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AN OVERVIEW OF THE CURRENT STATUS OF
RESONANCE THEORY IN REACTOR PHYSICS APPLICATIONS

by

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AN OVERVIEW OF THE CURRENT STATUS OF RESONANCE THEORY IN REACTOR PHYSICS APPLICATION

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I. 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 lattices become intertwined. The later requires the detailed knowledge of resonance structures of many nuclide of practical interest to the development of nuclear energy.

There has been a great deal of theoretical and practical interest in resonance reaction 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 a natural uranium fueled self-sustaining chain reaction. The observation by Fermi and Szilard 50 years ago, 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, signaled the beginning of the nuclear era. The practical needs have since provided with the motivation for better understanding of the resonance phenomena. Our knowledge in this area has been significantly enhanced by the development of reaction theory, physical theory of reactor, and other related subjects for the past decades. More recently, the significant advances in the new generation computers made possible the investigations of the extremely complex problems unimaginable in the earlier days. In parallel, a great deal of resonance data have become available during the past few years. One key factor responsible for the continuous efforts to improve the resonance data was the emergence of the fast reactor development which requires such information not only for all major actinides but also for structural material over considerably large energy span. Through the cooperative efforts of international nuclear data

communities, the evaluated cross section data and resonance parameters have been systematically compiled into various data files now in existence. Such a development, in turn, will undoubtedly provide the needed basis as well as incentives to further improve the estimations of parameters for the new generation nuclear reactors.

The key issue of the resonance treatment in reactor applications is directly associated with the use of the microscopic cross sections in the macroscopic reactor cells with a wide range of composition, temperature, and geometric configurations. It gives rise to the so called self-shielding effect. The accurate estimations of such an effect is essential not only in the calculation of the criticality of a reactor but also from the point of view of safety considerations. The latter manifests through the Doppler effect particularly crucial to the fast reactor development. The task of accurate treatment of the self-shielding effect, however, is by no means simple. In fact, it is perhaps the most complicated problem in neutron physics which, strictly speaking, requires the dependence of many physical variables. Two important elements of particular interest are : (1) a concise description of the resonance cross sections as a function of energy and temperature; (2) accurate estimation of the corresponding neutron flux where appropriate. These topics will be discussed from both the historical as well as the state-of-art perspectives.

II. GENERAL REMARKS ON SELF-SHIELDING EFFECTS

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. In the earlier days of reactor development 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 essentially 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. Fig.1 shows the behavior of the neutron flux as a function of energy in the vicinity of the U^{238} 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 behavior of flux and macroscopic cross section here clearly show that they are anti-correlated. The significant flux depression within the extent of the resonance in question indicates the existence of severe the energy self-shielding effect. The actual absorption rate is far less than what can be expected if the flux depression were not present. 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 in the vicinity of the same resonance. 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 a measure of the degree of the resonance self-shielding effect

$$f = \frac{\langle \sigma_a(E) \phi(E, \mathbf{r}) \rangle_{E, \mathbf{r}}}{\langle \sigma_a(E) \phi_{asym} \rangle_{E, \mathbf{r}}} \quad (1)$$

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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 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. The focus has since been centered around the intricate neutronic balance over a much larger energy span ranging from high keV region down to thermal energy with numerous number of nuclide that exhibit resonance behavior. Thus, one must also deal with interacting 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. Furthermore, it is also noteworthy 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. Secondly, there have been continuous and relentless efforts in the international nuclear data communities in recent years to systematically improve the data base required. 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, it is necessary to modify our 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 approaches on 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 methods 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,

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

over the energy group with width much greater than the extent of resonances for the actinides. 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 :

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

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 multivariant in nature. For the unresolved energy range, all averages must be treated statistically.

From Eq. 3, 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 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.

III. CROSS SECTION REPRESENTATIONS

III.1. A Brief Summary of R-Matrix Representations

In R-matrix theory, the reaction cross section for any incident channel c and exit channel c' is generally expressed in terms of the collision matrix $U_{cc'}$.^{1,2,3,4}

$$\sigma_{cc'} = \pi \lambda^2 g_c \left| \delta_{cc'} - U_{cc'} \right|^2 \quad (4)$$

where g_c and $\delta_{cc'}$ are the statistical factor and the Kronecker delta respectively. The unitary property of $U_{cc'}$ leads to the expression of the total cross section as a linear function of $U_{cc'}$,

$$\sigma_t = \sum_{c'} \sigma_{cc'} = 2\pi \lambda^2 g_c (1 - \Re U_{cc'}) \quad (5)$$

The collision matrix, in turn, can be expressed in terms of the resonance parameter matrix R according to Wigner and Eisenbud.¹

$$U_{cc'} = \exp[-i(\phi_c + \phi_{c'})] \left\{ \delta_{cc'} + iP_c^{1/2} \left[(I - R L^0)^{-1} R \right]_{cc'} P_{c'}^{1/2} \right\} \quad (6)$$

where

$$R_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E} \quad (7)$$

is a real symmetric matrix and

$$L_{cc'}^o = (S_c - B_c + i P_c)\delta_{cc'} \quad (8)$$

The energy-independent parameters $E_\lambda, \gamma_{\lambda c}$ and B_c denote the R-matrix state, reduced width amplitude and arbitrary boundary parameters respectively. Of all parameters given above, ϕ_c, S_c and P_c are momentum-dependent quantities. ϕ_c , hard-sphere phase shift factor, is directly related to the argument of the outgoing wave function at the channel radius whereas S_c , shift factor, and P_c , penetration factor, reflect the real and the imaginary parts of its logarithmic derivative respectively as defined in Table.1. These quantities along with the matrix R specifies the explicit energy dependence of the cross section.

The theories of Kapur-Peierls⁵ and of Humblet-Rosenfeld⁶ are alternatives to the R-matrix formalism, whereby the collision matrix can be expressed as linear combination of the Lorentzian type of rational terms. The principal difference between these two theories is that the Kapur-Peierls parameters⁵ are implicitly energy-dependent whereas the Humblet-Rosenfeld parameters⁶ are independent of energy and the matching radius; the latter, however, contains a 'background' term with unknown energy-dependence. Furthermore, another disadvantage of these formalism is that there is no conclusive statistical theory to describe the behavior of these parameters at present. These factors, in effect, hinder their wider usage in the practical applications. Nevertheless, these formalism are very attractive in the reactor applications because of the well-behaved nature of each Lorentzian terms that lead immediately to the well-known Voigt profile upon Doppler-broadening as one shall see.

III.2. Practical Formalism In Use

Although the formal R-matrix representation is rigorous on the theoretical ground, it is quite obvious that simplifications are apparently required before its deployment as the basis for

nuclear data evaluations and the subsequent usage in the reactor applications.. In the current ENDF/B format, four major formalism pertinent to the treatment of the resonance absorption are allowed, namely, the single level Breit-Wigner (SLBW), multilevel Breit-Wigner, Adler-Adler (AA)⁷ and Reich-Moore⁸ (RM) formalism. These formalism are based on the approximations of the formal R-Matrix theory to various degrees of sophistication. For our purposes here, it suffices to summarize their relevant connections to the theory and their characteristics pertinent to reactor applications.

With exception of the Reich-Moore⁸ formalism, all other three exhibit the similar form as a function of energy and can be considered as the consequences of the approximations of the Wigner' level matrix¹ under various assumptions. For our purposes here, it is convenient to cast them into the pole expansion form either in the energy domain or in the momentum domain (k-plane).

$$\sigma_x = \frac{1}{E} \sum_{f,\gamma} \sum_{\lambda} \Re e \left\{ \rho_{f,\gamma,\lambda}^{(x)} \cdot \frac{-i \sqrt{E}}{d_{\lambda} - E} \right\}; \quad \text{(Energy domain)}$$

$$= \frac{1}{E} \sum_{f,\gamma} \sum_{\lambda} \Re e \left\{ \frac{\rho_{f,\gamma,\lambda}^{(x)}}{2} \cdot \left[\frac{(-i)}{\zeta_{\lambda} - \sqrt{E}} - \frac{(-i)}{\zeta_{\lambda} + \sqrt{E}} \right] \right\}; \quad \text{(Momentum domain)}$$

where $\zeta_{\lambda}^2 = d_{\lambda}$, and the subscript x denotes the type of reaction under consideration. The subscripts f, γ and R will be used to denote fission, capture and compound nucleus (or total resonance) cross sections respectively.

Physically, each individual term retains the general features of a Breit-Wigner resonance upon which the traditional resonance integral concept was premised. The relationship between these pole and residue parameters and the traditional resonance parameters for three major formalism are tabulated in Table II. The use of the complex arithmetics here makes possible a direct comparison of these traditional formalism to the rigorous pole representation to be discussed later. $\rho_{f,\gamma,\lambda}^{(x)}$, however, are different and depend on the approximations assumed.

(1) Single level Breit-Wigner Approximation (SLBW)

It represents the limiting case when the resonances are well isolated. Thus, the level matrix A at a given E can be viewed as a matrix with only one element. In the earlier days of the reactor development, the resonance integrals were also treated as such as long as the neutron flux recovers between resonances. In reality, the resonance cross sections clearly can not be taken as a disjoint set of isolated resonances if the rigor and the continuity of flux are required. Ambiguity can arise as to what constitutes the macroscopic cross sections if one wishes to treat the neutron slowing-down problem in detail over an energy span consisting of many resonances of more than one nuclide. For this reason, the single level description used in practical applications such as that specified in the ENDF/B manual is often given in the context of Eq.9 as a linear combination of Breit-Wigner terms supplemented by the tabulated pointwise 'smooth' data so that the continuous nature of cross sections and thus the flux can be preserved.

(2) Multilevel Breit-Wigner Approximation (MLBW)

It corresponds to the situation in which the inverse of the level matrix is taken to be diagonal. One constraint for SLBW and MLBW of practical interest is that all parameters must be positive. It is worth noting that poles and residues are energy dependent although they are usually taken to be energy-independent in many applications. Otherwise additional terms in the \sqrt{E} -domain would result in all $\ell > 0$ sequences using SLBW and MLBW formalism.

