collision density is clearly reasonable for many fast reactor applications if the ultra-fine group structure is used. The effective cross sections for the unresolved resonances can also be determined in a similar way except on the statistical basis, as one shall see in the discussions later. These effective resonance cross sections along with remaining group constants with relatively smooth behavior within the group g provide sufficient information for the computation of the fine (or ultra-fine) group spectrum. For a homogeneous medium, the fundamental mode spectrum based on the consistent (or inconsistent) P_N or B_N approximation is usually assumed. Once this detailed spectrum becomes available, the broad group constants more suitable for applications can be obtained via the flux-collapsing technique. For the broad group effective cross sections for fission and capture, one has

$$\tilde{\sigma}_x^{(G)} = \frac{\sum_{g \in G} \tilde{\sigma}_x^{(g)} \phi^{(g)}}{\sum_{g \in G} \phi^{(g)}} \quad (\text{III.3.64})$$

where the constant lethargy width for g is assumed. It is noteworthy that, for the case of the

heterogeneous medium, the quantity $\phi^{(g)}$ becomes space-dependent and is usually calculated via the collision probability method. The collapsing procedure must include the spatial averaging.

Alternatively, the same procedure can also be carried out via a more accurate method based on the use of the continuous slowing-down approach described earlier. In this approach, the asymptotic slowing-down density for each group g without the contribution from the resolved resonances is computed first by using the extended Greuling-Goertzel approach capable of treating the fundamental mode spectrum with either the P_N or B_N approximations. The sequential attenuation of these asymptotic slowing-down densities by the escape probability past each resonance provides the basis for determining the weighting factor F_k in Eq. (III.3.62) and that for computing the flux $\phi^{(g)}$. The permission of the attenuation of collision density within the fine group enhances the fidelity of the absorption process within the group g . The method is usually applied only to the resolved energy region where the resonance escape probability is deterministic in nature.

Since the J_k^* -integral can be evaluated efficiently, the method described above provides a valuable means for treating the resonance self-shielding effect that includes the overlap effect to be carried out at run time. It has been incorporated into the MC²-2 code as an option for the routine applications.

III.4 Continuous Energy Approach

The inherent limitations of the resonance integral method for treating the problems with numerous overlapping resonances provided the incentive for the development of the continuous-energy approach whereby the rigor of neutron slowing-down properties and the cell heterogeneity effect can be preserved. Such a development was made possible by the availability of modern computing facilities and the use of efficient algorithms. For our purpose here, it suffices to focus on the case of the infinite homogeneous medium first.

The rigorous treatment of the resonance self-shielding effect for the homogeneous medium in the context of Eq. (III.2.21) requires the solution of the slowing-down equation at extremely fine mesh points and the subsequent reaction rates and flux must be integrated between any finite group boundaries specified by users. It amounts to the evaluation of a double integral with rapidly fluctuating integrands resulting from the possible presence of numerous of resonances. The problem of evaluating the slowing-down equation alone can become insurmountable via the traditional Simpson rule approach described earlier when multiple resonance absorbers and moderators are present. It is quite obvious that a highly efficient numerical algorithm is essential in spite of our ever-improving computing capability.

One method, sometimes referred to as the ‘hyper-fine group’ approach pioneered by Kier, is believed to be tailor-made for such a purpose. It is particularly attractive when used in conjunction with the traditional multigroup approach based on the effective cross section concept. Because it constitutes one of the most viable methods in existence, a brief discussion of its theoretical basis given below is believed to be of practical interest.

The idea is to divide the desired multigroup structure (i.e. broad, fine or ultra-fine group where appropriate) into the hyper-fine groups (hfg) with equal lethargy per given group J , Δu_J , in which the

resonance cross-sections and thus the flux can be considered as 'smooth'. The hfg is, of course, only pertinent to those groups containing the resolved resonances. To ensure the rigor, Δu_J clearly must be chosen to be much smaller than the smallest Doppler width of the nuclide in the mixture or the smallest total width of the resonance within the group J whichever is smaller. In addition, this hfg width must also be much smaller than $1/120$ when applied to the ultra-fine group approach described earlier. The extremely fine division of the lethargy domain into equal segments makes possible the discretization of the slowing-down equation defined by Eq. (III.2.21). For simplicity, all sources of non-elastic nature will be ignored in the following discussions although their inclusion does not present any serious problem in the practical applications.

The fundamental idea of the hfg approach can be best illustrated by considering the simplest possible case of one nuclide and uniform hyper-fine mesh Δu throughout the resolved energy range. The generalization to the case of multiple nuclides and broad group dependent hfg mesh is quite apparent.

To cast the continuous energy slowing-down process into the discretized hfg structure, one minor adjustment is required. The scattering interval ε must be adjusted slightly by making small changes to the atomic weight A so that L , the total number of hfg within ε defined as

$$L = \frac{\varepsilon}{\Delta u} \quad (\text{III.4.1})$$

is an integer. Hence, the maximum energy loss per collision becomes

$$\alpha = \exp(-L \Delta u) \quad (\text{III.4.2})$$

To discretize the slowing-down equation as defined in Eq. (III.2.21) requires the introduction of an effective scattering kernel $\bar{K}_l$ that signifies the probability of scattering down (or up in the lethargy domain) l hfg into the k -th hfg in question with low boundary u_k . $\bar{K}_l$ is non-zero in the range $1 \leq l \leq L$. It is quite apparent that

$$\begin{aligned} \bar{K}_l \Delta u &= \frac{1}{1-\alpha} \int_{u_k}^{u_k+\Delta u} du \int_{u_k-l\Delta u}^{u_k-(l-1)\Delta u} du' e^{-(u-u')} \\ &= \frac{(1-e^{-\Delta u})^2}{1-\alpha} e^{-(l-1)\Delta u} = (\bar{K}_1 \Delta u) e^{-(l-1)\Delta u}, \quad \text{for } 1 \leq l \leq L-1 \end{aligned} \quad (\text{III.4.3})$$

This leads to the identity that relates $\bar{K}_l$ to $\bar{K}_{l-1}$ in a simple way as follows

$$\bar{K}_l = \bar{K}_{l-1} e^{-\Delta u} \quad (\text{III.4.4})$$

This relationship provides the useful basis for development of the recurrence relation for solving the discretized slowing-down equation as one shall see.

It should be noted, however, that the above equation must be modified somewhat when the lowest

possible hfg within the scattering interval from the k -th (i.e., $l = L$) is considered. The reason is that not all neutrons with lethargy between $u_k - L\Delta u$ and $u_k - (L-1)\Delta u$ are energetically allowed to be scattered into the k -th hfg bound by u_k and $u_k + \Delta u$. This can be remedied readily by redefining the limits of the inner integral in Eq. (III.4.3) so that the effective scattering kernel for $l = L$ denoted by $\bar{K}_{LST}$ is

$$\bar{K}_{LST}\Delta u = \frac{1}{1-\alpha} \int_{u_k}^{u_k+\Delta u} du \int_{u-L\Delta u}^{u_k-(L-1)\Delta u} du' e^{-(u-u')} \quad (III.4.5)$$

For convenience, the above equation can be cast into the form similar to Eq. (III.4.3) by rearranging the inner integral to give

$$\begin{aligned} \bar{K}_{LST}\Delta u &= \frac{1}{1-\alpha} \int_{u_k}^{u_k+\Delta u} du \left[\int_{u_k-L\Delta u}^{u_k-(L-1)\Delta u} du' e^{-(u-u')} + \int_{u-L\Delta u}^{u_k-L\Delta u} du' e^{-(u-u')} \right] \\ &= \bar{K}_L\Delta u - \alpha \bar{K}_s\Delta u \end{aligned} \quad (III.4.6)$$

where $\bar{K}_L$ obeys Eq. (III.4.3) by setting $l = L$ and $\bar{K}_s$ physically corresponds to the effective probability of self-scattering in the k -th ufg in question as given by

$$\begin{aligned} \bar{K}_s\Delta u &= \int_{u_k}^{u_k+\Delta u} du \int_{u_k}^u du' e^{-(u-u')} \\ &= \frac{1}{1-\alpha} [\Delta u - 1 + e^{\Delta u}] \end{aligned} \quad (III.4.7)$$

In the limit of extremely small Δu , $\bar{K}_{LST}$ becomes identical to $\bar{K}_L$ as $\bar{K}_s$ approaches zero.

Thus, given the effective scattering kernels for all ufg's within one scattering interval, the discretized slowing-down equation for an infinite homogeneous medium consisting of one nuclide becomes

$$\begin{aligned} F_k &= \left\{ \sum_{l=1}^L (\Sigma_s \phi)_{k-l} \bar{K}_l e^{-(l-1)\Delta u} - \alpha (\Sigma_s \phi)_{k-L} \bar{K}_s \right\} + \bar{K}_s \frac{\Sigma_{sk}}{\Sigma_{tk}} F_k \\ &= S_k^{(in)} + S_k^{(self)} \end{aligned} \quad (III.4.8)$$

for any k -th hfg in question. Physically, the terms inside the bracket, denoted by $S_k^{(in)}$, signify the neutron source from all higher energy (or lower lethargy) hfg scattered elastically into the group k in question whereas the remaining term denoted by $S_k^{(self)}$, represents the contribution of self-scattering within the group k . For the case of a mixture consisting of many nuclides, the above equation can be modified readily by including the linear combination of the constituents corresponding to the discretized scattering process of each nuclide. The discretized slowing-down equation makes possible the step-wise evaluation of the detailed flux over the entire resolved energy range beginning from the energy region above the upper bound of the resonance range where the collision density can be taken to be constant.

It is important to realize, however, that the direct evaluation of Eq. (III.4.8) for each hfg would obviously be too time-consuming since numerous hfg's of lower lethargy can contribute to the scattering source in Eq. (III.4.8) for any k -th hfg in question especially when the mixture involves light-weight nuclide. The problem can be alleviated via the use of recurrence relationship made possible by the use of constant mesh spacing. By using Eq. (III.4.4), Eq. (III.4.8) can be rewritten in the form

$$F_k = \{F_{k-1}e^{-\Delta u} - (\bar{K}_1 - \bar{K}_s e^{-\Delta u})\alpha(\Sigma_s \phi)_{k-1-L} + \bar{K}_1(\Sigma_s \phi)_{k-1} - \alpha \bar{K}_s(\Sigma_s \phi)_{k-L}\} / (1 - r_k) \quad (\text{III.4.9})$$

where $r_k = \bar{K}_s[\Sigma_{sk} / \Sigma_{tk}]$. Hence, the collision density in the k -th hfg requires only that of the previous hfg ($k-1$) and the evaluation of a total of no more than four terms per nuclide in solving the integral equation on a step-by-step basis. In the limit of vanishingly small Δu , the problem becomes even much simpler as $\bar{K}_s$ approaches zero. Kier[26] has demonstrated the rigor and efficiency of such an approach. It was used as the basis in the development of the RABBLE-code which also treats the inter-intra cell transport effects to be addressed later. The same algorithm has also been incorporated into the RABANL option of the MC²-2 code. The latter also allows the inclusion of the inelastic scattering and fission sources on the ultra-fine group basis.

The 'continuous energy' approach described above provides the rigorous means of treating the slowing-down problem as well as the group constants. Once the collision density for each hfg is known, the corresponding flux ϕ_k can also be specified through Eq. (III.2.20). Therefore, the effective cross section for a given group G assumes the same form as defined by Eq. (III.3.64) if the hfg reaction cross section σ_{xk} and flux ϕ_k are used instead of those for the ufg structure. Unlike the case of using the resonance integral concept, the ambiguity resulting from the 'boundary' effect due to the extension of the limits of integration to $\pm\infty$ can be eliminated also. The rapidity by which the slowing-down equation can be solved makes possible the extension of such a scheme to the treatment of the heterogeneous reactor cell.

III.5 Doppler Reactivity

The reactivity of a reactor is generally viewed as the fractional change in the neutron population resulting from the change of the physical properties of the constituents in the system. For a critical reactor operated at the steady state condition, the reactivity signified by δk is the amount by which the multiplication factor k , sometimes referred to as k -effective, differs from unity. The change of temperature, for instance, can introduce several effects on the reactivity. The most common effects are the expansion effect attributed to the change in the densities of reactor material and the Doppler effect attributed directly to the change in the self-shielded cross sections. The latter is known as the Doppler reactivity.

The Doppler reactivity can be computed via either one of the two methods. The most direct method is to calculate the k values before and after the temperature change and δk is equal to the difference between these values. This method, however, provides very little analytical in-sight of the detailed physical processes taken place in energy as well as in space over the reactor system and can be numerically troublesome when δk is very small. An alternative of more theoretical interest is the perturbation approach. The reactor perturbation theory is essentially an extension of the Rayleigh-

Schrödinger theory in quantum mechanics whereby the quantity of interest, the reactivity in this case, can be expressed in terms of the perturbation series. In particular, the first term in the expansion is proportional to the perturbation itself. For practical purposes, one seldom ventures beyond the second order term. For the detailed descriptions of the theory and its applications, the reader is referred to Ref. 23. For our purposes here, it suffices to illustrate its usage in the calculations of the Doppler reactivity within the context of the multigroup approach based on the effective cross section concept.

The Doppler reactivity can be best illustrated via the use of the first order perturbation theory for a bare, homogeneous reactor in which the neutron fluxes and the corresponding adjoints are adequately described by the well-known fundamental-mode representations. Furthermore, if the multigroup fluxes ϕ_n and adjoints ϕ_n^* are so normalized that

$$\sum_{n=1}^N (\nu \Sigma_f)_n \phi_n = 1, \quad \sum_{n=1}^N \chi_n \phi_n^* = 1 \quad (\text{III.5.1})$$

where ν and χ_n are the average number of neutrons produced per fission and the fraction of the fission spectrum in group n respectively. Then the Doppler reactivity can be expressed as

$$\delta k = \sum_{n=1}^N \left\{ \delta(\nu \Sigma_f)_n \phi_n - \delta(\Sigma_a)_n \phi_n \phi_n^* - B^2 \delta \tilde{D}_n \phi_n \phi_n^* + \phi_n (\phi_{n+1}^* - \phi_n^*) \delta \Sigma_s(n \rightarrow n+1) \right\} \quad (\text{III.5.2})$$

where B^2 and $\tilde{D}_n$ denote the buckling and the diffusion coefficient for group n respectively. For simplicity, only $n \rightarrow n+1$ group transfers are considered here. It should be noted that the above expression must be integrated over the volume if the localized reactivity in a reactor is considered.

The physical meaning of each term in the above equation is quite transparent. The first two terms in the bracket on the right hand side of the equation represent the contributions attributed to the Doppler changes of the self-shielded, macroscopic fission and absorption cross sections respectively. The third and fourth terms signify the leakage and scattering components respectively as the result of Doppler effect. For most reactors of practical interest, the leakage terms are generally negligible as compared to the fission and absorption components because B^2 is generally small. Also, since, unlike the fluxes, the adjoints are relatively insensitive to energy groups especially when many groups are used, the scattering components are of little importance. Thus, the Doppler reactivity is dominated almost entirely by the fission and absorption components. It is interesting to note that they assume the opposite signs. The former contributes positively while the latter contributes negatively as temperature increases. In effect, these opposite effects, in part, cancel each other and the net effects depend solely on their relative importance. Such a behavior provides one of the most important criteria for the fast reactor design. From the point of view of reactor safety, it is essential to have a substantial negative Doppler reactivity feedback, which can provide the instantaneous response in the event of power excursion.

To achieve such a goal, the Doppler changes attributed to the fertile isotopes and structural material must be substantially greater than those of $\delta(\nu \Sigma_f)_n$ attributed to the fissionable isotopes. The magnitude of the negative Doppler reactivity is particularly dominant for reactors with relatively soft spectrum because $\delta(\Sigma_\gamma)_n$ for U^{238} exhibits [33] its highest values in the low energy region where the

resonances are extremely sharp. For this reason, the Doppler reactivity is sometimes used as an index for the relative softness of the spectrum of a reactor. For the highly enriched reactors, the net Doppler reactivity is most likely to be positive. Two factors that determine its outcome are the capture-to-fission ratio customarily denoted by α and the magnitude of the adjoint ϕ_n^* . The former is usually smaller than unity for all major fissionable nuclides with exception of perhaps the localized variations. The latter seldom exceeds 1.5 unless the adjoint exhibits significant peaking spatially in the middle of the fuel lumps.

In practical applications, the Doppler coefficient is often used as a measure of the Doppler effect in a reactor instead of the Doppler reactivity [34,35]. The Doppler Coefficient at a given temperature T is defined as the Doppler reactivity per one degree of temperature change in Kelvin from its original value, i.e. $\partial k / \partial T$. Alternatively, it is also sometimes referred to as $T \partial k / \partial T$ taking advantage of the approximate $1/T$ behavior of $\partial k / \partial T$ predicted for many large oxide-fueled fast reactors. Thus, the relationship between δk and $(\partial k / \partial T)$ is simply

$$\delta k = \int_{T_1}^{T_2} \left(\frac{\partial k}{\partial T} \right)_T dT, \quad T_1 \leq T \leq T_2 \quad (\text{III.5.3})$$

One convenient way to compute the derivative at a given temperature T is to assume that the temperature dependence of $(\partial k / \partial T)_T$ can be represented by a polynomial of the form $P_n(1/\sqrt{T})$ within the small temperature range under consideration based on the asymptotic temperature behavior of the resonance integral described earlier. The coefficients of this polynomial can be determined readily by the usual least-squared fitting to a handful of δk computed within T_1 and T_2 . Another simple alternative of practical interest is the analytical relationship derived from a simplified assumption of $(\partial k / \partial T)_T \approx C / T^x$. From Eq. (III.156), one obtains

$$(\delta k)_{T_1 \rightarrow T_2} = \begin{cases} \frac{C}{x-1} \left[\frac{1}{T_1^{x-1}} - \frac{1}{T_2^{x-1}} \right], & \text{for } x \neq 1 \\ C \ln \frac{T_2}{T_1}, & \text{for } x = 1 \end{cases} \quad (\text{III.5.4})$$

The temperature-independent parameters x for all $x \neq 1$ can be determined by knowing two δk values within T_1 and T_2 , i.e.

$$\frac{(\delta k)_{T_1 \rightarrow T_2}}{(\delta k)_{T_3 \rightarrow T_2}} = \frac{1 - (T_1/T_2)^{1-x}}{1 - (T_3/T_2)^{1-x}}, \quad T_1 \leq T_3 \leq T_2 \quad (\text{III.5.5})$$

By choosing $(T_3/T_2) = 2(T_1/T_2)$, x can be computed readily. Hence, this method provides an extremely simple means to deduce the Doppler coefficient from the values of Doppler reactivity.

Because of its practical importance to fast reactor safety, many Doppler experiments were carried out in

the 1960s, most notably those measurements performed in various fast critical assemblies. These results provide valuable reference to test our ability to estimate the Doppler coefficient of the liquid metal fast breeder reactors under consideration. Analyses of such measurements present challenges not only because it is difficult to isolate the Doppler effect of the sample from that of the heating wire and the expansion effect, but also it puts the calculational methods as well as nuclear data to a severe test. By and large, it was concluded that the discrepancies between the calculations and the measurements were of the order of 20% for the U^{238} samples and much greater for the samples of the fissionable isotopes based on the methodologies and nuclear data available in the late 1960s and early 1970s. For details, discussions on this subject can be found in Refs. 23, 24, 25, and 35. It is noteworthy that the great challenge of these analyses did provide the strong motivation for the subsequent improvement in the areas of calculational methods as well as in nuclear data.

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Chapter IV RESONANCE ABSORPTION IN HETEROGENEOUS MEDIA

Although the distribution of neutron flux in a heterogeneous system is, in principle, completely specified by the Boltzmann's equation [1-8], the treatment of resonance absorption in such a system is nevertheless a far more challenging task than that in the homogeneous media. The fact that a substantial reduction in resonance absorption can result from making the fuel into the form of lumps has provided strong motivation for a great deal of work in this area since the very beginning of the reactor development. It has been well recognized that such a reduction is primarily attributed to the change of the energy distribution of flux in the lump when a sharp resonance is present. However, unlike the case of infinite homogeneous media in which the energy distribution of flux is primarily characterized by the energy behavior of the macroscopic total cross section and the Placzek oscillations resulting from the elastic scattering process in the presence of a resonance, the energy and space dependence of flux in the present case becomes hopelessly intertwined as clearly indicated by the Boltzmann's equation defined previously. It is clearly unrealistic if the detailed distribution throughout the entire reactor must be specified simultaneously at every energy. Hence, the general starting point for all existing deterministic approaches is to focus on the examination of the resonance absorption within a localized unit cell. A realistic reactor can be generally viewed as an ensemble of unit cells consisting of one or more types of fuel lumps surrounded by cladding and moderator. These unit cells, in principle, can have either identical or different composition depending on the design under consideration. The resonance absorption in such a system is not only subject to the energy self-shielding effect but also to the spatial self-shielding effect attributed to the localized depression in flux. As discussed previously, such effects can be viewed conceptually as a measure of correlation between the microscopic cross section and neutron flux in energy and in space at a given temperature. This chapter deals with issues pertinent to the treatment of resonance absorption in reactor lattices, sometimes referred to as the 'lattice physics'. The objectives are to determine the effective resonance integrals and/or the effective group cross sections for various lattices from which the global resonance absorption throughout the reactor can be computed via the multigroup methods.

One convenient way to alleviate the entanglement of the energy and space dependence of the flux in a unit cell is via the use of the collision probability method derived on the basis of the mono-energetic neutron transport theory. The method provides a practical means to estimate the fractions of neutrons that suffer collision within a lump and that escape from it. One of the earliest works on the neutron behavior in a uranium lump was carried out by Peierls [9] using what was later known as the integral transport equation for the mono-energetic neutrons. The derivations of collision/escape probabilities for lumps of various geometries were systematically carried out later by Case et al [10]. It has since

become the primary tool for computing the resonance absorption in the fuel lump. The quantification of such a problem for a Breit-Wigner resonance was first investigated by Wigner et al. [11] in 1941 with their results published in 1955 and later extended by Dancoff and Ginsburg [12] to the case involving closely-packed fuel assemblies. Similar work was also carried out independently by Gurevich and Pomeranchouk [13] and others [14-19]. One development particularly worth noting is the two-region cell model pioneered by Chernick [20-22], which formally introduced the collision probability concept in conjunction to the treatment of multi-region slowing down problems in the presence of resonances. It provides a convenient basis which can readily lead to the equivalence relations not only in the slowing-down process between the homogeneous and heterogeneous media but also the corresponding resonance integrals. Because of their practical importance, the subject of collision probabilities and their applications to the resonance integral calculations have been an active area of research even to this date. A large body of articles on these subjects can be found in the open literature [23-59]. Comprehensive discussions of the earlier work on resonance absorption in the heterogeneous media were best summarized by Dresner [60], Nordheim [61] and Lukyanov [62].

The relatively limited computational capability and availability of high quality resonance data are directly responsible for three inevitable constraints in the earlier treatment of resonance absorption in the heterogeneous media : (1) considerations seldom go beyond the two-region unit cell embedded in an infinite array of reactor lattice; (2) the collision probability treatment is almost exclusively limited to a handful of simple configurations in one dimensional geometry; (3) each resonance is treated strictly as the Breit-Wigner type in the sense that it is physically disjoint with respect to any other resonances in the vicinity. The latter is, of course, the consequence of the emphasis that focused on the importance of the well-isolated and low-lying U^{238} resonances in thermal reactor applications.

The fast reactor development accompanied by our improved computational capabilities and better quality resonance data has certainly altered significantly our perception of resonance treatment. As described in the previous chapter, one distinctive characteristic that separates a fast reactor from the traditional thermal reactors is that U^{238} is no longer the only dominant resonant isotope in the reactor systems. From the perspective of the heterogeneity considerations, one is confronted with the presence of resonances of one or more isotopes not only in the fuel lump but also in the stainless steel cladding and the sodium coolant. An accurate account of the heterogeneity effects is particularly essential in computing pertinent reactor parameters for various fast critical assemblies, which consist of drawers made up with constituents in complex geometric arrangements, and in analysis of various measurements carried out in these systems. Because of its safety implication, one fast reactor parameter of particular interest is the Doppler coefficient discussed earlier. The need for analyzing the Doppler effect measurements in the highly heterogeneous system provided the strong motivation for the development of the continuous energy approaches for treating the complex cells with many regions [63-75]. The presence of a large number of resonances and spatial regions lead to the more frequent use of the effective cross section concept in addition to the traditional resonance integral approach. As discussed in Chapter I and Chapter III, the coexistence of the continuous energy approach and the traditional resonance integral approach is possible provided that all resonance cross sections are representable as a linear combination of the Breit-Wigner-like terms. This general criterion remains true for the heterogeneous treatment.

In the following discussions, a rather subjective overview on both the theoretical basis and practical means in dealing with this extremely complex subject will be presented.

IV.1 Fundamental Equations in Lattice Physics

The treatment of resonance absorption problems requires the knowledge of the neutron flux as a function of energy as well as space within a unit cell under consideration. The logical place to begin is, therefore, the basis by which the neutron flux is treated.

IV.1.1 Integral Transport Equation

With no loss of generality, the obvious starting point is Boltzmann's transport equation defined by Eq. (III.1). This equation, however, is not readily amenable to the problem at hand because of its complexity. It is quite obvious that simplifications are required. The first step is to cast the equation into an integral form. Since Eq. (III.1.1) is a linear first order partial differential equation, the solution is expressible in the form of the first order ordinary differential equation via the method of characteristics. This can be achieved by letting $\vec{r} = \vec{r}_0 + \zeta \vec{\Omega}$ and it follows [1-9] that

$$\phi(\vec{r}, \vec{\Omega}, E) = \int_0^\infty \exp \left[- \int_0^{\zeta'} \Sigma_t(\vec{r} - \zeta'' \vec{\Omega}, E) d\zeta'' \right] s(\vec{r} - \zeta' \vec{\Omega}, \vec{\Omega}, E) d\zeta' \quad (\text{IV.1.1})$$

This equation is generally referred to as the integral transport equation. The neutron flux in a given reactor cell, in principle, is completely specified once the source distributions and boundary conditions for the configuration in question are given. With exception of perhaps the Monte Carlo method, the expression is still far too complicated for routine applications which are almost exclusively based on the deterministic approaches particularly in conjunction with the resonance absorption. As discussed previously in the case of homogeneous media, one plausible assumption is that the scattering is taken to be isotropic. The isotropic scattering assumption allows the elimination of the angular dependence by integration of $\vec{\Omega}$ over all solid angles so that the scalar flux becomes a function of $\vec{r}$ and E only. Hence, the problem becomes more manageable if the application is limited to cells with convex geometries. Let

$$\vec{r}' = \vec{r} - \zeta' \vec{\Omega}; \quad d\vec{r}' = \zeta'^2 d\zeta' d\vec{\Omega} \quad (\text{IV.1.2})$$

where $\zeta' = |\vec{r} - \vec{r}'|$ and $d\vec{r}'$ is equivalent to the differential volume element dV' . The scalar flux after integrating over $\vec{\Omega}$ becomes

$$\phi(\vec{r}, E) = \int_{4\pi} \phi(\vec{r}, \vec{\Omega}, E) d\vec{\Omega} = \int \Lambda(|\vec{r} - \vec{r}'|) S(\vec{r}', E) d\vec{r}' \quad (\text{IV.1.3})$$

where $\Lambda(|\vec{r} - \vec{r}'|)$ is referred to as the transport kernel is defined as

$$\Lambda(|\vec{r} - \vec{r}'|) = \frac{1}{4\pi |\vec{r} - \vec{r}'|^2} \exp \left[- \int_0^{|\vec{r} - \vec{r}'|} d\zeta' \Sigma_t \left(\vec{r} - \zeta' \frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|}, E \right) \right] \quad (\text{IV.1.4})$$

Physically, Eq. (IV.1.3) represents the superposition of the neutron transport and slowing-down process. From the perspective of the resonance treatment, the use of the source attributed to the elastic

scattering should suffice. For practical purposes, the problem is still far too complicated unless its energy and space dependence are discretized. The discretization of the energy and space coordinates into fine meshes, in which the macroscopic cross sections can be considered as constants, makes possible the separation of the energy and space dependence in the integral transport equation defined by Eq. (IV.1.3). This leads to the widely used collision probability method and the interface current method whereby the intra-cell neutron transport at a given energy meshes can be viewed in terms of the collision probabilities and/or transmission probabilities from one region to the others as one shall see.

