APPLICATION OF FOURIER TRANSFORM METHODS TO RESONANCE ABSORPTION PHENOMENA IN NUCLEAR REACTORS

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DECLARATION

The author hereby declares that the work presented in this thesis is original and has not been submitted for the award of any degree or diploma or distinction to this or any other university.

S. V. G. Menon
(Candidate)

DECLARATION

I, hereby declare that the candidate worked for this thesis under my guidance from October 1975 to June 1978. The work presented in this thesis is original and has not been submitted for the award of any degree at this or any other university.

DR. S. V. Lawande
(Research Guide)

STATEMENT REGARDING NEW FACTS ETC.,
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In this thesis a new formulation of the problem of resonance absorption has been presented. The method employs the Fourier transformation of the slowing down equation. It is general in the sense that the procedure can be used in all situations where the Fourier transformation of the resonance cross-sections can be obtained.

The analytical expressions obtained for the zero temperature resonance integrals are new and have general applicability. A new formulation of the intermediate resonance approximation has also been given.

A new method using the Gauss-Hermite quadrature formulae for the evaluation of temperature dependent resonance integrals has been formulated and verified. As a bi-product, a fast and accurate method for the evaluation of the J-function has been justified.

A new formulation and method of solution of the problem of overlapping resonances of an absorber has been given. Finally, a new interpretation of the normalization condition based on the theory of distributions was found which allows the use of Fourier transformation methods for solving the homogenous form of the integral equation of the slowing down theory.

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S. V. G. Menon

ELECTRONIC VERSION

This electronics version of this thesis was prepared for submission to the Digital Archive of theses being prepared by SIRD, BARC. Smt Sobhana Nair, Senior, P.A., ThPD, put up a lot of time and efforts to prepare this version, as scanning from the original thesis produced a copy of poor quality. I am extremely grateful to Sobhana for her initiative, and hard work.

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CHAPTER-I

INTRODUCTION

A. Introduction to Slowing Down Theory:

The basic aspect of nuclear reactor theory is the study of the neutron density distribution which gives information on the average behavior of neutrons in the reactor system. In the general situation, the neutron density is a function of time and phase space co-ordinates. It satisfies the neutron transport equation, which is a linear form of the Boltzmann equation, stating neutron conservation in an elemental volume of phase space [1,2]. In this approach to reactor theory, it is tacitly assumed that neutron density is sufficiently large (~ 10^8 /c.c) so that the study of the average behavior is adequate for many purposes. At the same time it is also implied that the neutron density is much smaller than the density of reactor medium nuclei (~ 10^{22}/c.c) so that the rate of neutron-neutron interactions is negligible in comparison to that with the nuclei. The simplification offered by this approximation is the linearity of the transport equation in neutron density.

The nature of neutron-nucleus interactions enters into the transport equation as cross-sections, and usually the interactions due to the magnetic moment of the neutron are neglected. Even though the interaction cross-sections have their origin in quantum mechanical principles, the description offered by the transport equation is purely classical in the sense that neutrons are considered as point particles.

These assumptions mentioned so far are quite adequate for most of the reactor applications. Even then the transport equation poses many problems, partly due to its mathematical structure and partly due to the heterogeneous arrangement of materials in the reactor and the complicated dependence of the cross-sections on neutron energy. These facts necessitate the introduction of further simplifications. For instance, one considers an infinite homogeneous medium and investigates the distribution of neutrons in energy. Similarly, to gain insight in to the spatial and angular distribution of neutrons, one usually assumes that they can be classified as belonging to one or two energy groups.

The energy range of interest in reactor physics can be broadly classified as fast, resonance and thermal regions. In the energy range covering the first two regions, usually known as slowing down region, neutrons can only loose their energy in scattering collisions. In the third region, known as thermal region, they ca either lose or gain energy in scattering collisions. This happens due to the thermal motion of the scattering nuclei.

Main difficulty in the analytical treatment of neutron slowing down originates from the resonance structure of the cross-sections foe neutron interaction with fissile and fertile nuclei. Usually in nuclear reactors, resonance absorbers are lumped to reduce neutron capture in these resonances. Hence a rigorous treatment of the problem should start from the space dependent form of the transport equation. However, it has been shown by several investigators [3-6] that, to a good accuracy, this space dependent problem can be reduced to an equivalent infinite homogeneous medium problem.

The necessary steps involved to show this equivalence are the introduction of the "flat flux" approximation in the moderator and absorber regions and the asymptotic or unperturbed form of neutron energy distribution function in the moderator collision integrals of the transport equation. This enables one to write the equation in terms of the "first flight escape probability" for neutrons from the absorber regions. Use of the rational forms for the escape probability makes further simplifications. Then the problem becomes identical to that in an infinite medium where the resonance absorber and a fictitious moderator with energy independent scattering cross-section are homogeneously mixed together. At any rate, space independent equation will be the starting point for the discussion of even space dependent resonance absorption problems.

Foe the case of an infinite homogeneous medium, in the time independent situation, the neutron transport equation reduces to an integral equation for the neutron flux. The kernel of this integral equation has discontinuities arising from the finite energy loss suffered by a neutron in a scattering collision with the nuclide (except in the case of scattering from protons). The physical reason for this originates from the laws of conservation of energy and linear momentum in collisions. The doubly discontinuous nature of the kernel makes the integral equation of slowing down theory different from the class of integral equations well studied extensively in mathematical physics, viz., the Fredholm and Voltera equations. It turns out that in just two situations, the slowing down equation can be solved exactly. Firstly, when the moderating medium contains only hydrogen nuclei, with arbitrary energy dependence for cross-sections, an exact solution can be obtained [2]. The second situation arises when the medium contains one moderating element having energy independent cross-sections [7, 8].

In the fast energy range, presence of inelastic mode of energy degradation [9], and the anisotropic scattering [2, 10] in the centre of mass system complicates the kernel of the integral equation. However, in the energy range extending up to a few keV, the complications introduced by these processes can be neglected.

In the next few sections, we introduce the problem of resonance absorption through a discussion of the resonance cross-sections, the slowing down equation, etc,. This will be followed by a review of the presently known methods of treating this problem. Towards the end of the Chapter, we will be giving a brief summary of the present work.

B. Resonance Cross-Sections:

The low energy resonances in the neutron cross-section of fertile elements can be well represented by the single level Breit-Wigner formulae. The macroscopic scattering and absorption cross-sections corresponding to neutron energy e are given by

(1.1) $$\sigma_s(e) = \pi\lambda\!\!\!^{-2} g_J \frac{\Gamma_n^2 + 4\Gamma_n(e-e_r)R/\lambda\!\!\!^{-}}{(e-e_r)^2 + (\Gamma/2)^2} + 4\pi R^2$$

(1.2) $$\sigma_a(e) = \pi\lambda\!\!\!^{-2} g_J \frac{\Gamma_n \Gamma_r}{(e-e_r)^2 + (\Gamma/2)^2}$$

Here, $\lambda\!\!\!^{-}$, which equals $\lambda / 2\pi$, denotes the reduced de Broglie wavelength. Γ, Γ_n and Γ_r are, respectively, the total, scattering and absorption width of the resonance and e_r is the resonance energy. R is the potential scattering radius of the nuclide and the statistical spin factor of the nucleus g_J equals $(2J+1)/(2I+1)$ where I and J, respectively, denote the spin quantum number of the compound nucleus and target nucleus states. The energy dependence of the scattering width is expressed as $\Gamma_n=\Gamma_n(e_r)(e/e_r)^{1/2}$, but that of the total width can be neglected for most of the resonances of importance [1]. With the introduction of the quantities like peak cross-section σ_0, potential scattering cross-section σ_p, etc., defined by the relations:

(1.3) $$\sigma_0 = 4\pi\lambda\!\!\!^{-2} e_r g_J \Gamma_n(e_r)/\Gamma$$

$$\sigma_p = 4\pi R^2 \tag{1.4}$$

$$\sigma_{op} = \left[\sigma_0 \sigma_p g_J \, \Gamma_n(e_r)/\Gamma\right]^{1/2} \tag{1.5}$$

$$x = 2(e - e_r)/\Gamma \tag{1.6}$$

the expressions for the macroscopic cross-sections can be rewritten as

$$\sigma_s(x) = \sigma_0 \frac{\Gamma_n}{\Gamma} \frac{1}{1+x^2} + \sigma_{0p} \frac{2x}{1+x^2} + \sigma_p \tag{1.7}$$

$$\sigma_a(x) = \sigma_0 \frac{\Gamma_r}{\Gamma} \frac{1}{1+x^2} \tag{1.8}$$

The factor $(e/e_r)^{1/2}$ appearing in the expression for σ_a gives rise to the "*1/*v" variation of the absorption cross-section far away from the resonance. In the following parts of the thesis, we will equate this factor to unity, assuming that the contributrion from this "*1/*v" absorption cross-section can be added separately to that due to the resonance structure in cross-sections. All the other parameters appearing in the above two equations are energy independent. The energy variable *e* appearing in equations (1.1) and (1.2) is the energy of the neutron nucleus pair in the centre of mass system. If the nucleus is assumed to be at rest before the collision, *e* is proportional to the energy of the neutron in the laboratory co-ordinate system. The proportionality constant is related to the mass number of the nucleus M_N, and equals $M_N/(M_N+1)$. For heavy elements, the factor is very close to unity and the energy variable appearing the expression for cross-sections can be taken to be the neutron energy in the laboratory system. These formulae are applicable when the medium containing the resonance absorbers is at absolute zero temperature. When the medium is at any finite temperature, the nuclei are in motion and have an energy distribution corresponding to the temperature of the medium. For a neutron energy e_0, the energy *e* of the neutron nucleus pair will vary with the thermal energy of the nucleus. This effect is usually termed as Doppler-effect. Therefore, the cross-sections are to be averaged over the energy distribution of the nuclei. The velocity ($\vec{V}$) distribution of the nuclei can be assumed to be represented by the Maxwellian distribution function corresponding to the physical temperature of the medium [1, 2]. The resonance cross-sections can be thus be defined as

$$v\,\sigma_x^{eff}(e) = \int \sigma_x(e) \left|\vec{v} - \vec{V}\right| P(\vec{V},T)\, d\vec{V} \tag{1.8'}$$

Introducing the Maxwellian velocity distribution function corresponding to the temperature *T*,

$$P(\vec{V},T)=\left(\frac{M_N}{2\pi kT}\right)^{3/2}\exp\left[-M_NV^2/2kT\right] \tag{1.9}$$