(3) Adler-Adler Approximation⁷ (A-A)

The diagonalization of the inverse level matrix A^{-1} leads directly to the pole expansion defined by Eq.9. Adler-Adler approximation⁷ is equivalent to the Kapur-Peierls⁵ representation in which the poles and residues are assumed to be energy independent⁷. In the context of the

forgoing discussion, it is equivalent to assume the energy - independence of L° in Eq. 8 when the inverse of A^{-1} is considered. The approximation is usually restricted to the s-wave sequences of the fissionable isotopes in the low energy region where the assumption is valid.

(4) Reich-Moore Formalism⁸

For practical applications, the formal R-Matrix representation is obviously difficult to use when many levels and channels are present. The problem has been significantly simplified by the method proposed by Reich and Moore⁸. The only significant assumption made is

$$\sum_{c \in \gamma} \gamma_{\lambda c} L_{cc'}^{\circ} \gamma_{\mu c'} \approx \delta_{\lambda \mu} \sum_{c \in \gamma} \gamma_{\lambda c}^2 L_c^{\circ} \quad (10)$$

which utilizes the presence of large number of capture channels and the random sign of $\gamma_{\lambda c}$. It is consistent with the observed fact that the total capture width distribution is generally very narrow. If one partitions the collision matrix into a 2x2 block matrix arranged in such a way that the upper and lower diagonal blocks consist of only non-capture and capture channels respectively and utilizes Eq.10 as well as Wigner's identity between the channel matrix and the level matrix, the collision matrix can be reduced to the order of $m \times m$ where m is the total number of non-capture channels. The 'reduced' collision matrix remains in the same form except that the real matrix R is replaced by a complex matrix R' and

$$R'_{cc'} = \sum_{\lambda} \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_{\lambda} - E - i \Gamma_{\lambda \gamma} / 2} \quad (11)$$

One consequence of the approximation is that the reduced collision matrix is no longer unitary because $R'_{cc'}$ is complex. For practical applications, it presents no problem since the total cross section can be preserved if the capture cross section is defined as

$$\sigma_{\gamma} = \sigma_t - \sum_{c' \in \gamma} \sigma_{cc'} \quad (12)$$

All parameters retain the physical as well as statistical properties specified by the formal R-matrix theory. The order of the channel matrix is usually no greater than 3x3. Hence, the method is attractive in the data evaluations and, in fact, Reich-Moore parameters have become the backbone of the new ENDF/B-VI data.

However, unlike the other three formalism, resonances defined by the Reich-Moore formalism⁸ can no longer be perceived in the context upon which the traditional resonance theory in reactor physics was based. The direct application of this formalism to reactor calculations not only requires the entry of excessive files of pre-computed, numerically Doppler-broadened pointwise cross sections at various temperature, but also renders useless many well-established methods based on the resonance integral concept. Hence, there is strong motivation to seek remedies so that the newly released Reich-Moore can be fully utilized within the frame work of the existing methodologies.

III.3. Generalization of The Pole Representation

Although any given set of R-matrix parameters including those in the Reich-Moore⁸ form can be numerically converted into parameters of the Kapur-Peierls type⁹, the parameters so obtained, however, are implicitly energy-dependent. With exception of low-lying resonances of few fissionable isotopes, such dependence is generally not negligible. Thus, from practical point of view, the route via the traditional pole expansion is not useful for most of nuclide of interest. However, the desirable representations directly compatible to the traditional forms given by Eq.9 can be derived if the pole expansion is cast into somewhat different light.

(1) Rigorous pole representation¹⁰

One attractive means to preserve the general features of Eq.x and the rigor of the R-matrix description of cross sections is to perform the pole expansion in the k-plane (or momentum domain). The theoretical justification of such a representation is based on the

rationale that the collision matrix must be single-valued and meromorphic in the momentum domain. Any function that exhibits such properties must be a rational function according to the well known theorem in complex analysis. The rational function characteristics are quite apparent if one examines the explicit \sqrt{E} -dependence of the collision matrix U_{cc} defined by Eq.6. By substituting S_l and P_l into Eq.6 and Eq.8, the quantity U_{cc} is expressible in terms of a rational function of order $2(l+1)N$ where N is total number of resonances. This reflects the polynomial nature of the cofactor and the determinant of the inverse level matrix . Thus, one obtains via partial fraction¹⁰,

$$\sigma_t = \sigma_p + \frac{1}{E} \sum_{l,j} \sum_{\lambda=1}^N \sum_{j=1}^{2(l+1)} \Re \left\{ [R_{l,j,\lambda}^{(t)} \cdot e^{-i2\phi_l}] \cdot \frac{(-i)}{p_\lambda^{(t)*} - \sqrt{E}} \right\} \quad (13)$$

and similarly,

$$\sigma_x = \frac{1}{E} \sum_{l,j} \sum_{\lambda=1}^N \sum_{j=1}^{2(l+1)} \Re \left\{ R_{l,j,\lambda}^{(x)} \cdot \frac{(-i)}{p_\lambda^{(t)*} - \sqrt{E}} \right\} \quad (14)$$

for the reaction cross section of process x where $R_{l,j,\lambda}^{(x)}$ and $p_\lambda^{(t)}$ are pole and residue respectively. Note that the complex conjugate of $p_\lambda^{(t)}$ is used here in order to cast the expressions into the form defined by Eq.9. These equations can be viewed as the generalized pole expansion in which all parameters are genuine energy independent and the energy dependence of cross sections is specified explicitly by the rational terms alone.

By comparing Eq. 9 to Eq.13, one is led to the following observation: (1) For the s-wave, both the rigorous pole representation and the traditional formalism consist of identical number of terms with the same functional form in the momentum domain. In particular, the Adler-Adler formalism³ for the s-wave can be considered as the special case of the former when $p_\lambda^{(1)} = -p_\lambda^{(2)}$ and $R_{l,j,1,\lambda}^{(x)} = R_{l,j,2,\lambda}^{(x)}$; (2) For higher angular momentum states, Eq. 13 consists of

$2\ell N$ more terms than those defined by Eq.9. The difference, however, is only superficial. The same number of terms would have been resulted if the detailed energy dependence of the penetration factor and the shift factor had been included in Eq.9. Thus, the traditional formalism, can be considered as the special cases Eq.x under various physical conditions.

Eq.13 and Eq.14 provide the basis whereby any given set of R-matrix parameters, in principle, can be converted into pole parameters although it may not be an easy task in practice. The recent availability of R-matrix parameters in the Reich-Moore form greatly alleviates the numerical difficulties for such conversion process. A computer code WHOPPER based on the Newton-Raphson technique was developed for this purpose. The viability of this procedure has since been demonstrated.

One obvious disadvantage of this method is that as many as $2(\ell+1)$ terms must be considered for each resonance if the cross section is to be evaluated in momentum domain. This is obviously undesirable from the point-of-views of computing efficiency, storage requirement and its amenability to the existing codes for reactor calculations. It is clearly desirable to find the potential means to simplify Eq.14 without sacrificing the needed accuracies.

(2) Simplified Pole Representation¹⁰

To simplify the problems resulting from excessive number of multipole parameters requires better understanding of their fundamental properties. The $2(\ell+1)N$ poles for a given ℓ and J defined in Eq.13 and Eq.14 can be divided into two distinct classes. There are $2N$ s-wave-like poles with sharp peaks and distinct spacings while the remaining $2\ell N$ poles are closely spaced and are characterized by their extremely large imaginary components (or widths). In fact, the contributions of the latter to the sums are practically without any resonance-like fluctuations as if they were a 'smooth' constituent. On the other hand, the s-wave like poles always appear in pairs with opposite signs but not necessarily with the same magnitude. These characteristics provide the valuable basis for simplification.

Let $q_\ell^{(x)}(\sqrt{E})$ denote the contributions from those $2\ell N$ terms involving poles with giant 'width'. Eq.14 can be cast into the same form as that of Humblet-Rosenfeld.⁶

$$\text{where } \sigma_x = \frac{1}{E} \sum_l \Re e \left\{ \sum_J \sum_{\lambda=1}^N \left[R_{\ell,J,1,\lambda}^{(x)} \cdot \frac{2(-i)\sqrt{E}}{(p_\lambda^{(1)})^2 - E} \right] + s_\ell^{(x)}(\sqrt{E}) + q_\ell^{(x)}(\sqrt{E}) \cdot \delta_\ell \right\} ; \sqrt{E} > 0 \quad (15)$$

$$\text{and } s_\ell^{(x)}(\sqrt{E}) = 0 \text{ and } \delta_\ell = \sum_{\lambda=1}^N \sum_{\lambda'=1}^N \left[\frac{R_{\ell,J,2,\lambda}^{(x)}(-i)}{p_\lambda^{(2)}} \text{ for } \sqrt{E} > 0, \frac{R_{\ell,J,1,\lambda}^{(x)}(-i)}{(-p_\lambda^{(1)}) - \sqrt{E}} \right] \quad (16)$$

Hence, for a given range of practical interest, the rigorous pole representation can be viewed as a combination of a 'fluctuating' term consisting of N poles with $\Re p_\lambda^{(1)} > 0$ expressed in the energy domain consistent with the traditional formalism and two 'non-fluctuating' (or 'background') terms attributed to the tails of outlying poles (in reference to the domain $\sqrt{E} > 0$ where calculations are to take place) with negative real component and the poles with extremely large 'width' (or $|\Im p_\lambda^{(i)}|$) for $\ell > 0$ states respectively. The striking behavior of the 'fluctuating' and 'non-fluctuating' components have been confirmed in recent calculations for all major nuclide specified by the Reich-Moore parameters in the ENDF/B VI files.