IV.1.2 Collision Probability and Interface Current Approaches

The collision probability approach can be viewed as an obvious consequence of the discretization of the integral transport equation defined by Eq. (IV.1.3) in energy as well as in space. In the earlier days of reactor physics development, this concept was first introduced by Chernick [20,21] in conjunction with the treatment of resonance absorption in reactor cells consisting of two regions, i.e., fuel pin surrounded by the moderator. The method has since been generalized to many reactor physics applications as a powerful means for dealing with the heterogeneous nature of reactor lattices. A thorough review on this subject can be found in the article by Sanchez and McCormick [76]. Because of the important role that this simple yet extremely useful model has played in the theory of resonance absorption, specific discussions will be given in the following sections. With no loss of generality, it suffices to begin with the generalized description of the conceptual aspects of the method first. For a unit cell consisting of N homogeneous regions, the average flux for any region i at a given energy mesh E is simply

$$\phi_i(E) = \frac{1}{V_i} \int_{V_i} d\vec{r} \phi(\vec{r}, E) \quad (\text{IV.1.5})$$

Thus, the neutron transport behavior within a unit cell at a given E as inferred by Eq. (IV.1.3) can be described by a system of N linear equations

$$\sum_{ii} V_i \phi_i(E) = \sum_{j=1}^N V_j S_j(E) P_{i \leftarrow j}(E) \quad (\text{IV.1.6})$$

where $P_{i \leftarrow j}(E)$ is referred to as the collision probability defined as⁶

$$P_{i \leftarrow j}(E) = \frac{\Sigma_{ij}(E)}{V_j} \int_{V_j} d\vec{r} \int_{V_i} d\vec{r}' \Lambda(|\vec{r} - \vec{r}'|) \quad (\text{IV.1.7})$$

Physically, $P_{i \leftarrow j}(E)$ signifies the probability that neutrons initiated in region j will reach region i and suffer their next collision there. To account for the inter-cell transport effects attributed to the neighboring unit cells, appropriate boundary conditions are apparently required. The specific issues on the subject of collision probability will be addressed in the next section.

Eq. (IV.1.6) provides a convenient means whereby the neutron transport and slowing-down processes in

a cell can be treated separately. The source term $S_j(E)$, like the case of infinite homogeneous media, is dominated by the elastic slowing-down source for most of the energy region of interest to the studies of resonance absorption and is usually set to be equal to the collision density defined by Eq. (III.2.20). Thus, strictly speaking, it amounts to the solution of N slowing-down equations in which $P_{i \leftarrow j}(E)$ serves as the weights to indicate the relative contributions from each region in the cell. The problem is, in principle, completely specified once the inter-cell boundary condition at the outer surface is imposed. Two remaining problems are: (1) evaluation of the collision probability matrix $P_{i \leftarrow j}(E)$; (2) solution of the slowing-down equation. Since the treatment of the slowing-down equation has already been extensively discussed in the previous chapter, it suffices to focus only on the subjects of collision probability and other related topics in the following discussions.

Aside from the collision probability approach defined by Eq. (IV.1.6) based on the intra-cell fluxes, the neutron transport process can also be treated from the perspective of the intra-cell currents [41,77]. The same logic analogous to that in deriving Eq. (IV.1.6) applies. Consider a unit cell consisting of N homogeneous regions and a total of M surfaces. If J_k^+ and J_k^- denote the currents impinging on the inner and outer surfaces of the k^{th} surface respectively, the neutron conservation can be represented by

$$J_k^+(E) = \sum_{j=1}^N V_j S_j(E) P_{k \leftarrow j}^{S \leftarrow V}(E) + \sum_{l=1}^M A_l J_l^-(E) T_{k \leftarrow l}^{S \leftarrow S}(E), \quad k \in M \quad (IV.1.8)$$

subject to the following boundary condition

$$J_k^+ = \sum_{l=1}^M B_{kl} J_l^- \quad (IV.1.9)$$

where P and T denote the collision and transmission probabilities, respectively. Traditionally, the former is always attributed to those originated from a unit volume source whereas the latter is attributed to those originated from a unit surface source. The precise definition and their relationship of these quantities will be described in the next section. For sake of clarity, the superscripts $V \leftarrow V$ and $S \leftarrow S$ denote the volume-to-volume and surface-to-surface transfer respectively. As a general rule, a given region is always surrounded by one or more surfaces. Hence, the evaluation of the current requires the solution of a system of $2M$ linear equations. Once these currents are known, the flux of any region i can be obtained via the determination of the collision rate $C_i(E)$ defined as

$$C_i(E) = \sum_{j=1}^N V_j S_j(E) P_{i \leftarrow j}^{V \leftarrow V}(E) + \sum_{l=1}^M A_l J_l^-(E) P_{i \leftarrow l}^{V \leftarrow S}(E), \quad i \in M \quad (IV.1.10)$$

where the corresponding flux is related to $C_i(E)$ as follows

$$\phi_i(E) = \frac{C_i(E)}{\Sigma_{ti}(E)} \quad (\text{IV.1.11})$$

In contrast to the collision probability method, the major advantage of this approach is the relative ease by which various probabilities can be computed. For most of the cases of practical interest, a given unit cell can be viewed as a superposition of discretized sub-regions with convex geometries and each sub-region is bound by two surfaces, i.e., $N = 1$ and $M = 2$ in the context of Eq. (IV.1.8). The direct utilization of this method in association with the rigorous numerical approach for solving the slowing-down equation described in chapter III was pioneered by Kier [74]. Its viability to the resonance treatment has been well-demonstrated by the RABBLE [71] and MC²-2 codes [75] that are still considered among the most sophisticated benchmark tools to this day. Unlike the collision probability method in which the evaluation of each $P_{i \leftarrow j}$ must account for the intra-cell neutron transport in all sub-regions between i and j , all pertinent probabilities defined in Eq. (IV.1.8), on the other hand, are only dependent on the optical path within a sub-region in question. The intra-cell effects for this case are accounted for by the boundary conditions imposed. The obvious trade-off here is that the validity of the isotropic (or cosine current) assumption at each interface is required. The simplification of the intra-cell transport effects can also lead to a system of linear equations in neutron current much more amenable to numerical solution than those defined by Eq. (IV.1.6) as one shall see.

The collision probability method and the inter-face current method are considered as the fundamental starting point for the lattice physics whenever the deterministic approach is used. For applications in resonance theory, many simplifications are obviously required. In the following discussions, issues pertinent to the treatment of resonance absorption will be addressed where appropriate.

IV.2 General Features of Collision and Transmission Probabilities

Because the concept of collision/transmission probabilities provides a convenient means to discretize the otherwise unmanageable spatial configuration throughout a reactor, there have been significant advances in the area of utilizing such a concept for reactor applications. The amazing improvement in our computational tools makes possible the development of a large number of methodologies for computing collision probabilities to various degrees of sophistication. In many instances, the treatment of cells with arbitrary geometries in the multi-dimensional domain is within reach. The rigorous methods for treating the multi-dimensional collision probabilities, however, are still restricted to the problems with limited number of energy groups. With exception of the Monte Carlo approach, the application of the collision probability method to the resonance treatment still relies exclusively on the assumption of one-dimensional geometries.

For our purpose here, the general characteristics of collision probabilities will be addressed first. The discussion will be followed by their practical usage in conjunction to the treatment of resonance absorption in reaction lattices. For the sake of convenience, the energy dependence and the direction indicator $\leftarrow$ used to symbolize the collision and transmission probabilities will henceforth be dropped.

IV.2.1 General Remarks of Collision and Transmission Probabilities in an Isolated Lump

For illustrative purposes here, let us first consider a case of the mono-energetic (or 'one group')

transport theory for an isolated lump with convex geometry surrounded by moderator of infinite extent. In the context of Eq.IV.1.6, it corresponds to the case of neutron transport in the most elementary two-region cell. This simple case provides the analytical insight and the basis needed for the development of the collision probability methods for treating resonance absorption in the reactor lattices.

Assume that the composition is uniform and the source is isotropic, similar to the case investigated by Peierls in the earlier days. With no loss of generality, the integral transport equation described earlier can be cast into the following form:

$$\phi_0(\vec{r}) = \Sigma_s \int_V \phi_0(\vec{r}') \Lambda(|\vec{r} - \vec{r}'|) d\vec{r}' + Q(\vec{r}) \quad (\text{IV.2.1})$$

where $Q(\vec{r})$ denotes the ‘fixed’ source consisting of two potential types, namely

$$Q(\vec{r}) = \int_V q(\vec{r}') \Lambda(|\vec{r} - \vec{r}'|) d\vec{r}' + \int_S \varphi(\vec{r}_s') (\vec{\Omega} \cdot \vec{n}') \Lambda(|\vec{r} - \vec{r}_s'|) d\vec{r}_s' \quad (\text{IV.2.2})$$

The above equation is sometimes referred to as Peierls equation [9]. Physically, the first term represents the contribution attributed to the scattering in the energy ‘group’ in question or generally referred to as the ‘self-scattering’ term whereas the integrals in Eq. (IV.2.2) denote the contributions from certain ‘fixed’ volume source and surface source respectively. The quantity $(\vec{\Omega} \cdot \vec{n}')$ is the cosine of the angle between the vector $\vec{r} - \vec{r}_s'$ and the normal at the point $\vec{r}_s'$ on the surface. For a purely absorbing lump in which $\Sigma_t \approx \Sigma_a$, the term attributed to ‘in-group’ scattering vanishes and Eq. (IV.2.1) becomes conceptually simpler. The kernel $\Lambda(|\vec{r} - \vec{r}'|)$ must obviously be symmetric with respect to any coordinate system considered. Thus, the flux at $\vec{r}$ resulting from a unit source placed at $\vec{r}'$ is equal to that at $\vec{r}'$ if the unit source is placed at $\vec{r}$ instead. This symmetric property eventually leads to the reciprocity relation of the collision probability to be addressed.

From the perspective of resonance treatment in which the energy mesh under consideration is generally much finer than the extent of the resonance as discussed in the previous chapter, any collision taken place at a given hyper-fine group is practically equivalent to that of a pure absorber in the sense that the collision will remove a neutron from the energy range in question. It is, therefore, possible to derive the first-flight collision and transmission probabilities for a given energy mesh on this basis.

The first-flight collision probability for a lump is defined as the average collision rate corresponding to the uniform source of $q(\vec{r}') = 1$ and $\varphi(\vec{r}_s') = 0$, i.e.

$$P_c = \frac{1}{V} \int_V \Sigma_t \phi_0(\vec{r}) d\vec{r} = \frac{\Sigma_t}{V} \int_V d\vec{r} \int_V d\vec{r}' \Lambda(|\vec{r} - \vec{r}'|) \quad (\text{IV.2.3})$$

The corresponding escape probability is simply

$$P_{esc} = 1 - P_c \quad (\text{IV.2.4})$$

The volume integral in Eq. (IV.2.3) can be transformed into the form of a surface integral by utilizing the Gauss-Ostrogradski theorem whereby

$$\Sigma_t \int_V d\vec{r}' \Lambda(|\vec{r} - \vec{r}'|) = 1 - \int_S \Lambda(|\vec{r} - \vec{r}'_s|) (\vec{\Omega} \cdot \vec{n}') d\vec{r}'_s \quad (\text{IV.2.5})$$

Hence, the escape probability for a lump can be written as

$$\begin{aligned} P_{esc} &= \frac{1}{V} \int_V d\vec{r} \int_S d\vec{r}'_s (\vec{\Omega} \cdot \vec{n}') \Lambda(|\vec{r} - \vec{r}'_s|) \\ &= \frac{1}{2\pi V \Sigma_t} \int_S d\vec{r}_s \int_{\vec{\Omega} \cdot \vec{n}' > 0} d\vec{\Omega} (\vec{\Omega} \cdot \vec{n}') [1 - \exp(-\Sigma_t |\vec{r}_s - \vec{r}'_s|)] \end{aligned} \quad (\text{IV.2.6})$$

where $|\vec{r}_s - \vec{r}'_s|$ is an arbitrary chord on the surface that connects two points defined by $\vec{r}_s$ and $\vec{r}'_s$. For convenience, let $l = |\vec{r}_s - \vec{r}'_s|$. This quantity must be specified in the coordinate system amenable to practical applications. It is a common practice to study the collision probability problems in either the cylindrical or spherical coordinate systems. The chord length for a lump of convex geometries is completely specified by $\vec{r}'_s$ and the direction of $\vec{\Omega}$. In particular, for the configurations of practical interest such as slab, sphere, cylinder and tube, it is related to the physical dimension and the solid angle in a relatively simple way as one shall see. In such geometries, the cosine term $(\vec{\Omega} \cdot \vec{n}')$ in the integrand is independent of $d\vec{r}'_s$ and the integration yields

$$P_{esc} = \frac{1}{4\pi V \Sigma_t} \int_{\vec{\Omega} \cdot \vec{n}' > 0} d\vec{\Omega} (\vec{\Omega} \cdot \vec{n}') [1 - \exp(-\Sigma_t l)] \quad (\text{IV.2.7})$$

where the chord length, $l(d, \Omega)$, is a function of diameter (or thickness where appropriate) and angle. Table IV.1 shows examples of those variables that appear in the integrand of Eq. (IV.18) for three widely used fuel configurations. Here, φ is the azimuthal angle between the chord l and the z-axis and ϕ is the angle between the norm and the projection of l on the xy -plane.

With no loss of generality, it is useful at this point to introduce the generalized expressions for the surface and volume in any coordinate system. These quantities for a lump in question are given respectively as follows.

$$S = \frac{1}{\pi} \int d\vec{r}_s \int d\vec{\Omega} (\vec{\Omega} \cdot \vec{n}), \quad V = \frac{1}{4\pi} \int d\vec{r}_s \int d\vec{\Omega} (\vec{\Omega} \cdot \vec{n}) l(d, \vec{\Omega}) \quad (\text{IV.2.8})$$

Hence, the average chord length $\bar{l}$ is simply

$$\bar{l} = \frac{4V}{S} \quad (\text{IV.2.9})$$

The average chord length $\bar{l}$ is of great practical importance because the dimensionless quantity, $\Sigma_t \bar{l}$ known as the 'optical thickness,' is a convenient measure to study the general characteristics of the escape probability. Fig. IV.1 shows the behavior of P_{esc} as a function of $\Sigma_t \bar{l}$ for slab, cylinder, and sphere on the same plot. By and large, with exception of perhaps the intermediate values of $\Sigma_t \bar{l}$, all curves show striking resemblance. Thus, it follows that

$$P_{esc} = \frac{1}{\Sigma_t \bar{l}} (1 - e^{-\Sigma_t \bar{l}}) \quad (IV.2.10)$$

must provide a good approximation since it reproduces the exact values at both small and large values of optical thickness (or commonly referred to as white and black limits) for all configurations. This approximation is surprisingly accurate. For spherical and cylindrical geometries, for instance, the maximum error does not exceed 5% as illustrated in Fig. IV.1. Hence, it was used by Gurevich and Pomeranchouk [13] for treating the resonance absorption in the fuel lump, which led to one of the simple means to analyze the effective resonance integral in a fuel lump. Another even simpler function that exhibits the same limiting properties is the rational function of the form

$$P_{esc} = \frac{1}{1 + \Sigma_t \bar{l}} \quad (IV.2.11)$$

as first pointed out by Wigner. Although Eq. (IV.2.11) is less accurate than Eq. (IV.2.10), its rational form has been proved to be of great practical significance since the early days of reactor development. Its implications will be further addressed.

Figure IV. 1 Escape Probabilities from a Lump

Aside from the collision probability, another quantity of practical interest is the transmission probability T defined as the fraction of neutrons initiated from a uniform and isotropic surface source passing through the lump without suffering a collision. By using the same logic analogous to that in deriving the collision probability, it is quite obvious from Eq. (IV.2.2) that the first-flight transmission probability attributed to such a source is

$$T = \frac{1}{S\pi} \int_S d\vec{r}_s \int_{\vec{\Omega} \cdot \vec{n}' > 0} d\vec{\Omega} (\vec{\Omega} \cdot \vec{n}') \exp(-\Sigma_t |\vec{r}_s - \vec{r}'_s|) \quad (\text{IV.2.12})$$

Physically, the exponential term within the double integral signifies the transmission probability along the straight line between two points on the surface defined by $\vec{r}_s$ and $\vec{r}'_s$, and T is the fraction of neutrons transmitted through the lump without any collision. Alternatively, T also represents the current of unit strength at the surface that passes through the lump without being collided. By comparing Eq. (IV.2.12) to Eq. (IV.2.6), one obtains the reciprocity relation of the form

$$(1 - T) = (\Sigma_t \bar{l}) P_{esc} \quad (\text{IV.2.13})$$

The quantity $(1 - T)$ can be perceived as the net current initiated by a unit surface source and eventually passing through the lump in question. Because of their relative simplicity, these probabilities provide a convenient basis for utilization of the collision probability method as well as the interface-current method described in the previous section. The explicit representations of these quantities obviously depend on the geometric configuration of the lump under consideration. Relevant derivations will be carried out in the following discussions where appropriate.

IV.2.2 General Features of Traditional Treatment of Collision Probability in a Closely Packed Lattice

A reactor lattice consisting of many closely-packed fuel pins embedded in the coolant is certainly the most commonly encountered situation in reactor applications. Although it can be viewed as an ensemble of two-region unit cell in an infinite lattice, the existence of the neighboring pins will affect the escape probability of the pin in question. Unlike the case of the isolated fuel lump, neutrons that escape from it may not necessarily suffer their next collision in the surrounding moderator. This issue was first addressed by Dancoff and Ginsburg [12]. The ‘shadowing’ effect attributed to the neighboring fuel pins on the escape probability of the pin in question has henceforth been referred to as the Dancoff effect. There are two ways for treating the intra- and inter-cell transport effects, namely: (1) the use of the interface-current method based on the transmission and collision probabilities of an isolated region [71]; (2) the use of the modified collision probabilities in conjunction with the traditional two-region cell treatment, i.e., Eq. (IV.1.6) with $N = 2$. The former, which accounts for the intra- and inter-cell transport effects via the use of the boundary conditions on neutron current at each surface, will be addressed later along with the continuous energy approach. The latter, which has been used as the fundamental basis for the development of the effective resonance integral concept, will be discussed

first.

The most comprehensive discussions on the subject of the escape probability for a closely-packed reactor lattice are believed to be those given by Rothenstein [26,27], Nordheim [61] and Lukyanov [62]. The physical attributes of this phenomenon can be best illustrated by following a straight line trajectory of the neutron path through the absorber lumps and the surrounding moderator (or coolant). With no loss of generality, Fig. IV.2 shows a schematic description of such a path in a lattice. Let 0 denote the initial absorber lump in question and $2, 4, \dots, 2N$ denote all other absorber lumps while the regions sandwiched between the absorber lumps are signified by $1, 3, 5, \dots, 2N + 1$. If l_n is the chord length in region n , the transmission probability between the two end points of this chord is simply given by $\exp[-\Sigma_t^{(n)} l_n]$ as discussed in the foregoing section. For convenience, define

$$Y_n = \exp[-\Sigma_t^{(n)} l_n] \quad (\text{IV.2.14})$$

so that the average transmission probability through the surface of the n -th region is $T_n = \langle Y_n \rangle$ in the same context as that defined by Eq. (IV.2.12) for an isolated lump. Hence, in the notation above, the escape probability defined by Eq. (IV.2.13) becomes

$$P_0^{(iso)} = \frac{1}{\Sigma_t^{(0)} l_0} (1 - \langle Y_0 \rangle) \quad (\text{IV.2.15})$$

in the absence of the neighboring absorber lumps. The escape probability in this case is physically equivalent to the collision probability for the surrounding moderator. In the presence of neighboring absorber lumps, on the other hand, the above quantity must be modified by taking into account the probability of neutrons that survive without suffering any collision with other absorber lumps along the trajectory through all successive regions. Let P_0^* denote the modified escape probability for lump 0 in such a lattice. It is not difficult to see that P_0^* can be expressed symbolically in the general form as follows [26,27,61].

$$P_0^* = \frac{1}{\Sigma_t^{(0)} l_0} \langle (1 - Y_0)[(1 - Y_1) + Y_1 Y_2 (1 - Y_3) + \dots] \rangle \quad (\text{IV.2.16})$$

where the average is taken to be in the same context as that defined by Eq. (IV.2.12). Similarly, the escape probability of the moderator, P_1^* , can be obtained by interchanging the indices of the fuel and moderator regions in Eq. (IV.2.16). The above equation is obviously too general to be useful for practical applications unless some simplifying assumptions are introduced. One commonly used assumption in the earlier days is that all absorbers are identical in composition and geometric configuration equally spaced in a sea of moderator. Such an arrangement is often referred to as infinite lattice with repeated cells. Since the environment of every absorber is taken to be the same, it follows that the transmission probabilities between the surface within a given absorber and those between the surfaces of two absorbers become

$$\langle Y_{2n} \rangle = \langle Y_0 \rangle = T_0, \quad n = 1, 2, 3, \dots, N \quad (\text{IV.2.17})$$

and

$$\langle Y_{2n+1} \rangle = \langle Y_1 \rangle = T_1 \quad (\text{IV.2.18})$$

where T_0 is the same as that defined by Eq. (IV.2.12) and T_1 , analogous to T_0 , can be expressed in a general form⁶²

$$T_1 = \frac{1}{\pi S_0} \int_{S_0} d\vec{r}_{s0} \int_{S_1} d\vec{r}_{s1} (\vec{\Omega}_0 \cdot \vec{n}_0)(\vec{\Omega}_1 \cdot \vec{n}_1) \frac{\exp(-\Sigma_t^{(1)} |\vec{r}_{s0} - \vec{r}_{s1}|)}{|\vec{r}_{s0} - \vec{r}_{s1}|^2} \quad (\text{IV.2.19})$$

The repeated cell assumption leads to four approximations most frequently used in reactor applications. In particular, the first two of these provide the theoretical basis for the well-known rational approximation to be addressed later.

Figure IV. 2 Schematic Illustration of Neutron Transport in a Medium with Multiple Absorbers

(1) Black Limit

If the total cross sections of the absorbers are large, all higher order terms in the above equation diminish with exception of the linear term. In addition, if the average of the product is replaced by the product of the averages, one obtains

$$P_0^* = \frac{1}{\Sigma_t^{(0)} \bar{l}_0} (1 - \langle Y_0 \rangle)(1 - \langle Y_1 \rangle) = P_0^{(iso)} (1 - C) \quad (IV.2.20)$$

where $C = \langle Y_1 \rangle = T_1$ is often referred to as the Dancoff correction factor. Physically, it is equivalent to assume the neutron paths in the absorber and the moderator, are uncorrelated in the context of Eq. (IV.2.16) under the black limit. The factor $1 - C$ represents the fractional reduction of neutron collision in the moderator due to the presence of the neighboring absorber. The above relation between P_0^* and $P_0^{(iso)}$ provides the simplest illustration of the Dancoff effect attributed to the neighboring absorber.

(2) Nordheim's Approximation

In practical situations, the absorbers may not always be considered as 'black'. However, since the linear term is generally the dominant term in the sum, Eq. (IV.2.16) can be adequately approximated by replacing the average of the higher order products with the product of averages as pointed out by Nordheim⁶¹. Thus, upon the substitution of Eq. (IV.2.17) and Eq. (IV.2.18) into Eq. (IV.2.16), it becomes

$$P_0^* = \frac{1}{\Sigma_t^{(0)} \bar{l}_0} (1 - \langle Y_0 \rangle)(1 - \langle Y_1 \rangle)[1 + \langle Y_0 \rangle \langle Y_1 \rangle + \langle Y_0 \rangle^2 \langle Y_1 \rangle^2 + \dots] \quad (IV.2.21)$$

Note that the above equation represents a geometric series which can be recombined into the following closed form:

$$P_0^* = \frac{1}{\Sigma_t^{(0)} \bar{l}_0} \frac{(1 - \langle Y_0 \rangle)(1 - \langle Y_1 \rangle)}{1 - \langle Y_0 \rangle \langle Y_1 \rangle} = \frac{(1 - C)P_0^{(iso)}}{1 - (1 - \Sigma_t^{(0)} \bar{l}_0 P_0^{(iso)})C} \quad (IV.2.22)$$

It is interesting to note that the above equation can be cast into a somewhat different form, namely

$$\frac{1}{P_0^*} = \frac{1}{P_0^{(iso)}} + \frac{\bar{l}_0 \Sigma_t^{(0)} C}{1 - C} \quad (IV.2.23)$$

Hence, in contrast to Eq. (IV.2.20), the inverse of P_0^* is linear with respect to the corresponding inverse of $P_0^{(iso)}$ with a constant correction term. This expression provides a useful basis for the widely-used rational approximation to be discussed later.