The temperature dependent cross-section can be written in terms of the familiar ψ and χ function [1]

$$\sigma_s(x)=\sigma_0\frac{\Gamma_n}{\Gamma}\psi(x,\xi)+\sigma_{0p}\ \chi(x,\xi)+\sigma_p \tag{1.10}$$

$$\sigma_a(x)=\sigma_0\frac{\Gamma_r}{\Gamma}\psi(x,\xi) \tag{1.11}$$

Here ξ is a parameter depending on the temperature of the medium, and is given by the expression $\Gamma/(4e_rkT/M_N)^{1/2}$. The ψ and χ functions have only their integral representations given by

$$\psi(x,\xi)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\exp\left[-(x-y)^2\xi^2/4\right]\frac{1}{1+y^2}dy \tag{1.12}$$

$$\chi(x,\xi)=\frac{\xi}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\exp\left[-(x-y)^2\xi^2/4\right]\frac{2y}{1+y^2}dy \tag{1.13}$$

The non-availability of analytical expressions for these functions constitutes one of the difficulties in the development of analytical methods for treating the slowing down problems in presence of resonance absorbers [11]. It is useful to note that as *T* goes to zero, ξ tends to ∞ and

$$Lim_{\xi\to\infty}\frac{\xi}{2\sqrt{\pi}}\exp[-(x-y)^2\xi^2/4]=\delta(x-y) \tag{1.14}$$

where $\delta(x-y)$ is the Dirac delta function. Thus in the limit of zero temperature of the medium, the ψ and χ functions tend to the Lorentzian forms, and the cross-sections assume the Breit-Wigner shapes given by equations (1.7) and (1.8).

C. The Infinite Medium Slowing Down Equation:

As was pointed out earlier, to determine the energy distribution of neutrons in an infinite homogeneous medium, one has to start with the space independent transport equation. For the case of a mixture of a resonance absorber and a moderator, the time independent equation (assuming isotropic scattering in the centre of mass system) is given by [1, 2]

$$\left[\Sigma_a(e)+\Sigma_s(e)+\Sigma_m\right]\Phi(e)=S(e)+\int_e^{e/\alpha_m}\frac{\Sigma_m\Phi(e')}{(1-\alpha_m)}\frac{de'}{e'}+\int_e^{e/\alpha}\frac{\Sigma_s\Phi(e')}{(1-\alpha)}\frac{de'}{e'} \tag{1.15}$$

where $\Phi(e)$ is the neutron flux in unit energy interval at e. $S(e)$ is the source of neutrons appearing in unit energy interval at e, while Σ_m and $\Sigma_s(e)$ are, respectively, the macroscopic scattering cross-section of the moderator and absorber. $\Sigma_a(e)$ is the macroscopic absorption cross-section of the absorber. α_m and α are, respectively, related to the mass number of the moderator and absorber nuclides. For example, α is given by $(M_N-1)^2/(M_N+1)^2$. In writing equation (1.15), we have assumed that the moderator does not absorb neutrons, and have an energy independent scattering cross-section. In the resonance energy region, both these assumptions can be seen to be applicable to the moderators of interest in reactor physics.

Fission neutrons are distributed in energy, the average energy is about 2 MeV. These neutrons in a reactor medium do not contribute directly to the neutron flux in the energy region of isolated resonances of the absorber. Further, it is well known that, in the absence of absorption and far away from resonances, the neutron flux distribution has a "1/*e*" behavior., Thus in resonance absorption theory one is left to solving the homogeneous part of equation (1.15) with the normalization condition that the flux has a "1/*e*" shape above the resonance.

The resonances of the absorber are said to be well separated if the separation between two resonances is more than three or four times the average logarithmic energy decrement. For such resonances, one introduces the assumption of recovery of the asymptotic distribution between the resonances. This makes it possible to calculate the neutron absorption rate in these resonances independently. The average separation (in lethargy space for resolved resonances of U^{238} is of the order of 4.5, and is several times the average logarithmic energy decrement 0.0084. Thus the assumption of the flux recovery is indeed satisfied here. Over, a major part of this thesis, we shall be working under this approximation.

Dividing by the number of absorber nuclei in unit volume N_f, the homogeneous part of equation (1.15) becomes

$$\left[\sigma_a(e)+\sigma_s(e)+\sigma_m\right]\Phi(e)=\int_e^{e/\alpha_m}\frac{\sigma_m\Phi(e')}{(1-\alpha_m)}\,\frac{de'}{e'}+\int_e^{e/\alpha}\frac{\sigma_s\Phi(e')}{(1-\alpha)}\,\frac{de'}{e'} \tag{1.16}$$

Here we have introduced the quantity σ_m which is the macroscopic moderator scattering cross-section per absorber nucleus. That is $\sigma_m=\Sigma_m/N_f$.

The resonance cross-sections take a simplified form in the variable x rather than e. Therefore, it is natural to change the variable in equation (1.16) from e to x [12, 13]. To do this, we define the variable $f(e)= e\,\Phi(e)$. The equation for $f(e)$ becomes

$$\left[\sigma_a(e)+\sigma_s(e)+\sigma_m\right]f(e)=\int_e^{e/\alpha_m}\frac{\sigma_m f(e')}{(1-\alpha_m)}\left(\frac{e}{e'}\right)de'+\int_e^{e/\alpha}\frac{\sigma_s f(e')}{(1-\alpha)}\left(\frac{e}{e'}\right)de' \tag{1.17}$$

It is clear that the form of $f(e)$ far away from the resonance should be independent of e. Changing to the variable x in equation (1.17) we get

$$\begin{aligned}\left[\sigma_a(x)+\sigma_s(x)+\sigma_m\right]f(x)=&\int_x^{(x+\varepsilon_m)/\alpha_m}\frac{\sigma_m f(y)}{\varepsilon_m}\left(\frac{1+\Gamma x/2e_r}{1+\Gamma y/2e_r}\right)\frac{dy}{1+\Gamma y/2e_r}+\\&+\int_x^{(x+\varepsilon)/\alpha}\frac{\sigma_s f(y)}{\varepsilon}\left(\frac{1+\Gamma x/2e_r}{1+\Gamma y/2e_r}\right)\frac{dy}{1+\Gamma y/2e_r}\end{aligned} \tag{1.18}$$

where we have introduced the quantities ε_m and ε

$$\varepsilon_m=2e_r\frac{1-\alpha_m}{\Gamma} \tag{1.19}$$

$$\varepsilon=2e_r\frac{1-\alpha}{\Gamma} \tag{1.20}$$

The resonance absorber is a heavy element and α is close to unity. Therefore the upper limit in the second integral term in equation (1.18), viz., $(x+\varepsilon)/\alpha$, can be approximated by

$$\frac{x+\varepsilon}{\alpha}\approx x+\varepsilon \tag{1.21}$$

The accuracy obtained on employing the same approximation in the upper limit of the moderator collision integral term may at first seem to be quite doubtful. However, the moderator collision integral affects $f(x)$ in a very minor way only. This happens because

ε_m itself is a large quantity due to the small value of α_m. Further, over major part of the range of integration of this term, *f(x)* has its asymptotic form. Comparisons of the resonance integral obtained from the numerical solution of equation (1.18) with and without the approximation

$$\frac{x+\varepsilon_m}{\alpha_m} \approx x+\varepsilon_m \tag{1.22}$$

have shown that the error introduced by this is negligible [14].

The ratio of the natural width of the resonance to the resonance-energy Γ/e_r is very small for almost all resonances in the resonance region. Therefore factors like $(1+\Gamma x/2e_r)$ appearing in the integral terms of equation (1.18) can be approximated to unity [12,14]. Thus one obtains the following simplified equation for *f(x)*

$$\left[\sigma_a(x)+\sigma_s(x)+\sigma_m\right] f(x) = \frac{1}{\varepsilon_m}\int_x^{x+\varepsilon_m} \sigma_m f(y)\,dy + \frac{1}{\varepsilon}\int_x^{x+\varepsilon} \sigma_s(y) f(y)\,dy \tag{1.23}$$

As has been pointed out by several investigators [12,14,15], the implicit assumption in deriving the above equation is the approximation of the integral operators in the slowing does equation. For instance, the absorber collision integral is replaced as

$$\int_e^{e/\alpha} \frac{\sigma_s(e')\Phi(e')de'}{(1-\alpha)e'} \cong \frac{1}{\varepsilon}\int_x^{x+\varepsilon} \sigma_s(y) f(y)\,dy \tag{1.24}$$

The above replacement does not give the asymptotic value of the neutron flux well below the resonance [15]. It is well known that the magnitude of the neutron flux well below the resonance differs from that above the resonance by a factor which equals the resonance escape probability [2]. The modified form of the integral operator makes the asymptotic values of the neutron flux above the below the resonance same. The error introduced by this in evaluating the absorption rate in resonances in the epithermal region has been well established and has been found to be negligible [14,15]. We shall base all our further discussions on equation (1.23)

D. Resonance Escape Probablity And Resonance Integral:

Even though the quantity of prime interest is the neutron energy distribution in the resonance energy region, the integral parameters like resonance escape probability and resonance integral directly give the relevance of resonance absorption in reactor systems.

If the source of energy well above the resonance emits one neutron per second, the resonance escape probability is given by

(1.25) $$p = 1 - A$$

where A is the fraction of neutrons absorbed in the resonance. It is given by

(1.26) $$A = \int_{resonance} N_f \sigma_a(e)\Phi(e)de$$

Assuming that A is much smaller than 1, the expression for p can be written as [2]

(1.27) $$p \cong \exp(-A)$$

Defining the effective resonance integral as

(1.28) $$I_{eff} = \langle \xi \Sigma_s \rangle \int_{resonance} \sigma_a(e)\Phi(e)de$$

where $\langle \xi \Sigma_s \rangle$ is the average slowing down power of the mixture of elements, the resonance escape probability becomes

(1.29) $$p = \exp\left[-\frac{N_f}{\langle \xi \Sigma_s \rangle} I_{eff} \right]$$

When the source emits one neutron per second in an infinite non-absorbing homogeneous medium, the flux distribution away from the source neutron energy becomes $1/\langle \xi \Sigma_s \rangle e$ [2]. When expressed in the lethargy variable it becomes the constant value $1/\langle \xi \Sigma_s \rangle$ [2]. Thus the effective resonance integral is so defined that on multiplication with the asymptotic flux distribution in the lethargy variable it gives the absorption rate in the resonance.