The smooth behavior of these terms clearly suggests that their energy dependence can obviously be reproduced by other simpler functions within the finite interval of practical interest. It is well known in numerical analysis that the rational functions are best suited to approximate a well behaved function within a finite range. Hence, the obvious choice is to set the approximate functions $\hat{s}_\ell^{(x)}(\sqrt{E})$ and $\hat{q}_\ell^{(x)}(\sqrt{E})$ to be rational functions of arbitrary order. Mathematically, they can be view as the analytic continuations of the original functions $s_\ell^{(x)}(\sqrt{E})$ and $q_\ell^{(x)}(\sqrt{E})$ within domain $\sqrt{E} > 0$. One attractive feature of the proposed method is that the rational functions so obtained can be again expressed in the form of pole expansion via partial fraction, i.e.,

$$\hat{s}_l^{(x)}(\sqrt{E}) = \frac{P_{MM}(\sqrt{E})}{Q_{NN}(\sqrt{E})} = \sum_{\lambda=1}^{NN} \frac{r_{\lambda}^{(x)}(-i)}{\alpha_{\lambda}^* - \sqrt{E}} \quad (17)$$

$$\hat{q}_l^{(x)}(\sqrt{E}) = \sum_{\lambda=1}^{NN} \frac{b_{\lambda}^{(x)}(-i)}{\xi_{\lambda}^* - \sqrt{E}} \quad (18)$$

if $NN > MM$.

The pole and residue parameters so obtained can be viewed as 'pseudo' pole parameters. A code¹⁰ (WHOPJR) based on the MINPACK-package¹¹ has been developed to compute these 'pseudo' pole parameters. To provide sufficient accuracy to cross sections, NN of no greater than 3 is required. Thus, the procedure is conceptually equivalent to conversion of a given set of R-matrix parameters into the Humblet-Rosenfeld-type parameters with the 'background' term explicitly defined.

To verify the viability of the proposed method, extensive studies have been made for practically all nuclide with resonance data specified in the Reich-Moore type that are available in the ENDF/B VI files. With perhaps the only exception of U^{238} , the maximum relative error compared to the exact Reich-Moore cross sections were found to be of the order of 10^{-7} or better. Even for the case of U^{238} , the maximum relative errors seldom exceed 10^{-5} as reported in Ref.10.

III.4. Doppler-Broadening of the Generalized Pole Representation

Either one of the two approaches are usually taken depending on the rigor required. The rigorous broadening must be carried out in the momentum domain whereas the simplified broadening is based on the approximate kernel in the energy domain. In the following discussions, the Doppler-broadened cross sections based on the traditional formalism and the

generalized pole representation will be compared.

(1) Exact Doppler-Broadening

Solbrig¹² has shown that the Maxwell-Boltzmann kernel can be rigorously expressed as

$$S(\sqrt{E}, \sqrt{E'}) = \frac{\sqrt{E'}}{(\pi E)^{1/2} \Delta_m} \left\{ \exp\left[-\frac{(\sqrt{E} - \sqrt{E'})^2}{\Delta_m^2}\right] - \exp\left[-\frac{(\sqrt{E} + \sqrt{E'})^2}{\Delta_m^2}\right] \right\} \quad (19)$$

where

$$\Delta_m = \sqrt{\frac{k T}{A}} = \text{'Doppler width' in momentum space} \quad (20)$$

k - Boltzmann's constant

T - temperature, °K

A - atomic weight

The Doppler broadening of $\sqrt{E}' \sigma_x(\sqrt{E}')$ defined by Eq.9 in the momentum space and that defined by Eq.14 leads immediately to :

Traditional Representation

$$\sigma_x(\sqrt{E}, T) = \frac{1}{E} \sum_{i,j} \sum_{\lambda=1}^N \Re e \left\{ \frac{\rho_{i,j,\lambda}^{(x)}}{2} \frac{\sqrt{\pi}}{\Delta_m} \left[W\left(\frac{\sqrt{E}-\zeta_\lambda}{\Delta_m}\right) - W^*\left(\frac{\sqrt{E}+\zeta_\lambda^*}{\Delta_m}\right) \right] \right\} \quad (21)$$

Generalized Pole Representation

$$\sigma_x(\sqrt{E}, T) = \frac{1}{E} \sum_i \Re e \left\{ \sum_j \sum_{\lambda=1}^N \sum_{j=1}^2 R_{i,j,\lambda,j}^{(x)} \left[\frac{\sqrt{\pi}}{\Delta_m} W\left(\frac{\sqrt{E}-p_\lambda^{(j)*}}{\Delta_m}\right) \right] + q_i^{(x)}(\sqrt{E}) \delta_i \right\} \quad (22)$$

where $W(z)$ is the complex probability integral and is directly related to the usual Doppler-

broadened line shape functions via the following relation

$$W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t} dt \quad (23)$$

$$\Psi(x,y) + i\chi(x,y) = \sqrt{\pi} y W(z) \quad (24)$$

and

$$z = x + iy$$

Under the single level limit, Eq.21 is equivalent to the generalized form of the exact Doppler-broadening defined by Ishiguro¹³. Thus, except for the superficial difference leading to the 'smooth' term $q_i^{(s)}(\sqrt{E})\delta_i$, Eq.21 and Eq.22 have the same functional form, but are characterized by different parameters. From a practical point of view, the computational costs for these equations are expected to be comparable if the 'smooth' term is replaced by the approximation defined by Eq.17 and Eq.18.

(2) Approximate Doppler-Broadening

For most of the existing codes based on the traditional formalism, the Doppler-broadening is generally based on the approximate Gauss kernel defined in the energy domain rather than Solbrig's kernel.¹²

$$M(E_\lambda - E) \approx \frac{1}{\sqrt{\pi}\Delta_E} \exp \left[- \frac{(E_\lambda - E)^2}{\Delta_E} \right] \quad (25)$$

where $\Delta_E = \sqrt{\frac{4kTE}{A}}$ is the Doppler width in the energy domain.

The validity of such a approximation requires the criterion $E \gg \Delta_m$. It has been well established that the use of the Gauss kernel in the energy domain is generally satisfactory for $E > 1$ eV. Thus, only to the Voigt profile per resonance (or pole) is required for any pole representation in the energy domain. The Doppler-broadened cross sections become :

Traditional Formalism

$$\sigma_x^{(x)}(E,T) = \frac{1}{E} \sum_{IJ} \sum_{\lambda=1}^N \Re e \left\{ \sqrt{E} \rho_{IJ,\lambda}^{(x)} \frac{\sqrt{\pi}}{\Delta_E} W \left(\frac{E-d_\lambda}{\Delta_E} \right) \right\} \quad (26)$$

Generalized Pole Representation After Simplification

$$\sigma_x^{(x)}(E,T) = \frac{1}{E} \sum_I \Re e \left\{ \sum_J \sum_{\lambda=1}^N 2\sqrt{E} R_{IJ,\lambda}^{(x)} \frac{\sqrt{\pi}}{\Delta_E} W \left(\frac{E-\epsilon_\lambda}{\Delta_E} \right) + \hat{s}_I^{(x)}(\sqrt{E},T) + \hat{q}_I^{(x)}(E) \cdot \delta_I \right\} \quad (27)$$

where

$$\hat{s}_I^{(x)}(\sqrt{E},T) = \sum_{k=1}^{NN} r_k^{(x)} \left[\frac{\sqrt{\pi}}{\Delta_m} W \left(\frac{\sqrt{E} - \alpha_k^*}{\Delta_m} \right) \right] \quad ; \quad \epsilon_\lambda = [p_\lambda^{(1)*}]^2 \quad (28)$$

Thus, the utilization of the simplified pole representation in the context described above is not only compatible to but also not much more costlier than the traditional methods when the smooth contributions are effectively accounted for.

IV. FLUX DISTRIBUTION IN A REACTOR LATTICE

Once all neutron cross sections as a function of energy and temperature are specified, the flux distribution in a reactor is, in principle, obtainable via the use of the Boltzmann's transport equation. The case in point involves two general problems : (1) determination of the spatial distribution of flux at a given energy resulting from the heterogeneous nature of the reactor lattice; (2) determination of the source distribution as a function of energy at various locations of the lattice. In the following discussion, a brief summary on the practical treatment of this subject will be presented with emphasis on the conceptual aspects of the problem.

IV.1. Integral Transport Equation

The determination of the detailed flux distribution as a function of energy and space over

the entire reactor is generally a insurmountable task. Some simplified assumptions are apparently required. For practical applications, 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. Without loss of generality, the obvious starting point is the steady-state Boltzmann's transport equation¹⁴. Because it is a linear first order partial differential equation, the solution can be cast into the following form via the method of characteristics.

$$\phi(\bar{r}, \bar{\Omega}, E) = \int_0^\infty \exp\left[-\int_0^{\zeta'} \Sigma_t(\bar{r}-\zeta'' \bar{\Omega}, E) d\zeta''\right] s(\bar{r}-\zeta' \bar{\Omega}, \bar{\Omega}, E) d\zeta' \quad (29)$$

where

$$s(\mathbf{r}, \mathbf{\Omega}, E) = \int \int dE' d\mathbf{\Omega}' \Sigma_s(\mathbf{r}, E') f(\mathbf{r}, E' \rightarrow E, \mathbf{\Omega}' \rightarrow \mathbf{\Omega}) \phi(\mathbf{r}, \mathbf{\Omega}, E') + Q(\mathbf{r}, \mathbf{\Omega}, E) \quad (30)$$

is the source term consisting of that due to elastic scattering as denoted by the term with double integrals, and that due to inelastic scattering and fission processes as denoted by $Q(\mathbf{r}, \mathbf{\Omega}, E)$. $\Sigma_t(\mathbf{r}, E)$ and $\Sigma_s(\mathbf{r}, E)$ are the macroscopic total and elastic scattering cross sections respectively.