(3) Infinite Slabs

Eq. (IV.2.16) again becomes manageable if an infinite-repeated lattice consists of absorber and moderator configured as infinite slabs. Let φ be the azimuthal angle between a neutron path and the

vertical axis along the center of the absorber slab in question. The directional cosine and the chord length are related to φ and the thickness of the slab in a simple way as specified in Table IV.1. If the absorber and moderator with the thicknesses of t_0 and t_1 , respectively, are either in a periodic (or in a reflective) arrangement, it can be shown readily that Eq. (IV.2.16) can be reduced to the following form as pointed out by Corngold²³ and Rothenstein⁶⁰

$$P_0^* = \frac{2}{\Sigma_t^{(0)} l_0} \int_0^{\pi/2} \frac{[1 - \exp(-\Sigma_t^{(0)} t_0 / \sin \varphi)] [1 - \exp(-\Sigma_t^{(1)} t_1 / \sin \varphi)]}{1 - \exp[-(\Sigma_t^{(0)} t_0 + \Sigma_t^{(1)} t_1) / \sin \varphi]} \sin \varphi \cos \varphi d\varphi \quad (\text{IV.2.24})$$

where the factor 2 signifies the symmetry on both side of the absorber plate.

$$P_0^{(iso)} = \frac{1}{2\Sigma_t^{(0)} t_0} [1 - 2E_3(\Sigma_t^{(0)} t_0)] \quad (\text{IV.2.25})$$

where $E_3(x)$ is the exponential integral of order 3 defined as

$$E_n(x) = \int_1^\infty \frac{\exp(-xt)}{t^n} dt \quad (\text{IV.2.26})$$

On the other hand, under the black limit in the context described in the foregoing discussions, the Dancoff correction for this case is simply

$$C = 2E_3(\Sigma_t^{(0)} t_0) \quad (\text{IV.2.27})$$

Eq. (IV.2.25) can also be cast into the form of an infinite series in terms of the exponential integrals of order 3 if one expands the integrand into a geometric series, namely [23,60]

$$P_0^* = \frac{1}{2\Sigma_t^{(0)} t_0} \left\{ 1 - 2 \sum_{n=0}^{\infty} \{ E_3[(n+1)\tau_0 + n\tau_1] + E_3[n\tau_0 + (n+1)\tau_1] - 2E_3[(n+1)(\tau_0 + \tau_1)] \} \right\} \quad (\text{IV.2.28})$$

where $\tau_0 = \Sigma_t^{(0)} t_0$ and $\tau_1 = \Sigma_t^{(1)} t_1$ are the optical thicknesses of the absorber and the moderator respectively. Because of its simplicity, the above equation provides the most vivid illustration of the physical relationship between the collision probabilities and the inter-region currents in a multi-region cell. The rearrangement of the terms in the summation leads immediately to the physically obvious conclusion that

$$P_0^* = \sum_{n=1}^{all} P_{n \leftarrow 0} \quad (\text{IV.2.29})$$

where $P_{n \leftarrow 0}$ is the probability for neutrons initiated from an isotropic unit volume source in region 0 that will suffer their first collision in region n . These collision probabilities as inferred by Eq. (IV.2.28) are

defined in order as follows.

$$\begin{aligned}
 P_{1 \leftarrow 0} &= \frac{2}{2\Sigma_t^{(0)}t_0} \{E_3(0) - E_3(\tau_0)\} - \frac{2}{2\Sigma_t^{(0)}t_0} \{E_3(\tau_1) - E_3(\tau_0 + \tau_1)\} \\
 &= 2\{\vec{J}(0, \tau_0) - \vec{J}(\tau_1, \tau_0)\}
 \end{aligned} \tag{IV.2.30}$$

$$\begin{aligned}
 P_{2 \leftarrow 0} &= \frac{2}{2\Sigma_t^{(0)}t_0} \{E_3(\tau_0 + \tau_1) - E_3(2\tau_0 + \tau_1)\} - \frac{2}{2\Sigma_t^{(0)}t_0} \{E_3(\tau_0 + 2\tau_1) - E_3(2\tau_0 + 2\tau_1)\} \\
 &= 2\{\vec{J}(\tau_0 + \tau_1, \tau_0) - \vec{J}(\tau_0 + 2\tau_1, \tau_0)\}
 \end{aligned} \tag{IV.2.31}$$

$$\begin{aligned}
 P_{n \leftarrow 0} &= \frac{2}{2\Sigma_t^{(0)}t_0} \{E_3(\tau) - E_3(\tau + \tau_{m-1})\} - \frac{2}{2\Sigma_t^{(0)}t_0} \{E_3(\tau + \tau_m) - E_3(\tau + \tau_{m-1})\} \\
 &= 2\{\vec{J}(\tau, \tau_0) - \vec{J}(\tau + \tau_m, \tau_0)\}
 \end{aligned} \tag{IV.2.32}$$

where $\tau_m = \Sigma_t^{(m)}t_m$ is the mean-free path through plate m (with m equal to 1 for odd n and equal to 0 for even n), τ is the total optical distance between the inner surface of plate n and the reference interface of the nearest neighbor and the plate 0 in question, and $\vec{J}(\tau, \tau_0)$ signifies the interface-current at the inner surface of plate n resulting from an isotropic unit source in region 0. Physically, $-\vec{J}(\tau + \tau_m, \tau_0) = \vec{J}(\tau + \tau_m, \tau_0)$ is equivalent to a 'negative' source impinging on the far surface of plate n . The notations used here are consistent with those used by Olson [72] for treating the generalized cell with infinite slabs to be discussed in the next section. Thus, the collision probability $P_{n \leftarrow 0}$ can be construed as the net neutron current on the surfaces of region n for neutrons originated from region 0, which, in turn, can be identified with the collision rate in that region in conjunction with the neutron source of unit strength from region 0. These relationships are conceptually important to from much of the applications of the collision probability method to the resonance treatment in various critical assemblies to be addressed later.

(4) Cylindricized Two-Region Cell

The cell configuration most commonly encountered in reactor applications is that with fuel rod surrounded by moderator. The problem can be significantly simplified by cylindricizing the moderator around each fuel rod. Thus, the infinite lattice can be viewed as an ensemble of unit cell consisting of two coaxial regions. In reference to Eq. (IV.2.16) and the solid angle pertinent to the infinite cylinder listed in Table IV.1, it is possible to derive the similar type of expression as that for the infinite slabs as discussed by Takahashi [52] and also by Rothenstein [26],

$$P_0^* = \frac{2}{\Sigma_t^{(0)}r_0} \int_0^{\pi/2} \cos \phi d\phi \int_0^{\pi/2} \frac{\left[1 - \exp\left(-\frac{2\tau_0 \cos \phi}{\sin \phi}\right)\right] \left[1 - \exp\left(-\frac{2\tau_1 \zeta}{\sin \phi}\right)\right]}{1 - \exp\left[-\frac{2(\tau_0 \cos \phi + \tau_1 \zeta)}{\sin \phi}\right]} \sin^2 \phi d\phi \tag{IV.2.33}$$

where $\tau_0 = \Sigma_t^{(0)} r_0$, $\tau_1 = \Sigma_t^{(1)} r_1$, r_0 and r_1 are the radii of the fuel and the moderator, respectively, and

$$\zeta = \tau_1 [\sqrt{1 - a^2 \sin^2 \phi} - a \cos \phi], \quad a = r_0 / r_1 \quad (\text{IV.2.34})$$

In contrast to the case of the infinite slabs, the escape probability here involves a double integral which is obviously more difficult to evaluate. The inner integral, like the previous case, again can be cast into an infinite series of integrals. Each integral, however, is identifiable with the Bickley-Naylor [78] function of order 3 in the same context as the slab case with respect to the E_3 -function. Because of its important role in the practical applications, much of the following discussions will be devoted to the lattice in the cylindrical coordinate system.

It is worth noting that Eq. (IV.2.33) must approach Eq. (IV.2.28) asymptotically on physical grounds as r_0 and r_1 approach infinity. Mathematical proof of such a physical phenomenon will be presented later in conjunction with the transmission probabilities in an annulus.

Table IV. 1 Geometric Parameters for Three Most Commonly Considered Configurations.

Geometric Configurations	$(\vec{\Omega}, \vec{n})$	$d\vec{\Omega}$	$l(d, \Omega)$
Infinite slab, thickness t	$\cos \varphi$	$\sin \varphi d\varphi d\phi$	$t / \sin \varphi$
Infinite rod, diameter d	$\sin \varphi \cos \varphi$	$\sin \varphi d\varphi d\phi$	$d \cos \phi / \sin \varphi$
Sphere, diameter d_s	$\cos \varphi$	$\sin \varphi d\varphi d\phi$	$d_s \cos \varphi$

IV.2.3 General Features of Collision Probabilities in a Cell with Many Regions

Reactor lattices of practical interest can consist of cells with multiple regions of different compositions and geometric configurations. Strictly speaking, the determination of the collision probabilities in a multi-region cell involves the evaluation of integral of the type defined by Eq. (IV.2.16) over a three-dimensional domain, which can be an insurmountable task especially when the resonance behavior of the cross sections must be taking into account. Simplified assumptions are apparently required before the concept can be deployed in reactor applications. At this point in time, the multi-dimensional considerations of the collision probabilities are still off-limits for all deterministic methods in so far as the resonance treatment is concerned. Even for the case of a simple cell configuration, the computation can be prohibitive as long as the intra- and inter-cell neutron transport must be accounted for in great detail as evidenced by Eq. (IV.2.16). For this reason, the treatment of the multi-region cell in conjunction with the continuous energy approach usually resorts to the use of the interface current method whereby the complexity of evaluating the collision probabilities can be minimized as one shall see in the later section.

One special case particularly worth noting on both theoretical and practical grounds is a multi-region cell consisting of infinite slabs in which the collision probabilities for each plate can be derived analytically in a compact form similar to that of Eq. (IV.2.28). One typical example of such a configuration is a drawer that constitutes the basic building blocks of a critical assembly. Each drawer may consist of multiple fuel, stainless steel and sodium plates. The importance of the heterogeneity effect in such a system has been of great concern. In the first part of the following discussions, it will be shown how Eq. (IV.2.28) can be extended to accommodate such a multi-region system. Thus, one does not have to resort to the use of the interface current method at the expense of the isotropic current assumption across all boundaries once the multi-region collision probabilities are known.

Although the multi-dimensional collision probability approach has not been used in the presence of many resonances over a large energy span on a continuous energy basis, its applicability in the near future is clearly anticipated in light of the availability of the relatively inexpensive yet highly efficient computing facilities. Furthermore, the general features of collision probabilities in the multi-dimensional domain can provide better understandings of the phenomena of neutron transport in a complex cell. Of particular practical interest is the 2-dimensional collision probability approach in the cylindrical coordinate system pioneered by Carlvik [79]. For these reasons, the general features of the 2-dimensional collision probabilities will be discussed in the second part of this section.

(1) Cell Consisting of Many Plates

A drawer in a fast critical assembly is an example of a 'cell' consisting of multiple plates with different composition and thickness. Typically, there are at least two fuel plates accompanied by plates of stainless steel, sodium and depleted uranium. Similar to the two-region cell considered previously, a reactor lattice here can be viewed as an ensemble of an infinite number of repeated drawers arranged in either periodic or reflective arrangement. If the plates in question are again considered as infinite slabs, it is not difficult to see that the same principle can be extended to such a system as pointed out by Olson [72].

In the context of Eq. (IV.2.32), the collision probability from a plate j to another plate i within the same drawer is equivalent to the net current through the surfaces of region i resulting from a unit

neutron source originated from region j . For a periodic drawer arrangement, it can be shown readily by using the same logic leading to Eq. (IV.2.32) that

$$P_{i \leftarrow j} = \sum_{m=0}^{\infty} \{ [\bar{J}(\tau_r + mh, \tau_j) - \bar{J}(\tau_r + \tau_i + mh, \tau_j)] + [\bar{J}(\tau_l + mh, \tau_j) - \bar{J}(\tau_l + \tau_i + mh, \tau_j)] \} \quad (\text{IV.2.35})$$

where τ_r and τ_l are the optical paths from the right and the left surfaces of plate j to the next i plate respectively in lieu of the symmetry assumed for the simple case, h , the optical thickness of the drawer, and

$$\bar{J}(\tau + mh, \tau_j) = E_3(\tau + mh) - E_3(\tau + mh + \tau_j) \quad (\text{IV.2.36})$$

Note that the infinite sum involving E_3 -function can be cast into an integral of a closed form similar to Eq. (IV.2.24), i.e.

$$\int_1^{\infty} \frac{\exp(-zt)}{[1 - \exp(-ht)]t^3} dt = \sum_{k=0}^{\infty} E_3(z + kh) \quad (\text{IV.2.37})$$

The above equation amounts to no more than an empty form unless the integral can be evaluated efficiently. For this reason, a general Gauss quadrature specifically aiming for integrals of the following form was developed by Olson [72] such that

$$\int_1^{\infty} \frac{\exp(-x)f(x)}{x^n} dx = \sum_{i=1}^M w_{n,i} f(x_{n,i}) + R_M \quad (\text{IV.2.38})$$

where $w_{n,i}$, $x_{n,i}$ and R_M are the quadrature weight, quadrature points and remainder respectively. For the case under consideration, n is equal to 3. The quadrature approach was found to be exceedingly accurate and efficient so that it was incorporated into the RAB1D code [72] as well as the MC²-2 code [75] for routine applications in the analysis of various critical assemblies. To our knowledge, this is probably the only case applied to the continuous energy approach in the presence of resonances without resorting to any further approximation.

(2) Generalized Collision Probabilities in the Two-Dimensional Domain

Strictly speaking, the determination of the collision probability involves the evaluation of integral of the type defined by Eq. (IV.2.3) over a three-dimensional domain, which can be an insurmountable task especially when the resonance behavior of the cross sections and the geometric complexity must be taking into account. Simplified assumptions are apparently required before the concept can be deployed in reactor applications. One most commonly used starting point for studying the general features of the multi-dimensional collision probabilities is to examine the problem from the perspective of the cylindrical coordinate system in which the neutron flux is taken to be constant along the z -axis such as that leading to Eq. (IV.2.33). Thus, the axial dependence of the integral can be eliminated and the problem becomes two dimensional in nature. The general idea of utilizing such a coordinate system was

pioneered by Bonalumi [30] and was later generalized by Carlvik [55,79] to account for many possible situations of practical interest. This reduces the integral into a more manageable form readily amenable to numerical quadratures and makes further simplification more transparent for many cases of practical interest.

The problem can be best illustrated by examining the integral for a lump defined by Eq. (IV.2.12) and Eq. (IV.2.7). Let l be the chord length and θ be the azimuthal angle between l and the z-axis as before. It follows that l is related to its projection on the xy -plane, say a , by $l = a / \sin \theta$. If $(\vec{\Omega}_A, \vec{n}_A)$ denotes the directional cosine of a at the end of the chord on the xy -plane, the integrals defined by Eq. (IV.2.12) can be treated in the two-dimensional domain by integrating over the azimuthal angle if the symmetry along z-axis is assumed. From the perspective of the transmission probability, one obtains

$$T = \frac{1}{\pi S} \int_{\vec{\Omega}_A \cdot \vec{n}_A > 0} d\Omega_A (\vec{\Omega}_A \cdot \vec{n}_A) Ki_3(\Sigma_t a) \quad (IV.2.39)$$

where $Ki_n(x)$ is known as the Bickley-Naylor function [78] defined as

$$Ki_n(x) = \int_0^\pi \exp\left(-\frac{x}{\sin \varphi}\right) \sin^{n-1} \varphi d\varphi = \int_1^\infty \frac{\exp(-xt)}{t^n \sqrt{t^2 - 1}} dt \quad (IV.2.40)$$

subject to the following recurrence relations:

$$Ki_0(z) = K_0(z), \quad Ki_1(z) = \int_z^\infty Ki_0(t) dt, \quad \dots, \quad Ki_n(z) = \int_z^\infty Ki_{n-1}(t) dt \quad (IV.2.41)$$

$$nKi_{n+1}(z) = -zKi_n(z) + (n-1)Ki_{n-1}(z) + zKi_{n-2}(z) \quad (IV.2.42)$$

where $K_0(x)$ is the modified Bessel function of zeroth order.

Physically, the quantity $Ki_3(\Sigma_t a)$ signifies the probability for neutrons travelling a distance of a in a uniform region on the xy -plane with constant Σ_t without suffering any collision. One convenient quantity widely used in the collision probability studies is the 'optical' thickness τ , defined as the product of the total macroscopic cross section and the distance within the region in question. In this particular case, $\tau = a\Sigma_t$.

Similarly, the collision probability defined by Eq. (IV.2.7) can be simplified to the following form

$$P_c = 1 - \frac{1}{2\pi V} \int_{\Omega_A} d\Omega_A (\vec{\Omega}_A \cdot \vec{n}_A) \int_0^{\pi/2} d\theta \sin^2 \theta \int_0^a dx \frac{1}{\sin \theta} \exp\left[-\frac{\Sigma_t}{\sin \theta} (a-x)\right] \quad (IV.2.43)$$

By changing the order of integration, one has

$$\begin{aligned}
P_c &= 1 - \frac{1}{2\pi V} \int_{\Omega_A} d\Omega_A (\vec{\Omega}_A \cdot \vec{n}_A) \int_0^a dx Ki_2[\Sigma_t(a-x)] \\
&= 1 - \frac{1}{2\pi V \Sigma_t} \int_{\Omega_A} d\Omega_A (\vec{\Omega}_A \cdot \vec{n}_A) [Ki_3(0) - Ki_3(\Sigma_t a)]
\end{aligned}
\tag{IV.2.44}$$

Physically, the inner integral in the above equation signifies the escape probability along the chord of length a in question in a region of convex geometry.

The same idea can be readily extended to the collision probabilities in a multiple region lattice. One most notable method for the rigorous treatment of such a problem was first proposed by Carlvik [82]. Again, if the symmetry along the z -axis is assumed, the collision probabilities in the xy -plane can be expressed in terms of integrals involving the Bickley-Naylor functions [78]. The only difference is that the non-convex nature of the multi-region lattice must be taken into account. The Carlvik's approach [79] can be best illustrated by the geometric considerations given by Fig. IV.3. Here, the objective is to find the collision probability in an arbitrary region i characterized by macroscopic cross section Σ_{ti} for neutrons initiated from an arbitrary region j with macroscopic total cross section Σ_{tj} . For simplicity, let τ_i , τ_j , and $\tau_{i,j}$ be the optical lengths along a straight line at an angle of α in the polar coordinate system. Analogous to the case of a single region leading to Eq. (IV.2.44), the probability for neutrons starting along line with length a in region j to make the next collision in region i is

Figure IV. 3 Schematic Illustration of Carlvik's Approach

$$\begin{aligned}
P_{i,j}(a, y) &= \frac{1}{a} \int_0^a \{Ki_2[\Sigma_{ij}(a-x) + \tau_{i,j}] - Ki_2[\Sigma_{ij}(a-x) + \tau_{i,j} + \tau_i]\} dx \\
&= \frac{1}{\Sigma_{ij}a} [Ki_3(\tau_{i,j}) - Ki_3(\tau_{i,j} + \tau_j) - Ki_3(\tau_{i,j} + \tau_i) + Ki_3(\tau_{i,j} + \tau_j + \tau_i)]
\end{aligned}
\tag{IV.2.45}$$

where the x - and y -axis are taken to be co-linear and perpendicular to the line a respectively. Thus, the total collision probability P_{ij} can be obtained by multiplying both side of Eq. (IV.2.45) by the volume element $a dy$ and the angular element $d\alpha$ and integrating over the volume of region j . The resulting P_{ij} becomes

$$P_{ij} = \frac{1}{2\pi\Sigma_{ij}V_j} \int d\alpha \int dy [Ki_3(\tau_{i,j}) - Ki_3(\tau_{i,j} + \tau_j) - Ki_3(\tau_{i,j} + \tau_i) + Ki_3(\tau_{i,j} + \tau_j + \tau_i)]
\tag{IV.2.46}$$

The above equation clearly indicates that the quantity $\Sigma_{ij}V_jP_{ij}$ is symmetric with respect to index i and j . Hence, it follows that the reciprocity relation

$$\Sigma_{ij}V_jP_{ij} = \Sigma_{ji}V_iP_{ji}
\tag{IV.2.47}$$

is generally valid even for a complex cell. The practical importance of this reciprocity relation is quite apparent. For a $N \times N$ collision probability matrix, only $N(N+1)/2$ elements require the direct numerical treatment while the remaining elements are obtainable via the above relationship. Thus, the computational efficiencies can be significantly enhanced. Furthermore, it also leads to the 'equivalence' relation of great practical importance to be addressed later.

From Eq. (IV.2.44), it is quite clear that the corresponding diagonal element P_{ii} in conjunction with the coordinates described above is simply

$$P_{ii} = 1 - \frac{1}{2\pi\Sigma_{ii}V_i} \int d\alpha \int dy [Ki_3(0) - Ki_3(\tau_i)]
\tag{IV.2.48}$$

analogous to what one expects for the case of an isolated lump discussed previously. Physically, the differences of the Ki_3 -functions in the integrands of Eq. (IV.2.44) and Eq. (IV.2.48) signify the transmission probabilities along the straight line connecting two points on a given surface.

Numerically, the evaluation of Eq. (IV.2.46) and Eq. (IV.2.48) can be readily accomplished by discretizing the variables y and α as illustrated in Fig. IV.3. By drawing parallel lines with equal spacing Δy at a given value of angle α that intersect both region i and j , the inner integral can be computed once the all the intersections with boundaries are known. The integration over α can be carried out by repeating the same procedure at various angles.

It is important to know that the intra-cell collision probabilities described above implicitly require that the neutron flux vanishes at the outer boundary of the unit cell. The latter is commonly referred to as the 'black' boundary condition. To allow for neutrons passing and/or returning through the outer boundary, a boundary condition is required to account for the inter-cell transport effects. One commonly used boundary condition is the so-called 'white' boundary condition whereby all neutrons going through the outer boundary will return with the angular distribution as if it were from a constant source outside of the boundary. Carlvik [79] introduced a parameter R_j signifying the fraction of neutrons initiated from the region j that will pass through the outer boundary as

$$R_j = \Sigma_{tj} V_j - \sum_i \Sigma_{tj} V_j P_{ij}^{(black)} \quad (IV.2.49)$$

By utilizing the reciprocity relation, the collision probabilities under the 'white' boundary condition can be related to that under the 'black' condition via the following relation

$$\Sigma_{tj} V_j P_{ij}^{(white)} = \Sigma_{tj} V_j P_{ij}^{(black)} + \frac{R_i R_j}{\sum_j R_j} \quad (IV.2.50)$$

according to Carlvik.

Thus, the collision probabilities for a unit cell with symmetry along the z-axis, in principle, can be determined numerically via the technique described above in spite of the potential complexity of the cell. Carlvik's method [79] is conceptually simple and the collision probabilities can be readily reduced to the case of co-axial cylinders such as that defined by Eq. (IV.2.33) if symmetry with respect to α is assumed. For a given α , the most essential requirement is to find the intersections between the equally spaced rays and the surfaces of various regions within the cell. The procedure is obviously tailor-made for the ray-tracing technic pioneered by Zolotukhin and Maiorov [83] for the Monte Carlo method. Such an approach essentially removes the long-standing difficulties attributed to complex geometries. The GTRAN2 code recently developed by Vujic [81,82] has incorporated the ray-tracing features in conjunction with the 2-dimensional collision probability method for treating the reactor lattices with complicated geometries. So far, such a method is still limited to applications at the multigroup level. The possibility of its utilization to the resonance treatment is apparently on horizon in view of our vastly improved computational capability in the past few years.

IV.3 Traditional Collision Probability Method for a Two-Region Cell

So far, the above discussions have been focused on the general features of the collision and transmission probabilities. Discussions henceforth will concentrate on their applications to the slowing-down process and the subsequent of resonance absorption in the heterogeneous media. The simplest case of the collision probability method for treating the neutron transport as well as slowing-down processes defined by Eq. (IV.2.6) is a unit cell consisting of a fuel lump surrounded by a moderator region. One fundamental assumption is that the reactor lattice consists of an infinite number of repeated unit cells of the same kind. The earlier development of resonance theory for reactor lattices was almost exclusively based on such a cell configuration. The simplicity of the geometry provides a great deal of analytical in-sight to the otherwise extremely difficult problem. Therefore, such a classical

case still plays an important role in reactor physics to this day.

Like the case of the homogeneous media, the resonance integral concept to be discussed in this section also reflects the earlier emphasis focused on a well-isolated Breit-Wigner resonance.

IV.3.1 Fundamental Equations

The application of the collision probability method for treating the resonance absorption in a two-region cell embedded in an infinite reactor lattice was pioneered by Chernick. The cell under consideration consists of a fuel region and a moderator region designated by 0 and 1, respectively. If $F_0(u)$ and $F_1(u)$ represent the collision densities in these regions respectively, the fundamental integral transport equation from the perspective of the collision probability method are specified by the following coupled integral equations

$$\begin{aligned} V_0 F_0(u) = & (1 - P_0) \sum_i^{fuel} \frac{1}{1 - \alpha_i} \int_{u-\varepsilon_i}^u e^{-(u-u')} \frac{\Sigma_{si}^{(0)}(u')}{\Sigma_t^{(0)}(u')} V_0 F_0(u') du' \\ & + P_1 \sum_j^{fuel} \frac{1}{1 - \alpha_j} \int_{u-\varepsilon_j}^u e^{-(u-u')} \frac{\Sigma_{sj}^{(1)}(u')}{\Sigma_t^{(1)}(u')} V_1 F_1(u') du' \end{aligned} \quad (IV.3.1)$$

and

$$\begin{aligned} V_1 F_1(u) = & (1 - P_1) \sum_j^{mod} \frac{1}{1 - \alpha_j} \int_{u-\varepsilon_j}^u e^{-(u-u')} \frac{\Sigma_{sj}^{(1)}(u')}{\Sigma_t^{(1)}(u')} V_1 F_1(u') du' \\ & + P_0 \sum_i^{fuel} \frac{1}{1 - \alpha_i} \int_{u-\varepsilon_i}^u e^{-(u-u')} \frac{\Sigma_{si}^{(0)}(u')}{\Sigma_t^{(0)}(u')} V_0 F_0(u') du' \end{aligned} \quad (IV.3.2)$$

where the summations are over nuclides in these regions respectively and

P_0, P_1 are escape probabilities;

V_0, V_1 are volumes; and

$\varepsilon_i, \varepsilon_j$ are maximum lethargy increments per collision respectively.

Physically, these coupled integral equations signify the conservation of neutrons at a given energy mesh. Except for the interaction between two regions, the nature of the slowing-down equation and pertinent parameters resulting from the elastic scattering process remains the same as that defined by Eq. (III.3.1). Here, the escape probabilities serve as vehicles to distinguish the elastic scattering sources within the region in question and those coming from outside. Thus, once the escape (or collision) probabilities as functions of optical thicknesses in the configuration are known, the requirement for the solution of the slowing-down equation is not different from what was described in the previous chapter. The only complication here is that one is dealing with coupled integral equations instead. Numerically, such a process must be repeated at each extremely fine energy mesh required for the subsequent calculations

of resonance integrals. Although it may not be a prohibitive task by current standard, it was certainly insurmountable in the early days. Simplifications of the coupled equations are apparently required before they are deployed for the resonance treatment.