It is useful to normalize the source strength to $\langle \xi \Sigma_s \rangle$ so that the asymptotic flux distribution above the resonance is $1/e$, in energy space or just 1 in lethargy space. If $\Phi(e)$ is obtained from equation (1.16) with this normalization, the constant factor appearing in the expression for I_{eff} drops out. We shall be following this convention in the following parts of the thesis. In terms of the quantity $f(x)$ the expression for I_{eff} becomes

(1.30) $$I_{eff} = \langle \xi \Sigma_s \rangle \int_{resonance} \sigma_a(x) f(x) \frac{\Gamma}{2e_r} \frac{dx}{1 + \Gamma x / 2e_r}$$

As was explained in the last section of the factor $(1+\Gamma x/2e_r)$ can be approximated to unity. Using the expression for σ_a given in equation (1.11), we find that

$$I_{eff}(\xi)=\frac{\sigma_0\Gamma_r}{2e_r}\int_{resonance}\psi(x,\xi)\,f(x)\,dx \tag{1.31}$$

The absorption cross-section or equivalently the ψ function goes to negligible values beyond the region of influence of the resonance. Therefore the limits of integration in the above expression can be extended to cover the entire range of x. Introducing the infinite dilution integral I_o, which equals $\pi\sigma_0\Gamma_r/2e_r$, the expression for I_{eff} becomes

$$I_{eff}(\xi)=\frac{I_0}{\pi}\int_{-\infty}^{\infty}\psi(x,\xi)\,f(x)\,dx \tag{1.31}$$

It can be seen from equation (1.16) that in the limit of infinite dilution of the absorber, $\Phi(e)$ approaches the $1/e$ form. Alternatively $f(x)$ tends to 1 and the effective resonance integral becomes I_o. In obtaining the above result one should make use of the fact that the integral of the ψ function is π [2]. Thus we are left with the problem of evaluating the effective resonance integral from equation (1.32) and $f(x)$ is obtained as the solution of equation (1.23) with the condition that it goes to 1 when $x \to \infty$. In the remaining part of this chapter, we shall briefly discuss the well known approximation techniques developed for this purpose.

E. Well Known Approximation Methods for Evaluating the Resonance Integral:

Since the difficulty in solving the integral equation (1.23) is with the collision integral terms, approximation methods have been designed to simplify them. The earliest and those obtained from considerations of the nature of the resonance are due to Wigner [16, 17]. They are known as narrow resonance (N.R.) and wide resonance (W.R.) approximations.

1. Narrow resonance and Wide resonance approximations:

For the purpose of identifying a resonance as narrow or wide Wigner introduced the concept of practical width Γ_P. This is defined as the part of the energy region over which the total resonance cross-section is more than the potential scattering cross-section. Neglecting resonance potential interference scattering term from the expression for σ_S, it is readily seen that this definition for the practical width gives the expression [2].

(1.32) $$\Gamma_P = \Gamma\sqrt{\frac{\sigma_0}{\sigma_p} - 1}$$

However, this definition does not include the effect of the scatterer on the resonance. To include this effect, Bell and Glasstone [1] defines practical width as the energy region over which the neutron flux distribution differs from the unperturbed distribution by a factor of 2 or more. They give the expression

(1.33) $$\Gamma_P = \Gamma\sqrt{\frac{\sigma_0}{(\sigma_p + \sigma_m)} - 1}$$

The maximum energy that a neutron of resonance energy can lose in a scattering collision with the absorber nuclide is $e_r(1-\alpha)$. If Γ_P is much smaller than $e_r(1-\alpha)$, the resonance is said to be narrow. It can be seen from equation (1.23) that the region of influence of resonances of this type is much smaller than the range of integration in the collision terms. That is, the number of neutrons scattered in to an infinitesimal interval *de* at *e* is not affected by the presence of the resonance. For such resonances the integral term *P*

(1.35) $$P = \frac{1}{\varepsilon}\int_{x}^{x+\varepsilon} \sigma_s(y) f(y)\, dy$$

can be simplified by substituting the asymptotic values of σ_S and *f(x),* that is, σ_P and 1, respectively, inside the integral. Thus in the narrow resonance approximation, the integral term becomes

(1.36) $$P_{N.R} = \sigma_p$$

Because of the low mass of the moderator nuclide, it becomes immediately obvious that this approximation will be quite adequate for the moderator collision integral term. It has been pointed out by Goldstein [18], Seghal [19] and Ishiguro [14] that, with scatters like oxygen, carbon etc, narrow-resonance approximation can lead to an overestimation of resonance integrals of the low lying resonances by a few percent when σ_m is small. In any case, this approximation is excellent for scattering by hydrogen. Introduction of narrow resonance approximation for the moderator collision integral term reduces equation (1.23) to

(1.37) $$\left[\sigma_a(x)+\sigma_s(x)+\sigma_m\right]f(x)=\sigma_m+\frac{1}{\varepsilon}\int_{x}^{x+\varepsilon}\sigma_s(y)f(y)\,dy$$

It may be useful to point out an important difference between equations (1.23) and (1.37). In the process of applying the narrow resonance approximation to be moderator collision term, we have made use of the normalization condition on *f(x)*. Therefore, equation (1.37) appears as an inhomogeneous equation. On the other hand, equation (1.23) is a homogenous equation and in obtaining its solution we have to employ the normalization condition on *f(x)*.

Even though the resonance absorbers of prime interest in reactor physics are heavy elements, there are quite a few resonances especially over the higher end of the resonance region for which the narrow resonance approximation can be applied [1,2]. This arises due to the fact that for higher energy resonances, $e_r(1-\alpha)$ increases and the condition for the applicability of this approximation becomes more and more satisfactory. The narrow resonance approximation to the absorber collision integral term also in equation (1.37) gives the following expression for *f(x):*

(1.38) $$f_{N.R}(x)=\frac{\sigma_m+\sigma_p}{\sigma_a(x)+\sigma_s(x)+\sigma_m}$$

The wide resonance approximation can be considered to be more or less the opposite of the narrow resonance approximation. It corresponds to the situation when $\Gamma_P >> e_r(1-\alpha)$. In this situation it can be assumed that over the energy region from which neutrons are scattered to an infinitesimal energy interval *de* at *e*, the scattering collision density is constant. In other words the region of integration in the collision integral is much smaller than the region of influence of the resonance. Thus the integrand does not vary appreciably and can be taken outside the integral sign. Thus the wide resonance approximation to the collision integral provides (with narrow resonance approximation for moderator collision integral)

(1.39) $$P_{N.R}=\sigma_p$$

and the following expression for *f(x)*

(1.40) $$f_{W.R}(x)=\frac{\sigma_m}{\sigma_a(x)+\sigma_P+\sigma_m}$$

With the above expressions for *f(x)* the effective resonance integral can be evaluated. Substituting for σ_a and σ_s from equations (1.10) and (1.11), the resonance integral in the narrow resonance approximation becomes

$$I_{eff}^{N.R}(\xi) = \frac{2}{\pi}\frac{I_0}{\gamma_1^2} J\left(\xi, 1/\gamma_1^2, a\right) \tag{1.41}$$

where γ_1^2 and a are given by

$$\gamma_1^2 = \frac{\sigma_0}{\left(\sigma_P + \sigma_m\right)}, \quad a = \frac{\sigma_0}{\gamma_1^2\left(\sigma_P + \sigma_m\right)} \tag{1.42}$$

$J(\xi, \beta, a)$ is the function defined by Dresner [17] as

$$J(\xi, \beta, a) = \frac{1}{2}\int_{-\infty}^{\infty} \frac{\psi(x,\xi)\,dx}{\beta + \psi(x,\xi) + a\,\chi(x,\xi)} \tag{1.43}$$

In the wide resonance approximation, the resonance integral becomes

$$I_{eff}^{N.R}(\xi) = \frac{2}{\pi}\frac{I_0}{\gamma_0^2} J\left(\xi, 1/\gamma_0^2, a\right) \tag{1.44}$$

where γ_0^2 is given by

$$\gamma_0^2 = \frac{\sigma_0}{\sigma_m}\frac{\Gamma_r}{\Gamma} \tag{1.45}$$

The $J(\xi, \beta, a)$ function can be evaluated analytically only in the limit of zero temperature. We shall give the resulting expressions for the zero temperature resonance integrals later on.

2. Improvements to narrow resonance and wide resonance approximation:

(a) Improved narrow resonance approximation:

Spiney [30] and Chernic and Vernon [3] had developed formulae for the resonance integrals which are improvements over that provided by equations (1.41) and (1.44). Spiney's improvement was on the narrow resonance approximation. He used the fact that if resonance potential interference scattering is neglected and the condition

$$\frac{\Gamma_n}{\Gamma} = \frac{\sigma_P}{\sigma_m + \sigma_P} \tag{1.46}$$

is satisfied, equation (1.37) can be solved exactly. To see this let us rewrite equation (1.37) with the explicit form of the cross-sections

(1.47) $$\left[\sigma_0\psi(\xi,x)+\sigma_P+\sigma_m\right]f(x)=\sigma_m+\frac{1}{\varepsilon}\int_x^{x+\varepsilon}\left[\sigma_0\tfrac{\Gamma_n}{\Gamma}\psi(\xi,x)+\sigma_P\right]f(y)\,dy$$

by defining the quantity γ_λ^2 for λ=0, 1 and ∞ by the equation

(1.48) $$\gamma_\lambda^2=\frac{\sigma_0}{(\lambda\sigma_P+\sigma_m)}\frac{(\Gamma_r+\lambda\Gamma_n)}{\Gamma}$$

we can rewrite equation (1.47) as

(1.49) $$\left[1+\gamma_1^2\psi(\xi,x)\right]f(x)=\frac{\sigma_m}{\sigma_m+\sigma_P}+\frac{\sigma_P}{\sigma_m+\sigma_P}\frac{1}{\varepsilon}\int_x^{x+\varepsilon}\left[1+\gamma_\infty^2\psi(\xi,y)\right]f(y)\,dy$$

It is seen from the definition of γ_λ^2 that when the condition given by equation (1.46) is satisfied, $\gamma_1^2=\gamma_\infty^2$. Hence it is natural to rewrite equation (1.49) as