This equation is generally referred to as the integral transport equation. With exception of perhaps the Monte Carlo method, the expression involving extremely complex dependence in phase space is obviously far too complicated for routine applications. One plausible simplification is to assume that the scattering is taken to be isotropic. The isotropic scattering assumption allows the elimination of the angular dependence by integration of $\bar{\Omega}$ over all solid angles so that the scalar flux becomes a function of \bar{r} and E only. The scalar flux after integrating over $\bar{\Omega}$ becomes¹⁴

$$\phi(\bar{r}, E) = \int_{4\pi} \phi(\bar{r}, \bar{\Omega}, E) d\bar{\Omega} = \int \Lambda(|\bar{r}-\bar{r}'|) S(\bar{r}', E) d\bar{r}' \quad (31)$$

where $\Lambda(|\bar{r}-\bar{r}'|)$ usually referred to as the transport kernel is defined as

$$\Delta(|\vec{r}-\vec{r}'|) = \frac{\exp[-\Sigma_t(\vec{r}, E) |\vec{r}-\vec{r}'|]}{|\vec{r}-\vec{r}'|^2} \quad (32)$$

Physically, Eq.31 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. Thus, the determination of the detailed flux distribution require a the computation of the elastic scattering source and that of the inter- and intra-cell neutron transport. For practical purposes, the problem is still far to too complicated because the space and energy dependence are still hopelessly inter-twined. One convenient way to alleviate the problem is to discretise the energy and space dependence. The discretization of its spatial dependence leads to the widely used collision probability method and the interface current method.

IV.2. Collision And Transmission Probabilities in A Lump

Conceptually, 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 defined in Eq. 31. For our purpose here, it suffices to focus on the theoretical basis leading to various methods currently in use.

From the perspective of resonance treatment in which the energy mesh under consideration is generally much finer than the extent of the resonance, 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 probability¹⁵ for a lump is defined as the average collision rate corresponding to the uniform source of unit strength, i.e.

$$J_k^+(E) = \sum_{j=1}^N V_j S_j(E) P_{k \leftarrow j}^{v \leftarrow v}(E) + \sum_{t=1}^M A_t J_t^-(E) T_{k \leftarrow t}^{s \leftarrow s}(E) ; \quad k \in M \quad (40)$$

subject to the following boundary condition

$$J_k^+ = \sum_{t=1}^M B_{kt} J_t^- \quad (41)$$

where N and M are the total number of regions and surfaces respectively. For the sake of clarity, the superscripts V←V and S←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 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

$$C_i(E) = \sum_{j=1}^N V_j S_j(E) P_{i \leftarrow j}^{v \leftarrow v}(E) + \sum_{t=1}^M A_t J_t^-(E) P_{i \leftarrow t}^{v \leftarrow s}(E) ; \quad i \in N \quad (42)$$

where the corresponding flux is related to $C_i(E)$ as follows

$$\phi_i(E) = \frac{C_i(E)}{\Sigma_i(E)} \quad (43)$$

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 .40. 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 here 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.35 as one shall see.

IV.3. Slowing-Down of Neutrons By Elastic Scattering

In the resonance region of practical interest, the neutron source term defined in Eq.35 is dominated by that attributed to the elastic scattering process. Under the assumption of isotropic scattering, the elastic scattering source is expressible by the following integral equation of the convolution type in the lethargy (logarithmic in energy) domain^{14,17},

$$F(u) = \sum_{i=1}^I \int_{u-\epsilon_i}^u du' F(u') \frac{\Sigma_{si}(u')}{\Sigma_i(u')} K_i(u-u') \quad (44)$$

where $F(u) = \Sigma_i(u) \cdot \phi(u)$ is known as the collision density and I is the total number of nuclide in the mixture. The quantity K is the scattering kernel defined by

$$K_i(u-u') = \begin{cases} \frac{e^{-(u-u')}}{1-\alpha_i} du, & 0 \leq u-u' \leq \epsilon_i \\ 0, & elsewhere \end{cases} \quad (45)$$

where ϵ_i denotes the maximum scattering interval of the i^{th} nuclide in the lethargy domain.

Because of the complex nature of the Doppler-broadened cross sections in the presence of resonances, no rigorous analytical solution appears feasible. Therefore, one must resort to the use of numerical solution at the energy meshes much finer than the extent of a resonance if rigor is required. Otherwise, one must rely approximate methods at the expense of rigor. In fact, the accurate account of such a problem constituted one of the greatest obstacles in the treatment of the resonance absorption in the earlier days of the reactor development.

In the past decade, however, the astounding advances in our computational capabilities along with the development of highly efficient numerical algorithms, has made such a problem much less inhibitive.

IV.4. Approximation of Neutron Flux

In the earlier days of reactor development, two crucial areas required simplifications before the resonance treatment could be carried out. One area was a viable but simple solution to the slowing-down equation and another area was an approximate means to account for the collision probability in a unit reactor cell. These approximations are physically equivalent to the parameterization of the flux distribution in energy and space.

1. Neutron Slowing-Down In Infinite Homogeneous Medium

The usual starting point¹⁷ is to examine the distribution in an infinite homogeneous medium consisting of background material with 'constant' cross section along with fuel in which the absorption is attributed to an isolated resonance.

(1) Narrow-Resonance (NR-) Approximation¹⁷

By examining an isolated resonance in an infinite-homogeneous mixture with its extent much smaller than the maximum energy loss due to elastic scattering, it is quite obvious that the first order approximation to the slowing-down equation defined by Eq.44 can be taken to be constant. It follows immediately that the flux for such a simple case must be inversely proportional to the macroscopic total cross section according to the definition of the collision density, i.e.

$$\phi(E) \propto \frac{1}{\Sigma_t(E) E} \quad (46)$$

This is generally referred to as the narrow-resonance (or NR-) approximation. Physically, it provides an extremely simple illustration of the fact that the flux and the resonance cross section are anti-correlated. This method is particularly useful in the fast reactor applications where the assumption is valid for the majority of resonances considered.

(2) Infinite Mass Approximation¹⁷

In another extreme when the mass of the absorber atom approach infinity, the corresponding scattering kernel in the slowing-down equation becomes a δ -function. Consequently, the flux is reduced to a form similar to Eq.46, i.e.

$$\phi(E) = \frac{1}{[\Sigma_p^{(bk)} + \Sigma_a(E)] E} \quad (47)$$

where $\Sigma_p^{(bk)}$ is the macroscopic potential scattering cross section of the background material only.

The only difference between Eq.46 and Eq.47 is the absence of the scattering cross section of the absorber. Physically, it is equivalent to the situation where the extent of the resonance becomes large compared to the scattering interval. Therefore, it is sometimes referred to as the 'wide-resonance' approximation. Mathematically, it retains the similar functional form which can be used as the basis for a more realistic approximation.

(3) Intermediate Resonance (IR-) Approximation

Another widely used approximation is the 'intermediate resonance' approximation pioneered by Goldstein and Cohen¹⁸. The rationale is to utilize a parameterization scheme to unify the strikingly similar flux shapes exhibited by narrow and wide resonances. It is reasonable to conjecture that the neutron flux across a resonance generally resembles the following approximate form

$$\phi(E) = \frac{\Sigma_p^{(bg)} + \lambda \Sigma_p^{(r)}}{[\Sigma_p^{(bg)} + \Sigma_a^{(r)}(E) + \lambda \Sigma_s^{(r)}(E)] E} \quad (48)$$

where λ is a parameter characteristic of the resonance in question yet to be determined. The expression obviously satisfies the narrow and wide-resonance limits as λ approaches 1 and 0 respectively. Hence, the key question here is how to define λ in order to reflect the characteristics of the resonance in the slowing-down process. Goldstein and Cohen¹⁸ argued that one way to determine it is via a transcendental equation of the form

$$\int_{-\infty}^{\infty} \Sigma_a^{(r)}(E) \phi^{(1)}(E) dE = \int_{-\infty}^{\infty} \Sigma_a^{(r)}(E) \phi^{(2)}(E) dE \quad (49)$$

where $\phi^{(1)}(E)$ is the first order iterant taken to be that defined by Eq.48 and $\phi^{(2)}(E)$ is the second order iterant upon substitution of the former into the slowing-down equation. Thus, the parameter λ serves as a vehicle to account, at least in part, for the higher order effects of the elastic scattering process sometimes referred to as the Placzek oscillations. It should be noted that the solution of the transcendental equation is by no means simple unless the integral can be

evaluated analytically. One obvious that hinders such a procedure is the complexity of the Doppler-broadened line-shape functions. Therefore, the evaluation of λ in most of practical applications is either based on the Lorentzian shape functions at zero temperature or on the approximate broadening functions.

2. Rational Approximation of Collision Probability And Equivalence Relation

Another important development in the earlier days is the approximate means of treating the neutron transport problems in a reactor cell, particularly those in a two region cell consisting of a fuel pin surrounded by moderator. From practical point of view, two essential elements are¹⁷ : (1) simplification of the method for evaluating the collision probabilities; (2) an approximate model to represent the flux distribution in both energy and space. The former can be accomplished via the use of rational approximation while the latter is the natural consequence of applying the rational approximation to the two-region slowing-down equation defined by Eq.35. The original development leading to these approximations was pioneered by Wigner.

From the definition of the escape probability, Wigner conjectured that one plausible approximation for P_{esc} is a simple rational function in terms of the mean-free path across the region in question, i.e.

$$P_{esc} \approx \frac{1}{1 + \Sigma_i(E) l} \quad (50)$$

The obvious rationale was based on the fact that the above expression simultaneously satisfies the small argument limit commonly referred to as 'white' limit as well as the asymptotic limit also known as the 'black' limit, namely, $\lim_{\Sigma_i l \rightarrow \infty} P_{esc} \approx 1 - \Sigma_i(E) l$ and $\lim_{\Sigma_i l \rightarrow 0} P_{esc} \approx 1 / \Sigma_i(E) l$

respectively. One most striking consequence of this rational approximation is that it leads to the so-called equivalence relation, whereby the two-region coupled slowing-down equation implied by Eq.35 reduces unambiguously to the form of Eq.44 if the collision density in the moderator is taken to be constant. The only difference between the resulting integral equation and that for infinite homogeneous medium is that one must replace Σ_p for the homogeneous medium by $\Sigma_p^{pin} + 1/l$. Thus, the equivalence relation provides an extremely simple vehicle to account for the

neutron transport from a fuel pin to the moderator in terms of its average chord length while the slowing-down equation retains the same form as the case of the infinite homogeneous medium.