One of the most important properties of the escape probabilities is the reciprocity relation generally defined by Eq. (IV.2.47). For the two-region cell, the quantity P_0 is related to P_1 through the following identity

$$\frac{P_0}{P_1} = \frac{\Sigma_t^{(1)}(u)V_1}{\Sigma_t^{(0)}(u)V} \quad (\text{IV.3.3})$$

so that P_1 can be computed readily once P_0 is known.

Another simplification is plausible by taking advantage of the fact that the moderator cross sections outside of the fuel region usually exhibit weak dependence on energy. It is, therefore, possible to assume the NR-approximation in the moderator. By taking $F_1(u) = \Sigma_t^{(1)}$, the coupled is reduced to the form similar to that for the homogeneous media,

$$V_0 F_0(u) = (1 - P_0) \sum_i^{\text{fuel}} \frac{1}{1 - \alpha_i} \int_{u-\varepsilon_i}^u e^{-(u-u')} \frac{\Sigma_{si}^{(0)}(u')}{\Sigma_t^{(0)}(u')} V_0 F_0(u') du' + P_0 V_0 \Sigma_t^{(0)}(u) \quad (\text{IV.3.4})$$

The above equation shows a great deal of similarity to the corresponding slowing-down equation for the homogeneous medium. The difference is that one must evaluate P_0 as a function of $\Sigma_t^{(0)}(u)$ and the configuration of fuel lump, and the additional source term $P_0 \Sigma_t^{(0)}(u)$. Eq. (IV.3.4) is generally considered as the starting point from which many simplified methods can be derived.

From the perspective of our computational capabilities available today, the numerical solution of the above equation does not present a serious problem especially in conjunction with the use of the hyper-fine group approach described in the previous chapter. However, it was obviously prohibitive in the earlier days without any simplified assumptions on the slowing-down equation specified by Eq. (IV.3.4). Like the treatment of slowing-down equation in the homogeneous media, one approximation that simplifies this equation considerably is the NR-approximation for the diluents in the fuel. Thus, the sum in Eq. (IV.3.4) involves only the heavy nuclides that exhibit extensive resonant behavior. In particular, if the fuel is dominated by one resonance absorber such as U^{238} , Eq. (IV.3.4) becomes [61]

$$F_0(u) = (1 - P_0) \frac{1}{1 - \alpha} \int_{u-\varepsilon}^u e^{-(u-u')} \frac{\Sigma_s^{(r)}(u')}{\Sigma_t^{(0)}(u')} F_0(u') du' + P_0 \Sigma_t^{(r)}(u) + \Sigma_m \quad (\text{IV.3.5})$$

where $\Sigma_t^{(r)}(u)$ and Σ_m are the macroscopic total cross sections of the resonance absorber and diluents respectively. Hence, given values of P_0 , the solution of Eq. (IV.3.5) is no different than that for the simplified slowing-down equation in homogeneous media as defined by Eq. (III.3.1).

IV.3.2 Historical Notes on the Resonance Treatment for an Isolated Lump

The simplest possible two-region cell is the one consisting of an isolated absorber surrounded by moderator of infinite extent. It was the first scenario of the heterogeneous treatment in the presence of a Breit-Wigner resonance examined independently by Wigner et al. [11] and by Gurevich and Pomeranchouk [13] in early days of reactor development. The results deduced from these approximate methods have played an important role in the analysis of the resonance integral measurements. In particular, the dependence of the effective resonance integral as a function of the surface to mass ratio has been used extensively in practical applications. From the perspective of our current resonance theory, it is still of some theoretical interest if we put the fundamental basis of these earlier approximations in the context of our existing knowledge today.

The starting point can be viewed as a special case defined by Eq.IV.3.5 in which either one of the two simplified assumptions are made, namely: (1) the flux of the absorber being determined by the NR-approximation, or alternatively, (2) the NRIM-(or WR-) approximation. In the following discussions, various results based on the NR- and NRIM-approximations will be addressed separately.

(1) NR Approximation

Let $\phi_0(u)$ denote the flux of the absorber. Under the NR-approximation, Eq. (IV.66) for a single absorber nuclide admixed with diluent becomes

$$\Sigma_t^{(0)}(u)\phi_0(u) = (1 - P_0)\Sigma_p^{(0)} + P_0\Sigma_t^{(0)}(u) \quad (\text{IV.3.6})$$

Thus, the corresponding resonance integral can be expressed in terms of two integrals with different physical meaning, i.e.

$$RI = \Sigma_p^{(0)} \int_0^\infty \frac{\sigma_a^{(0)}(u)}{\Sigma_t^{(0)}(u)} du + \int_0^\infty \frac{P_0\sigma_a^{(0)}(u)\Sigma_r^{(0)}}{\Sigma_t^{(0)}(u)} du = I_v + I_s \quad (\text{IV.3.7})$$

where $\Sigma_p^{(0)}$ and $\Sigma_r^{(0)}$ are the total macroscopic potential scattering cross section and total macroscopic resonance cross section respectively. The quantities I_v and I_s are referred to as the ‘volume’ integral and ‘surface’ integral respectively according to Wigner et al. [11]. The substitution of Eq. (IV.2.7) into Eq. (IV.3.7) yields

$$I_s = \frac{S_0}{4V_0} \left\langle \int_0^\infty \frac{\sigma_a^{(0)}\Sigma_r^{(0)}}{[\Sigma_t^{(0)}(u)]^2} [1 - \exp(-\Sigma_t^{(0)}(u)l)] du \right\rangle \quad (\text{IV.3.8})$$

where $\langle \rangle$ denotes the integration over the geometric configuration of the absorber in the context of Eq. (IV.2.7). The volume integral I_v , on the other hand, is no different than that for homogeneous media. Physically, I_v should dominate whenever a weak resonance is considered as the self-shielding effects in energy and space diminish. On the other hand, the second order term I_s can play an important role

when a strong resonance is encountered.

For the computational capability available today, the above equation obviously does not pose any problem and can be determined numerically as a function of traditional resonance integral parameters β_k , θ_k and $\bar{l}$. However, it is not analytically integrable unless some pertinent approximations are introduced. The simplest possible approximation is the direct substitution of the Wigner's rational approximation defined by Eq. (IV.2.11) into Eq. (IV.3.7) whereby the resulting resonance integral becomes

$$(RI)_k = \frac{(\Sigma_p^{(0)} + 1/\bar{l})\Gamma_a}{N_0 \cos(2\phi_l)E_0} J(\beta'_k, \theta_k, a_k) \quad (IV.3.9)$$

where $\beta'_k = (\Sigma_p^{(0)} + 1/\bar{l})/[N_0\sigma_{0k} \cos(2\phi_l)]$ and N_0 is the concentration of the absorber. The expression is identical to that defined for homogeneous media except for the presence of $\bar{l}$ accounting for the heterogeneous nature of the lump. It was the earliest version of the 'equivalence relation' observed by Wigner et al [11], which was later generalized to the closely-packed lattice also as one shall see. If one neglects the temperature dependence and the asymmetric term in the integrand of the J -integral, Eq. (IV.3.9) immediately reduces to a much simpler form from which physical interpretation becomes quite apparent.

$$(RI)_k = \frac{(\Sigma_p^{(0)} + 1/\bar{l})\Gamma_a}{N_0 \cos \phi_l E_0} J(\beta'_k, 0, a_k) = \frac{\pi \Gamma_a \sigma_{0k}}{2 E_0} \sqrt{\frac{\beta'_k}{1 + \beta'_k - a_k^2 / \beta'_k}} \quad (IV.3.10)$$

In the limit of a strong resonance in the low energy region, the above expression can be approximated by

$$(RI)_k \geq \text{const.} \sqrt{\Sigma_p^{(0)} + \frac{S_0}{4V_0}} \propto \sqrt{A + B \frac{S_0}{M}} \propto A' + B' \sqrt{\frac{S_0}{M}} \quad (IV.3.11)$$

Similar results can also be obtained if the Wigner approximation is used in conjunction with Eq. (IV.3.7) in which the volume and the surface integrals are evaluated separately. The above equation provides a simple basis for analyzing the resonance integral measurements and has been widely used for such a purpose. It gives excellent fit to data over a large range of surface to mass ratios. It is interesting to note that the resonance integral would appear to be a linear function of S_0/M if P_0 in Eq. (IV.3.7) were replaced by $1/\bar{l}$, the limiting case for Wigner approximation for a dilute lump. Such a limiting case is also derivable from the above equation via the binomial expansion. Hence, the square root variation is primarily attributed to the resonance-dependent portion of the escape probability.

Similar results were also derived independently by Gourevich and Pomeranchouk [13] from a somewhat different perspective. By assuming that $\Sigma_t^{(0)}(u) \approx \Sigma_a^{(0)}(u)$, they obtain from Eq. (IV.3.6)

$$RI = \frac{1}{N_0 \bar{l}} \int_0^\infty \langle 1 - \exp(\Sigma_a^{(0)}(u)l) \rangle du \quad (\text{IV.3.12})$$

where $\langle \rangle$ denotes the integration over the appropriate geometric parameters of the lump described previously.

According to the rationale of Gourevich and Pomeranchouk [13], resonances can be divided into two general classes, one weak and the other strong. In the limit of small $\Sigma_a^{(0)}(u)l$, it is quite obvious that the above equation will become independent of the heterogeneous nature of the lump as the exponential term in the integrand approaches its linear limit. Of more practical interest is the asymptotic limit under the condition of strong absorption. The derivation of the latter is obviously difficult to derive because of the complicated dependence of the absorption cross section on energy and temperature. However, the analytical expression is obtainable if one neglects the temperature dependence of the absorption cross section. The formal derivation of Eq. (IV.3.12) for the zero temperature case was first presented by Lukyanov [62] and the resulting expression approaches those of Gourevich and Pomeranchouk [13] asymptotically in the limit of strong absorption. In the following discussions, the integral of interest will be cast in the form of the Euler integral which plays an important role in computing the transmission probabilities from mathematical point of view as one shall see in Section IV.4.

The substitution of the Lorentzian form for absorption cross section at zero temperature into Eq. (IV.3.12) yields

$$\begin{aligned} (RI)_k &= \frac{c_1}{N_0 \bar{l}} \langle \int_0^\infty dw \int_0^\infty dx \frac{c_0}{1+x^2} \exp\left(-\frac{c_0 w}{1+x^2}\right) \rangle \\ &= \frac{\text{const.}}{N_0 \bar{l}} \langle \int_0^\infty dw \int_0^1 dv \frac{\exp(-c_0 wv)}{v^{1/2} \sqrt{1-v}} \rangle \end{aligned} \quad (\text{IV.3.13})$$

where $c_0 = \sigma_{0k} \Gamma_{ak} / \Gamma_{tk}$, $c_1 = \Gamma_{tk} / E_0$, and the new variable of integration $v = 1 / (1+x^2)$. The inner integral can be readily identified with the well-known Laplace transform identity of the general form [83]

$$\int_0^{2b} dt e^{-pt} (2bt - t^2)^{\nu-1/2} = \sqrt{\pi} \Gamma(\nu+1/2) \left(\frac{2b}{p}\right)^\nu e^{-bp} I_\nu(bp) \quad (\text{IV.3.14})$$

where $I_\nu(x)$ is the modified Bessel function of an arbitrary order ν . The above integral is one type of Euler integral that one often encounters in treating the transmission probabilities. By substituting Eq. (IV.3.14) and the following integral identity for the modified Bessel functions [84]

$$\int_0^z dt e^{\pm t} t^\nu I_\nu(t) = \frac{e^{\pm z} z^{\nu+1}}{2\nu+1} [I_\nu(z) + I_{\nu+1}(z)] \quad (\text{IV.3.15})$$

into Eq. (IV.3.13), one obtains

$$(RI)_k = \frac{c_1 \pi}{N_0 l} < \frac{c_0 l}{2} e^{-c_0 l / 2} [I_0(c_0 l / 2) + I_1(c_0 l / 2)] > \quad (IV.3.16)$$

In the limit of a strong resonance, the modified function asymptotically approaches the well-known limit, i.e., $I_\nu(x) \approx e^{-x} / \sqrt{2\pi x}$. Hence, the corresponding resonance integral becomes

$$\lim_{\Sigma_a^{(0)} l \rightarrow \infty} (RI)_k = \frac{const. < l^{1/2} >}{\sqrt{l}} \frac{1}{l^{1/2}} \quad (IV.3.17)$$

where the ratio $< l^{1/2} > / \bar{l}^{1/2}$ is characteristic of the geometric configuration of the lump. For instance, it is equal to 0.983, 0.975 and 0.945 for sphere, slab and cylindrical rod respectively. Thus, the superimposition of a group consisting of both strong as well as weak resonances leads to the same S_0 / M dependence specified by Eq. (IV.3.11).

The inclusion of the Doppler-broadening will undoubtedly complicate the problem. By and large, its influence is likely to be more significant on the strongly absorbing resonances than those weak ones. Hence, the general behavior of resonance integral as a function of the surface to mass ratio is not expected to change dramatically. A simple scheme for parameterization purposes widely used in analysis of the measurements is assumed to have the following form

$$(RI)_k = A + B \sqrt{\frac{S_0}{M}} \left[1 + \alpha \left(\sqrt{\frac{T}{T_0}} - 1 \right) \right] \quad (IV.3.18)$$

where T_0 is taken to be the room temperature. Various values of these parameters were recommended by Hellstrand⁵¹ via the fitting of the experimental results for both uranium metal and oxide within finite range of practical interest. For our purpose here, the conceptual aspects discussed above should suffice.

(2) NRIM (or WR) Approximation

In contrast to the NR-approximation, the flux under the NRIM-(or WR-) approximation in the same context described in Chapter III must assume the following form

$$\Sigma_t^{(0)}(u) \phi_0(u) = (1 - P_0) [\Sigma_s^{(0)}(u) - \Sigma_m^{(0)}] \phi_0(u) + P_0 [\Sigma_t^{(0)}(u) - \Sigma_m^{(0)}] + \Sigma_m^{(0)} \quad (IV.3.19)$$

so that the corresponding resonance integral becomes

$$(RI)_k \approx \Sigma_m^{(0)} \int_0^\infty \frac{\sigma_a(u)}{\Sigma_a^{(0)}(u) + \Sigma_m^{(0)}} du + N_0 \int_0^\infty \frac{P_0 [\sigma_a(u)]^2}{\Sigma_a^{(0)}(u) + \Sigma_m^{(0)}} du \quad (IV.3.20)$$

in lieu of scattering contributions from the absorber, where $\Sigma_m^{(0)}$ is the macroscopic cross section of the diluents. Similar to the NR-approximation, the above equation also encompasses a volume integral and a surface integral. In absence of diluents, the resonance integral based on Eq. (IV.3.19) assumes the form originally derived by Wigner et al [11,60]

$$(RI)_k = \int_0^\infty \frac{P_0 \sigma_a(u) \Sigma_t^{(0)}(u)}{\Sigma_t^{(0)}(u) - (1 - P_0) \Sigma_s^{(0)}(u)} du \quad (IV.3.21)$$

where the volume integral drops out. The above surface integrals are generally difficult to evaluate as described in the foregoing discussions. Again, if the Wigner's approximation [11] is used, the above integral reduces to the identical form as Eq. (IV.3.9)

$$(RI)_k = \frac{(\Sigma_m^{(0)} + 1/\bar{l}) \Gamma_t}{N_0 E_0} J(\beta'_k, \theta_k) \quad (IV.3.22)$$

except that β_k must be redefined as

$$\beta'_k = \frac{\Sigma_m^{(0)} + 1/\bar{l}}{N_0 \sigma_{0k}} \quad (IV.3.23)$$

and the asymmetric term no longer present in the J -integral because the diluents with macroscopic cross section $\Sigma_m^{(0)}$ is solely responsible for the elastic scattering process in the lump. Thus, it follows that, analogous to the case of the NR-approximation, the resonance integral at zero temperature assumes the form of Eq. (IV.3.10) except that $\Sigma_p^{(0)}$ is replaced by $\Sigma_m^{(0)}$. The qualitative nature remains unchanged, i.e.

$$(RI)_k = \frac{\pi}{2} \frac{\Gamma_a \sigma_{0k}}{E_0} \sqrt{\frac{\beta'_k}{1 + \beta'_k}} \quad (IV.3.24)$$

The above discussions provide an overview of the earlier work with the emphasis on the qualitative nature of the resonance integral pertinent to interpretation of the measurements. In the following sections, our attention will focus on the treatment of resonance absorption in realistic reactor lattices.

IV.3.3 Nordheim's Method for Treating Resonance Absorption in a Two-Region Cell

The treatment of resonance absorption became the center of attention in reactor physics communities around the globe when the commercial power development reached its peak in the early 1960s. Although many methods for treating Eq. (IV.3.5) and the corresponding resonance integrals to various degrees of sophistication were developed, very few nevertheless, were based on the direct numerical approach without further assumptions. One notable numerical method for solving such an equation and for computing the resonance integral subsequently was first developed by Nordheim and Kuncir [29].

The method was by far the most rigorous means for solving such a problem at that time. It encompasses the successive solution of the integral equation starting with the asymptotic flux above the resonance via the Simpson's rule coupled with the flux recovery assumption for an isolated resonance described in the previous chapter and the use of the escape probability P_0^* defined by Eq. (IV.2.22). A priori based on the flux recovery assumption valid only for an isolated resonance reflects the fundamental difference between this method and the continuous energy approach to be described in Section IV.2.29. For an isolated resonance, the only significant assumption of this method is the flux recovery that leads to the 'tail' corrections defined by Eq. (III.3.25). One unique feature of Nordheim's method worth noting is that the quantity P_0^* is expressed in terms of two decoupled quantities $P_0^{(iso)}$ and C in the context given by Eq. (IV.2.22). The decoupling of these quantities makes possible the separate treatment of them with individualized degrees of sophistication. For most of the fuel configurations of practical interest, the former is usually representable as a function of τ_0 in a closed analytical form, as compiled by Case et al [10]. Mathematical derivations of the commonly used escape probabilities for the isolated lumps will be presented in Section IV.5.2 from a somewhat different perspective. On the other hand, the latter, as generally defined by Eq. (IV.2.20) in accordance with the 'black' limit, is much less troublesome because the macroscopic total cross section of the moderator is usually insensitive to energy. Thus, one computation of C for a given reactor lattice may suffice for many cases of interest. In fact, the Dancoff factor was taken to be a user's input quantity in the original code developed by Nordheim and Kuncir [29]. The fact that the Dancoff correction can be treated separately independent of the resonance structures of the fuel provides great flexibility. Aside from the Carlvik's method [79] described earlier, a great deal of work on this subject can be found in the literature. In light of the significant advances in our computing capabilities, the Monte Carlo approach can also be used for this purpose as one shall see. For our purpose here, we shall focus on few simple cases that can shed some analytical insight to its role in resonance absorption.

The availability of the more efficient treatment of the slowing-down equation on the basis of the continuous energy hyper-fine group approach developed by Kier [71], as described in Chapter III, in effect eliminates the needs for all assumptions inherently required in Nordheim's method [29]. Given the escape probability, the rigorous treatment of Eq. (IV.3.4) and the subsequent treatment of the effective resonance cross sections are no longer prohibitive as one shall see in Section IV.4.

IV.3.4 Equivalence Relation and Rational Approximations

One of the most interesting developments in the earlier days of reactor physics is the equivalence relation between the slowing-down equation in a heterogeneous lattice consisting of two-region cells and that for an infinite homogeneous medium. Such a relation was first observed by Wigner [11] when the escape probability in Eq. (IV.3.5) was replaced by the rational approximation given by Eq. (IV.2.11). Because of its practical implications, this subject has been studied exhaustively by many reactor physicists in the attempt to improve the accuracy of the rational approximation more suitable for configurations of practical interest. In the following discussions, the subjects of equivalence relation and of rational approximations will be addressed separately.

(1) Equivalence Relation

With no loss of generality, let the one-term rational approximation be represented by a generic form

$$P_0 = \frac{\Sigma_e}{\Sigma_e + \Sigma_t^{(r)}(u)} \quad (\text{IV.3.25})$$

where Σ_e , usually referred as the ‘escape’ cross section, is independent of $\Sigma_t^{(r)}(u)$ and can be identified with $1/\bar{l}$ if the Wigner approximation for an isolated lump is used. The substitution of Eq. (IV.3.25) into Eq. (IV.3.4) gives

$$F^{(eq)}(u) = \frac{1}{1-\alpha} \int_{u-\varepsilon}^u e^{-(u-u')} \frac{\Sigma_s^{(r)}(u')}{\Sigma_e + \Sigma_t^{(r)}(u')} F^{(eq)}(u') du' + \Sigma_m^{(eq)} \quad (\text{IV.3.26})$$

where

$$F_0^{(eq)}(u) = [\Sigma_e + \Sigma_t^{(0)}(u)]\phi(u) \quad (\text{IV.3.27})$$

and $\Sigma_m^{(eq)} = \Sigma_e + \Sigma_m$ can be viewed as the ‘equivalent’ background cross section for all diluents.

Eq. (IV.3.26) exhibits the identical form as the slowing-down equation for homogeneous media defined by Eq. (III.3.1). Hence, all numerical as well as analytical approximations for treating such an equation and the subsequent resonance integrals described in Chapter III are equally applicable to the equivalent equation above simply by redefining the total macroscopic cross section of the fuel or moderator. If the NR-approximation for the diluents is assumed, as is in Nordheim's approach [29], Eq. (IV.3.26) will reduce to the same form given by Eq. (III.3.1). The benefits of the equivalence relation are quite evident both on theoretical as well as practical grounds. The reliability of the results based on the above equation is, of course, dependent on the accuracy of the rational approximation used.

(2) Rational Approximations for Practical Applications

Rational approximations currently in use can be divided into two general classes, namely, one-term rational approximation and multiple-term rational approximation. The former represents the traditional form defined by Eq. (IV.3.25) used strictly within the context of the equivalence relation described above. One obvious physical constraint is that Σ_e must be positive to be meaningful. The latter, on the other hand, can be generally regarded as a Pade approximation of the collision and/or escape probabilities for a given reactor lattice. Unlike the former, strictly speaking, the higher order rational functions generally do not lead to the equivalence relation defined by Eq. (IV.3.26), although it is potentially far more accurate for obvious reasons. In this section, we shall focus on the one-term approximation while the multiple-term approximations will be addressed separately in Section IV.3.6.

The simplest possible rational approximation is Wigner's, defined by Eq. (IV.2.11) intended for the isolated fuel lumps. Although this expression reproduces the expected values in the limits of both small and large optical thickness of the fuel lump, inaccuracies do occur with intermediate ones. Another potential shortcoming of this approach is that it does not account for the Dancoff effect due to neighboring absorbers. These issues can be greatly alleviated via pertinent remedies discussed in order as follows.

The Nordheim approximation [29,61] given by Eq. (IV.2.22) provides a good starting point. By substituting Eq. (IV.3.25) into Eq. (IV.2.22), one obtains

$$P_0^* = \frac{(S_0 / 4V_0)(1-C)}{\Sigma_t^{(0)} + (S_0 / 4V_0)(1-C)} \quad (\text{IV.3.28})$$

Thus, the above equation leads to a simple physical interpretation that the Dancoff effect is effectively equivalent to the reduction of the surface area of an absorber as if it were isolated. This simple model is conceptually useful but the accuracy of the Wigner approximation is still at issue.

One way to improve the Wigner's approximation was proposed by Levine [50] -- the introduction of an additional parameter a , so that it assumes a slightly modified form

$$P_0^{(iso)} = \frac{a / \bar{l}}{a / \bar{l} + \Sigma_t^{(0)}} \quad (\text{IV.3.29})$$

Strictly speaking, a , sometimes referred to as the Bell-Levine factor [25,50], must be a function of the total cross section as well as the geometric configuration of the isolated lump. Clearly, the approximation is no longer useful within the context of the equivalence relation if this multivariate dependence is maintained. For this reason, the assignment of constant values of 1.35 and 1.1 to pin and plate geometries respectively appears to be satisfactory, as deduced from the trial and error method [50]. The issue was further examined by Otter [85]. It was suggested that a mean value a be defined for each resonance by, in effect, integrating over the resonance by breaking it into several intervals, in each of which Eq. (IV.3.29) is applied with appropriate constant value of parameters. However, it was found that such an exercise is not necessary because Levine's assumption [50] of a constant value for a given configuration actually gave good results even when applied to all resonances. An alternative for determining a pursued more recently was via a least-squared fitting of a set of $P_0^{(iso)}$ values for the configuration in question based on representative values of total cross sections between the maximum peak value and the minimum value of the absorber [86]. In any case, the heuristic nature of this parameter a reflects the inherent inadequacy of the one-term rational approximation when used to simulate the otherwise very complicated function.

Thus, by substituting Eq. (IV.3.29) into Eq. (IV.2.22) and equating the result to the generic form given by Eq. (IV.3.25), one obtains [87]

$$\Sigma_e = \frac{1}{\bar{l}} \frac{a(1-C)}{1+(a-1)C} \quad (\text{IV.3.30})$$

The above equation can be considered as a generic form for the 'escape' cross section for the one-term rational approximation, allowing for corrections for the Wigner approximation as well as the Dancoff effect. The quantities a and C are considered as input parameters in many production codes for flexibility [75]. For many practical applications, the Dancoff factor can also be cast into simple rational form analogous to that of the escape probability if one does not wish to use the rigorous treatment. In analogy to Eq. (IV.3.29), the simplest possible form is

$$\gamma_B = 1 - C = \frac{\bar{l} \Sigma_t^{(1)}}{1 + \bar{l} \Sigma_t^{(1)}} \quad (\text{IV.3.31})$$

as given by Bell [25]. However, extensive studies by Leslie et al [45] and also by Pennington [88,89] have shown that the above equation can significantly underestimate the value of $1 - C$, especially in the range of $\bar{l} \Sigma_t^{(1)} \approx 2$ to 3. Hummel et al [87] have found that the accuracy of Eq. (IV.3.30) can be significantly enhanced by the following modification:

$$1 - C \approx \gamma_B + \gamma_B^4 (1 - \gamma_B) \quad (\text{IV.3.32})$$

The above approximation was found to yield a much more satisfactory fit to the Monte Carlo results given by Leslie et al [45] and to the results of Pennington [88,89] based on deterministic method.

The procedure of finding Σ_e can also be viewed as a means of parameterization given the knowledge of the escape probability. Any viable value of Σ_e must approximately satisfy the following equation under the NR-approximation, i.e.,

$$\phi(u) = (1 - P_0) \frac{\Sigma_p^{(0)}}{\Sigma_t^{(0)}} + P_0 \approx \frac{\Sigma_e + \Sigma_p}{\Sigma_e + \Sigma_t^{(0)}} \quad (\text{IV.3.33})$$

Given the geometric configuration and composition of a lattice, the direct computation of the flux or P_0 for a range of $\Sigma_t^{(0)}(u)$ values of interest via either Monte Carlo or deterministic methods no longer presents a serious problem in view of today's computational capabilities. In this context, Σ_e can also be considered as a fitted parameter for a particular cell of interest.