(1.50) $$\left[1+\gamma_1^2\psi(\xi,x)\right]f(x)=\frac{\sigma_m}{\sigma_m+\sigma_P}+\frac{\sigma_P}{\sigma_m+\sigma_P}\frac{1}{\varepsilon}\int_x^{x+\varepsilon}\left[1+\gamma_1^2\psi(\xi,y)\right]f(y)\,dy$$
$$+\frac{\sigma_P}{\sigma_m+\sigma_P}\left(\gamma_\infty^2-\gamma_1^2\right)\frac{1}{\varepsilon}\int_x^{x+\varepsilon}\left[1+\gamma_1^2\psi(\xi,y)\right]f(y)\,dy$$

The last term on the RHS of equation (1.50) is considered as a perturbation and neglected in obtaining the first order approximation to *f(x)*. Then the first order approximation f_1 is readily found to be given by

(1.51) $$f_1(x)=\frac{1}{1+\gamma_1^2\psi(\xi,x)}$$

It may be noted that $f_1(x)$ is same as the expression obtained in the narrow resonance approximation. Substituting $f_1(x)$ for *f(x)* on the R.H.S. of equation (1.50) we get a second order approximation to *f (x)*. Denoting this by $f_2(x)$ we find that

(1.52) $$f_2(x)=\frac{1}{1+\gamma_1^2\psi(\xi,x)}\left[1+\frac{\sigma_P}{\sigma_m+\sigma_P}\left(\gamma_\infty^2-\gamma_1^2\right)\frac{1}{\varepsilon}\int_x^{x+\varepsilon}\frac{\psi(\xi,y)}{1+\gamma_1^2\psi(\xi,y)}\,dy\right]$$

Spinney obtained the improved formula for the resonance integral with the above approximation to *f(x)*. It is given by [17]

(1.53) $$I_{eff}^{SP}(\xi)=I_{eff}^{N.R}(\xi)\left[1+\frac{\sigma_P}{\sigma_m+\sigma_P}\left(\gamma_\infty^2-\gamma_1^2\right)\frac{\pi}{2\varepsilon}\frac{I_{eff}^{N.R}(\xi)}{I_0}\right]$$

(b) Improved wide resonance approximation:

Chernic and Vernon's improvement was on the wide resonance approximation. They considered $f_{WR}(x)$ as the first order approximation to $f(x)$. That is,

$$f_1(x) = f_{W.R}(x) = \frac{1}{1+\gamma_0^2\,\psi(\xi,x)} \tag{1.54}$$

A second order approximation to $f(x)$ is obtained by substituting it for $f(x)$ on the R.H.S. of equation (1.49). The second order approximation is then found to be

$$f_2(x) = \frac{1}{1+\gamma_1^2\,\psi(\xi,x)}\left[\frac{\sigma_m}{\sigma_m+\sigma_P} + \frac{\sigma_P}{\sigma_m+\sigma_P}\,\frac{1}{\varepsilon}\int_x^{x+\varepsilon} \frac{1+\gamma_\infty^2\psi(\xi,y)}{1+\gamma_0^2\psi(\xi,y)}\,dy\right] \tag{1.55}$$

Since the above approximation is an improvement over the wide resonance approximation, the integrand in the RHS of equation (1.55) may be expanded in a Taylor series about *x*. Neglecting terms beyond third order in the series expansion, it can be shown that the resonance integral is given by [17]

$$I_{eff}^{CV}(\xi) = I_{eff}^{W.R}(\xi) + \frac{I_0}{\pi}\left(\frac{\sigma_P}{\sigma_m+\sigma_P}\right)^2 \frac{\varepsilon^2}{b}\int_{-\infty}^{\infty} dx\,\frac{\psi(\xi,y)}{1+\gamma_0^2\psi(\xi,y)}\,\frac{d^2}{dx^2}\left[\frac{1+\gamma_\infty^2\psi(\xi,y)}{1+\gamma_0^2\psi(\xi,y)}\right] \tag{1.56}$$

The integral on the RHS of the above expression can be analytically evaluated only in the limit of zero temperature. In this situation one gets [17]

$$I_{eff}^{CV}(\infty) = I_{eff}^{W.R}(\infty) - \frac{I_0}{3}\left(\frac{\sigma_P}{\sigma_m+\sigma_P}\right)\varepsilon^2\,\frac{1}{\gamma_1\gamma_0}\,\frac{\gamma_\infty^2-\gamma_0^2}{(\gamma_1+\gamma_0)^3} \tag{1.57}$$

It has been found that the improved narrow resonance formula derived by Spinney is applicable to more situations than to which the above formula applies.

3. Intermediate resonance approximation:

Even though the above discussed approximations are applicable to certain resonances, strictly speaking, they are only limiting situations. Further, there are many resonances of absorbers for which these approximations are not applicable [2]. Goldstein and Cohen [12, 21] developed the intermediate resonance (I.R.) approximation in which they assumed that the collision integral term can be considered as a linear combination of the approximate forms resulting from the narrow resonance and wide resonance approximations. Thus they introduced an interpolation parameter λ with which the collision integral term is approximated to be

$$P_{I.R} = \lambda\,P_{N.R} + (1-\lambda)\,P_{W.R} \tag{1.58}$$

The interpolation parameter λ is to be determined. It can be seen that the limits λ=1 and λ=0, respectively, produce the narrow resonance and wide resonance approximations. Substitution of the expressions for P_{NR} and P_{WR} in to the above equation gives

$$P_{I.R} = \sigma_S(x)\,f(x) + \lambda\left[\sigma_P - \sigma_S\,f(x)\right] \tag{1.59}$$

Therefore, equation (1.37) gives

$$f_{I.R}(x) = \frac{\sigma_m + \lambda\,\sigma_p}{\sigma_a(x) + \lambda\,\sigma_s(x) + \sigma_m} \tag{1.60}$$

Goldstein and Cohen also considered an approach in which the intermediate resonance approximation for *f(x)* is taken as a linear combination of f_{NR} and f_{WR}. However, the former approach in which the interpolation parameter λ appears in the expression for f_{IR} in a non-linear fashion has been found to be superior to the latter [12]

Substitution of the expression for f_{IR} *(x)* in the equation (1.32) gives [21]

$$I_{eff}^{I.R}(\xi) = \frac{I_0}{\pi}\int_{-\infty}^{\infty}\frac{(\sigma_m + \lambda\sigma_P)\psi(x,\xi)}{\sigma_a(x) + \lambda\sigma_S(x) + \sigma_m}dx \tag{1.61}$$

Introduction of the expressions for $\sigma_a(x)$ and $\sigma_S(x)$ gives

$$I_{eff}^{I.R}(\xi) = \frac{2}{\pi}\frac{I_0}{\gamma_\lambda^2}J\left(\xi, 1/\gamma_\lambda^2, a_\lambda\right) \tag{1.62}$$

where J and γ_λ^2 are respectively given by equations (1.43) and (1.48) and a_λ is given by

$$a_\lambda = \frac{\lambda}{\gamma_\lambda^2}\frac{\sigma_{0P}}{(\lambda\,\sigma_P + \sigma_m)} \tag{1.63}$$

In the limit of zero temperature, the *J*-function can be evaluated analytically and we get

$$I_{eff}^{I.R}(\xi) = \frac{I_0}{\sqrt{\beta_\lambda^2 - \eta_\lambda^2}} \tag{1.64}$$

where β_λ^2 and $\widehat{\eta}_\lambda$ are defined by

$$\beta_\lambda^2 = 1 + \gamma_\lambda^2 \tag{1.65}$$

$$\eta_\lambda = \frac{\lambda\,\sigma_{0P}}{(\lambda\,\sigma_P + \sigma_m)} \tag{1.66}$$

The limits λ=1 and λ=0, respectively, give the resonance integral in the narrow resonance and wide resonance approximations. Thus, in the zero temperature-limit we get

(1.67) $$I_{eff}^{N.R}(\infty) = \frac{I_0}{\sqrt{\beta_1^2 - \eta_1^2}}$$

(1.68) $$I_{eff}^{N.R}(\infty) = \frac{I_0}{\beta_0}$$

The procedure given by Goldstein [22, 23] to determine the interpolation parameter λ is the following. Equation (1.37) may be rewritten as

(1.69) $$\left[\sigma_a(x) + \lambda\sigma_s(x) + \sigma_m\right] f(x) = \left(\sigma_m + \lambda\sigma_P\right) + (\lambda - 1)\left[\sigma_s(x) f(x) - \sigma_P\right] + \frac{1}{\varepsilon}\int_x^{x+\varepsilon}\left[\sigma_s(y) f(y) - \sigma_P\right]dy$$

A first order approximation to *f(x)* is obtained by neglecting the terms in the square bracket on the RHS of the above equation. It is seen to be same as f_{IR} given by equation (1.60). A second order approximation to *f(x)* is obtained by substituting f_{IR} for *f(x)* on the *RHS* of equation (1.69). It is found to be

(1.70) $$f_{I.R}^{*} = f_{I.R}\left[1 + \frac{1}{\sigma_m + \lambda\sigma_P}\left\{(\lambda - 1)\left(\sigma_s(x) f(x) - \sigma_P\right) + \frac{1}{\varepsilon}\int_x^{x+\varepsilon}\left(\sigma_s(y) f(y) - \sigma_P\right)dy\right\}\right]$$

Goldstein obtains an equation for λ by equating the resonance integrals obtained with these two successive approximations to *f(x)*. Thus he obtains

(1.71) $$\lambda = 1 - \frac{\int_{-\infty}^{\infty}\sigma_a(x)dx\frac{1}{\varepsilon}\int_x^{x+\varepsilon}\left[\sigma_s(y) f_{I.R}(y) - \sigma_P\right]dy}{\int_{-\infty}^{\infty}\sigma_a(x)\left[\sigma_s(x) f_{I.R}(x) - \sigma_P\right]dx}$$

The integrals in equation (1.71) can be analytically evaluated only in the limit of zero temperature. Thus in the zero temperature limit we get

(1.72) $$\lambda = 1 - \frac{1}{\delta_\lambda}\tan^{-1}(\delta_\lambda) - \frac{\eta_1\sqrt{\beta_\lambda^2 - \eta_\lambda^2}}{\beta_1^2 - \beta_0^2 - 2\eta_1\eta_\lambda}\frac{1}{\delta_\lambda}\log\left(1 + \delta_\lambda{}^2\right)$$

$$\delta_\lambda = \frac{\varepsilon}{2\sqrt{\beta_\lambda^2 - \eta_\lambda^2}}$$

When λ is evaluated as the solution of this transcendental equation, the resonance integral can be readily obtained from equation (1.64).