The 'equivalent' slowing-down equation is obviously amenable to all approximations described above. For convenience, a quantity known as 'equivalent' potential scattering cross section, denoted by $\sigma_p^{(eq)}$, was introduced for application of the equivalence relation,

$$\sigma_p^{(eq)} = \frac{\Sigma_p^{(pin)} + \Sigma_{esc}}{N^{(ab)}} \quad (51)$$

where Σ_{esc} , referred to as 'escape cross section', is equal to $1/\bar{l}$ if the Wigner approximation is used and $N^{(abs)}$ is the concentration of the absorber.

The significant simplification demonstrated by such an approach had motivated a great deal of work to improve the accuracy of the Wigner approximation. The most commonly used method is to introduce additional correction factors into the original expression of Σ_{esc} so that¹⁹

$$\Sigma_{esc} = \frac{1}{l} \frac{a(1-C)}{1+(a-1)C} \quad (52)$$

where C and a are generally referred to as the Dancoff factor^{16,20} and Bell factor respectively. Physically, the Dancoff factor represents the probability that a neutron leaving the surface of the pin in question will reach any neighboring pin without suffering any collision in the moderator. The fact that this quantity is a function of the optical path of the moderator alone and, thus, can be considered as energy independent greatly simplifies the problem involved. The Bell factor, on the other hand, represents the correction attributed to the 'non-black' nature of the neighbor pins so that a neutron still can re-enter into the moderator. For the repeated-infinite lattice usually assumed, a is taken to be constant depending only on the configuration of the fuel lump. The parameterization of this type no longer poses a great deal of problem since the availability of many Monte Carlo codes with great flexibility on the geometric configuration of the lattices. Since Eq.52 does not change the basic feature of the rational approximation, the equivalence relation for a two region cell remains valid.

Another approach to approximate the collision (or escape) probability is to use the multiple rational terms numerically equivalent to the well-known Pade approximation where $\Sigma_i(E)$ is the variable. From the point of view of accuracy, the higher order rational function can clearly provide better estimate of the quantity in question. Nevertheless, the method is not free of other complication. It should be noted that the equivalence relation can no longer be rigorously derived beyond the NR-approximation if the collision probability is represented by more than one single rational term. Generally speaking, the validity of the equivalence relation become less apparent for unit cells containing more than one region with different resonance absorbers if one ventures beyond the NR- approximation.

V. METHODS FOR TREATING RESONANCE ABSORPTION

Various deterministic methods differ only in the rigor by which the detailed flux is computed. They are either used in conjunction with the multi-group approach based on the effective cross section concept or the continuous slowing-down approach based on the resonance integral concept. In the following discussions, a brief summary is presented with emphasis on the conceptual aspects of the method.

V.1. Integral Transport Theory Approach

In principle, the most rigorous method for computing the effective resonance cross sections is via the use of the integral transport method along with the numerical solution of the slowing-down equation at extremely fine mesh interval compared to the extent of each resonance (or pole where appropriate). At this point in time, the detailed resonance treatment is still limited to the idealized case of repeated unit cell with convex geometries in the one-dimensional domain.

One the most attractive method of treating the detailed flux in a unit cell to date is via the use of the interface-current approach described earlier. Because of its importance to reactor applications, a brief summary is presented.

(1) Neutron Transport In A Generic Configuration

One of the most useful unit cell configurations of practical interest is the case of an infinite cylinder discretized into tubular regions. From the perspective of collision/transmission probability evaluations, the neutron transport within the cell is determined by the dimension and composition each annular region in the polar coordinate system if the integration of Eq.33 is carried out along the axial direction. An annular segment can be considered as the most generic configuration in reactor applications because of its unique properties^{21,22}. In the limit when both the 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 reactor applications.

To compute the detailed flux distribution, a cell can be divided into a total of K annuli. In the context of Eq.40, any annular region k is sandwiched between the inner and outer surfaces; i.e. $N=1$ and $M=2$. Thus, the pertinent collision and transmission probabilities depend on the macroscopic cross section, inner and outer radii of the annulus in question while the interaction effects between regions manifest through the simple boundary condition imposed. The resulting current equations can be symbolically represented in the following matrix form^{19,22},

$$T J = P S \tag{52a}$$

where T , P , J and S denote the transmission probability, collision probability, current and neutron source respectively. It should be noted that the current for any given region k consists of an outgoing component as well as an incoming component impinging on the outer surface. Hence, Eq.52a represents a system of $2K$ linear equations. As described in Ref.21 and Ref.22, the transmission probability T is specified by three elements, namely, T^{oo} , T_k^{oi} and T_k^{io} which represent the transmission probabilities from outer-to-outer, inner-to-outer, and outer-to-inner respectively. These integrals can be written in the form of the 'incomplete' integral of Euler-type as a function of the mean free path and radii of the region. The corresponding collision probability of the region P_k can be obtained via the reciprocity relation defined by Eq.40. Thus, within the context of Eq.x, T for the annulus bound by two surfaces must be tri-diagonal in nature so that Eq.x is readily amenable to the numerical solution via the simple Gauss elimination procedure followed by backward substitution once the source at a given energy mesh is known. This method, along with the rigorous numerical algorithm for solving the slowing-down equation

described in the following section, has been successfully deployed in the RABBLE-code as well as the RABANL option of the MC^2-2 code for routine reactor applications.

(2) Numerical Solution of the Slowing-Down Equation

One representative algorithm²² that had successfully demonstrated its worth in treating the slowing-down equation was developed by Kier and was subsequently incorporated into the MC^2-2 code¹⁹. The method is exceeding efficient inspite of its surprising simplicity.

The basic assumption is to divide the lethargy domain into equally-spaced hyper-fine groups (hfg) with width Δu much smaller compared to the extend of any resonance in question so that the macroscopic cross sections and thus the collision density can be taken as constant within such an interval. Hence, it is possible to discretize the collision density defined by Eq.44 in terms of average quantities for the hfg under consideration. It was shown that the computation of the discretized slowing-down equation can be significantly expedited via the following recurrence relation

$$F_j = \{F_{j-1} e^{-\Delta u} - (\bar{K}_1 - \bar{K}_s e^{-\Delta u}) \alpha (\Sigma_s \phi)_{j-1-L} + \bar{K}_1 (\Sigma_s \phi)_{j-1} - \alpha \bar{K}_s (\Sigma_s \phi)_{j-L}\} / [1-r_j] \quad (53)$$

where $r_j = \bar{K}_s [\Sigma_s / \Sigma_{tj}]$ and $\bar{K}_1 = (1 - e^{-\Delta u})^2 / (1 - \alpha)$. \bar{K}_s here denotes the average scattering kernel corresponding to the effective probability of self-scattering within the j^{th} hfg in question and L is the total number of number of hyper-fine group within the scattering interval of a nuclide. For the case of a mixture consisting of maay nuclide, the above equation must include the linear combination of the appropriate constituents. Hence, the collision density in the j^{th} hfg requires only that of the previous hfg ($j-1$) 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.

V.2 Resonance Integral Concept

In contrast to the more rigorous approach, the more widely used resonance integral concept provides better analytical in-sight on the subject of resonance absorption. The fundamental idea was premised on the assumption that the resonance absorption can be treated

individually for each contributing resonance with known physical attributes as a function of energy and temperature. For an isolated resonance in an infinite homogeneous medium illustrated in Fig.1, the resonance escape probability, which serves as a measure of the fraction of neutrons scattered past the resonance without being absorbed, can be simply expressed as¹⁷

$$P_{esc} = 1 - \int_{-\infty}^{\infty} \Sigma_a(E) \phi(E) dE \quad (54)$$

where the integral is commonly referred to as the absorption probability for an isolated resonance. That is to say that the initial neutron source must be attenuated by P_{esc} when neutrons are slowed down past the resonance via elastic scattering. For an energy interval containing more than one resonance, the flux distribution can be obtained via the step-wise attenuation the initial source by the product $\prod_i P_{esc}^{(i)}$. This provides a simplistic description of the role of each resonance and

becomes the basis of the continuous slowing-down approach widely used in reactor applications.

Traditionally, the resonance integral that characterizes the absorption process is defined as the absorption rate attributed to a given resonance, i.e. the integral in Eq.54, normalized by the asymptotic flux above the resonance. Analytical behavior becomes more transparent if one of the approximate methods described earlier is introduced. Since all three approximations exhibit the same basic form as a function of $\Sigma_a(E)$ and are equally amenable to the use of the equivalence relation, it should suffice to examine the case on the basis of the NR-approximation for illustration purposes.

If the Briet-Wigner representation is assumed, the resonance integral for a given resonance r in an infinite homogeneous medium is defined as¹⁷

$$(RI)_{NR} = \frac{\sigma_p \Gamma_{ar}}{E_r} J(\theta_r, \beta_r, a_r) = \frac{\sigma_p \Gamma_{ar}}{E_r} \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\theta_r, x)}{\beta_r + \psi(\theta_r, x) + a_r \chi(\theta_r, x)} dx \quad (55)$$

where $\Gamma_{ar} = \Gamma_{\gamma r} + \Gamma_{fr}$, $\beta_r = \Sigma_p / [\Sigma_{0r} \cos 2\phi_l]$ and $a_r = \tan 2\phi_l$. Here, Σ_{0r} is the total macroscopic peak resonance cross section of the level r and σ_p is the macroscopic potential scattering cross section per absorber atom. hence, the J-integral provides a concise mathematical description of

resonance absorption as a function of reactor composition as well as temperature.