From the above discussions, it is quite apparent the equivalence relation makes possible the unified treatment of resonance absorption in both homogeneous and heterogeneous media. It is particularly so when applied in conjunction to the resonance integral calculations and the Bondarenko type of approach [90].

IV.3.5 Equivalence Relation Based Resonance Integrals for Two-Region Cells

The equivalence relation in the context of Eq. (IV.3.26) has provided the basis for a wide range of applications to various degrees of sophistication just like the case of the homogeneous media described in the previous chapter. The accuracy of the resonance integrals in this case depend on the rigor by which the slowing-down equation and the escape probability P_0 are treated.

(1) Direct Numerical Approaches

Since the 'equivalent' slowing-down equation is no different from that for the homogeneous media, all direct numerical methods described in Chapter III are readily applicable. The equivalence relation, in

effect, eliminates the difficulties usually associated with the computation of the collision probabilities and makes the direct numerical approach more attractive than before. For computation of resonance integral in conjunction with an isolated integral, Nordheim's method [29] is clearly amenable to the homogeneous-like equation. For the continuous energy approach over a large energy interval with many resonances present, the method such as that proposed by Kier [71] is obviously preferred as the means of computing the effective resonance cross sections. One special feature of the equivalence-relation based approaches of particular practical interest is that the resulting resonance integrals and effective cross sections at a given temperature are again a function of a simple parameter, namely, $\sigma_p = (\Sigma_p + \Sigma_e)$ in unit of barns per atom of the absorber. Thus, the widely used Bondarenko scheme [90] is also applicable to all equivalence-relation-based results. For example, the SHIELD code [91] based on the rigorous solution of Eq. (IV.3.26) was developed just for this purpose.

(2) The WR-, NR- and IR-Approximations

The 'equivalence' equation defined by Eq. (IV.3.26) obviously leads to three widely used approximations described in the previous chapter. In the same context as the slowing-down equation for the infinite homogeneous media, the approximate fluxes become:

(1) NR-Approximation

$$\phi(u) = \frac{\Sigma_p^{(eq)}}{\Sigma_p^{(eq)} + \Sigma_t(u)}, \quad \Sigma_p^{(eq)} = \Sigma_p + \Sigma_e \quad (\text{IV.3.34})$$

(2) NRIM-approximation (or WR-)

$$\phi(u) = \frac{\Sigma_m^{(eq)}}{\Sigma_m^{(eq)} + \Sigma_a(u)}, \quad \Sigma_m^{(eq)} = \Sigma_m + \Sigma_e \quad (\text{IV.3.35})$$

(3) IR-Approximation

$$\phi(u) = \frac{\Sigma_m^{(eq)} + \lambda \Sigma_p^{(r)}}{\Sigma_m^{(eq)} + \Sigma_a^{(r)}(u) + \lambda \Sigma_s^{(r)}(u)}, \quad \Sigma_m^{(eq)} = \Sigma_m + \Sigma_e$$

analogous to the original derivation by Goldstein and Cohen [95] intended for the homogeneous media which was later extended to the heterogeneous media by Sehgal and Goldstein [96]. Alternatively, if the NR-approximation for the diluents is not assumed, one obtains

$$\phi(u) = \frac{\Sigma_p^{(eq)}}{\Sigma_p^{(eq)} + \Sigma_a(u) + \eta_r \Sigma_{sr}(u)}, \quad \Sigma_p^{(eq)} = \Sigma_e + \sum_i \eta_i \Sigma_{pi} \quad (\text{IV.3.36})$$

analogous to the expression by Ishiguru [94] and Lukyanov [62] intended for the homogeneous media, where $\Sigma_{sr}(u)$ is the macroscopic resonance scattering cross section for the absorber.

The only difference between the above equations and those defined in Chapter III for the homogeneous media under the same assumptions is that Σ_p (or Σ_m) is now replaced by $\Sigma_p^{(eq)}$ (or $\Sigma_m^{(eq)}$) where appropriate. Thus, for a Breit-Wigner resonance, the resulting resonance integrals exhibit precisely the same form as the traditional expression in terms of $J_k(\theta_k, \beta'_k, a_k)$ defined by Eq. (III.3.5) or $K_k(h'_k, \theta_k, l'_k)$ defined by Eq. (III.3.6) as if they were for the homogeneous media. Here, all the primed parameters are based on the 'equivalent' cross sections according to the approximation used. Similarly, the same principle is applicable in conjunction with the generalized J_k^* -integral [95] including the overlap effects from the neighboring resonances as long as the resonance cross sections are representable by the linear combination of the Breit-Wigner like terms as discussed in the previous chapter. The latter is usually used along with the NR-approximation for fast reactor applications where the overlap effect can play an important role. It is quite apparent that the equivalence relation is tailor-made for the Bondarenko scheme widely used in routine reactor applications. The self-shielding factors at a given temperature can be pre-calculated and tabulated as a function of $\Sigma_p^{(eq)}$ prior to their deployment. A priori for these approximations is, of course, contingent upon the validity of Eq. (IV.3.25) in which Σ_e must be independent of the resonance in question, as outlined in the previous section.

IV.3.6 Multiple-Term Rational Approximations

The inherent limitation of the one-term rational approximation defined by Eq. (IV.3.25) should be recognized. It is quite obvious that the astounding result dramatized by the equivalence relation could not have been accomplished without some degrees of compromise in rigor. One way to improve the approximation is to use a generalized rational function, commonly referred to as the Pade approximation in numerical analysis, in place of Eq. (IV.3.25). From the point of view of parameterization, accuracy can obviously be enhanced if a higher order rational approximation for P_0 is used. The reason is that the presence of more parameters provides more 'degrees of freedom' for the approximation. A rational function of arbitrary order subject to certain physical constraints can be expressed as a linear combination of terms similar to that given by Eq. (IV.3.25). With no loss of generality, the collision probability can be approximated by

$$1 - P_0 \approx \Sigma_t^{(0)} r_n(\Sigma_t^{(0)}) \quad (IV.3.37)$$

where $r_n(x)$ is a rational function specified by the ratio of a polynomial of x of order $n-1$ to that of order n . The generalized rational approximation above still exhibits the same characteristics of Eq. (IV.3.25) under the 'white' and 'black' limits. It follows, from Eq. (IV.3.4), that

$$\phi_0(u) = r_n(\Sigma_t^{(0)}(u)) \sum_i^{fuel} \frac{1}{1 - \alpha_i} \int_{u-\epsilon_i}^u e^{-(u-u')} \frac{\Sigma_{si}^{(0)}(u')}{\Sigma_t^{(0)}(u')} F_0(u') du' + [1 - \Sigma_t^{(0)}(u) r_n(\Sigma_t^{(0)}(u))] \quad (IV.3.38)$$

The above equation clearly does not lead to the traditional equivalence relation defined by Eq. (IV.3.26) unless $n=1$. Thus, the trade-off here is that one must deal with a somewhat more complicated slowing-down equation. Like the case of one-term approximation, the parameterization via the higher order rational function is system-dependent. In view of the availability of many deterministic as well as

Monte Carlo tools for computing the collision probabilities today, the procedure is in principle no different than the usual Pade approximation for a reasonably well-behaved function.

Although Eq. (IV.3.38) no longer exhibits the equivalence relation specified by Eq. (IV.3.26), it, nevertheless, still retains certain attributes of the latter that are essential to the numerical as well as analytical approximations. Numerically, methods for treating the resonance absorption in the homogeneous media are still applicable here with some minor modifications. Analytically, the above equation is equally susceptible to approximations based on the characteristics of resonances in question provided that the rational function is subject to certain constraints. In particular, the roots of the polynomial in the denominator of the rational function must be single-valued and real but negative so that the escape probability, upon partial fraction, is expressible as a linear combination of terms having the same general features of Eq. (IV.3.25). These requirements are obviously important when the traditional NR-, NRIM- and IR-approximations are applied to Eq. (IV.3.38). They are the necessary conditions to ensure that the subsequent resonance integrals are still representable via the well-known J -integrals or K -integrals described in Chapter III.

The fact that the resulting resonance integrals retain the same traditional forms makes the multiple-term rational approximations attractive when applied to the three widely used approximations. The trade-off here is that it requires the evaluation of at least n traditional J -integrals for each resonance considered. For this reason, the rational function seldom exceeds $n = 2$. For instance, a two-term rational approximation based on the IR-approximation of Eq. (IV.3.38) was developed by Ishiguro and Takano [96] in the late 1960s. More recently, the method was further examined by Chen and Gelbard [97] utilizing the NR-flux computed by the Monte Carlo method which is much less inhibited by the geometric complexity of the lattice. For illustrative purposes here, the general features of the latter which provide some analytical insights to the higher order scheme will be presented as follows.

The NR-flux defined by Eq. IV.3.6 can be rearranged into the following form [86,97]:

$$\phi(u) = \frac{\Sigma_p}{\Sigma_t^{(0)}(u)} + \left(1 - \frac{\Sigma_p}{\Sigma_t^{(0)}(u)} \right) P_0 \quad (\text{IV.3.39})$$

where P_0 in the context of the NR-approximation can also be physically identified as the flux attributed to the source outside of the fuel region. In the method of Chen and Gelbard, P_0 is taken to be of the form

$$P_0 = \frac{(a + C_1 C_2 C_3 x)}{(C_1 + C_1 C_3 x)(1 + C_2 C_3 x)} \quad (\text{IV.3.40})$$

where $x = \bar{l} \Sigma_t(u)$. Here, a , C_1 , C_2 , and C_3 are fitting parameters subject to the following criteria: (a) They must be real and positive; (b) $C_1 \neq C_2$; substantial difference is preferred.

Within the constraint of these criteria, it is necessary to use four parameters to fit three flux values corresponding to three pre-determined $\Sigma_t^{(0)}(u)$ values. In Ref. 100, an iterative strategy was developed

for solving three equations of P_0 determined by the Monte Carlo calculation at the chosen values of $\Sigma_t^{(0)}(u)$. The accuracy of the flux (or P_0) as a function of $\Sigma_t^{(0)}(u)$ as defined by Eq. (IV.3.40) was found to be sensitive to the choice of $\Sigma_t^{(0)}(u)$'s for the fitted parameters. One effective strategy proposed was to set $\Sigma_t^{(0)}(u_1)$ close to Σ_p value and $\Sigma_t^{(0)}(u_3)$ close to the maximum possible value of the peak resonance cross section while determining $\Sigma_t^{(0)}(u_2)$ as reported.

For resonance integral calculations based on the NR-approximation, it is necessary to cast Eq. (IV.3.40) into a more convenient form. By partial fraction, it can be shown readily that

$$\phi(u) = \frac{a_1}{b_1 + \Sigma_t(u)} + \frac{a_2}{b_2 + \Sigma_t(u)} + \frac{(1-a)\Sigma_p}{\Sigma_t(u)} \quad (\text{IV.3.41})$$

where

$$b_1 = \frac{1}{C_1 C_3 \bar{l}} \quad (\text{IV.3.42})$$

$$b_2 = \frac{1}{C_2 C_3 \bar{l}} \quad (\text{IV.3.43})$$

$$a_1 = \frac{1}{b_1} \left[\left(\frac{C_1 a - C_1 C_2}{C_1 - C_2} \right) (1 + C_3 \Sigma_p \bar{l} C_1) \right] \quad (\text{IV.3.44})$$

$$a_2 = \frac{1}{b_2} \left[\left(\frac{C_1 C_2 - a C_2}{C_1 - C_2} \right) (1 + C_3 \Sigma_p \bar{l} C_2) \right] \quad (\text{IV.3.45})$$

Thus, the trade-off here is that evaluation of three integrals is required when Eq. (IV.3.41) is applied to the resonance integral calculations. On the other hand, a noticeable improvement over the one-term rational approximation can be achieved. Typically, the relative errors in resonance integrals are of the order of 1% or better as reported in Ref. 89 if the NR-approximation is used.

IV.4 Recent Collision Probability Methods for a Multiple-Region Cell with Many Resonant Isotopes

The treatment of resonance absorption in a multiple-region cell consisting of more than one resonant isotope, whether physically separated or otherwise, is apparently beyond the reach of various approximate methods described in the previous section if one wishes to preserve the rigor. The only alternative is the direct numerical approach. The purpose of this section is to present an overview of a few of the most advanced methodologies currently available for routine reactor applications.

The requirement of extremely fine energy mesh points in solving the slowing-down equations and in computing the accompanying collision probabilities defined by Eq. (IV.1.6) has always been considered as the major roadblock that can hinder the rigorous resonance treatment in a complex cell. As discussed in Chapter III, the availability of the hyper-fine group method [71,75] along with the power of modern computing facilities has, to a great extent, alleviated the difficulties associated with the numerical solutions in the presence of many resonant isotopes. However, the application of this method along with the multi-dimensional collision probability treatment remains prohibitive to this day.

For our purpose, discussions will focus on the collision probability method in association with the hyper-fine group approach for treating resonance absorption in a one dimensional cell with many regions. Such a problem can also be treated by the interface-current method to be described in the next section.

IV.4.1 Discretized Slowing-Down Equation for a Multi-Region Cell

The application of collision probability method in conjunction with the continuous energy hyper-fine group approach requires the discretization of Eq. (IV.1.6) in the lethargy domain and the specification of the collision probability matrix for a cell in question. The former can be accomplished by utilizing the discretized slow-down equation given by Eq. (III.4.8) while the latter depends on the cell configuration in question. The fundamental equation for the collision probability approach defined by Eq. (IV.1.6) must be modified when applied in the context of the ‘hyper-fine’ group scheme described in Chapter III. Because of the finite width associated with the group, a self-scattering term [71,72,75] is, in principle, always present in the discretized slowing-down equation as specified by Eq. (III.4.8). The term vanishes if and only if the width becomes infinitesimally small. Hence, by applying the same logic of Eq. (III.4.8) to Eq. (IV.1.6), one obtains, in matrix notation [75],

$$C^{(k)} = \frac{P^{(k)} S_k^{(in)}}{1 - P^{(k)} r_k} \quad (IV.4.1)$$

where $C^{(k)}$ is a vector denoting the collision rate evaluated at a given hyper-fine group k with its element in a spatial region i specified by

$$C_i^{(k)} = V_i F_i^{(k)} \quad (IV.4.2)$$

and $P^{(k)}$ is $N \times N$ collision probability matrix at the k -th hyper-fine group for a cell with N regions and r_k is a diagonal matrix with its elements defined by Eq. (III.4.7) signifying the contribution resulting from the self-scattering with the k -th hyper-fine group. It should be noted that in principle, the source term should also include those groups attributed to inelastic scattering, fission and others [75]. For our purpose here, the dominant elastic scattering source should suffice.

Thus, given the collision probability matrix, the solution of Eq. (IV.4.1) requires the inversion of a $N \times N$ matrix for each hyper-fine group, which can be costly. On the other hand, the need for inversion can be avoided if one chooses an extremely small hyper-fine group width so that r_k vanishes.

IV.4.2 Collision Probabilities for Practical Geometries

Because the solution of Eq. (IV.4.1) must be carried out at each hyper-fine group over an exceedingly large energy range dictated by our ever-increasing resolved resonance data, the complexity associated with the evaluation of collision probabilities can make such a procedure impractical. Therefore, the multiple-region cells considered in the rigorous resonance treatment are still limited to three commonly used configurations at this point in time, namely, infinite slabs, cylindricized two-region cell and cell with multiple annuli. While the explicit derivations of collision probabilities for these geometries have already been presented in Section IV.2 and further discussions will be given in the next section devoted to the interface-current method, some practical considerations pertinent to their applications are summarized as follows.

The practical applications of the collision probability method to a highly heterogeneous cell can be best illustrated by its extensive usage in the analysis of the measurements in various fast critical assemblies [64-70]. For the ZPR and ZPPR assemblies, a typical drawer encompasses two fuel plates sandwiched between plates of stainless steel and sodium. The collision probabilities for infinite slabs given in Section IV.2.3 are tailor-made for such applications. In fact, the efficient quadrature for computing these quantities defined in Eq. (IV.2.38) by Olson [72] was motivated by the need of the rigorous hyper-fine group approach outlined in the foregoing section. The case of infinite slabs is probably the simplest possible scenario in which the quantities in question are representable in terms of a simple expression that is relatively easy to evaluate. The hyper-fine group approach for infinite slabs has since been incorporated into the RABANL option of the MC²-2 code [75] for routine applications.

The collision probabilities for a cylindricized two-region cell bear a great deal of resemblance to cells with infinite slabs as discussed in Section IV.2.2. The difference is that one either has to evaluate the double integral or an infinite sum involving single integrals of the Bickley-Naylor function [78] of the order 3. It is clearly more difficult to evaluate than that for the infinite slabs.

The collision probabilities for a cell with multiple annuli can be considered as a limiting case of those described by Carlvik [79] for the two dimensional domain. It is equivalent to the case in which the symmetry with respect to the angle α in Eq. (IV.2.46) is assumed. Thus, Eq. (IV.2.46) can be expressed explicitly in terms of a sum of single integrals of Bickley-Naylor function of the order 3, also similar to the case of multiple slabs. Each element of the collision probability matrix requires the evaluation of M integrals of that type where M is the total number of surfaces traversed by a neutron trajectory between region j to region i . It is not difficult to see that the hyper-fine group scheme defined by Eq. (IV.4.1) can become prohibitive if the total number of regions is large.

The practical difficulties for applying the collision probability method in the context of hyper-fine group treatment beyond the case of infinite slabs provide the strong motivation to seek other alternatives. One of the most attractive alternatives is the use of the interface-current method in which the problem related to the computational efficiencies can be alleviated significantly at a reasonable sacrifice in rigor as one shall see.

IV.5 Interface-Current Method for a Multi-Region Cell With Many Resonant Isotopes

As discussed in Section IV.1.2, one attractive alternative is the use of the interface current method. The main advantage of this method is the relative ease by which the pertinent probabilities are evaluated. In

contrast to the collision probability approach where the evaluation of any P_{ij} may require the integration over several regions as clearly indicated by the Carlvik's method [79], the inter-face current method usually only requires the knowledge of the escape probabilities of each individual region and the transmission probabilities between surfaces of a region in question. The intra-cell transfer is accounted for via the boundary condition defined by Eq. (IV.1.9). This is, of course, accomplished at the expense of the assumption that the neutron current must be isotropic (or cosine current assumption) at the boundaries. The method is particularly effective for a convex region with two surfaces, i.e., $N = 1$ and $M = 2$ in the context of Eq. (IV.1.8). The fact that the evaluation of various probabilities for an isolated region is far simpler than those where the neutron path can cross into many regions clearly simplifies the numerical problems involved.

One of the most useful unit cell configurations of practical interest is the case of an infinite cylinder discretized into tubular regions. In the polar coordinate system in the two-dimensional domain, it consists of an ensemble of annuli signifying the spatial regions to be examined. The unit cell of circular symmetry is usually referred to as the Wigner-Seitz cell [98]. It is presumably analogous to the Wigner-Seitz approximation in band theory of solid in which the potential is taken to be spherically symmetric throughout all polyhedron surfaces surrounding an atom. In the same context, a uniform current at each surface of the annular region is also assumed. An annular segment can be considered as the most generic configuration in reactor physics applications because of its unique properties. In the limit when both inner and outer radii approach infinity, it becomes a plate. On the other hand, it becomes a pin when the inner radius vanishes. Thus, to specify the neutron transport properties in an annulus amounts to the specification of those in all three configurations most commonly encountered in lattice physics calculations. In the following discussions, we will focus on the unit cell consisting of multiple annuli pioneered by Kier and Robba [71].

IV.5.1 Neutron Transport in a Generic Unit Cell

Let r_i and r_{i-1} be the outer and inner radius of an annulus designated by i . From the perspective of the interface current approach, the specification of the neutronic balance requires the knowledge of the following quantities using the notation of Kier and Robba [71]:

J_i^+ and J_i^- – the neutron current impinging on the inner surface of the annulus $i+1$ (in the increasing radial direction) and the outer surface of the annulus i (in the decreasing radial direction), respectively.

P_i^+ and P_i^- – the first-flight escape probabilities of the annulus i through the outer and inner surfaces, respectively.

T_i^{OI} , T_i^{IO} and T_i^{OO} – the first-flight transmission probabilities from inner-to-outer, outer-to-inner, and outer-to-outer of annulus i , respectively.

S_i – the neutron source in annulus i , usually to be the elastic scattering source defined by the slowing-down equation.

If the mesh interval is ordered from the inside out, it is quite apparent, on physical grounds, that the

conservation of neutrons at each surface can be characterized by a system of linear equations given as follows [71,75].

$$J_i^+ = \begin{cases} T_i^{OO} J_i^- + P_i^+ S_i, & i=1 \\ T_i^{OI} J_{i-1}^+ + T_i^{OO} J_i^- + P_i^+ S_i, & i=2, \dots, N \end{cases} \quad (\text{IV.5.1a})$$

and

$$J_i^- = \begin{cases} T_{i+1}^{IO} J_{i+1}^- + P_{i+1}^- S_{i+1}, & i=1, \dots, N-1 \\ J_i^+, & i=N \end{cases} \quad (\text{IV.5.1b})$$

With no loss of generality, the above equations can be represented in the matrix notation:

$$T\vec{J} = P\vec{S} \quad (\text{IV.5.2})$$

where the vectors $\vec{J}$ and $\vec{S}$ contain $2N$ elements and the corresponding matrices T and P are matrices of order $2N \times 2N$ with special characteristics. From the perspective of matrix algebra, it is most convenient to order $\vec{J}$ and $\vec{S}$ so that $J_1^-, J_1^+, J_2^-, J_2^+, \dots, J_N^-, J_N^+$ and similarly, $S_1, S_2, S_2, S_3, S_3, \dots, S_N, S_N, 0$. It is easy to visualize that the corresponding matrix T must be a tri-diagonal matrix of the following form

$$T = \begin{bmatrix} T_1^{OO} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 1 & 0 & T_2^{IO} & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & T_2^{OI} & T_2^{OO} & 1 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 1 & 0 & T_3^{IO} & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & T_3^{OI} & T_3^{OO} & 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & T_4^{IO} & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 1 & -1 \end{bmatrix} \quad (\text{IV.5.3})$$

and the matrix P must be diagonal with elements $P_1^+, P_2^-, P_2^+, P_3^-, P_3^+, \dots, P_N^-, P_N^+, 0$ in order to reproduce Eq. (IV.4.3) and Eq. (IV.4.4).

Thus, from the point of view of computation, the inversion of a tri-diagonal matrix is known to be relatively simple once the transmission probabilities are specified. The obvious way to accomplish this goal is via the Gauss elimination procedure followed by the backward substitution widely used for such a purpose. Furthermore, it should be noted that the escape probabilities are related to the transmission probabilities via the reciprocity relation defined by Eq. (IV.2.13). For the case in point here, they are

$$P_i^+ = \frac{1}{\sum_{ii} \bar{l}^+} (1 - T_i^{oo} - T_i^{io}) \quad (\text{IV.5.4})$$

$$P_i^- = \frac{1}{\sum_{ii} \bar{l}^-} (1 - T_i^{oi}) \quad (\text{IV.5.5})$$

where $\bar{l}^+$ and $\bar{l}^-$ are the average outward and inward chord lengths respectively.

Having solved for the interface currents J_i^- and J_i^+ , one can readily obtain the collision rate for each annulus via the neutron balance relation below

$$C_i = \begin{cases} S_1 + J_1^- - J_1^+, & i = 1 \\ S_i + J_i^- - J_i^+ + J_{i-1}^+ - J_{i-1}^-, & i = 2, \dots, N \end{cases} \quad (\text{IV.5.6})$$

from which the flux for region i can be determined according to Eq. (IV.1.11). Thus, the same procedure can be repeated for each energy mesh where the slowing-down equation can be solved recursively by using the numerical scheme defined by Eq. (III.4.9) of chapter III.

The efficiency by which the inversion of a tri-diagonal matrix can be computed makes the above method extremely attractive especially when used in conjunction with the resonance treatment. The routine applications using numerous spatial regions have been demonstrated by the RABBLE [71] and MC²-2 [75] codes. In the limit of $N = 2$, for example, the unique feature of this method can be best understood. Unlike the Chernick' approach in which the inter-cell Dancoff effects on the collision probability must be accounted for, the inter-face current here implicitly relies on the boundary condition for the inter-cell effects.

It is worth noting that the above scheme can also be used as a means of computing collision probabilities. Physically, the element P_{ij} is equivalent to the collision rate in region i per unit volume attributed to a unit source initiated from region j . Thus, P_{ij} can be obtained via the procedure above by setting $S_j = \delta_{ij}$. Once the collision probabilities are specified, one can use them directly in conjunction with Eq. (IV.4.1).

In the following discussions, the analytical as well as practical aspects of transmission probabilities will be addressed.

IV.5.2 Collision and Transmission Probabilities for Geometries of Practical Interest

One type of cell configuration of particular interest in the treatment of resonance absorption is that consisting of multiple tubes with infinite length. It can be viewed as the most generic and representative unit cell in the collision probability calculation. The traditional pin cell and plate cell can be considered as special cases in which the inner radius approaches zero and both inner as well as outer radii approach infinity. Within the context of one-dimensional geometry, one only needs to consider a cell with

multiple annuli. For our purpose here, it suffices to begin with the rigorous determination of the collision and transmission probabilities of a single annulus first. It will be shown later how these quantities can be used to a cell with multiple annuli.

(1) Neutron Transport in an Annular Region

The treatment of transmission/collision probabilities in an annulus intended specifically for resonance calculations was pioneered by Kier [71]. The transmission probabilities of an infinite cylinder or tube in the form defined by Eq. (IV.2.12) can be simplified significantly upon performing the integration over the azimuthal angle in the cylindrical coordinate system. The neutron transport behavior in an annulus is completely specified by three types of transmission probabilities. They are: (1) transmission probability from the outer surface to the outer surface of the given annulus i to be denoted by T_i^{OO} ; (2) transmission probability from the inner to the outer surface of the given annulus i , to be denoted by T_i^{OI} ; (3) transmission probability from the outer to inner surface of the given annulus i , to be denoted by T_i^{IO} . Also of practical interest are two escape probabilities, P_i^+ and P_i^- , that signify the fraction of neutron initiated from the uniform volume source in the region escape from the outer and inner surfaces respectively. These latter quantities can be obtained by the reciprocity relation defined by Eq. (IV.2.13) once all transmission probabilities are known.