For many resonances of fertile materials of interest, the resonance potential interference term in the scattering cross-section can be neglected. This happens because of the smallness of Γ_n in comparison to Γ [24, 25]. In this situation, the transcendental equation (1.72) for λ simplifies to

$$\lambda = 1 - \frac{2\beta_\lambda}{\varepsilon}\tan^{-1}\left[\frac{\varepsilon}{2\beta_\lambda}\right] \tag{1.73}$$

The expression for the resonance integral also gets simplified to

$$I_{eff}^{I.R}(\infty) = \frac{I_0}{\beta_\lambda} \tag{1.74}$$

It can be seen from the transcendental equations (1.72) and (1.73) that the narrow resonance and wide resonance limits of λ, viz., 1 and 0, respectively, are obtained in the limits ε tending to ∞ and 0.

It is natural to seek the consequences if the equation for λ is determined by equating the resonance integral obtained by the first order approximation and, say, the third order approximation. Dyos and Keane [26] have investigated this problem in the simplified situation when the resonance potential interference scattering is neglected. They have observed that the convergence of the scheme of determining λ by equating resonance integral in the first order approximation to that obtained in higher order approximations in rather slow when $\Gamma_n > \Gamma_r$.

The major problem in the intermediate resonance approximation has been found to be the range of the interpolation parameter when resonance potential interference scattering is present [14]. Usually, one expects the actual resonance integral to lie between those calculated in the limiting narrow resonance and wide resonance approximations. But when resonance potential interference scattering is present, for certain situations depending on the value of σ_m and the relative magnitudes of Γ_n and Γ_r this does not happen. The actual resonance integral goes outside the limits given by the narrow resonance and wide resonance approximations. Consequently, the interpolations parameter goes outside its expected range between 0 to 1 [14]. Therefore, Goldstein's procedure becomes an extrapolation rather than an interpolation. Further, the transcendental equation (1.72) for determining λ is somewhat complicated and gives rise to more than one solution on the real axis and sometimes just one solution. The changeover from interpolation to extrapolation and the difficulty in determining the roots of the transcendental equation have been discussed in detail by Mikkelson [27].

The generalization of Goldstein's method of determining λ to include temperature dependence of resonance cross-sections is not straightforward. Because of the complicated form of the cross-sections, one is not able to get an equation for λ as in the case of zero temperature. However, with certain approximations, Goldstein [21, 28] evaluates the integrals in equation (1.71) and provides an equation for λ in terms of the tabulated functions like $J(\xi,\beta,a)$. He has shown that the resulting equation for λ reproduces the equation (1.72) in the zero temperature limit. But the possibility of solving this general transcendental equation for all situations has not been clearly shown. Many authors have investigated the possibility of using the interpolation parameter λ determined from zero temperature calculations directly in the temperature dependent resonance integrals [29,27,14]. That is, if λ is evaluated from the transcendental equation (1.73), the temperature dependent resonance integral is given by

$$I_{eff}^{I.R}(\xi)=\frac{2}{\pi}\frac{I_0}{\gamma_\lambda^2}J\left(\xi,1/\gamma_\lambda^2\right) \tag{1.75}$$

where γ_λ^2 is given by equation (1.48) and $J(\xi,\beta)$ is the function defined as [17]

$$J(\xi,\beta)=\int_0^\infty \frac{\psi(x,\xi)}{\beta+\psi(x,\xi)}dx \tag{1.76}$$

Of course, if resonance potential interference scattering is included and λ is obtained from equation (1.72), the expression for the resonance integral given by equation (1.62) will have to be used.

It was observed by Goldstein [15] that if resonance potential interference scattering is neglected, the first order approximation to $f(x)$ becomes symmetric about the origin. It can be readily seen from equation (1.49) that $f(x)$ is a symmetric function only when $\gamma_1^2=\gamma_\infty^2$. However, the second and higher order approximations show the expected behavior of $f(x)$ [15,30]. Pomeraning and Dyos [31] tried to remove the symmetric nature of the first order approximation by introducing one more interpolation parameter. They have shown that this improves the accuracy of the intermediate resonance approximation.

Goldstein [18], Seghal [19] and Ishiguro [14] have generalized the intermediate resonance approximation to remove the narrow resonance approximation for the moderator collision integral by introducing two interpolation parameters.

We feel that when generalizations are attempted the intermediate resonance approximation is not free from difficulties. Nevertheless, the intermediate resonance approximation is an important step in the development of techniques of solution to the resonance absorption problems.

F: Other Methods Of Solving The Slowing Down Equation:

In the previous section we considered some of the methods which are specifically aimed at evaluating the resonance integral. In this section we shall briefly outline some of the general attempts in solving the slowing down equation.

1. Weinberg and Wigner – Corngold equation:

An altogether different approach to the solution of the slowing down equation was given by Weinberg and Wigner [32]. They considered neutron absorption as a negative source and reformulated the slowing down equation using the solution in the non-absorbing situation as a Green's function. Equation (1.16) with a mono-energetic source emitting neutrons of energy $e*$ may be rewritten as

$$(1.77)\quad [\sigma_s(e)+\sigma_m]\,\Phi(e)=\delta(e-e*)-\sigma_a(e)\Phi(e)+\int_e^{e/\alpha_m}\frac{\sigma_m\Phi(e')}{(1-\alpha_m)}\,\frac{de'}{e'}+\int_e^{e/\alpha}\frac{\sigma_s\Phi(e')}{(1-\alpha)}\,\frac{de'}{e'}$$

Now let us denote by *g(e,e*)* the solution of equation (1.77) in the situation when the absorption cross-section is zero. The solution *g(e,e*)* is also known as Placzek funcftion [2,33]. The principle of superposition of the solutions of linear equations may be employed to reformulate equation (1.77) as

$$(1.78)\qquad \Phi(e)=g(e,e*)-\int_e^{e*}\sigma_a(e')\,\Phi(e')\,g(e,e')\,de'$$

An important point to be noticed in this formulation is that the above integral equation for $\Phi(e)$ is of the Volterra type. However, it is very complicated because its kernel is the Placzek function having discontinuities in all orders of derivatives [2]. Therefore, it is necessary to resort to approximation techniques for its solution. It has been pointed out that it is quite suitable for obtaining solutions by iteration [2,33]. Proceeding on these lines, Weinberg and Wigner obtained a correction factor in the expression for the resonance escape probability given by the narrow resonance approximation.

Subsequently, using Laplace transforms, Corngold [34] gave a rigorous and more general formulation of the problem in terms of Green's functions. Then he set up a variational principle for the resonance escape probability in terms of the neutron flux and its adjoint function and showed that quite accurate estimates of this parameter could be obtained with simple trial functions. Further, using this variational approach he estimated the effects of the assumption of asymptotic flux recovery between neighboring resonances of the absorber [35]. To employ analytical treatment of this problem, Corngold used only representative forms of the resonance cross-sections such as rectangular shapes in the lethargy space and hence the conclusions drawn are only of a general nature.

2. Synthetic kernel approach to the solution of the slowing down equation:

There had been a continuing attempt in developing approximate forms of the kernel of the slowing down equation so as to get analytical solutions. Three well known approximate kernels, also known as synthetic kernels, are due to Fermi [36,2], Wigner [2,32] and Goertzel and Greuling [37]. The synthetic kernels reduce the slowing down dequation to Volterra equations whose solutions can be analytically obtained. These kernels are derived under the approximation that the collision density is a slowly varying function of lethargy variable and they contain the first two moments of the slowing down kernel as parameters. This approach to the solution of the slowing down equation has been improved by Stacey [39] by redefining the parameters of the approximate kernel. The main aim is to enlarge the applicability of the theory to situations having at lease weak resonances in cross-sections. The improvement by Yamamura et al [39,40] to include higher moments of the slowing down kernel has been found to destroy the basic analytical nature of the method. However, it has provided very fast algorithms for the computation of fast reactor spectra. Recently, Yamamura et al [41, 42] have developed a scheme in which the parameters of the synthetic kernel are themselves functions of the solution of the equation and to be obtained in an iterative manner. The present status of the synthetic kernel approach is that in the simplest form it can not be applied to the resonance absorption problem while the sophisticated versions though accurate require a good amount of numerical work. The extension of this formalism to include anisotropic scattering in the centre of mass system, inelastic mode of energy degradation, time dependence, etc. have also been attempted. These are summarized by Stacey in a recent review article [43].

G: Summary of the Present Work:

The work presented in this thesis represents a new attempt to solve the slowing down equation when the resonance cross-sections can be represented by the single level Breit-Wigner formulae. The idea we have exploited is that the discontinuous nature of the kernel of the slowing down equation can be removed by going over to the Fourier transform space. It may be appropriate to remark here that similar approach was used for solving the neutron transport equation in finite systems in single as well as multi-dimensional situations [44, 45]. Our method uses the fact that the Fourier transforms of ψ and χ functions have very simple analytical forms and thus circumvents the difficulties arising from the non-availability of the analytical expressions for the temperature dependent resonance cross-sections. Further, the method is specifically aimed at obtaining the integral parameter of interest, viz. the resonance integral, directly rather than first obtaining the neutron flux distribution in the resonance and then calculating this parameter. This is achieved by carefully defining the unknown function in the transform variable.

Chapter-II is devoted to the development of the most important ideas of the present work. In order to simplify the treatment we introduce two assumptions, viz. that the resonance potential interference scattering can be neglected and that the moderator collision integral can be treated in the narrow resonance approximation. Thus we treat equation (1.47). Introducing the Fourier representation of the discontinuity factor we convert equation (1.47) to a Fredholm integral equation of second kind with a continuous kernel over the interval $(-\infty,\infty)$ [46]. In this process, the unknown function $\theta(k,\xi)$ in the transform variable k is defined such that its value at the origin ($k=0$) is directly proportional to the resonance integral.

Thereafter the main task is to solve this integral equation and obtain the resonance integral. However, a simplification arises in the limit of zero temperature. It is shown that in this limit, the kernel of the integral equation becomes a Green’s function of a second order differential operator and therefore the equation for $\theta(k,\infty)$ can be reduced to a second order differential equation [46, 47]. The narrow resonance, wide resonance and intermediate resonance approximations are shown to correspond to approximating a function $g(k,\varepsilon)$ depending on the resonance parameters by various constant values. Next we develop a *WKB* solution to the differential equation and obtain a new expression for the resonance integral [47]. This formula is applied to some of the typical resonances of U^{238} nucleus in a homogenous mixture with hydrogen. The numerical values of the resonance integral are compared with those obtained by other methods.