The emergence of fast reactor development has introduced a somewhat different scenario that clearly affects our perception of the resonance integral concept. The question arises as to whether a resonance can always be treated as isolated. This makes necessary the inclusion of the mutual self-shielding effect attributed to the neighboring resonances. Another potential problem resulting from the relatively more important role for the fissionable isotopes is the questionable validity of the Breit-Wigner representation when applied to the more closely spaced resonances. The only consolation is that the NR-approximation is likely to be more plausible for majority of resonances in the relatively high energy region.

For these reasons, a plausible means to resolve these problems was proposed²³. The most important criterion for generalization of the resonance integral concept is that one must be able to represent the cross section in terms of linear combination of the Breit-Wigner terms generally achievable via the pole expansion scheme described in section III. Thus, each resonance or pole still retains the same physical properties as those of a Breit-Wigner resonance. From the perspective of resonance integral, each term still can be considered as 'separate' entity provided that the overlapping effects of the neighboring resonances are taken into account in the evaluation of the detailed flux. It follows that, through the use of the approximate flux in rational form, a generalized J-integral denoted by J^* can be expressed as²³

$$J_k^* = J_k(\beta_k, \theta_k, a_k, b_k) - \sum_{k' \in k} O_{kk'} \quad (56)$$

where

$$J(\beta_k, \theta_k, a_k, b_k) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\theta_k x_k) + b_k \chi(\theta_k x_k)}{\beta_k + \psi(\theta_k x_k) + a_k \chi(\theta_k x_k)} dx_k \quad (57)$$

$$J_k(\beta_k, \theta_k, a_k, b_k) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{\psi(\theta_k x_k) + b_k \chi(\theta_k x_k)}{\beta_k + \psi(\theta_k x_k) + a_k \chi(\theta_k x_k)} dx_k \quad (58)$$

$$r_{k'} = \frac{\psi(\theta_{k'}, x_{k'}) + a_{k'} \chi(\theta_{k'}, x_{k'})}{\beta_k + \psi(\theta_k, x_k) + a_k \chi(\theta_k, x_k) + \sum_{k' \in k} A_{k'} [\psi(\theta_{k'}, x_{k'}) + a_{k'} \chi(\theta_{k'}, x_{k'})]} \quad (59)$$

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 imaginary part of the k th residue for the absorption cross section to that of the real part if the pole representation or the Adler-Adler approximation are used, is zero otherwise. All parameters retain the same physical meaning described previously according to the type of representation used. Physically, the generalized J^* -integral consists of an 'isolate' 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 $\sum_{k' \in k} O_{kk'}$ to

account for the mutual self-shielding effect due to the neighboring poles. All these integrals are readily amenable to the efficient quadrature described in Ref.23.

Thus, the coexistence of the resonance integral approach and the more rigorous integral transport theory approach is possible as long as the cross sections can be represented by the linear combination of the Breit-Wigner-like terms.

VI. 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 application. The methods for treating this phenomenon can be viewed as a natural extension of the statistical theories of average cross sections. More recently, new frontiers on this subject appear to be on the horizon as the work pioneered by Fröhner²⁴ on the basis of information theory and that by Lukyanov et al^{25,26} using the 'characteristic' function concept have offered 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 calculational methods.

VI.1 Nature of the Problem

Two average quantities of interest in reactor calculations are $\langle \sigma_x \phi \rangle_{E,F}$ and $\langle \phi \rangle_{E,F}$ which represent the expectation values 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} respectively. From the statistical theory of spectra, the distributions of these parameters are well-known. The distribution of E_i for a given spin state is characterized by the Wigner distribution and by the long-range correlation described by Dyson²⁷. γ_{ci} 's are statistically independent and normally distributed with zero means and variance of unity according to Porter and Thomas²⁸. 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 $\langle \gamma_{ci}^2 \rangle$ and through the explicit knowledge of the behavior of σ_x and ϕ , the expectation values of interest are, in principle, completely specified.

Two special problems must be considered in the applications of the statistical theory to the self-shielded cross sections. First, the attenuation of flux within the region under consideration, strictly speaking, implies that the events are actually deterministic in nature. It should be noted that the statistical averaging implicitly requires the stationarity of the quantity within the energy interval under consideration. The question may arise since the flux will attenuate within the interval containing many resonances. The statistical description 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 measurements such

as the Doppler reactivity experiments. One closest analogy is perhaps the transmission and self-indication measurements which, 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 bench-marking purposes.

VI.2 Existing Methods---Basis And Problems

The averages of interest can be either cast into the form of Riemann integral or that of Lebesgue integral 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 which, 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.

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 and the integral method.

(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.

Once these resonance sequences (or ladders) are generated, the subsequent calculations are the same as those for the resolved resonances. Thus, the method is applicable to all methods to various degrees of sophistication described previously. Unfortunately, considerable uncertainties in the self-shielding are expected especially when the total number of resonances is small or the flux attenuation is substantial within the given energy interval. From a practical point of view, some bias in the selection process is obviously required in order to reproduce the observed physical phenomena such as the Doppler effect. It is believed that the problem can be greatly alleviated if the results from accurate self-indication experiments are used directly as one of the

criteria. This is because these observed quantities inherently contain the information directly related to the self-shielding effect of a nuclide at a given temperature.

(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 simplified 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. Since the detailed descriptions of this method had already be given in Ref.23, a brief summary here should suffice.

Under the above assumptions, the expectation values of interest can be represented in relatively simple forms²³ :

$$\langle \sigma_x \phi \rangle_{E_0} = \sum \frac{\sigma_p^{(eq)} \langle \Gamma_x J^* \rangle_{E_0}}{\langle D \rangle} \quad ; \quad \langle \phi \rangle_{E_0} = 1 - \sum \frac{\langle \Gamma_x J^* \rangle_{E_0}}{\langle D \rangle} \quad (60)$$

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 the reaction rate is over the l- and J-states of the nuclide in question while that in 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 integrals 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 form²³

$$\langle q_k \rangle = \prod_J \frac{1}{\langle D_J \rangle} \int_{-\infty}^{\infty} \Omega(D_J) dD_J \prod_x \frac{1}{\langle \Gamma_x \rangle} \int_0^{\infty} d\Gamma_x P_v \left(\frac{\Gamma_x}{\langle \Gamma_x \rangle} \right) q_k(D_J, \Gamma_x) \quad (61)$$

where $P_v(\Gamma_x / \langle \Gamma_x \rangle)$ and $\Omega(D_J / \langle D_J \rangle)$ are the χ^2 -distribution of v-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, $\Gamma_{ci}^{(x)} \propto \gamma_{ci}^2$ and $\Gamma_x = \sum_{c=1}^v \Gamma_{ci}^{(x)}$, 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. 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 nuclide, 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.

(1) Direct Numerical Approach

If one neglects the long range correlation of Dyson, the function $\Omega(y)$ must satisfy the following integral equation of the convolution type

$$\Omega(x) = W(x) + \int_0^x dt \Omega(x-t)W(t) \quad (62)$$

where $W(y)$ is the Wigner distribution defined as

$$W(y) dy = \frac{\pi}{2} y \exp[-\frac{\pi}{4}y^2] dy \quad (63)$$

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.62.

(2) Analytical Approximation

The solution to Eq.62 becomes significantly simplified if the Wigner distribution is replaced by a χ^2 -distribution $P_\nu(y)$. For the convolution integral equation of this type, it is most readily amenable to the use of 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

$$\Omega(y) = \frac{e^{-\frac{\nu}{2}y}}{2\pi i} \left(\frac{\nu}{2}\right) \int_{c-i\infty}^{c+i\infty} \frac{e^{\frac{\nu p}{2}y} dp}{p^{\frac{\nu}{2}} - 1} \quad (64)$$

whereby, for all even $\nu \geq 2$, $\Omega(y)$ is expressible in terms of the analytical function of the closed form in terms of the damped-oscillatory terms as can be readily seen via the Cauchy integral formula. In particular, the χ^2 -distributions of 8 or 10 degrees of freedom exhibit the closest resemblance to the Wigner distribution. The former is especially suitable for practical applications because of its relatively simple form as given below.

$$\Omega(y) = 1 - e^{-8y} - 2 e^{-4y} \sin(4y) \quad (65)$$

The above equation was extensively used in the earlier studies of the Doppler effect contributions attributed to the unresolved resonances.

(3) Dyson's Two-Level Correlation Function

Another alternative is to identify $\Omega(y)$ directly with Dyson's two-level correlation function defined as

$$\Omega(y) = 1 - [s(y)]^2 - \frac{ds(y)}{dy} \int_y^\infty s(t) dt \quad (66)$$

where $s(y) = \frac{\sin(\pi y)}{\pi y}$. In Ref.23, a numerical algorithm specifically developed for treating the

integrals defined by Eq.66 and Eq.61 was proposed and has been incorporated into the MC²-2 code¹⁹ used for routine applications.

From a practical point of view, the multiple integral defined in Eq.61 is obviously still too cumbersome to evaluate since the problems of interest inevitably involve many uncorrelated resonance sequences in the mix. One simplified approximation²³ that can simplify the problem drastically is the separability assumption on the NR-flux. This can be accomplished by noting that

$$\phi \sim \frac{1}{\Sigma_t} \approx \frac{1}{\Sigma_p + \Sigma_R^{(j)}} \left[1 - \sum_{j \neq J} \frac{\Sigma_R^{(j)}}{\Sigma_p + \Sigma_R^{(j)}} \right] \quad (67)$$

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 form²³

$$\langle \sigma_x^{(j)} \phi \rangle = \left\langle \frac{\sigma_x^{(j)}}{\Sigma_p + \Sigma_R^{(j)}} \right\rangle \left[1 - \sum_{j \neq} \left\langle \frac{\Sigma_R^{(j)}}{\Sigma_p + \Sigma_R^{(j)}} \right\rangle \right] \quad (68)$$

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^{19,23}

$$\tilde{\sigma}_x = \sum_{JJ} \frac{\frac{\sigma_p^{(eq)}}{\langle D \rangle} \langle \Gamma_x(J-O_{kk'}) \rangle}{1 - \frac{1}{\langle D \rangle} \langle \Gamma_i(J-O_{kk'}) \rangle} \quad (69)$$

whereby each uncorrelated sequences 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 expedite considerably.