Neutron transmission in an annular region can be best illustrated graphically. Fig. IV.4 shows an annulus with an outer radius r_i and an inner radius r_{i-1} . Two most essential quantities are T_i^{OI} and T_i^{OO} from which other probabilities can be derived via the reciprocity relation. Neutrons which originate from an arbitrary point A on the outer surface of the annulus may travel through the region under consideration via various paths. For T_i^{OI} , the minimum and maximum neutron paths are represented by AB and AD respectively but in reverse direction from C to A. The former is co-linear with the radius AO while the latter is a line tangent to the inner surface. Thus, any neutron path $CA = |\vec{r}_s - \vec{r}'_s|$ within these limits must be of the following form according to the law of cosines

$$|\vec{r}_s - \vec{r}'_s| = (r_i^2 - r_{i-1}^2 \sin^2 \phi)^{1/2} - r_{i-1} \cos \phi \quad (\text{IV.5.7})$$

where ϕ is the angle between the line AC and the normal at point C. For convenience, define $b_i = 2\Sigma_i r_i$ and $a_i = (r_{i-1} / r_i)$. It follows from Eq. (IV.2.12) that T_i^{OI} can be expressed as a function of the dimensionless quantities a_i and b_i . For convenience, let $z = b_i(1 - a_i) / 2$. One obtains [71,98]

$$\begin{aligned} T_i^{OI} &= \frac{4}{\pi} \int_0^{\pi/2} d\phi \cos \phi K i_3(\Sigma_i |\vec{r}_s - \vec{r}'_s|) \\ &= \frac{4}{\pi} \int_0^1 dx K i_3 \left[\frac{z}{1 - a_i} \left(\sqrt{1 - a_i^2 x^2} - a_i \sqrt{1 - x^2} \right) \right] \\ &= \frac{4}{\pi} \frac{1 + a_i}{2a_i} \int_1^{\sqrt{1/\gamma_i}} dx \frac{1 - x^4 \gamma_i^2}{x^2 \sqrt{x^2 - 1} \sqrt{1 - x^2 \gamma_i^2}} K i_3 \left[\frac{b_i}{2} (1 - a_i) x \right] \end{aligned} \quad (\text{IV.5.8})$$

where $\gamma_i = (1 - a_i) / (1 + a_i)$.

Figure IV. 4 Neutron Path in Annular Geometry

For T_i^{oo} , the minimum and maximum neutron paths are specified by the lines tangent to the outer and inner surfaces respectively. In particular, AE is equal to twice AD and the angle $\angle ADO$ is a right angle. Define $\alpha_i = \sqrt{1 - a_i^2}$. Thus, any neutron path $AF = |\vec{r}_s - \vec{r}'_s|$ can be expressed in terms of the obvious relation

$$|\vec{r}_s - \vec{r}'_s| = 2r_i \cos \phi \quad (\text{IV.5.9})$$

where ϕ here is the angle between AF and the normal at A. It follows from Eq. (IV.2.12) that [99]

$$\begin{aligned} T_i^{oo} &= \frac{4}{\pi} \int_{\sin^{-1}(r_{i-1}/r_i)}^{\pi/2} d\phi \cos \phi K i_3(2\Sigma_i r_i \cos \phi) \\ &= \frac{4}{\pi} \int_0^{\alpha_i} dx \frac{x}{\sqrt{1-x^2}} K i_3(b_i x) \\ &= \frac{4}{\pi} \left\{ \int_0^1 dx \frac{x}{\sqrt{1-x^2}} K i_3(b_i x) - a_i \int_0^1 dx \frac{x}{\sqrt{1-x^2}} K i_3[b_i a_i \sqrt{(\alpha_i/a_i)^2 + x^2}] \right\} \end{aligned} \quad (\text{IV.5.10})$$

Physically, T_i^{oo} can be viewed as a combination of an 'asymptotic' and a 'non-asymptotic' term. The former signifies the limiting case of a solid fuel rod corresponding to the vanishing inner radius, i.e. $a_i = 0$. It will be shown that the integration of this integral can be carried out analytically. The latter

signifies the correction required for the annulus when the inner radius is not small. It will be shown that the integral is readily amenable to numerical quadrature.

From geometric considerations, it is obvious that the mathematical behavior of T_i^{OO} and T_i^{OI} must be significantly different. T_i^{OI} must vanish rapidly if $b_i(1-a_i)/2$ becomes very large. In contrast, T_i^{OO} does not vanish rapidly no matter how thick the annular region is since there is always the possibility that neutrons may skim through the annulus near the outer surface. Eq. (IV.5.8) and Eq. (IV.5.10) completely specify all transmission and collision probabilities as functions of two variables because the remaining quantities can be obtained via the following reciprocity relations

$$T_i^{IO} = \left(\frac{r_{i-1}}{r_i} \right) T_i^{OI} \quad (\text{IV.5.11})$$

$$P_i^- = \frac{r_{i-1}(1-T_i^{OI})}{2\Sigma_{it}(r_i^2 - r_{i-1}^2)} \quad (\text{IV.5.12})$$

$$P_i^+ = \frac{r_{i-1}(1-T_i^{OO} - T_i^{IO})}{2\Sigma_{it}(r_i^2 - r_{i-1}^2)} \quad (\text{IV.5.13})$$

In the following discussions, various analytical behavior and their practical implications will be addressed.

(2) Asymptotic Behavior of These Transmission Probabilities

One of the most intriguing mathematical properties of these transmission probabilities is their asymptotic behavior [99]. The generic nature of the annular configuration and its importance to the resonance treatment in a reactor cell can be best illustrated by considering two limiting cases.

(a) Pin Geometry ($r_{i-1} \rightarrow 0$)

A mathematical proof of the physically obvious consequence that the collision probability P_i^+ must become equal to that of the pin geometry under such a condition is of great theoretical as well as practical interest. Let $F(b_i)$ represent the transmission probability T_i^{OO} as the inner radius vanishes. Integrating by parts, one can readily show that

$$\begin{aligned} \lim_{a_i \rightarrow 0} T_i^{OO} &= F(b_i) = \frac{4}{\pi} \int_0^1 dx \frac{x}{\sqrt{1-x^2}} Ki_3(b_i x) \\ &= 1 - \frac{4}{\pi} b_i^2 \int_{b_i}^{\infty} \frac{dz}{z} \int_0^1 dx x \sqrt{1-x^2} K_1(zx) \end{aligned} \quad (\text{IV.5.14})$$

where $K_1(y)$ is the modified Bessel function of order 1. The inner integral is analytically integrable via the use of the K-transform identity and the subsequent integration over the variable z can also be carried out by using the Wronskian relation of the modified Bessel functions [84]. Hence, $F(b_i)$ becomes

$$\begin{aligned}
 F(b_i) &= 1 - b_i^2 \int_{b_i/2}^{\infty} \frac{d\xi}{\xi^2} I_1(\xi) K_1(\xi) \\
 &= 1 - \frac{2}{3} b_i^2 \left\{ \frac{1}{b_i} I_1\left(\frac{b_i}{2}\right) K_1\left(\frac{b_i}{2}\right) \right. \\
 &\quad \left. + \left(\frac{b_i}{2} \left[I_1\left(\frac{b_i}{2}\right) K_1\left(\frac{b_i}{2}\right) + I_0\left(\frac{b_i}{2}\right) K_0\left(\frac{b_i}{2}\right) \right] - 1 \right) + \left[I_0\left(\frac{b_i}{2}\right) K_1\left(\frac{b_i}{2}\right) - \frac{1}{b_i} \right] \right\}
 \end{aligned} \tag{IV.5.15}$$

where $I_n(y)$ and $K_n(y)$ are the modified Bessel functions of the first and second kind, respectively. It is interesting to note that, by substituting Eq. (IV.5.15) into the reciprocity relation defined by Eq. (IV.5.4), one obtains the identical result for an isolated pin as derived by Inglis.

From Eq. (IV.5.8), the corresponding T_i^{OI} under the same condition is simply

$$\lim_{a_i \rightarrow 0} T_i^{OI} = \frac{4}{\pi} Ki_3(b_i) \tag{IV.5.16}$$

Physically, the above equation indicates the obvious fact that the transmission probability from any point on the centerline of an infinite cylinder to another point on the surface along the normal path is expressible in terms of the Bickley function [78] of order 3. On the other hand, T_i^{IO} for neutrons on the reverse path must vanish according to the reciprocity relation defined by Eq. (IV.5.11).

It is interesting to note that $F(b_i)$ is a relatively slowly varying function of b_i characterized by the following asymptotic series characteristics of the modified Bessel function

$$F(b_i) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k+1} \frac{1 \cdot 3 \cdot 5 \cdots (2k-1)}{2 \cdot 4 \cdot 6 \cdots (2k)} \frac{(\mu-1)(\mu-3^2) \cdots [\mu-(2k-1)^2]}{b_i^{2k}} \tag{IV.5.17}$$

where $\mu = 4$. As b_i becomes very large, $F(b_i)$ is further reduced to a very simple form

$$F(b_i) = \frac{3}{4b_i^2} \tag{IV.5.18}$$

It should be noted that Eq. (IV.5.18) is equally applicable to the case of large value of $(b_i \alpha_i)$ even if the inner radius is not zero. That is to say that for an annular region with large optical path, there is little

difference between the annulus and a circle in so far as T_i^{oo} is concerned.

(b) Plate Limit

Another physical situation of practical interest is the plate limit. Although it is quite apparent from the perspective of geometry that an annulus is equivalent to a circle, it is much less obvious from the functional behavior of the transmission/collision probabilities. Therefore, a mathematical proof is of great theoretical interest. The quantity T_i^{OI} defined by Eq. (IV.3.10) under the condition of $a_i \rightarrow 1$ can be derived based on L'Hospital's rule. One obtains [99]

$$\lim_{a_i \rightarrow 1} T_i^{OI} = h(z) = \frac{4}{\pi} \int_0^1 dx Ki_3 \left(\frac{z}{\sqrt{1-x^2}} \right) = \frac{4}{\pi} \int_1^\infty dt \frac{Ki_2(zt)}{t^3 \sqrt{t^2-1}} \quad (IV.5.19)$$

By using the recurrence relation of $Ki_n(x)$ and the K-transform identity, one can readily show that

$$h(z) = \frac{4}{\pi} z^2 \int_z^\infty dy \int_1^\infty dw w \sqrt{w^2-1} \frac{K_1(yw)}{yw} = 2E_3(z) \quad (IV.5.20)$$

where $E_3(z)$ is the exponential integral of order 3. Thus, T_i^{OI} approaches the traditional transmission probability of an infinite slab derived in Section IV.2.2. Eq. (IV.5.20), in effect, establishes the fact that $E_3(z)$ is one special case of integrals involving Ki_3 -function.

(c) Relation to Hypergeometric Functions

Conceptually, the transmission and collision probabilities for neutron transport in a reactor cell can be generally viewed as integrals of generalized hypergeometric functions. The relationship between the Ki_3 -function and the Meijer's G-function [101,102] was first pointed out by Milgram [103]. Various mathematical properties of transmission probabilities are the natural consequences characterized by the special integrals involving the G-functions. Utilization of the hypergeometric functions in practical applications had not received much attention until the extensive studies by Luke [102,104] became available. In the following discussion, a brief description is given in order to shed some light on this subject.

The Ki_3 -function is related to the G-function as follows [103]

$$Ki_3(x) = \frac{1}{4} G_{13}^{21} \left(\frac{x^2}{4} \middle| \begin{matrix} -1 \\ 0, 0, -2 \end{matrix} \right) \quad (IV.5.21)$$

In general, the function $G_{p,q}^{m,n} \left(z \middle| \begin{matrix} a_p \\ b_q \end{matrix} \right)$ is an analytic function of z with a branch point at origin and is

characterized by parameters $a_1, a_2, \dots, a_n$; $a_{n+1}, \dots, a_p$; $b_1, b_2, \dots, b_m$; and $b_{m+1}, \dots, b_q$. One property of the G-function of great importance is its characteristics when subject to the Euler transformation. The transformation usually can be expressed in either one of the two forms [102]

$$\int_0^1 dy y^{-\alpha} (1-y)^{\alpha-\beta-1} G_{pq}^{mn} \left(zy \left| \begin{matrix} a_p \\ b_q \end{matrix} \right. \right) = \Gamma(\alpha - \beta) G_{p+1, q+1}^{m, n+1} \left(z \left| \begin{matrix} \alpha, a_p \\ b_q, \beta \end{matrix} \right. \right) \quad (\text{IV.5.22})$$

where $0 \leq n \leq p < q$; $1 \leq m \leq q$ and $\Re(\beta) < \Re(\alpha) < \Re(b_j) + 1$. Or, alternatively,

$$\int_1^\infty dy y^{-\alpha} (y-1)^{\alpha-\beta-1} G_{pq}^{mn} \left(zy \left| \begin{matrix} a_p \\ b_q \end{matrix} \right. \right) = \Gamma(\alpha - \beta) G_{p+1, q+1}^{m+1, n} \left(z \left| \begin{matrix} a_p, \alpha \\ \beta, b_q \end{matrix} \right. \right) \quad (\text{IV.5.23})$$

From our perspective here, the transmission probabilities for two simple geometries defined by Eq. (IV.5.12) and Eq. (IV.5.17) are just the Euler transformation of the Ki_3 -function. In particular, it is sufficient to record that

$$T_{pin} = \frac{1}{\sqrt{\pi}} G_{2,4}^{3,1} \left(\frac{b_i}{4} \left| \begin{matrix} 1/2, 2 \\ 3/2, 0, 1/2, 0 \end{matrix} \right. \right) = F(b_i) \quad (\text{IV.5.24})$$

Similar relation for T_{pl} or E_3 to the G-function can also be derived. For more complicated geometry such as annulus, the transmission probabilities are related to the hypergeometric of the form

$$\int_B^A dy y^{-\alpha} (1-y)^{\alpha-\beta-1} G_{pq}^{mn} \left(zy \left| \begin{matrix} a_p \\ b_q \end{matrix} \right. \right) \quad (\text{IV.5.25})$$

which can be viewed as an ‘incomplete’ G-function in the same context as the incomplete Bessel function. Milgram [103] has explored various mathematical properties of the G-function and has demonstrated the numerical means to compute the transmission probabilities for the annular geometry. It is quite obvious that further exploration in this area will be of some practical interest, especially for use in problems involving more complex geometries.

(d) Evaluations of Transmission Probabilities for Practical Applications

The well-defined analytical properties such as the small argument limits and the asymptotic limits of transmission probabilities described above makes the evaluations of these integrals relatively simple. In practical applications, two approaches, one based on pre-computed tables [71] and the other based on the low-order quadratures [99], are most commonly used.

Since the transmission probabilities can be considered as a function of two variables, a_i and b_i , described earlier, the pre-computed tables can be constructed in the finite domain outside of those

where the limiting approximations become valid. A two-dimensional interpolation routine is all it requires at run time if the tabulated values are used.

Alternatively, the low-order quadrature has also been shown [99] to provide the comparable efficiency as well as accuracy of the table method. In spite of their mathematical behavior discussed previously, T_i^{OO} and T_i^{OI} do have some desirable numerical characteristics in common. These quantities in their integral form are both amenable to the general form of the Gauss-Jacobi quadrature, namely

$$\int_{c_1}^{c_2} (c_1 - x)^\zeta (x - c_2)^\eta f[g(x)] dx = \left(\frac{c_1 - c_2}{2} \right)^{\zeta + \eta + 1} \sum_{j=1}^N w_j f \left[g \left(\frac{c_1 + c_2}{2} + \frac{c_1 - c_2}{2} x_j \right) \right] \quad (\text{IV.5.26})$$

where w_j and x_j are weights and abscissae associated with the Jacobi-polynomial $P_N^{(\zeta, \eta)}(x)$. For T_i^{OI} , $\zeta = -1/2$, and $\eta = 1$ while $\zeta = -1/2$ and $\eta = 0$ are appropriate for the non-asymptotic term for T_i^{OO} . The fact that the integrand $f[g(x)]$ is specified in terms of the Ki_3 -function readily amenable to the interpolation scheme from the pre-computed tables makes the quadrature approach plausible. It is important to realize, however, that Eq. (IV.5.26) is of practical interest if and only if the total number in the sum is small. As reported in Ref. 102, $N = 3$ was found to be satisfactory and the resulting computing time requirement is comparable to the scheme based on 6-point interpolation from the direct tabulation of the integrals in the two-dimensional arrays.

As discussed earlier, the integrals under consideration can be viewed as the hyper-geometric integrals with the integrands defined by the Meijer's G-function. Computer programs based on such an approach have been developed by Milgram [103], and their applicability to practical applications has been demonstrated. In view of significant developments on the theory of the hypergeometric functions in recent years [102,104], it is an area that may produce advances in the general treatment of the collision probability method, from the mathematical point of view.

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Chapter V STATISTICAL TREATMENT OF UNRESOLVED RESONANCES

The treatment of resonance self-shielding effect in the unresolved energy range constitutes one of the most important links in the fast reactor applications. The range under consideration is usually defined as the energy span between the upper boundary of the resolved energy region and an upper bound beyond which the self-shielding effect becomes unimportant. For major actinides, it spans from the low keV region up to about 100 keV at present. The methods for treating this phenomenon can be viewed as a natural extension of the statistical theories of average cross sections such as those described by Moldauer [1,2] and Ericson [3]. More recently, new frontiers on this subject appear to be on the horizon as the work pioneered by Fröhner [4] on the basis of information theory and that by Lukyanov et al [5,6] using the 'characteristic' function concept have offered other potential alternatives to the traditional approaches. Since the theoretical foundations may often be obscured in routine applications, it is useful to summarize briefly some conceptual aspects of the problem prior to the discussions of the basis for the computational methods.

V.1 Nature of the Problem

Two average quantities of interest in reactor calculations are $\langle \sigma_x \phi \rangle_{E,r}$ and $\langle \phi \rangle_{E,r}$ which represent the expectation values of the reaction rate of a given reaction process x and the neutron flux, respectively, over a large number of events within a given energy and spatial interval. As discussed earlier, the flux depends on the macroscopic total and scattering cross sections as specified by the integral transport equation. Unlike the cases considered in the theory of average cross sections, the averages here are clearly multi-variant in nature. Without loss of generality, each microscopic cross section is represented by the R-matrix formalism defined previously in terms of parameters E_i and γ_{ci} which signifies the R-matrix state and the reduced width amplitude for various channels c respectively. The statistical properties of these parameters provide a convenient basis for the evaluation of the averages. From the statistical theory of spectra⁷, the distributions of these parameters are well-known. The distribution of E_i for a given spin state is characterized by the Wigner distribution [7,8,9] and/or by the long-range correlations described by Dyson [7,10]. The former, commonly referred to as the 'Gaussian ensemble', was derived on the premise that an ensemble of elements of a real symmetric Hamiltonian is normally distributed and statistically independent [7,8,9]. The resulting distribution of level spacing is expressible in terms of a simple analytical form particularly useful for practical applications, as one shall see. In contrast, the latter, usually referred to as the 'Gaussian orthogonal ensemble' (or G.O.E.) [7,10], is free from the assumption of the former. The system under consideration here is not the Hamiltonian but the complex eigenvalues of a unitary matrix of the form $\exp(i\theta_j)$, with θ_j uniformly distributed around a unit circle. The unitary matrix S is taken to be a function of the Hamiltonian H so that θ_j is a function of E_j . Over a small range of angles, E_j and θ_j are approximately linear. The other parameters, γ_{ci} 's, are statistically independent and normally distributed with zero means and variance of unity according to Porter and Thomas [11]. For detailed discussions on these subjects, readers are referred to Ref.7. These distributions, in effect, define the joint density function (j.d.f.) required for evaluating the averages. Given information of $\langle |E_i - E_{i+1}| \rangle$ and $\langle \gamma_{ci}^2 \rangle$

through the explicit knowledge of the behavior of σ_x and ϕ , the expectation values of interest are, in principle, completely specified from the point of view of statistical theory.

It should be noted that problems do arise when the statistical treatment of average cross sections is extended to that of the self-shielding effects characterized by the macroscopic nature of the reactor lattices. Two special problems must be considered in such applications. First, the attenuation of flux within the region under consideration implies that the events are actually deterministic in nature. By nature, the self-shielding effects are strongly energy-dependent. By and large, the degree of such effects becomes much more important in the relatively low energy region where resonances are sharp whereas the effects diminish gradually as resonances become less sharp in the high energy region due partly to the general reduction in their peak values and partly to the extreme Doppler-broadening. A large self-shielding effect is often accompanied by greater attenuation in neutron flux in the macroscopic reactor lattices. It is important to realize, however, that the statistical averaging implicitly requires the assumptions of ergodicity and stationarity [1,2,12] of the samples within the energy interval under consideration. The dilemma here is that these assumptions are, strictly speaking, questionable whenever the self-shielding effects are still significant enough to be of practical interest. The question will arise as long as the flux attenuates within the interval containing a handful of resonances that exhibit appreciable self-shielding effect. The statistical description, of course, becomes meaningless if the flux attenuates too rapidly. Consequently, significantly large uncertainties in the estimated self-shielding effect are expected if the statistical method is applied to the low energy region where the resonance absorption is substantial. In fact, this has motivated the continuous efforts to extend the resolved energy regions for all major actinides in the past decades. Secondly, there does not appear any simple way to relate the statistical behavior of the self-shielding effect in the complex reactor lattice directly to the observed measurement such as the Doppler reactivity experiments. One closest analogy is perhaps the transmission and self-indication measurements that in effect, provide the information of the correlation between the transmission and absorption ratios of a simple foil containing one nuclide at a given temperature. It is equivalent to the self-shielding effect in its simplest form. Therefore, these measurements can serve as useful guides for benchmarking purposes.

V.2 Existing Methods---Basis and Problems

The averages of interest can be either cast into the form of Riemann integrals or that of Lebesgue integrals, depending on the philosophy of how the joint density function is defined. The former is the consequence of the direct use of the statistical distributions of the resonance parameters while the latter results from using the conditional probabilities of partial and total cross sections themselves that in principle, can be derived via the transformation of variables. Two forms of the j.d.f. provide the theoretical basis for all existing methods in existence. In the following discussion, a brief summary is presented.

V.2.1 Methods Based on Distributions of Resonance Parameters

There are two methods originated via the direct use of the probability distributions of the resonance parameters, namely, the ladder method [13,14,15,16] and the integral method [17,18].

(1) Ladder Method

This method is conceptually the most straightforward. Discrete resonance sequences for each J -state

can be constructed directly by sampling from the cumulative density functions of γ_{ci} (or γ_{ci}^2) and level spacing with the standard technique widely used in the Monte Carlo approach [19]. Once these resonance sequences (or ladders) are generated, the subsequent calculations are the same as those for the resolved resonances [13,14,15,16]. Thus, the method is applicable to all methods to various degrees of sophistication described previously. For applications using the Breit-Wigner approximation, this procedure is most transparent. Once resonance sequences are generated, they can be used directly in conjunction with various deterministic methods for the group-constant generation or Monte Carlo approaches. For applications using the R-matrix representations, it is most convenient to convert the statistically generated parameters into the pole parameters that are more amenable for practical calculations described earlier. The MATDIAG code [20], which allows the conversion of the R-matrix parameters with arbitrary numbers of channels and levels, has been used for this purpose. Alternatively, the POLLA code [21] for converting the Reich-Moore [22] type of parameters into the Kapur-Peierls [23] type parameters is particularly suitable for practical applications.

Unfortunately, considerable uncertainties in the subsequent self-shielding effect calculations are still expected for two reasons. First, a statistically generated 'ladder' from the distributions of resonance parameters may not necessarily reflect accurately the averages under consideration without some viable selection criteria especially in the energy intervals containing only a handful of resonances. Secondly, the inherent problem attributed to the non-statistical nature of the self-shielding effect described in the foregoing section is always present whenever the effect is appreciable.

The problem of statistical nature, in principle, can be alleviated somewhat although not totally removed by various improved sampling techniques. Dyos [15] has suggested two criteria for selecting resonance ladders. First, the means and variances of the parameters for the selected ladder must match the corresponding theoretical values derived from various distributions. Secondly, the unshielded average cross sections within the given energy interval must be substantially the same as the 'observed' values inferred by the evaluators of the data file. Although these procedures help make the ladder method more realistic, large uncertainties may still be present when the Doppler effect is considered. This is apparently attributed to the multi-variant nature of the problem as pointed out in Ref. 24 and Ref. 25. Alternatively, a scheme of stratified random ladders was proposed by Ribon [26] based on the stratified sampling techniques widely used in the Monte Carlo approach. By utilizing the stratified samples taken from the distributions of resonance parameters, Ribon [26] has shown that the variances can be significantly reduced. Also included in his approach is a numerical means whereby resonance levels can be generated directly based on the 'Gaussian orthogonal ensemble' surmise of Dyson [10] instead of the Wigner distribution commonly used. Excellent agreement between the results of his method and those of the integral method to be described was reported.

As discussed in the previous section, the problem of non-statistical nature can only be lessened via the further extension of the resolved energy range and making use of other physical measurements directly related to the self-shielding effect in the energy region of interest.

(2) Integral Method

In contrast to the ladder method, the averages of interest, in principle can also be obtained by direct integration over the prescribed joint density function. However, the problem is obviously too complicated in practice unless some simplifying assumptions are made. To utilize this method for practical applications usually requires three basic assumptions not required by the ladder method: (1)

validity of the Breit-Wigner approximation for cross sections; (2) validity of the NR-approximation; (3) validity of the equivalence relation. Assumptions (2) and (3) here appear to be mandatory in conjunction with the practical use of this method. Inevitably, questions have been raised as to the possibility of extending its applicability beyond the Breit-Wigner approximation. The issues concerning the multilevel effects will be addressed separately in section (b).

(a) Approach based on the Breit-Wigner Approximation

Detailed descriptions of this method have been presented in Refs.17 and 18. For our purpose here, a brief discussion with emphasis on the conceptual aspects should suffice.

Under the above assumptions, the expectation values of interest can be represented in relatively simple forms:

$$\langle \sigma_x \phi \rangle_{E_0} = \sum \frac{\sigma_p^{(eq)} \langle \Gamma_x J^* \rangle_{E_0}}{\langle D \rangle}, \quad \langle \phi \rangle_{E_0} = 1 - \sum \frac{\langle \Gamma_x J^* \rangle_{E_0}}{\langle D \rangle} \quad (\text{V.2.1})$$

where $\sigma_p^{(eq)}$ and $\langle D \rangle$ are the 'equivalent' potential scattering cross section per absorber atom and average level spacing respectively. The summation in average reaction rate is over the I - and J -states of the nuclide in question while that in average flux is over all resonance sequences for the mixture. The angular bracket $\langle \rangle$ signifies the population average for an ensemble of stationary samples of resonance integral which are specified by the statistical properties of resonances parameters in the vicinity of E_0 . In terms of the known distributions explicitly, such an average can be represented by multiple integral of the form

$$\langle q_k \rangle = \prod_j \frac{1}{\langle D_j \rangle} \int_{-\infty}^{\infty} \Omega\left(\frac{D_j}{\langle D_j \rangle}\right) dD_j \prod_x \frac{1}{\langle \Gamma_x \rangle} \int_0^{\infty} d\Gamma_x P_\nu\left(\frac{\Gamma_x}{\langle \Gamma_x \rangle}\right) q_k(D_j, \Gamma_x) \quad (\text{V.2.2})$$

where $P_\nu(\Gamma_x / \langle \Gamma_x \rangle)$ and $\Omega(D_j / \langle D_j \rangle)$ are the χ^2 -distribution of ν -degree of freedom and the level correlation function, respectively, and q_k denotes the quantity to be averaged. Since the partial width for a given channel c of the reaction process x is $\Gamma_{ci}^{(x)} \propto \gamma_{ci}^2$ and $\Gamma_x = \sum_{c=1}^{\nu} \Gamma_{ci}^{(x)}$, it follows from the elementary statistical theory that $P_\nu(y)$ is the distribution for the partial width consisting of ν channels with equal strength as defined by

$$P_\nu(y) dy = \frac{\nu}{2\Gamma(\nu/2)} \left(\frac{\nu}{2} y\right)^{\nu/2-1} e^{-\nu y/2} dy \quad (\text{V.2.3})$$

Physically, the level correlation function $\Omega(y)$ is equivalent to the probability of finding any level within an interval $d | E_k - E_{k'} |$ at a distance of $D = | E_k - E_{k'} |$ from a given level k . If k and k' belong to

resonances of two different J -state or different nuclides, the levels are statistically uncorrelated so that $\Omega(y) = 1$. On the other hand, if k and k' belong to the same J -state of the same nuclide, they are subject to Wigner's level repulsion and/or Dyson's description of level correlation. For practical applications, there are three ways by which $\Omega(y)$ can be evaluated.