Subsequently we concentrate on the temperature dependent problem [46]. Here it is found that the kernel of the integral equation contains a factor $exp\ (-k^2/\xi^{\ 2})$. Therefore the equation can be solved by employing the Gauss-Hermite quadrature formulae except for large values of ξ which correspond to low temperatures. So the zero temperature part of the solution is separated and the temperature dependent correction alone is obtained with the use of the quadrature formulae.

Earlier we have seen that in the classical approximations, viz., the narrow resonance, wide resonance and intermediate resonance approximations, the temperature dependent resonance integral is proportional to the resonance integral function $J(\xi,\beta)$. Therefore, our method of solving the integral equation of slowing down theory gives a procedure to evaluate this function when we make suitable approximations in the equations [46]. By comparing the $J(\xi,\beta)$ function calculated by this method with the numerical computations over a wide range of ξ and β values, we obtain a fairly good estimate of the accuracy of this method. Finally, the method is applied for evaluating the Doppler coefficients of some of the resonances of U^{238} nucleus in a homogeneous mixture with hydrogen. These results are compared with those obtained by the intermediate resonance approximation and Monte Carlo calculations.

In Chapter III, the method is generalized to include resonances potential interference scattering [48]. Thus we treat equation (1.37) when σ_a and σ_s are given by equations (1.10) and (1.11). For the temperature dependent problem it is shown that an integral equation for a function related to $\theta(k,\xi)$ can be obtained. Again we consider the integral equation in the zero temperature-limit and obtain a second order differential equation for $\theta(k,\infty)$. Applying the *WKB* method to obtain the solution, a new expression for the resonance integral including the resonance potential interference scattering effects is derived. We then analyze the intermediate resonance approximation through the solution of this differential equation. Introducing two interpolation parameters a set of two coupled transcendental equations are obtained. These equations are derived by equating $\theta(k,\infty)$ and its derivative at $k=0$ obtained in two successive orders of approximation. It is found that these equations are easier to solve numerically compared to Goldstein's equation and yield fairly accurate values for the resonance integral. This discussion is concluded with a comparison of the numerical values of zero temperature resonance integrals of U^{238} nucleus.

Because of the nature of certain terms present due to the inclusion of resonance potential interference scattering, we notice that it is not appropriate to employ the Gauss-Hermite quadrature formulae for the solution of the general integral equation. Therefore, we examine the approach wherein the solution is expanded in terms of a set of polynomials related to Hermite polynomials. It is shown that the matrix elements of the resulting system of equation determining the expansion coefficients can be evaluated using suitable recurrence relations.

So far we were working under the assumption that the resonances are sufficiently separated in energy and used the unperturbed neutron flux distribution viz. the '1/*e*' distribution above the resonance. When the resonances of the absorber are closely spaced, the presence of one resonance perturbs the flux distribution in the other resonance. This interaction between the resonances leads to a reduction in the overall resonance absorption and modifies the Doppler broadening effect considerably. The effect of interaction is of second order in magnitude and obtaining it even from a direct numerical solution of the slowing down equation would be difficult. This is because the Doppler broadened functions are also to be computed numerically.

In Chapter-IV, we generalize the Fourier transform method for an estimation of these effects [50]. In the energy region of interfering resonances, the scattering and absorption cross-sections of the absorber are given by superposition of the cross-sections for individual resonances. For the case of two interacting resonances, the problem of obtaining the resonance integral (including the interaction effect) is reduced to the solution of a Fredholm integral equation. In the zero temperature-limit, the equations in the transform variable are shown to reduce to two coupled second order differential equations. A method of solving these equations is developed in the *WKB* approximation and applied to the two interfering low-energy resonances of Th^{232} [50]. Thereafter we consider the temperature dependent problem. It is well known that in the narrow resonance approximation the resonance integral including the interaction effect is proportional to be generalized *J*-function [51]. We make suitable approximations in the integral equation so that its solution at $k=0$ is proportional to this function. Employing the Gauss-Hermite quadrature formulae to obtain the solution of the resulting integral equation, we calculate the Doppler coefficients of Th^{232} resonances. It is seen that the interaction between the resonances leads to destructive interference and consequent reduction in Doppler coefficient for low temperature.

In Chapter-V we develop the Fourier transform method relaxing the assumption of narrow resonance approximation for the moderator collision-integral. There is an important difference between equation (1.23) to be treated in this situation and those encountered in earlier chapters. Equation (11.23) is a homogenous equation in $f(x)$ and is to be solved with the normalization condition that $f(x)$ goes to unity when $x\rightarrow\infty$. In the equations treated earlier, together with the narrow resonance approximation for moderator collision integral, this normalization condition had been employed and therefore they appeared as inhomogeneous equations. In converting the initial value problem posed by equation (1.23) together with the normalization condition to an integral equation in the Fourier transform space, we find it necessary to introduce elementary ideas from the theory of distributions [52]. The situation encountered is similar to that occurring in Case's method of solving the neutron transport equation in plane geometry [53]. In later part of this Chapter we consider the integral equation in the limiting situation of zero temperature and show that a second order differential equation can be obtained.

In conclusion, it may be said that we have given a new formulation of the problem of resonance absorption in reactor physics. Using Fourier transforms, we convert the slowing down equation with resonance cross-sections to Fredholm integral equations of second kind. The equations reduce to second order differential equations in the limit of zero temperature. The important feature of our method has been the reduction of the slowing down integral equation with discontinuous kernel to equations of the type well studied in mathematical physics. The methods attempted to solving the equations in the transformed space do indicate the applicability of this approach to the evaluation of resonance integrals accurately.

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CHAPTER-II

FOURIER TRANSFORM METHOD FOR EVALUATING RESONANCE INTEGRALS – PART I

In this Chapter we shall develop some of the salient features of the Fourier transform method for evaluating resonance integrals. For the sake of simplicity it will be assumed that the resonance potential interference scattering can be neglected and that the moderator collision integral can be treated in the narrow resonance approximation.

A: <u>Derivation of the Freedom Integral Equation</u>:

We shall proceed with the temperature dependent cross-sections and show that the slowing down equation can be transformed to a Fredholm integral equation [46]. Introducing the constant *A* defined as

$$A=\frac{\sigma_P}{\sigma_m+\sigma_P} \tag{2.1}$$

equation (1.49) can be rewritten as

$$\left[1+\gamma_1^2\,\psi(x,\xi)\right]f(x)=(1-A)+\frac{A}{\varepsilon}\int_x^{x+\varepsilon}\left[1+\gamma_\infty^2\,\psi(y,\xi)\right]f(y)\,dy \tag{2.2}$$

Our aim is to obtain the resonance integral defined din terms of *f(x)* in equation (1.32). As have been already emphasized, one of the difficulties in dealing with the above integral equation is the doubly discontinuous nature of its kernel. To remove this we introduce the discontinuity factor,

$$\begin{aligned} H(x,y,\varepsilon)&=0,\;\; y<x \\ &=1,\;\; x<y<x+\varepsilon \\ &=0,\;\; y>x+\varepsilon \end{aligned} \tag{2.3}$$

Using $H(x,y,\varepsilon)$, equation (2.2) can be written as

$$\left[1+\gamma_1^2\,\psi(x,\xi)\right]f(x)=(1-A)+\frac{A}{\varepsilon}\int_{-\infty}^{\infty}\left[1+\gamma_\infty^2\,\psi(y,\xi)\right]H(x,y,\varepsilon)\,f(y)\,dy \tag{2.4}$$

$H(x,y,\varepsilon)$ *can* be expressed as

$$H(x,y,\varepsilon)=\int_x^{x+\varepsilon}\delta(y-z)\,dz \tag{2.5}$$

where $\delta(y-z)$ is the usual Dirac delta function. Using the Fourier integral representation of the delta function [52] we get

$$H(x,y,\varepsilon) = \int_{-\infty}^{\infty} dk'\nu(k',\varepsilon)\exp[ik'(y-x)]$$

where

$$\nu(k,\varepsilon) = \frac{(1-e^{-ik\varepsilon})}{ik\varepsilon} \tag{2.6}$$

The fact that this is indeed a representation of the discontinuity factor can be seen by considering it as a contour integral. Substituting for *H(x,y,ε)* in equation (2.4) we get

$$\left(1+\gamma_1^2\psi\right) f(x) = (1-A) + A\int_{-\infty}^{\infty} dk'\nu(k',\varepsilon)e^{-ikx}\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik'y}\left(1+\gamma_\infty^2\psi\right) f(y)\,dy \tag{2.7}$$

Defining the Fourier transforms

$$\theta(k,\xi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\, f(x)\psi(x,\xi)\,dx \tag{2.8}$$

$$F(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\, f(x)\; dx \tag{2.9}$$

equation (2,7) can be rewritten as

$$\left[1+\gamma_1^2\psi(x,\xi)\right] f(x) = (1-A) + A\int_{-\infty}^{\infty} dk'\nu(k',\varepsilon)e^{-ik'x}\left[F(k')+\gamma_\infty^2\theta(k',\xi)\right] \tag{2.10}$$

Fourier transformation of this equation gives

$$F(k)+\gamma_1^2\,\theta(k,\xi) = (1-A)\delta(k) + A\nu(k,\varepsilon)\left[F(k)+\gamma_\infty^2\theta(k,\xi)\right] \tag{2.11}$$

In obtaining this relation between *F(k)* and *θ(k,ξ)* we have used the Fourier integral representation of the delta function. The above equation can be rewritten as

$$F(k)+\frac{\gamma_1^2-\gamma_\infty^2\nu(k,\varepsilon)}{1-A\nu(k,\varepsilon)}\theta(k,\xi) = \frac{(1-A)}{1-A\nu(k,\varepsilon)}\delta(k) \equiv \delta(k) \tag{2.12}$$

It is now appropriate to look closely into the definition of the transforms *F(k)* and *θ(k,ξ)*. We have seen that *f(x)* goes to unity as $x \to \pm\infty$. Therefore its Fourier transform *F(k)* will contain a delta function as has been obtained in equation (2.12).