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

$$h(\sigma_x, \sigma_s, \sigma_t) = h_t(\sigma_t) h_x(\sigma_x | \sigma_t) h_s(\sigma_s | \sigma_x, \sigma_t) \quad (70)$$

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. Hence, the

problem is reduced to the specifications of 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. 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.

One direct means of evaluating these distributions widely used in reactor applications is via the numerical techniques originally proposed by Levitt²⁹. The procedure involves generations of many resonance 'ladders' from the known distributions of resonance parameters described previously, whereby $h_i(\sigma_i)$ and conditional distributions can be computed numerically in various energy intervals covering the unresolved energy range. 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 $h_i(\sigma_i)$ 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

$$\left\langle \frac{\sigma_x}{\Sigma_t} \right\rangle_{E_0} = \int_0^{\sigma_t^{(max)}} \frac{E[h_x(\sigma_x|\sigma_t)]h_t(\sigma_t)}{\Sigma_t} d\sigma_t \quad ; \quad \left\langle \frac{1}{\Sigma_t} \right\rangle = \int_0^{\sigma_t^{(max)}} h_t(\sigma_t) d\sigma_t \quad (71)$$

where the conditional means of the partial cross section is defined as

$$E[h_x(\sigma_x|\sigma_t)] = \int_0^{\sigma_t^{(max)}} \sigma_x h_x(\sigma_x|\sigma_t) d\sigma_x \quad (72)$$

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' method²⁹. It is theoretically equivalent to converting the Riemann integrals defined by Eq.x to the form of Lebesgue's integrals by transformation of variables through numerical means. The widely used sub-group method 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. It should be noted that this method is not without its shortcomings. The conditional means so obtained are usually accompanied by large statistical uncertainties as expected for quantities generated from the second order distributions. This motivates further explorations of other possibilities of treating this intriguing problem.

VI.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. For our purposes here, it suffices to summarize the theoretical basis of these methods and their practical implications.

1. Method Based on Information Theory

As discussed in Sec.III, two matrices that determine the properties of the cross section are R_{cc} and U_{cc} (or S_{cc} using Fröhner's notation^{4,24}). 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 aprioi, $d[S]$ equivalent the invariant (differential) volume element in the sample space of S . By utilizing the maximizing of the information entropy and the elegant mathematical theory matrix developed by Hau Lo-Ken³⁰, Fröhner²⁴ 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 Shannon³¹ and the ideal was later adopted by Jaynes³² 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 which satisfy the known macroscopic information on one hand while maintaining the maximum unbiased stance with respect to the unknown knowledge on the other hand.

For a continuous probability distribution $p(x)$ of a physical quantity x with equally probable apriori within a differential segment dx , the information entropy is defined as

$$H = - \int dx p(x) \ln[p(x)] \quad (73)$$

The known macroscopic information is assumed to be the average values $\langle f_k(x) \rangle$ given by

$$\langle f_k(x) \rangle = \int dx p(x) f_k(x) \quad ; \quad k = 1, 2, \dots, K \quad (74)$$

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.x is tailor-made for the method of LaGrange's multiplier with result

$$p(x) = \frac{1}{z} \exp[-\sum_k \lambda_k f_k(x)] \quad (75)$$

where the normalization function z , also known as the partition function, is defined as

$$z = \int dx \exp[-\sum_k \lambda_k f_k(x)] \quad (76)$$

and the LaGrange's multiplier λ_k can be determined from a system of equations (usually non-linear)

$$\langle f_k(x) \rangle = -\frac{\partial}{\partial \lambda_k} [\ln(z)] \quad (77)$$

Hence, the desirable distribution can be derived via this procedure.

For our case here involving a $n \times n$ complex matrix (or real for R), the problem is obviously much more difficult. To define such a distribution, one must define a reference coordinate system by which the a priori can be specified. Furthermore, one must also choose a viable constraint through which the procedure of the method based on the LaGrange multiplier can be carried out.

Based on the work of Hua³⁰, Fröhner²⁴ derived the pertinent expressions for the differential volume elements $d[R]$ and $d[S]$ in the generalized polar coordinate system for the real symmetric matrix R and the complex unitary as well as symmetric matrix S . The coordinate system is defined in terms of eigen values and eigen vectors of these matrices as given below.

$$d[R] = 2^{n(n-1)/2} \prod_c dR_c \prod_{a < b} |R_a - R_b| \delta O_{ab} \quad ; \quad -\infty < R_1 < R_2 < \dots < R_n \quad ; \quad a < b \quad (78)$$

and

$$d[S] = 2^{n(n-1)/2} \prod_c d\theta_c \prod_{a < b} | \exp(i\theta_a) - \exp(i\theta_b) | \delta O_{ab} \quad ; \quad -\pi < \theta_1 < \theta_2 \dots < \pi \quad (79)$$

where R_c and $\exp(i\theta_c)$ are eigen values of R and S respectively. δO_{ab} here is a skew symmetric matrix introduced by Hua³⁰ and is related to the orthogonal transformation O that diagonalizes R , i.e.

$$\delta O = O^T dO = - \delta O^T \quad (80)$$

It should be noted that the commutative property of R and S are implicitly utilized so that δO is common to both expressions.

For the required constraint, Fröhner²⁴ chose $f(S)$ of the form

$$f(S) = \ln | \det(S - \bar{S}) |^2 \quad (81)$$

so that the constraint becomes

$$\langle f(S) \rangle = 2 \ln (\det T) \quad (82)$$

where

$$T = I - \bar{S}^* \bar{S} \quad (83)$$

is also known as Satchler's transmission matrix. 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 usual t-distribution. In particular, the latter is given by

$$p(S | \bar{S}) d[S] = C_n' \left[\frac{\det T}{\det | I - \bar{S}^* \bar{S} |^2} \right]^{(n+1)/2} d[S] \quad (84)$$

where C_n' is a normalization constant. In the limit of one channel (or pure scattering case), the above expression reduces to the Poisson's distribution and becomes the same as that derived by Lopez, Mello and Seligman³³.

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, further exploration is apparently required before such a method can be deployed for two reasons. 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 to be useful.

2. Method Based on Characteristic Function

Like the method of Fröhner, another unconventional approach based on the 'characteristic function' concept to examine the statistical properties of cross sections was recently developed by Lukyanov et al^{25,26}. 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 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

$$\langle (1 - iR)^{-1} \rangle = \int_0^{\infty} e^{-t} \langle e^{iRt} \rangle dt \quad (85)$$

where the average on the right hand side is more amenable to the integration over the Porter-Thomas distribution. By carrying out the averaging process before integration, the average is likely to be easier to evaluate. The quantity $\langle e^{iRt} \rangle$ is referred to as the 'characteristic' function which can serve another purpose beside the evaluation of the average defined in Eq.85. Since the average implies that

$$\langle e^{-t+iRt} \rangle = \int_{-\infty}^{\infty} e^{-t+iRt} p(R) dR \quad (86)$$

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 quite obvious that these distributions will become Poisson's distribution same as those derived by Fröhner if the characteristic function remains in the exponential form.

As pointed out by Lukyanov et al, 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 distribution of each resonance into a function of the closed form. It was shown that the characteristic function can be evaluated analytically with the result given as follows.

$$\langle e^{iRt} \rangle = e^{-\pi s_n t} \quad (87)$$

where $s_n = \frac{\langle \Gamma_n \rangle}{\langle D \rangle}$ is the strength function. It follows that $\langle S_{nn} \rangle$ is immediately reduced to the

familiar result given by

$$\langle S_{nn} \rangle = e^{-i2\phi} \frac{1 - \pi S_n}{1 + \pi S_n} . \quad (88)$$

It is also note-worthy that the above scheme can be readily used to confirm the validity of the causality relation

$$\langle S_{nn}^k \rangle = \langle S_{nn} \rangle^k \quad (89)$$

even if the Reich-Moore approximation is assumed.

The characteristic function approach has since been extended to the two channel case using the same basic assumptions. Its potential importance as a possible alternative to the numerically-based probability table method is very much in evidence. It is important to realize, however, that further explorations especially in the area to account for the Doppler -broadening are apparently needed.

VII. CONCLUSIONS

A rather subjective overview on the current status of resonance theory for reactor physics applications has been presented. The state-of-art developments were discussed along with the historical perspective on this subject.

For the past decades, there have been significant advances in all areas pertinent to this intriguing subjects. These include the improvements on our better understanding of the basic theories, our capabilities of dealing with extremely complex problems and the quality of resonance data. Three general areas are believed to be still worthy of further explorations. First, the deterministic methods to this date are still limited to infinite-repeated reactor lattices based on the 1-dimensional cell configuration at the resonance level. Further exploration into the feasibility of treating the problems in multi-dimensional geometries will undoubtedly be of some practical interest. Secondly, extensive bench-mark studies to verify our ability to predict the self-shielding effect and its associated Doppler-effect are apparently lacking. One idea place to begin is to utilize the existing results of various transmission and self-indication measurements. Thirdly, the statistical theory for treating the unresolved resonances is also worthy of further exploration.