(i) Direct Numerical Approach

If one neglects the long-range correlation of Dyson [10], the function $\Omega(y)$ must satisfy the following integral equation of the convolution type

$$\Omega(x) = W(x) + \int_0^x \Omega(x-t)W(t)dt \quad (\text{V.2.4})$$

where $W(y)$ is the Wigner distribution [8] defined as

$$W(y)dy = \frac{\pi}{2} y \exp\left(-\frac{\pi}{4} y^2\right) dy \quad (\text{V.2.5})$$

The analytical solution to this equation in a closed form does not appear to be feasible. Hence, one has to resort to the use of numerical means when applied to the evaluation of Eq. (V.2.4).

(ii) Analytical Approximation

The solution to Eq. (V.2.4) becomes significantly simplified [17] if the Wigner distribution is replaced by a χ^2 -distribution $P_\nu(y)$. For a convolution integral equation of this type, it is most readily amenable to the Laplace transform method, provided that its inverse is derivable. The χ^2 -distribution used in this context leads immediately to the inverse transform defined by [17]

$$\Omega(y) = \frac{e^{-\nu y/2}}{2\pi i} \left(\frac{\nu}{2}\right) \int_{c-i\infty}^{c+i\infty} \frac{e^{(\nu p/2)y}}{p^{\nu/2}-1} dp \quad (\text{V.2.6})$$

whereby, for all even $\nu \geq 2$, $\Omega(y)$ is expressible in terms of the analytical function of the closed form, as can be readily seen via the Cauchy integral formula. The poles for all even integer ν are readily obtainable via the De Moivre's theorem in terms of linear combination of the damped oscillatory terms. In particular, the χ^2 -distributions of 8 or 10 degrees of freedom exhibit the greatest resemblance to the Wigner distribution. The former is especially suitable for practical applications because of its relatively simple form as given below [17].

$$\Omega(y) = 1 - e^{-8y} - 2e^{-4y} \sin(4y) \quad (\text{V.2.7})$$

The above equation was extensively used in the earlier studies of the Doppler effect contributions attributed to the unresolved resonances [17].

(iii) Dyson's Two-Level Correlation Function

Another alternative is to identify $\Omega(y)$ directly with Dyson's two-level correlation function defined as [10]

$$\Omega(y) = 1 - [s(y)]^2 - \frac{ds(y)}{dy} \int_y^\infty s(t) dt \quad (\text{V.2.8})$$

where $s(y) = \sin(\pi y) / \pi y$. Eq. (V.2.8) can be used directly in conjunction with the integral defined by Eq. (V.2.2) and the resulting integral can be carried out efficiently via the Fourier transform method to be described [18].

From a practical point of view, the multiple integral defined in Eq. (V.2.2) is obviously still too cumbersome to evaluate since the problems of interest inevitably involve many uncorrelated resonance sequences in the mix. One simplified approximation that can simplify the problem drastically is the separability assumption on the NR-flux. This can be accomplished by noting that [17,18]

$$\phi \approx \frac{1}{\Sigma_t} \approx \frac{1}{\Sigma_p + \Sigma_R^{(J)}} \left[1 - \sum_{j \neq J} \frac{\Sigma_R^{(j)}}{\Sigma_p + \Sigma_R^{(j)}} \right] \quad (\text{V.2.9})$$

Upon integrating over the uncorrelated level spacing of J and j , the reaction rate of a given sequence J is reduced to a much more manageable form

$$\langle \sigma_x^{(J)} \phi \rangle = \langle \frac{\sigma_x^{(J)}}{\Sigma_p + \Sigma_R^{(J)}} \rangle \left[1 - \sum_{j \neq J} \langle \frac{\Sigma_R^{(j)}}{\Sigma_p + \Sigma_R^{(j)}} \rangle \right] \quad (\text{V.2.10})$$

which provides a concise description of resonance overlapping effect attributed to other statistically uncorrelated sequences. Thus, it follows that the corresponding effective cross section for a given nuclide becomes [17,18]

$$\sigma_x \approx \sum_{J,l} \frac{(\sigma_p^{(eq)} / \langle D \rangle) \langle \Gamma_x (J - O_{kk'}) \rangle}{1 - (1 / \langle D \rangle) \langle \Gamma_t (J - O_{kk'}) \rangle} \quad (\text{V.2.11})$$

whereby each uncorrelated sequence can be evaluated separately in so far as the effective cross section is concerned. However, this is not to imply that the mutual self-shielding effect on the absorption rate is unimportant.

Thus, the simplified expression only requires the evaluations of the integral over the partial width distributions and the correlation function of each spin sequence in question so that computations can be expedited considerably. It was found [18] that these averages over various distributions can be carried out most accurately and efficiently via the use of numerical quadratures. For averages over χ^2 -distributions, the best results can be achieved by the use of the half-space Gauss-Hermite quadrature given by Steen et al [27] specifically intended for integral involving the Gaussian-like function in the

integrand. By transforming of the variables, all integral over the χ^2 -distribution can be expressed in the form readily amenable to the following quadrature

$$\int_0^\infty e^{-y^2} f(y) dy = \sum_{i=1}^N C_i f(y_i) + R_N \quad (\text{V.2.12})$$

where C_i , y_i and N are weight, quadrature point and remainder given by Ref. 27. On the other hand, the overlap integral involving the Dyson's two-level correlation [10] can be simplified somewhat via the utilization of Fourier transform identities. One such an identity of is the Fourier transform of the two-level correlation function given below [10,18].

$$\mathcal{F}\{1 - \Omega(|D|)\} = \begin{cases} \frac{\langle D \rangle}{\sqrt{2\pi}} \left\{ 1 - \left| \frac{\langle D \rangle \xi}{\pi} \right| + \left| \frac{\langle D \rangle \xi}{2\pi} \right| \ln \left[1 + \left| \frac{\langle D \rangle \xi}{\pi} \right| \right] \right\}, & \left| \frac{\langle D \rangle \xi}{2\pi} \right| \leq 1 \\ \frac{\langle D \rangle}{\sqrt{2\pi}} \left\{ -1 + \left| \frac{\langle D \rangle \xi}{2\pi} \right| \ln \left[\frac{|\langle D \rangle \xi / \pi| + 1}{|\langle D \rangle \xi / \pi| - 1} \right] \right\}, & \left| \frac{\langle D \rangle \xi}{2\pi} \right| > 1 \end{cases} \quad (\text{V.2.13})$$

Another pertinent Fourier transform identity is [18]

$$\tau(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\psi(\theta_k, x_k) \exp(i\xi x_k)}{\beta_k + \psi(\theta_k, x_k)} = \mathcal{F} \left\{ \frac{\psi(\theta_k, x_k)}{\beta_k + \psi(\theta_k, x_k)} \right\} \quad (\text{IV.2.14})$$

which satisfies a convolution integral equation of the following form [18]

$$\beta_k \tau(\xi) + \frac{1}{2} \int_{-\infty}^{\infty} \exp\left\{-[(\xi - t)^2 / \theta_k^2] - |\xi - t|\right\} \tau(t) dt = \sqrt{\frac{\pi}{2}} \exp\left\{-[\xi^2 / \theta_k^2] - |\xi|\right\} \quad (\text{IV.2.15})$$

As described in Ref.18, Eq. (V.2.13) through Eq. (V.2.15) leads to the efficient algorithms that have since been incorporated into the MC²-2 code [28] for routine applications.

(b) Statistical Behavior of the Kapur-Peierls Type Parameters

As discussed earlier, all resonance representations can be cast into the same general form consisting of a linear combination of the Breit-Wigner-like terms in the resolved energy region. Because of the obvious similarity within the context of the J^* -integral averages defined in Eq. (V.2.1), it is quite natural to ask whether the integral method described above can be extended to various pole representations in the unresolved region.

Unlike the treatment of the resolved resonances in which every conceivable effort was made to preserve the rigor of their energy dependence, the energy dependence here is only relevant in the vicinity of E_0 where statistical samples of resonance integral are taken to be stationary with respect to energy in the context defined by Eq. (V.2.1). Hence, all pole representations, in effect, assume the

Kapur-Peierls [23] form with energy-independent parameters (Adler-Adler approximation). Given the statistical distributions of the R-matrix parameters, the issue is whether it is feasible to deduce distributions of the corresponding Kapur-Peierls parameters in analytical forms whereby the above integral method can be utilized in the same manner. This issue was addressed in great detail in Ref. 29. For our purpose here, a brief discussion to illustrate the conceptual aspects of the problem should suffice.

The analytical nature of the problem can be best illustrated by considering a simple case involving two interfering levels and a single channel. The 2×2 level matrix can be evaluated analytically

$$A_{\mu\nu} = \frac{\text{adj}(A^{-1})}{\det(A^{-1})} \quad (\text{V.2.16})$$

By setting $\det(A^{-1}) = 0$, one obtains the complex poles d_λ via a quadratic equation, and the corresponding residue parameters can also be obtained. Let $D^{(S)}$ and $\Gamma_i^{(S)}$ be the Kapur-Peierls 'level' spacing $\text{Re}(d_1 - d_2)$ and 'level' width $\text{Im} d_i / 2$, respectively. The relationship between these parameters and the corresponding R-matrix parameters are given by

$$D^{(S)} = \pm \left[\frac{1}{2} \left(\left[D^2 - \frac{1}{4}(\Gamma_1 + \Gamma_2)^2 \right] + \left\{ \left[D^2 - \frac{1}{4}(\Gamma_1 + \Gamma_2)^2 \right]^2 + D^2(\Gamma_2 - \Gamma_1)^2 \right\}^{1/2} \right) \right]^{1/2} \quad (\text{V.2.17})$$

$$\Gamma_i^{(S)} = \frac{1}{2}(\Gamma_1 + \Gamma_2) \pm \left[\frac{1}{2} \left(\left[\frac{1}{4}(\Gamma_1 + \Gamma_2)^2 - D^2 \right] + \left\{ \left[D^2 - \frac{1}{4}(\Gamma_1 + \Gamma_2)^2 \right]^2 + D^2(\Gamma_2 - \Gamma_1)^2 \right\}^{1/2} \right) \right]^{1/2} \quad (\text{V.2.18})$$

Thus, deriving the joint distributions of $D^{(S)}$ and $\Gamma_i^{(S)}$ from those of D and Γ_i can be accomplished readily by a transformation of variables commonly used in statistical theory once the Jacobian is known from the equations above. Upon integration of the joint distribution so obtained, the probability density function for $D^{(S)}$ becomes [29]

$$f(z) = \frac{\pi}{2} z \exp\left(-\frac{\pi}{4} z^2\right) \frac{\tau(z)}{C} \quad (\text{V.2.19})$$

where $z = D^{(S)} / \langle D \rangle$ and

$$\tau(z) = \int_0^\infty d\alpha \frac{z^{-1} \exp\left[-\frac{\alpha \langle D \rangle}{2 \langle \Gamma \rangle} - \frac{\pi}{32} \alpha^2\right]}{(4z^2 + \alpha^2)^{1/2}} \left[I_0\left(\frac{\pi}{32} \alpha^2\right) \left(4z^2 + \frac{\alpha^2}{2}\right) + I_1\left(\frac{\pi}{32} \alpha^2\right) \frac{\alpha^2}{2} \right] \quad (\text{V.2.20})$$

Here, C and $I_n(x)$ denote the normalization constant and the modified Bessel function of the first kind, respectively. It is interesting to note that Eq. (V.2.19) physically represents the combination of the Wigner distribution previously defined and a correction factor $\tau(z)$, which in turn is strongly dependent upon the ratio of R-matrix average spacing to the corresponding average total width. In the limit of large $\langle D \rangle / \langle \Gamma \rangle$, the correction factor asymptotically approaches unity as $f(z)$ becomes equal to the usual Wigner distribution. It is also the obvious criterion that the Kapur-Peierls representation becomes identical to the Breit-Wigner approximation as levels are isolated from each other. On the other hand, $f(z)$ can be significantly different from the Wigner distribution as the ratio $\langle D \rangle / \langle \Gamma \rangle$ becomes small. Fig. V.1 illustrates the behavior of $f(z)$ as compared to the Wigner distribution and random (exponential) distribution at various values of the ratio of average spacing-to-width. Such behavior underlines the intrinsic effects attributed to the interference of the neighbor levels on the statistical distributions of the Kapur-Peierls type parameters. To quantify these effects, the averages and variances of various cases corresponding to Fig.V.1 are presented in Table V.1. It is seen that the averages of $f(z)$ are monotonically increasing function of $\langle D \rangle / \langle \Gamma \rangle$ while the variances decrease monotonically as the ratio decreases.

Figure V. 1 Analytical pdf for Kapur-Peierls Level Spacing Using Two Levels

Table V. 1 Average Spacing and Variances for Various Cases

Distribution Functions	$\frac{\langle D^{(S)} \rangle}{\langle D \rangle}$	$\frac{\langle (D^{(S)})^2 \rangle - \langle D^{(S)} \rangle^2}{\langle D^{(S)} \rangle^2}$
------------------------	---	---

Wigner	1.0	0.2732
Random	1.0	1.0
$f(z): \langle D \rangle / \langle \Gamma_i \rangle = \pi$	0.9587	0.3150
$f(z): \langle D \rangle / \langle \Gamma_i \rangle = 2.0$	0.9273	0.3444
$f(z): \langle D \rangle / \langle \Gamma_i \rangle = 1.0$	0.8603	0.4057
$f(z): \langle D \rangle / \langle \Gamma_i \rangle = 0.5$	0.7876	0.4700
$f(z): \langle D \rangle / \langle \Gamma_i \rangle = 0.1$	0.7140	0.4910

Similarly, the p.d.f. of $\Gamma^{(S)}$ can also be derived with the result given below [29]

$$h(\omega) = \frac{\exp(-\omega/2)}{(2\pi\omega)^{1/2}} \frac{\Xi(\omega)}{C'} \quad (\text{V.2.21})$$

where C' is the normalization constant, $\omega = \Gamma_i^{(S)} / \langle \Gamma_i \rangle$ and

$$\Xi(\omega) = \frac{\sqrt{2\pi}}{4} \int_0^\infty d\eta \frac{\exp\left[-\frac{\eta}{2} + \frac{\pi \langle \Gamma_i \rangle^2}{32 \langle D \rangle^2} (\eta + \omega) - \frac{\pi \langle \Gamma_i \rangle^2}{4 \langle D \rangle^2} \eta \omega\right]}{\sqrt{\eta}} g(\eta) \quad (\text{V.2.22})$$

$$g(\eta) = \left\{ K_0(\zeta) \left[\frac{(\omega - \eta)^2}{4} - \frac{(\omega + \eta)^2}{8} \right] + K_1(\zeta) \frac{(\omega + \eta)^2}{8} \right\} \quad (\text{V.2.23})$$

$$\zeta = \frac{\pi \langle \Gamma_i \rangle^2}{32 \langle D \rangle^2} (\eta + \omega)^2 \quad (\text{V.2.24})$$

Here, $K_n(x)$ is the modified Bessel function of the second order. Like the case of 'level' spacing, the Kapur-Peierls total width distribution is expressible as the Porter-Thomas distribution⁷ modified by a correction factor $\Xi(\omega)$. The latter is also strongly dependent on the average spacing-to-width ratio, and, in the limit of $\langle D \rangle / \langle \Gamma_i \rangle \rightarrow \infty$, it asymptotically approaches unity. Hence, the distributions of the Kapur-Peierls parameters are generally different from those specified for the R-matrix parameters unless the resonances are well separated to begin with.

The illustrative example given above signifies the complexities in deriving the distributions of the Kapur-Peierls parameters analytically even for simplest possible case consisting of two interfering levels and a single channel. The problem will undoubtedly become far more difficult as the number of levels and channels increases. Such difficulties apparently hinder the applications of the integral method beyond the Breit-Wigner approximation. In the following discussions, other numerical as well as analytical

means concerning the statistical treatment of the unresolved resonances will be described.

V.2.2 Method Based on Conditional Distributions of Cross Sections

One alternative to those methods discussed above is to utilize the statistical properties of cross sections directly if the probability distribution and the associated conditional distributions are known. The theoretical basis can be best illustrated by examining the case of a single nuclide.

Let $h(\sigma_x, \sigma_s, \sigma_t)$ be the joint density function for random variables σ_x , σ_s and σ_t corresponding to the absorption, scattering and total cross sections, respectively. With no loss of generality, it is related to the conditional distributions by

$$h(\sigma_x, \sigma_s, \sigma_t) = h_t(\sigma_t) h_x(\sigma_x | \sigma_t) h_s(\sigma_s | \sigma_x, \sigma_t) \quad (\text{V.2.25})$$

It should be noted that, for reactor applications, the only conditional distributions of interest are $h_x(\sigma_x | \sigma_t)$, and $h_s(\sigma_s | \sigma_t)$, pertinent to the evaluations of the reaction rates and flux. The latter is inferred by the fact that the neutron flux depends only on the scattering and total cross sections, as can be visualized from the slowing-down equation described previously. Hence, the problem is reduced to the specifications of the distribution of the total cross section and conditional distributions of partial cross sections for a given value of σ_t . Conceptually, these distributions, in principle, can be deduced from the known statistical properties of resonance parameters discussed in the previous section via the transformation of variables provided the pertinent Jacobian can be defined. The actual evaluations, however, are obviously difficult because of the extremely complex relationship between the cross section and the corresponding resonance parameters. The temperature dependence of cross sections further complicates the matter.

(1) Direct Numerical Method

One direct means of evaluating these distributions widely used in reactor applications is via the numerical techniques originally proposed by Levitt [30]. The procedure involves generations of many resonance 'ladders' from the known distributions of resonance parameters described previously, whereby $h_t(\sigma_t)$ and conditional distributions can be computed numerically in various energy intervals covering the unresolved energy range. The quantity $h_t(\sigma_t)$ signifies the probability of finding a value of total cross section between σ_t and $\sigma_t + d\sigma_t$ whereas the quantity $h_x(\sigma_x | \sigma_t)$ represents the probability of finding a value of the partial cross section of reaction process x between σ_x and $\sigma_x + d\sigma_x$ at the given value of σ_t . It is important to realize, however, that the conditional distributions so obtained must be stored in three-dimensional arrays, which can require exceedingly large storage space and multi-dimensional interpolation schemes when applied to practical calculations. Fortunately, for the purpose of computing flux and reaction rates, only $h_t(\sigma_t)$ and the conditional means are required. This can be readily illustrated by examining the simple case of the NR-approximation for the case of one nuclide

$$\langle \frac{\sigma_x}{\Sigma_t} \rangle_{E_0} = \int_0^{\sigma_t^{(\max)}} \frac{E[h_x(\sigma_x | \sigma_t)] h_t(\sigma_t)}{\Sigma_t} d\sigma_t, \quad \langle \frac{1}{\Sigma_t} \rangle_{E_0} = \int_0^{\sigma_t^{(\max)}} \frac{h_t(\sigma_t)}{\Sigma_t} d\sigma_t \quad (\text{V.2.26})$$

where the conditional means of the partial cross section is defined as

$$E[h_x(\sigma_x | \sigma_t)] = \int_0^{\sigma_x^{(\max)}} \sigma_x h_x(\sigma_x | \sigma_t) d\sigma_x \quad (\text{V.2.27})$$

Here, the relevant statistical descriptions of practical importance are the marginal probability distribution of the total cross section and the conditional means of the partial cross section, both of which are a function of σ_t alone. Thus, one only needs to pre-compute these quantities for each statistically uncorrelated nuclide at various energy intervals and a given temperature. The results can then be stored in simple tabulated forms in two-dimensional arrays from which the averages can be computed.

This method is commonly referred to as the ‘probability table’ method [30]. It is theoretically equivalent to converting the Riemann integral defined by Eq. (V.2.2) to the form of Lebesgue’s integral by transformation of variables through numerical means. The widely used sub-group method [31,32] can be considered as a subset of this method extended into the resolved region as well. From a practical point of view, it is apparently much more efficient than that based on the direct use of resonance ‘ladders’ and is particularly attractive in conjunction with applications using the Monte Carlo techniques. For the latter applications, it is most convenient to store the pre-computed cumulative distribution $H_t(\sigma_t)$ along with its corresponding conditional means at various energy and temperature intervals as a function of σ_t for various nuclides of interest. To ensure that the numerically generated values will reproduce the theoretical expectation values of $\langle \sigma_t \rangle$ and $\langle \sigma_x \rangle$ obtained by direct integration, they are normalized accordingly prior to their deployment. The numerical scheme of Levitt [30] has been used in the VIM-code for Monte Carlo calculations [33] in reactor applications.

(2) Moment Method

The numerical scheme, although conceptually simple, lacks the analytical insight to provide the in-depth understandings of its potential limitations. One attractive alternative to this method that, at least in part, remedies such a shortcoming was proposed by Ribon and Maillard [34]. Instead of generating the ‘probability tables’ from resonance ladders by brute-force, they are constructed by matching the moments of total cross sections and the ‘cross’ moments of partial and total cross sections. For total cross sections, the n^{th} order moment in the form of the Riemann integral is truncated into a form of the discretized Lebesgue integral

$$M_n = \frac{1}{\Delta E} \int_{\Delta E} \sigma_t^n(E) dE = \sum_{i=1}^N p_i \sigma_{ti}^n \quad (\text{V.2.28})$$

for $2N$ values of n with the range of $I < n < I + 2N - 1$ where I can be negative. In all methods discussed in this chapter, the validity of Eq. (V.2.28), of course, is contingent upon the implicit assumption stationarity of the resonance samples. Ribon and Maillard³⁴ conjectured that these

discretized quantities could be viewed as the Gauss quadrature points and weights in conjunction with another integral of the following form:

$$F(z) = \int_{\sigma_i} \frac{p(\sigma_i)}{1 - z\sigma_i} d\sigma_i = \sum_{i=1}^{2N} \frac{p_i}{1 - \sigma_{ii}z} + R_{2N} \quad (\text{V.2.29})$$

which in turn, can be defined unambiguously via the well-known Pade approximation. This can be accomplished by noting that

$$\begin{aligned} F(z) &= \int_{\sigma_i} p(\sigma_i) [1 + z\sigma_i + z^2\sigma_i^2 + \cdots + z^k\sigma_i^k + \cdots] d\sigma_i \\ &= M_0 + M_1z + M_2z^2 + \cdots + M_{2N-1}z^{2N-1} + R_{2N} \\ &= 1 + z \sum_{i=1}^N p_i\sigma_{ii} + z^2 \sum_{i=1}^N p_i\sigma_{ii}^2 + \cdots + z^{2N-1} \sum_{i=1}^N p_i\sigma_{ii}^{2N-1} + R_{2N} \end{aligned} \quad (\text{V.2.30})$$

The above equation serves two purposes. First, by knowing the exact values of $2N$ moments, it is possible to define a set of Gauss quadrature coordinates and weights rigorously so that, for sufficiently large number of N , the integral $F(z)$ can be evaluated accurately. Secondly, the equation also relates various moments in the quadrature form defined by Eq. (V.2.28) to the integral defined by Eq. (V.2.29). The assertion here is that, for sufficiently large N , the same set of (p_i, σ_{ii}) will also provide good estimate of M_n defined in Eq. (V.2.28) for $n < 2N$ as can be inferred by matching each z^k term in Eq. (V.2.30). Because the validity of Eq. (V.2.28) implies that the series defined in Eq. (V.2.30) must converge rapidly for sufficiently large value of $2N$, the latter can be viewed as a natural consequence of the former. The mathematical proof of the former can be shown rigorously as follows while the verification of the latter can certainly be carried out numerically once the set of (p_i, σ_{ii}) is defined.

The finite series of $2N$ terms of moments is expressible in terms of a rational function of order N in the following form according to the Pade-approximation

$$F(z) = \frac{a_0 + a_1z + a_2z^2 + \cdots + a_{N-1}z^{N-1}}{1 + b_1z + b_2z^2 + \cdots + b_Nz^N} = \sum_{i=1}^N \frac{w_i}{1 - z/z_i} + R_{2N} \quad (\text{V.2.31})$$

where z_i and w_i are identified with the poles and residues of the rational function, respectively. It follows, by comparing Eq. (V.2.29) to Eq. (V.2.31), that

$$p_i = w_i, \quad \sigma_{ii} = \frac{1}{z_i} \quad (\text{V.2.32})$$

and the coefficients of the rational function are determined by a system of $2N$ linear equations

$$\begin{cases} a_0 = M_0 \\ a_1 = M_1 + M_0 b_1 \\ \vdots \\ a_{N-1} = M_{N-1} + M_{N-2} b_1 + \cdots + M_0 b_{N-1} \end{cases} \quad (\text{V.2.33})$$

$$\begin{cases} M_N + M_{N-1} b_1 + \cdots + M_1 b_{N-1} + M_0 b_N = 0 \\ \vdots \\ M_{2N-1} + M_{2N-2} b_1 + \cdots + M_{N-1} b_N = 0 \end{cases} \quad (\text{V.2.34})$$

Once these coefficients are known, the poles can be computed by the root finder for the N -th order polynomial and, thus, the corresponding residues can be determined readily. It should be noted that, like other Gauss quadratures based on various orthogonal polynomials, the poles here are also single-valued and lying on the real z -axis. For all $p(\sigma_i) > 0$, p_i must also be greater than zero as pointed out by Ribon and Maillard [34].