The transform *θ(k,ξ)* is of particular interest because at k=0 it is proportional to the resonance integral. Equation (1.32) shows that

$$I_{eff}(\xi) = 2I_0\theta(0,\xi) \tag{2.13}$$

Thus it is natural to convert the relation (2.12) between *F(k)* and *θ(k,ξ)* into an equation in *θ(k,ξ)*. Thereafter the resonance integral can be obtained directly from its solution. To eliminate *F(k)* from equation (2.12) we need one more independent relation between *F(k)* and *θ(k,ξ)*. If we denote by $\overline{\psi}(k,\xi)$ the Fourier transform of the ψ function, the application of the convolution [52] theorem to equation (2.8) gives

$$\theta(k,\xi) = \int_{-\infty}^{\infty} F(k')\,\overline{\psi}(k-k',\xi)\,dk' \tag{2.14}$$

Changing the variable to k' in equation (2.12), multiplying by $\overline{\psi}(k-k',\xi)$ and integrating over k' we get

$$\theta(k,\xi) + \int_{-\infty}^{\infty} \overline{\psi}(k-k',\xi)\left[\frac{\gamma_1^2 - \gamma_\infty^2 \nu(k',\varepsilon)}{1 - A\nu(k',\varepsilon)}\right]\theta(k',\xi)\,dk' = \overline{\psi}(k,\xi) \tag{2.15}$$

To complete the derivation of the integral equation we have to evaluate the function $\overline{\psi}(k,\xi)$. The ψ function was defined as a convolution integral in equation (1.12). Therefore its transform can be obtained with the use of the converse of the convolution theorem [51,52].

$$\overline{\psi}(k,\xi) = \frac{1}{2}\exp(-|k|)\exp(-k^2/\xi^2) \tag{2.16}$$

Here $(1/2)\exp(-|k|)$ and $\exp(-k^2/\xi^2)$ are respectively the Fourier transforms of the Lorentzian and Gaussian functions. Substituting for $\overline{\psi}(k-k',\xi)$ in equation (2.15) we find

$$\begin{aligned} \theta(k,\xi) + \frac{1}{2}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - (k-k')^2/\xi^2\right] g(k',\varepsilon)\,\theta(k',\xi)\,dk' \\ = \frac{1}{2}\exp\left[-|k| - k^2/\xi^2\right] \end{aligned} \tag{2.17}$$

The function *g(k,ε)* is defined as

$$g(k,\varepsilon) = \frac{\gamma_1^2 - A\gamma_\infty^2\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)} \tag{2.18}$$

Thus the problem of solving the slowing down equation and evaluating the resonance integral (including its temperature dependence) has been reduced to the solution of the integral equation (2.17). It is a Fredholm integral equation of second kind with a continuous kernel over the interval (-∞,∞). It may be remarked that in the present method we have circumvented the difficulties arising from the non-availability of analytical expressions for the Doppler broadened functions. The fact that the ψ function has a simple analytical expression in the Fourier transform space has been exploited in our approach.

The flux distribution in the resonance, if required, can be obtained from the inverse transform:

$$f(x)\psi(x,\xi) = \int_{-\infty}^{\infty} e^{-ikx}\theta(k,\xi)\,dk \tag{2.19}$$

Before discussing the integral equation (2.17) further, we shall analyze the limiting zero temperature situation.

B. Resonance Integrals in the Zero Temperature Limit:

In Chapter-I we have seen that most of the analytical work on resonance absorption problems is limited to the zero temperature situation. This becomes possible due to the Lorentzian form of the Breit-Wigner cross-section. In the present method the integral equation gets simplified and a good amount of work can be carried out analytically.

(i) Derivation of a differential equation for θ

When the temperature of the medium goes to zero, the parameter $\xi \rightarrow \infty$. Therefore, equation (2.17) becomes

$$\theta(k,\infty)+\frac{1}{2}\int_{-\infty}^{\infty}\exp\left(-\left|k-k'\right|\right)g(k',\varepsilon)\ \theta(k',\infty)\,dk'=\frac{1}{2}\exp\left(-\left|k\right|\right) \tag{2.20}$$

Since the kernel of this integral equation happens to be the Green's function of a differential operator it can be reduced to a differential equation. That is [54],

$$\left(\frac{d^2}{dk^2}-1\right)\frac{1}{2}\exp\left(-\left|k-k'\right|\right)=-\delta(k-k') \tag{2.21}$$

Applying this operator on equation (2.20) we get

$$\left(\frac{d^2}{dk^2}-1\right)\theta(k,\infty)-g(k,\varepsilon)\theta(k,\infty)=-\delta(k) \tag{2.22}$$

This may be rewritten as [46,47]

$$\frac{d^2\theta}{dk^2}-\left[1+g(k,\varepsilon)\right]\theta(k,\infty)=-\delta(k) \tag{2.23}$$

Since the integral equation has been converted into a differential equation we have to provide the boundary conditions on $\theta(k,\infty)$. They are provided by putting $k=\pm\infty$ in equation (2.20),

$$\theta(k,\infty)=0, \qquad k=\pm\infty \tag{2.24}$$

Thus the problem of evaluating the zero temperature resonance integral has been reduced to the solution of a differential equation. Earlier, Spinrad, Chernic and Corngold [55] had barely outlined the possibility of deriving such a differential equation. But at the time of developing the method published in reference [47] we were completely unaware of the aforesaid work.

The delta function ion the R.H.S. of equation (2.23) shows that $d\theta/dk$ is discontinuous at $k=0$. The discontinuity can be obtained by integrating the equation near the origin:

$$\left.\frac{d\theta}{dk}\right|_{0+} - \left.\frac{d\theta}{dk}\right|_{0-} = -1 \tag{2.25}$$

Thus the problem reduces to the solution of the homogenous differential equation

$$\frac{d^2\theta}{dk^2} - \left[1 + g(k,\varepsilon)\right]\theta(k,\infty) = 0 \tag{2.26}$$

in the open interval $(0,\infty)$ and $(-\infty,0)$ satisfying the boundary condition

$$\theta(k,\infty) \to 0, \quad as \;\; k \to \pm\infty \qquad (a) \tag{2.27}$$

From the definition of $\theta(k,\infty)$, we know that it is continuous at $k=0$, that is,

$$\left.\theta(k,\infty)\right|_{0+} = \left.\theta(k,\infty)\right|_{0-} \qquad (b) \tag{2.28}$$

Finally we have

$$\left.\frac{d\theta}{dk}\right|_{0-} - \left.\frac{d\theta}{dk}\right|_{0+} = 1 \qquad (c) \tag{2.29}$$

Before attempting the general solution, we shall consider some limiting situations [47]

(ii) <u>Solutions of the differential equation in certain limiting situations</u>:

While discussing the intermediate resonance approximation we pointed out that the narrow resonance and wide resonance approximation can be obtained in the limits $\varepsilon\to\infty$ and $\varepsilon\to 0$. As $\varepsilon\to\infty$, the function $v(k,\varepsilon) \to 0$. Thus we get

$$g_{N.R}(k,\varepsilon) = \gamma_1^2 \tag{2.30}$$

The differential equation (2.26) becomes

$$\frac{d^2\theta_{N.R}}{dk^2} - \beta_1^2\,\theta_{N.R}(k,\infty) = 0 \tag{2.31}$$

with $\beta_1^2 = 1 + \gamma_1^2$. The general solution of this equation is

$$\theta_{N.R}(k,\infty) = C_+ \exp(-\beta_1 k) + C_- \exp(+\beta_1 k) \tag{2.32}$$

where $C_\pm$ are consonants. $\theta_{N.R}$ Satisfying the boundary conditions (2.27) is given by

$$\begin{aligned} \theta_{N.R}(k,\infty) &= C_+ \exp(-\beta_1 k)\,, \;\; k > 0 \\ \theta_{N.R}(k,\infty) &= C_- \exp(-\beta_1 k)\,, \;\; k < 0 \end{aligned} \tag{2.33}$$

The other conditions (2.28) and (2.29) give

$$\begin{aligned} &C_+ = C_- \\ &\frac{C_- + C_+}{\beta_1} = 1 \end{aligned} \tag{2.34}$$

which yield

(2.35) $$C_+ = C_- = \frac{1}{2\beta_1}$$

Finally

(2.36) $$\theta_{N.R}(k,\infty) = \frac{1}{2\beta_1}\exp(-\beta_1|k|)$$

The resonance integral in the narrow resonance approximation becomes

(2.37) $$I_{eff}^{N.R}(\infty) = 2I_0\theta_{N.R}(0,\infty) = \frac{I_0}{\beta_1}$$

and is found to be same as that given in equation (1.74).

As $\varepsilon \to 0$, the function $\nu(k,\varepsilon) \to 1$ and we get

(2.38) $$g_{W.R}(k,\varepsilon) = \frac{\gamma_1^2 - A\gamma_\infty^2}{1-A}$$

This is same as the quantity γ_0^2 according to the definition of γ_λ^2 given in equation (1.48). Thus we get

(2.39) $$\frac{d^2\theta_{W.R}}{dk^2} - \beta_0^2\,\theta_{W.R}(k,\infty) = 0$$

where $\beta_0^2 = 1 + \gamma_0^2$. Solution of this equation is

(2.40) $$\theta_{W.R}(k,\infty) = \frac{1}{2\beta_0}\exp(-\beta_0|k|)$$

and

(2.41) $$I_{eff}^{W.R}(\infty) = 2I_0\theta_{W.R}(0,\infty) = \frac{I_0}{\beta_0}$$

which is again the expression obtained earlier. Further the function $g(k,\varepsilon)$ can be rewritten as

(2.42) $$g(k,\varepsilon) = \gamma_1^2 + (\gamma_1^2 - \gamma_\infty^2)\frac{A\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)}$$

thus when $\gamma_1^2 = \gamma_\infty^2$, we again obtain the narrow resonance limit. Earlier we have seen that this is same as the condition $\Gamma_n/\Gamma = \sigma_P/(\sigma_P + \sigma_m)$ observed by Spinney [20].

The intermediate resonance approximation corresponds to the approximation

(2.43) $$g_{I.R}(k,\varepsilon) \cong \gamma_\lambda^2$$

Therefore we have

(2.44) $$\theta_{I.R}(k,\infty) = \frac{1}{2\beta_\lambda}\exp(-\beta_\lambda|k|)$$

and

(2.45) $$I_{eff}^{I.R}(\infty)=2I_0\theta_{I.R}(0,\infty)=\frac{I_0}{\beta_\lambda}$$

where $\beta_\lambda^2=1+\gamma_\lambda^2$. The constant γ_λ^2 or β_λ is as yet unspecified. The procedure given by Goldstein can be used to derive a transcendental equation for β_λ. Details of this derivation will be given in the next Chapter where we shall consider the general problem including resonance potential interference scattering.