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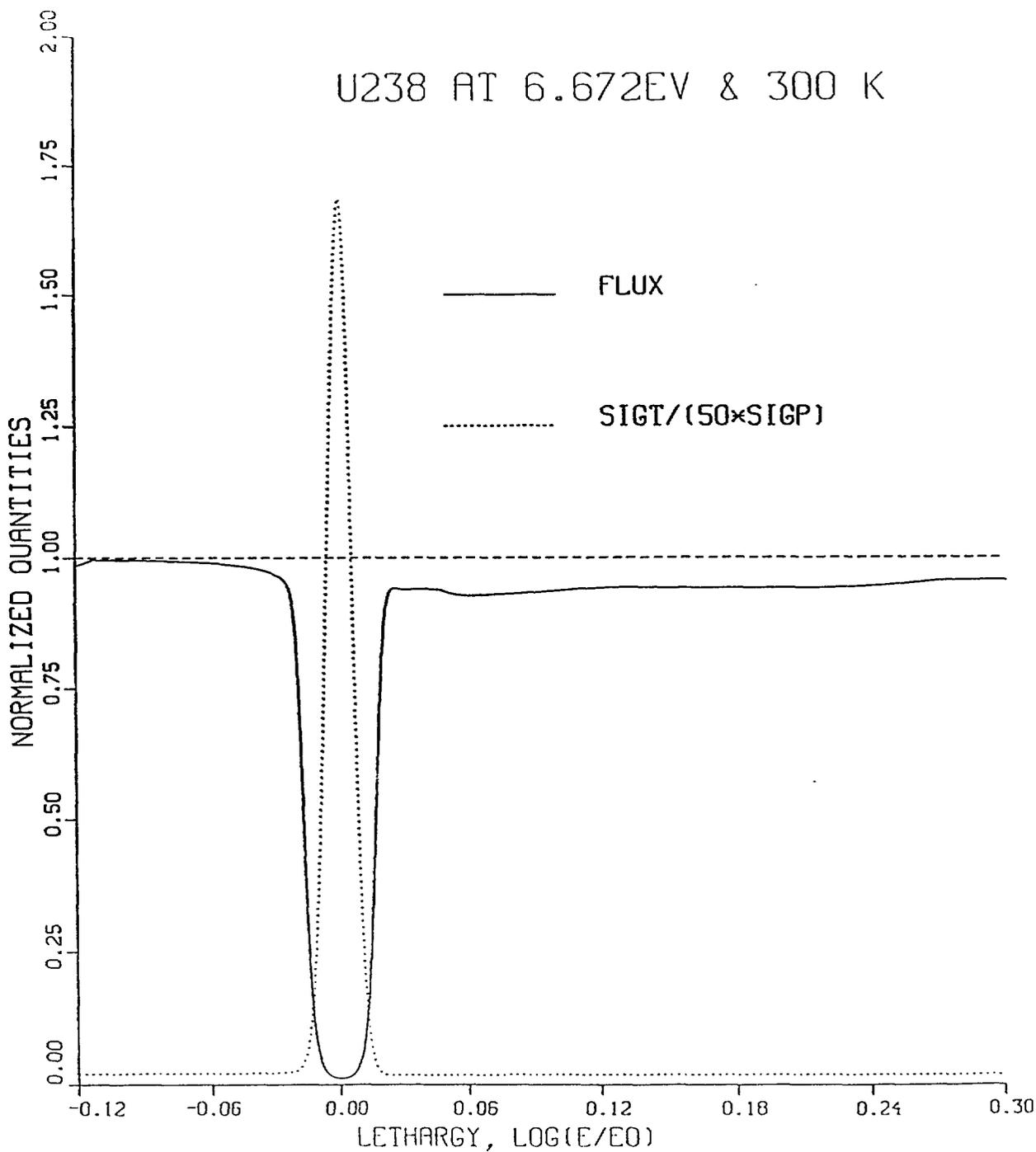


Figure 1. Flux and Σ_t for an Isolated Resonance in an Infinite Homogeneous Medium

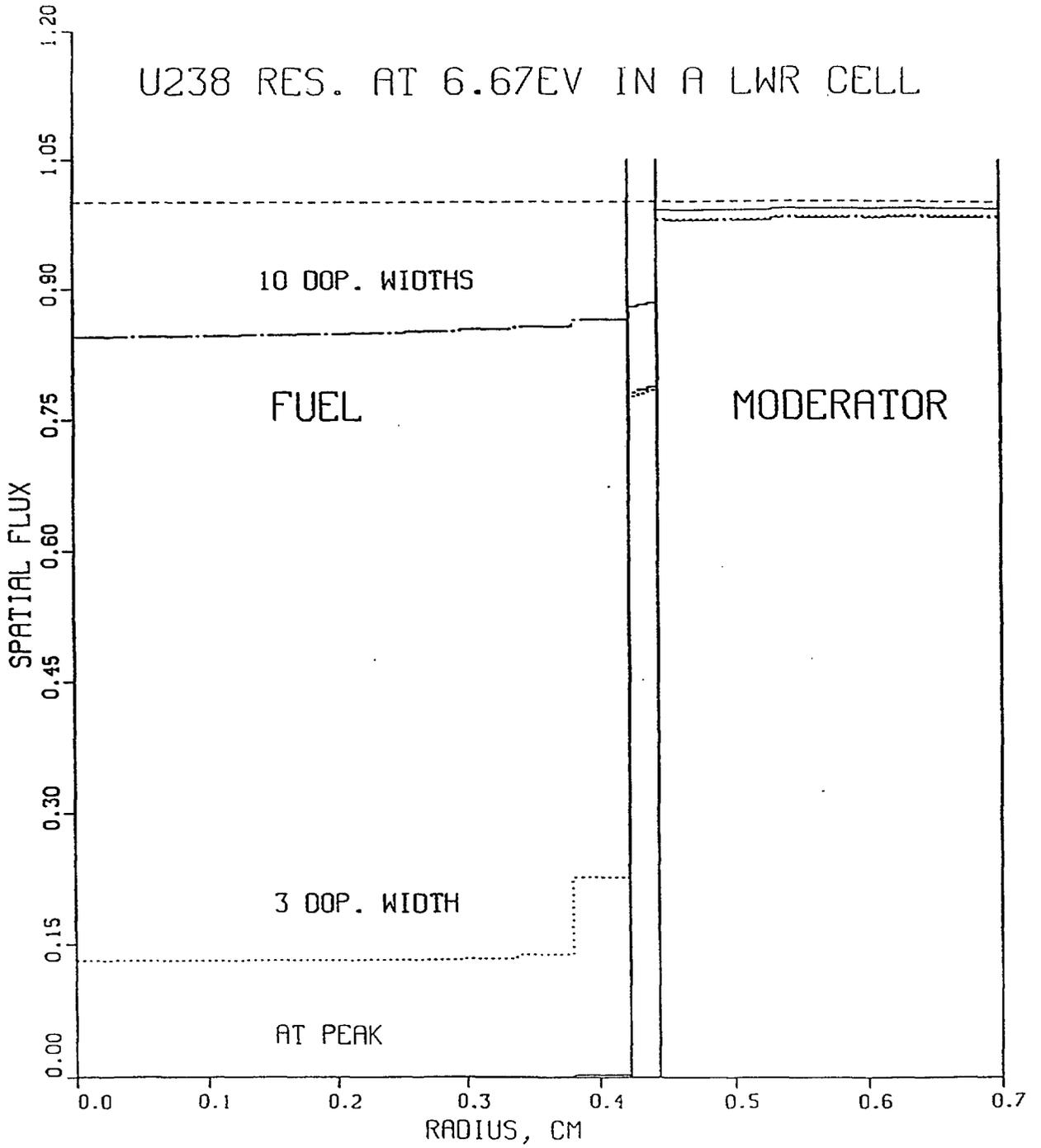


Figure 2. Flux Distribution in a Reactor Cell in the presence of an Isolated Resonance

Table 1. Momentum-Dependent Factors for Various ℓ -states Defined at Channel Radius r_c ($\rho = kr_c$).

| Factors | $\ell = 0$ | $\ell = 1$ | $\ell = 2$ | $\ell = 3$ |
|-------------|------------|---------------------------|---|---|
| P_ℓ | ρ | $\frac{\rho^3}{1+\rho^2}$ | $\frac{\rho^5}{9+3\rho^2+\rho^4}$ | $\frac{\rho^7}{225+45\rho^2+6\rho^4+\rho^6}$ |
| S_ℓ | 0 | $\frac{-1}{1+\rho^2}$ | $\frac{-(18+3\rho^2)}{9+3\rho^2+\rho^4}$ | $\frac{-(675+90\rho^2+6\rho^4)}{225+45\rho^2+6\rho^4+\rho^6}$ |
| ϕ_ℓ | ρ | $\rho - \tan^{-1}\rho$ | $\rho - \tan^{-1}\left(\frac{3\rho}{3-\rho^2}\right)$ | $\rho - \tan^{-1}\left(\frac{\rho(15-\rho^2)}{15-6\rho^2}\right)$ |

TABLE II. Poles and Residues for Traditional Formalism

| FORMALISM | POLES, d_λ | RESIDUES, $\rho_{ij,\lambda}^{(x)}$ |
|-------------|---|--|
| SLBW | $E_{0\lambda} - \frac{i\Gamma_{i\lambda}}{2}$ | $C g_J \frac{\Gamma_{x\lambda} \Gamma_{n\lambda}}{\Gamma_{i\lambda}/2} \frac{1}{\sqrt{E}} ; x \in f, \gamma$ $C g_J 2\Gamma_{n\lambda} \frac{1}{\sqrt{E}} \exp(-i2\phi_\lambda); x \in R$ |
| MLBW | Same as above | <p>Same as above if $x \in f, \gamma$</p> $C g_J 2\Gamma_{n\lambda} \frac{1}{\sqrt{E}} \{\exp(-i2\phi_\lambda) + W_{\lambda'}\}; X \in R$ <p>where</p> $W_{\lambda'} = \sum_{\lambda' \neq \lambda} \frac{i \Gamma_{n\lambda'}}{(E_\lambda - E_{\lambda'}) + i \left(\frac{\Gamma_{i\lambda} + \Gamma_{i\lambda'}}{2} \right)}$ |
| ADLER-ADLER | $\mu_\lambda - i v_\lambda$ | $C g_J [G_\lambda^{(x)} + iH_\lambda^{(x)}]; x \in f, \gamma$ $C g_J \exp(-i 2 \phi_\lambda) [G_\lambda^{(x)} + iH_\lambda^{(x)}]; x \in R$ |

$$C = \pi\lambda^2 \left(\frac{1+A}{A} \right)^2$$

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