As discussed earlier, the conditional distributions are much more difficult to deal with, independent of the method used, because of their multivariate nature. Fortunately, one is only concerned with the conditional means in reactor applications. In the context of the moment-matching method described above, the partial moment must be matched with the discretized quantities defined below

$$M_{n'}^{(x)} = \frac{1}{\Delta E} \int_{\Delta E} \sigma_x \sigma_t^{n'} d\sigma_t = \sum_{i=1}^N p_i x_i \sigma_{ii}^{n'} \quad (\text{V.2.35})$$

where $x_i = E(\sigma_x | \sigma_{ii})$ is the conditional means corresponding to a given value of σ_{ii} . In contrast to the determination of variables p_i and σ_{ii} that requires $2N$ moments, the determination of x_i only requires a total of N partial moments. Thus, given total moment M_n with n defined in the integer domain $D: I < n < I + 2N - 1$, the values of x_i are determined by matching the partial moments $M_{n'}$ with $J < n' < J + N - 1$ and $n' \in D$.

For practical applications, the key issue here is how to choose I and J that are suitable to the problems under consideration. Qualitatively, the physical aspects of interest can be best illustrated via the NR-approximation where $\phi \propto 1/(C + \sigma_t)$. Here, C denotes the constant 'background' cross section in barns per absorber atom for the mixture. In the limit of high dilution, the flux is essentially determined by the power series of σ_t . It follows that the positive moments as well as partial moments must play relatively important roles in the procedure described above. The same argument can be made for the high energy region or for extremely broadening where σ_t may also become relatively small compared to C . In the limit of high concentration, on the other hand, the negative moments may play a more prominent role as the flux is approaching the power series of $1/\sigma_t$. Hence, it is clearly desirable to choose I and J in such a way that both the extreme cases can be covered adequately. Quantitatively,

the choice of I is relatively straightforward because the discretized parameters are unambiguously defined by the quadrature procedure. The choice of J , however, is far more troublesome due to its non-unique nature. Given N , there are apparently many possible choices of J that satisfy the constraint $n' \in D$. Furthermore, the values of x_i must satisfy the following physical condition in order to ensure the internal consistency of the probability tables

$$\sigma_{ii} = \sum_x x_i \quad (\text{V.2.36})$$

where the sum is over all partial reaction processes. Another potential problem is that the positive nature of each individual x_i cannot be guaranteed even if the above condition is met.

For these reasons, extensive investigations have been carried out by Ribon and Maillard [34] to examine various problems pertinent to the applications of this method to reactor calculations. By imposing the conditions

$$\left\{ \begin{array}{l} \int \sigma_t^m dE = \int \sigma_t^{m-1} \sum_x x_i dE \\ \int \sigma_t^n dE = \int \sigma_t^{n-1} \sum_x x_i dE \end{array} \right. \quad (\text{V.2.37})$$

for $n \neq m$, they showed that the internal consistency required by Eq. (V.2.36) is automatically satisfied upon a proper choice of the order of partial moments to be matched. This can be best illustrated by a simple case involving only two entries of the probability tables. For such a case, Eq. (V.2.37) becomes

$$p_1 \sigma_{t1}^m + p_2 \sigma_{t2}^m = p_1 \sigma_{t1}^{m-1} \sum_x x_1 + p_2 \sigma_{t2}^{m-1} \sum_x x_2 \quad (\text{V.2.38})$$

$$p_1 \sigma_{t1}^n + p_2 \sigma_{t2}^n = p_1 \sigma_{t1}^{n-1} \sum_x x_1 + p_2 \sigma_{t2}^{n-1} \sum_x x_2 \quad (\text{V.2.39})$$

Multiplying Eq. (V.2.39) by σ_{t2}^{m-n} and subtracting it from Eq. (V.2.38), one obtains

$$p_1 \left[1 - \left(\frac{\sigma_{t1}}{\sigma_{t2}} \right)^{n-m} \right] \sigma_{t1}^m = p_1 p_1 \left[1 - \left(\frac{\sigma_{t1}}{\sigma_{t2}} \right)^{n-m} \right] \sigma_{t1}^{m-1} \sum_x x_1 \quad (\text{V.2.40})$$

It follows that

$$\sigma_{ii} = \sum_x x_i \quad (\text{V.2.41})$$

for all $n \neq m$ and $\sigma_{t1} \neq \sigma_{t2}$. By extending the argument to tables of arbitrary entries, Ribon and

Maillard³⁴ concluded that, for successive moments M_n of σ_i with n range between $I < n < I + 2N - 1$, one plausible choice is the consecutive order of partial moment n' with range of $J < n' < J + N - 1$ in which J is within the range of $I - 1 < J < I + N$. In the context of Eq. (V.2.37), the consecutive choice means $|m - n| = 1$. Therefore, for given value of I and N , there are several possible choices of n' for which $n' \in D$. Of these choices, one important constraint must be imposed for obvious reason; i.e. the consecutive n' must include the zeroth order moment M_0 in order to reproduce the infinitely dilute value of the partial cross section. Furthermore, the choice of I and J must also take into account the range of dilution signified by the 'background' cross sections in barns per absorber atom of practical interest as mentioned earlier. Upon extensive examinations, Ribon and Maillard [34] recommended that the use of $I = 1 - N$ and $J = -N / 2$ appear to be most satisfactory. They also concluded that the negative values of x_i 's, if any, are usually too small to be of practical concern. In short, the construction of the probability tables, in principle, can be optimized according to one's needs. Aside from providing a convincing mathematical basis for generating the probability tables, one obvious advantage of this moment-matching method over the brute-force method of Levitt [30] should be recognized. If the Breit-Wigner representation is assumed, one can actually evaluate all moments via the integral method presented in the previous section without resorting to the generation of ladders. Thus, a great deal of simplification in computation can be achieved and, at the same time, the statistical uncertainties associated with ladder generations can be avoided, at least for tables of individual nuclide.

Like the 'ladder' method described earlier, the probability table methods here are also subject to uncertainties of both statistical and non-statistical nature. The former are most likely to appear when more than one resonant nuclide appears in the mixture whereas the latter are usually associated with the accuracy of the numerical method used or the inherent non-statistical nature of the self-shielding effects particularly in the relatively low energy region.

V.3 Recent Advances in the Treatment of Unresolved Resonances

From the perspective of reactor applications, two recently developed methods deserve particular attention and further exploration. One method was pioneered by Fröhner [4] on the basis of maximization of the information entropy while the other was developed by Lukyanov et al [5,6] using the 'characteristic' function concept. For our purposes here, it suffices to summarize the theoretical basis of these methods and their practical implications.

V.3.1 Method Based on Information Theory

As discussed in Chapter II, two matrices that determine the properties of the cross section are $R_{cc'}$ and $U_{cc'}$ (or $S_{cc'}$ using Fröhner's notation⁴). Therefore, the statistical properties of the cross section are completely specified if joint density function of the matrix S and/or R are known. The latter can be picture as the product of a probability distribution $P(S | \bar{S})$ and an equally probable a priori, $d[S]$ equivalent to the invariant (differential) volume element in the sample space of S . By utilizing the maximizing of the information entropy and the elegant mathematical theory of matrices developed by Hua Lo-Ken [35], Fröhner [4] was able to derive the generalized distributions of $P(S | \bar{S})d[S]$ and

$P(R|\bar{R})d[R]$ analytically in the closed forms.

The information theory concept was originally developed by Shannon [36] and the idea was later adopted by Jaynes [37] and others for physics applications. One quantity that serves as a measure of indeterminacy of a given distribution in question is called information entropy. In lieu of complete information, one is led to choose a distribution that is maximally non-committal because any other choice would imply the knowledge that is lacking. The maximization of the information entropy subject to constraints of the known information given in terms of expectation values gives a powerful means to construct the probability distributions that satisfy the known macroscopic information on one hand while maintaining the maximum unbiased stance with respect to the unknown knowledge on the other hand. The general features of this approach can be summarized as follows.

For a continuous probability distribution $p(x)$ of a physical quantity x with equally probable a priori within a differential segment dx , the information entropy is defined as

$$H = -\int dx p(x) \ln[p(x)] \quad (\text{V.3.1})$$

The known macroscopic information is assumed the average values $\langle f_k(x) \rangle$ given by

$$\langle f_k(x) \rangle = \int dx p(x) f_k(x), \quad k = 1, 2, \dots, K \quad (\text{V.3.2})$$

where $f_k(x)$ is a known function of x for various events k . The problem of maximizing H subject to the constraint of Eq. (V.3.2) is tailor-made for the method of LaGrange's multiplier with result

$$p(x) = \frac{1}{z} \exp[-\sum_k \lambda_k f_k(x)] \quad (\text{V.3.3})$$

where the normalization function z , also known as the partition function, is defined as

$$z = \int dx \exp[-\sum_k \lambda_k f_k(x)] \quad (\text{V.3.4})$$

and the LaGrange's multiplier λ_k can be determined from a system of equations (usually non-linear)

$$\langle f_k(x) \rangle = -\frac{\partial}{\partial \lambda_k} [\ln(z)] \quad (\text{V.3.5})$$

Hence, the desirable distribution can be derived via this procedure.

Perhaps the most difficult aspect of Fröhner's derivation [4] is to determine the volume elements $d[R]$ and $d[S]$ corresponding to the equally probable a priori in the space of matrices R and S

respectively. As pointed out by Fröhner [4], the work of Hua Lo-Ken [35] turns out to be tailor-made for this purpose. The following discussions are a brief account of how the admirable development pioneered by Hua [35] can be utilized to the problem at hand.

If an arbitrary complex square matrix z of the order $n \times n$ is regarded as a point in $2n^2$ -dimensional real Euclidean space, then the quadratic form corresponding to the line element ds in this space can be written as

$$(ds)^2 = \text{tr}(dzdz^+) = \sum_{\mu, \nu} dx_{\mu} g_{\mu\nu} dx_{\nu} \quad (\text{V.3.6})$$

where z^+ denotes the conjugate transpose of z and $g_{\mu\nu}$ is a metric tensor that connects any differential element dx_{μ} and dx_{ν} with x_{μ} 's denoting all real and imaginary parts of matrix elements of z . The volume element $d[z]$ in the $2n^2$ -dimensional space is of the form

$$d[z] = \sqrt{\det(g)} \prod_{\mu} dx_{\mu} \quad (\text{V.3.7})$$

Such an element is invariant under translation and rotation in the prescribed space. Any other set of square matrices of a particular type forms a manifold in this space. For the present case, the matrices of interest are the real symmetric matrix R and the complex unitary-symmetric matrix S (or U defined previously by Eq. (II.1.17)). A real symmetric matrix of order n has only $n(n+1)/2$ independent elements and, therefore,

$$(ds)^2 = \sum_a (dR_{aa})^2 + 2 \sum_{a < b} (dR_{ab})^2 = \sum_{\mu, \nu} dx_{\mu} g_{\mu\nu} dx_{\nu} \quad (\text{V.3.8})$$

where

$$g = \begin{bmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 2 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 2 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 2 \end{bmatrix} \quad (\text{V.3.9})$$

and

$$\det(g) = 2^{n(n-1)/2} \quad (\text{V.3.10})$$

It follows that

$$d[R] = 2^{n(n-1)/4} \prod_{\mu < \nu} dR_{\mu\nu} \quad (\text{V.3.11})$$

The unitary-symmetric matrix S (or U) is related to R through Eq. (II.1.22). It is important to note that, with exception of the hard-sphere phase shift factor $\exp[-i(\varphi_c + \varphi_{c'})]$, R can be identified as what Hua [35] regarded as the parameter of S . The one-to-one correspondence between R and S is guaranteed for almost all matrices unless the matrix in question forms a manifold of dimension less than $n(n+1)/2$ according to Hua [35]. It is, therefore, possible to express $d[S]$ unambiguously in terms of $d[R]$ by differentiating Eq. (II.1.22) once the hard-sphere phase shift factor is fixed. Following the general description of Hua [35], Fröhner [4] showed that

$$dS_{ab} = 2i \exp[-i(\varphi_c + \varphi_{c'})] [(I - iR)^{-1} dR (I - iR)^{-1}]_{ab} \quad (\text{V.3.12})$$

from which the corresponding $(ds)^2$, $g_{\mu\nu}$ and, thus, $d[S]$ can be found. The resulting $d[S]$ is given as⁴

$$d[S] = 2^{n(n+1)/2} [\det(I + R^2)]^{(n+1)/2} d[R] \quad (\text{V.3.13})$$

which defines the relationship between $d[S]$ and $d[R]$ in the domain of unitary-symmetric matrices. For practical applications, however, Eq. (V.3.11) and Eq. (V.3.13) are inconvenient and it is more desirable to transform them into the ‘polar’ coordinate system defined by Hua [35] in terms of their eigenvalues and eigenvectors. For a real symmetric matrix R , it is possible to find a real orthogonal transformation O that diagonalizes R , i.e.

$$R = O \Lambda O^T \quad (\text{V.3.14})$$

where Λ is a diagonal matrix consisting of real eigenvalues R_a . For convenience, the eigenvalues can be ordered with $R_1 < R_2 < R_3 < \dots < R_n$. By differentiating Eq. (V.3.14), one can relate dR to dO , dR_a and dO^T . Utilizing the orthogonal condition, Hua³⁵ introduced a skew symmetric matrix δO with

$$\delta O = O^T dO = -\delta O^T \quad (\text{V.3.15})$$

so that the differentiation of Eq. (V.55) yields

$$dR = O[d\Lambda + \delta O \Lambda - \Lambda \delta O] O^T \quad (\text{V.3.16})$$

The square of the line segment ds becomes

$$(ds)^2 = \sum_c (dR_c)^2 + 2 \sum_{a < b} (R_a - R_b)^2 \delta O_{ab}^2 \quad (\text{V.3.17})$$

and the corresponding volume element $d[R]$ in the ‘polar’ coordinate system becomes

$$d[R] = 2^{n(n-1)/2} \prod_c dR_c \prod_{a < b} |R_a - R_b| \delta O_{ab}, \quad -\infty < R_1 < R_2 < \dots < R_n, \quad a < b \quad (\text{V.3.18})$$

according to Fröhner [4]. Once $d[R]$ is defined in the ‘polar’ coordinate system, the corresponding $d[S]$ can be specified by substituting Eq. (V.3.18) into Eq. (V.3.13) and by utilizing the following relations:

- (a) The eigenvalues of a unitary matrix are expressible in the form of $\exp(i\mathcal{G}_c)$.
- (b) The volume element is invariant under translation and rotation so that the presence of the hard-sphere phase shift should not alter the outcome. Thus, R_c can be replaced by

$$R_c = i \frac{1 - \exp(i\mathcal{G}_c)}{1 + \exp(i\mathcal{G}_c)} = \tan\left(\frac{\mathcal{G}_c}{2}\right) \quad (\text{V.3.19})$$

- (c) The relationship defined by Eq. (II.1.22) suggests that S (or U) is expressible in terms of power series of R . It follows that R and S are commutative. Hence, the same orthogonal transformation O also diagonalizes S and δO_{ab} remains the same in deriving $d[S]$.
- (d) The determinant of a matrix is equal to the products of its eigenvalues so that

$$\det(I + R^2) = \prod_c (1 + R_c^2) = \prod_c \sec^2 \frac{\mathcal{G}_c}{2} \quad (\text{V.3.20})$$

Thus, the volume element $d[S]$ in the ‘polar’ coordinate system becomes

$$d[S] = 2^{n(n-1)/2} \prod_c |\exp(i\theta_a) - \exp(i\theta_b)| \delta O_{ab}, \quad -\pi < \theta_1 < \theta_2 < \dots < \pi \quad (\text{V.3.21})$$

where R_c and $\exp(i\theta_c)$ are eigenvalues of R and S respectively.

It is interesting to note, as pointed out by Fröhner [4], that one general feature of these volume elements when cast into the ‘polar’ coordinate system is the presence of terms involving the differences in their respective eigenvalues. Mathematically, the eigenvalue repulsion can be viewed as a natural consequence generally encountered for a wide range of matrices whenever the ‘polar’ coordinates are introduced. Physically, as pointed out by Fröhner [4], Eq. (V.3.18) leads immediately to the well-known Wigner repulsion if R_{ab} is replaced by the Hamiltonian H_{ab} and R_c by E_λ respectively. This astounding result certainly can be considered to be one of the major developments in nuclear spectroscopy.

For the required constraint, Fröhner⁴ chooses $f(S)$ of the form

$$f(S) = \ln |\det(S - \bar{S})|^2 \quad (\text{V.3.22})$$

so that the constraint becomes

$$\langle f(S) \rangle = 2 \ln(\det T) \quad (\text{V.3.23})$$

where

$$T = I - \bar{S}^+ S \quad (\text{V.3.24})$$

is also known as Satchler's transmission matrix [38]. The quantity $f(S)$ here ensures the utilization of all possible moments of S and the causality relation inferred by the constraint.

Given $d[S]$ and the constraint required, Fröhner showed that both $P(R | \bar{R})d[R]$ and $P(S | \bar{S})d[S]$ can be expressed in terms of a generalized form of the Student's t-distribution. In particular, the latter is given by

$$P(S | \bar{S})d[S] = C'_n \left[\frac{\det T}{\det |I - \bar{S}^+ S|^2} \right]^{(n+1)/2} d[S] \quad (\text{V.3.25})$$

where

$$C'_n = 2^{-n(3n+1)/4} C_n \quad (\text{V.3.26})$$

$$C_n = \pi^{-n(n+1)/4} \frac{\Gamma(n+1)/4}{\Gamma(1/2)} \prod_{c=1}^n \frac{\Gamma(n-c+1)}{\Gamma[(n-c)/2+1]} \quad (\text{V.3.27})$$

In the limit of one channel (or pure scattering case), the above expression reduces to the Cauchy's distribution and becomes the same as that derived by Lopez, Mello and Seligman [39]. For this simplified case, the distribution of the cross section can be readily derived once $P(S | \bar{S})d[S]$ is specified.

The method, in principle, provides the vehicle to derive analytically the distributions for the 'probability table' method discussed previously. From a practical point of view, however, for two reasons, further exploration is apparently required before such a method can be deployed. First, the extension of this method beyond the simple case of pure scattering can be an insurmountable challenge. Secondly, the applicability of this method to reactor applications must be accompanied by the means to include the Doppler-broadening effect for it to be useful.

V.3.2 Method Based on Characteristic Function

Like the method of Fröhner [4], another unconventional approach based on the ‘characteristic function’ concept to examine the statistical properties of cross sections was recently developed by Lukyanov et al [5,6]. Its potential role for reactor applications also warrants further exploration. Unlike the former, the basic concept is relatively simple and much easier to understand.

The original idea was first conceived by examining the average cross section based on the Reich-Moore formalism [22] for the simple case of one channel. With no loss of generality, one observes that the statistical average of U_{nn} (or S_{nn}) requires the evaluation of $\langle (1-iR)^{-1} \rangle$ (or $\langle (1-iR')^{-1} \rangle$ if the Reich-Moore formalism is used), which can present a problem in the presence of many levels. This problem can be alleviated if one makes use of the relation

$$\langle (1-iR)^{-1} \rangle = \int_0^\infty e^{-t} \langle e^{iRt} \rangle dt \quad (\text{V.3.28})$$

where the average on the right hand side is more amenable to the integration over the Porter-Thomas [11] distribution. By carrying out the averaging process before integration over t , Eq. (V.3.28) is likely to be easier to evaluate. The quantity $\langle e^{iRt} \rangle$ is referred to as the ‘characteristic’ function that can serve another purpose beside the evaluation of the average defined in Eq. (V.3.28). Since the average implies that

$$\langle e^{-t+iRt} \rangle = \int_{-\infty}^\infty e^{-t+iRt} p(R) dR \quad (\text{V.3.29})$$

where $p(R)$ is the probability density function of R . Thus, by knowing the characteristic function, one can, in principle, deduce the probabilities $p(R)$ as well as $p(S)$ via the Fourier transform. For this particular case, it is obvious that these distributions will become Cauchy’s distribution same as those derived by Fröhner⁴ if the characteristic function retains the exponential form.

As pointed out by Lukyanov et al [5,6], the characteristic function concept can be best illustrated by examining a simple example based on the Reich-Moore approximation and the ‘picket fence’ model in which resonances are equally spaced. The equal-spacing assumption makes possible the subsequent combination of terms resulting from the integration over the Porter-Thomas [11] distribution of each resonance into a function of a closed form. This can be accomplished via the following steps: First, for convenience, the Reich-Moore [22] approximation for the case of one channel can be rearranged into the form

$$R' = \sum_{\lambda} \frac{s_n x_{\lambda}}{\varepsilon + \lambda - i s_{\gamma}} \quad (\text{V.3.30})$$

where $s_n = \langle \Gamma_n \rangle / \langle D \rangle$, $s_{\gamma} = \Gamma_{\gamma} / \langle D \rangle$, $\varepsilon = (E_0 - E) / \langle D \rangle$, and $\lambda = (E_{\lambda} - E_0) / \langle D \rangle$ is an integer between $-\infty$ and $+\infty$ if the ‘picket fence’ model is assumed.

Secondly, by substituting Eq. (V.3.30) into Eq. (V.3.28) and integrating over the χ^2 -distribution of one degree of freedom, one obtains [5,6]

$$\langle e^{itR'} \rangle = \int_{-1/2}^{1/2} d\varepsilon \prod_{\lambda=-\infty}^{\lambda=\infty} \left(1 - \frac{2its_n}{\varepsilon + \lambda - is_\gamma} \right)^{-1/2} \quad (\text{V.3.31})$$

It is interesting to note that the infinite product in the integrand can be identified with sinusoidal functions in the closed form given below.

$$\frac{\sin \pi(\varepsilon - is_\gamma - 2its_n)}{\sin \pi(\varepsilon - is_\gamma)} = \prod_{\lambda=-\infty}^{\lambda=\infty} \left(1 - \frac{2its_n}{\varepsilon + \lambda - is_\gamma} \right) \quad (\text{V.3.32})$$

The validity of the above equation can be readily shown by noting the well-known identities:

$$\frac{\sin \pi z}{\pi z} = \frac{1}{\Gamma(1+z)\Gamma(1-z)} \quad (\text{V.3.33})$$

$$\frac{1}{\Gamma(1+z)} = e^{\gamma z} \prod_{n=1}^{\infty} e^{-z/n} \left(1 + \frac{z}{n} \right) \quad (\text{V.3.34})$$

where $\Gamma(z)$ and γ are the gamma function and Euler's constant respectively. The substitution of Eq. (V.3.33) and Eq. (V.3.34) into the left hand of Eq. (V.3.32) will yield the result as given. Thus, the characteristic function becomes

$$\langle e^{itR'} \rangle = \int_{-1/2}^{1/2} d\varepsilon \sqrt{\frac{\sin \pi(\varepsilon - is_\gamma)}{\sin \pi(\varepsilon - is_\gamma - 2its_n)}} \quad (\text{V.3.35})$$

The above integral is readily amenable to the method of residues. It was shown [5,6] that the characteristic function can be evaluated analytically with the result given as follows.

$$\langle e^{iRt} \rangle = e^{-\pi s_n t} \quad (\text{V.3.36})$$

where s_n is the strength function previously defined. It follows that $\langle S_{nn} \rangle$ is immediately reduced to the familiar result given by

$$\langle S_{nn} \rangle = e^{-i2\phi} \frac{1 - \pi s_n}{1 + \pi s_n} \quad (\text{V.3.37})$$

It is also noteworthy that the above scheme can be readily used to confirm the validity causality relation

[6]

$$\langle S_{nn}^k \rangle = \langle S_{nn} \rangle^k \quad (\text{V.3.38})$$

even if the Reich-Moore approximation is assumed.

Similarly, the characteristic function approach can be readily extended to the evaluation of the corresponding average capture cross section by defining [5,6]

$$\begin{aligned} \langle \sigma_\gamma \rangle &= -2 \int_0^\infty dt \int_0^\infty dt' e^{-(t+t')} \left(\frac{\partial}{\partial t} + \frac{\partial}{\partial t'} \right) \langle e^{i(Rt - R^* t')} \rangle \\ &= -2 \int_0^\infty du e^{-u} \int_{-u}^u dv \frac{\partial}{\partial u} F(u, v) \end{aligned} \quad (\text{V.3.39})$$

where $u = t + t'$, $v = t - t'$ and $F(u, v)$ is taken to be the characteristic function for capture defined as

$$F(u, v) = \left\langle \exp \left[i \left(\frac{u+v}{2} R - \frac{u-v}{2} R^* \right) \right] \right\rangle \quad (\text{V.3.40})$$

Upon integration over the χ^2 -distribution of one degree of freedom, one obtains the characteristic function similar to that for the total cross section [5,6]

$$\begin{aligned} F(u, v) &= \int_{-1/2}^{1/2} d\varepsilon \prod_{\lambda=-\infty}^{\lambda=\infty} \left[1 - 2is_n \left(\frac{t}{\varepsilon + \lambda - is_\gamma} - \frac{t'}{\varepsilon + \lambda + is_\gamma} \right) \right]^{-1/2} \\ &= \int_{-\pi/2}^{\pi/2} dx \sqrt{\frac{\sin(x - iy) \sin(x + iy)}{\sin(x - ip) \sin(x + iq)}} \end{aligned} \quad (\text{V.3.41})$$

where $x = \pi\varepsilon$, $y = \pi s_\gamma$, $z = \pi s_n$, $f + zv = p$, and

$$f - zv = q, \quad f = \sqrt{z^2 v^2 + 2zyu + y^2} \quad (\text{V.3.42})$$

By substituting Eq. (V.3.41) into Eq. (V.3.42), one obtains

$$\langle \sigma_\gamma \rangle = \frac{1}{z} \int_y^\infty dp \int_y^\infty dq \exp \left[-\frac{(pq - y^2)}{2\pi s_n y} \right] \sinh(p + q) \phi(p, q) \quad (\text{V.3.43})$$

where

$$\phi(p, q) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} dx \sqrt{\frac{\sin(x-iy)\sin(x+iy)}{\sin^2(x-ip)\sin^3(x+iq)}} \quad (\text{V.3.44})$$

It was shown in Ref. 6 that the quantity $\phi(p, q)$ is directly identifiable with the usual elliptic integral via the following relation

$$\phi(p, q) = \frac{4}{\pi} \frac{\sqrt{\sinh(p+y)\sinh(q+y)}}{\sinh^2(p+q)} (1+\kappa) E\left(\frac{2\sqrt{\kappa}}{1+\kappa}\right) \quad (\text{V.3.45})$$

where

$$\kappa = \sqrt{\frac{\sinh(p-y)\sinh(q-y)}{\sinh(p+y)\sinh(q+y)}} \quad (\text{V.3.46})$$

and $E(X)$ is the elliptic integral of the second kind. Thus, all integrals are again reduced to manageable forms. The well-behaved nature of the elliptic integral can be utilized to simplify the integrand further if one wishes.

The characteristic function approach described above based on a single channel, in principle, can be extended to cases of arbitrary number of channels. The latter will obviously require the inclusion of the determinant and co-factors of the inverse matrix $(I - iR)^{-1}$ when the characteristic function is defined. In fact, it has since been extended to the two channel case by Lukyanov et al [40] using the same basic assumptions. Its potential importance as a possible alternative to the numerically based probability table method is very noticeable. It is important to realize, however, that further explorations, especially in the area of a means to account for the Doppler –broadening, are apparently needed.

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