(iii) WKB approximation for $\theta(k,\infty)$

Equation (2.26) being a second order differential equation with a variable coefficient can not be integrated exactly. One of the powerful methods for treating this equation is the WKB method [56]. We shall derive a new expression for I_{eff} by obtaining a WKB approximation to $\theta(k,\infty)$. Using equation (2.42), equation (2.26) can be written as

(2.46) $$\frac{d^2\theta}{dk^2}-\beta_1^2\,\theta(k,\infty)-(\gamma_1^2-\gamma_\infty^2)\frac{A\,\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}\theta(k,\infty)=0$$

It is seen that the coefficient of $\theta(k,\infty)$ in the last term goes to zero as k → ±∞. Therefore the asymptotic form of $\theta(k,\infty)$ is same as $\theta_{N.R}(k,\infty)$. To include this fact, we attempt a solution

(2.47) $$\theta(k,\infty)=C_+\exp\left[-\beta_1|k|+\int_k^\infty S^+(k')dk'\right],\ k>0$$

$$=C_-\exp\left[-\beta_1|k|+\int_{-\infty}^k S^-(k')dk'\right],\ k<0$$

The boundary conditions (2.27) require

(2.48) $$\int_k^\infty S^+(k')dk'\to 0\ \ as\ \ k\to\infty$$

$$\int_{-\infty}^k S^-(k')dk'\to 0\ \ as\ \ k\to-\infty$$

This implies that

(2.49) $$S^\pm(k')\to 0\ \ (faster\ \ than\ \ 1/k)\ as\ \ k\to\pm\infty$$

The continuity condition (2.28) gives

(2.50) $$C_+\exp\left[-\beta_1|k|+\int_0^\infty S^+(k')dk'\right]=C_-\exp\left[-\beta_1|k|+\int_{-\infty}^0 S^-(k')dk'\right]$$

The discontinuity condition (2.29) gives

(2.51) $$C_-\left[\beta_1 + S^-(0)\right]\exp\left[\int_{-\infty}^{0} S^-(k')dk'\right] - C_+\left[-\beta_1 - S^+(0)\right]\exp\left[\int_{0}^{\infty} S^+(k')dk'\right] = 1$$

Solving these equations, we get

(2.52) $$C_+ = \frac{1}{2\beta_1 + S^+(0) + S^-(0)}\exp\left[-\int_0^\infty S^+(k')dk'\right]$$

$$C_- = \frac{1}{2\beta_1 + S^+(0) + S^-(0)}\exp\left[-\int_{-\infty}^{0} S^-(k')dk'\right]$$

Substituting in equation (2.47), we obtain

(2.53) $$\theta(k,\infty) = \frac{1}{2\beta_1 + S^+(0) + S^-(0)}\exp\left[-\beta_1 k - \int_0^k S^+(k')dk'\right] \quad , \quad k > 0$$

$$= \frac{1}{2\beta_1 + S^+(0) + S^-(0)}\exp\left[+\beta_1 k - \int_k^0 S^-(k')dk'\right] \quad , \quad k < 0$$

Thus *θ(k,∞)* has been expressed in terms of $S^{\pm}(k)$. The resonance integral becomes

(2.54) $$I_{eff}(\infty) \; = \frac{2I_0}{2\beta_1 + S^+(0) + S^-(0)}$$

We now substitute from equations (2.53) in the differential equation (2.46) and get

(2.55) $$\mp\frac{dS^{\pm}}{dk} + 2\beta_1 S^{\pm}(k) + [S^{\pm}(k)]^2 = (\gamma_1^2 - \gamma_\infty^2)\frac{A\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)}$$

The upper sign stands for *k>0* and the lower sign for *k<0*. Since the above equations are nonlinear equations of the Ricatti type they can not be integrated exactly. We shall obtain their solutions by a perturbation expansion. The first order approximation is obtained by neglecting the quadratic terms in the equations. Integrating the resulting equation and using the boundary condition (2.49), we find

(2.56) $$S_1^+(k) = (\gamma_1^2 - \gamma_\infty^2)\int_k^\infty \exp[-2\beta_1(k'-k)]\frac{A\nu(k',\varepsilon)}{1 - A\,\nu(k',\varepsilon)}dk'$$

$$S_1^-(k) = (\gamma_1^2 - \gamma_\infty^2)\int_{-\infty}^{k} \exp[+2\beta_1(k'-k)]\frac{A\nu(k',\varepsilon)}{1 - A\,\nu(k',\varepsilon)}dk'$$

These solutions will be sufficiently accurate when $|S(k)| << 2\beta_1$ The second order approximation is obtained by substituting $S_1^{\pm}(k)$ in the quadratic terms in equations (2.55). Integrating the resulting equations we get

(2.56) $$S_2^+(k) = \int_k^\infty \exp[-2\beta_1(k'-k)]\left[(\gamma_1^2 - \gamma_\infty^2)\frac{A\nu(k',\varepsilon)}{1 - A\,\nu(k',\varepsilon)} - S_1^{+2}(k')\right]dk'$$

$$S_2^-(k) = \int_{-\infty}^{k} \exp[-2\beta_1(k'-k)]\left[(\gamma_1^2 - \gamma_\infty^2)\frac{A\,\nu(k',\varepsilon)}{1-A\,\nu(k',\varepsilon)} - S_1^{-2}(k')\right]dk'$$

Even though this process can be obtained, we shall restrict our further discussions up to the second order approximation. We find that the real and imaginary parts of $A\nu/(1-A\,\nu)$ are respectively even and odd functions. Therefore, $S_{nR}^{\pm}(k)$ and $S_{nI}^{\pm}(k)$, the real and imaginary parts of $S_n^{\pm}(k)$ *(n=1,2)* will also have the property

(2.58) $$S_{nR}^{+}(k) = +S_{nR}^{-}(-k)$$

$$S_{nI}^{+}(k) = -S_{nI}^{-}(-k)$$

Thus in the second order approximation (2.54) becomes

(2.59) $$I_{eff}(\infty) = \frac{I_0}{\beta_{eff}}$$

where

(2.60) $$\beta_{eff} = \beta_1 + S_{2R}^{+}(0)$$

Substituting for $S_1^{+}(k)$ in equation (2.57) and performing one integration by parts in the second integral, we get

(2.61) $$S_2^{+}(0) = (\gamma_1^2 - \gamma_\infty^2)\int_0^\infty \exp[-2\beta_1 k]\frac{A\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}dk + \frac{(\gamma_1^2-\gamma_\infty^2)^2}{2\beta_1}\times$$

$$\times\left[\left\{\int_0^\infty \exp[-2\beta_1 k]\frac{A\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}dk\right\}^2 - 2\int_0^\infty \frac{A\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}dk\int_k^\infty \exp[-2\beta_1 k']\frac{A\nu(k',\varepsilon)}{1-A\,\nu(k',\varepsilon)}dk'\right]$$

The integrals in this equation can not be evaluated analytically. However, we find that the integrands can be expanded in a convergent power series in *A*. By definition *A* is less than unity and so also is the magnitude of the term $\nu(k,\varepsilon)$. Therefore we write

(2.62) $$\frac{A\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)} = \sum_{n=1}^{\infty} A^n\,\nu^n(k,\varepsilon)$$

Substitution into equation (2.61) gives

(2.63) $$S_2^{+}(0) = \frac{(\gamma_1^2-\gamma_\infty^2)}{2\beta_1}\sum_{n=1}^{\infty} A^n\,I_n(c) + \frac{(\gamma_1^2-\gamma_\infty^2)^2}{8\beta_1^3}\times$$

$$\times\left[\left\{\sum_{n=1}^{\infty} A^n\,I_n(c) + \right\}^2 - 2\sum_{n=1}^{\infty} A^n \sum_{m=1}^{\infty} A^m\,V_{nm}(c)\right]$$

where $c=\varepsilon/2\beta_1$ and

(2.64) $$I_n(c) = \int_0^\infty \exp[-k]\, \nu^n(k,\varepsilon)\, dk$$

$$V_{nm}(c) = \int_0^\infty \nu^n(k,\varepsilon)\, dk \int_k^\infty \exp[-k']\, \nu^m(k',\varepsilon)\, dk'$$

On commuting the resonance integrals we have found that it is adequate to keep terms up to A^3. Therefore $S_{2R}^+(0)$ can be written as

(2.65) $$S_2^+(0) = \frac{(\gamma_1^2 - \gamma_\infty^2)}{2\beta_1} \sum_{n=1}^{3} A^n\, RI_n(c) + \frac{(\gamma_1^2 - \gamma_\infty^2)^2}{8\beta_1^3} \times$$

$$\times \left[A^2 \left\{RI_1^2 - II_1^2 - 2RV_{11}\right\} + 2A^3 \left\{RI_1 \times RI_2 - II_1 \times II_2 - RV_{12} - RV_{21}\right\}\right]$$

Here RI_n and II_n respectively denote the real and imaginary parts of $I_n(c)$. Similarly, RV_{nm} stands for the real part of V_{nm}. The required integrals to obtain $S_{2R}^+(0)$ have been evaluated in Appendix-I

The expression for $\theta(k,\infty)$ in the second order approximation is given by equations (2.53) and (2.57). $S_2^\pm(k)$ can not be evaluated analytically for non-zero values of k and obtaining $\theta(k,\infty)$ from these equations would involve lot of numerical work. However, an expression which coincides with this function at $k=0$ and hence reproduces the resonance integrals is

(2.66) $$\theta_{WKB}(k,\infty) \cong \frac{1}{2\beta_{eff}} \exp(-\beta_{eff}|k|)$$

It can be seen from the previous sub-section that this form of $\theta(k,\infty)$ is very much similar to that obtained in the intermediate resonance approximation. In fact it corresponds to replacing $g(k,\varepsilon)$ by

(2.67) $$g(k,\varepsilon) \cong \beta_{eff}^2 - 1$$

(iv) Comparison of various methods:

Here we shall establish the accuracy of the above derived expressions for the resonance integral by numerical comparison. In this section we shall also include results obtained from the other formulae derived in Chapter-I. We choose the first ten low energy resonances of U^{238} nucleus. The resonance parameters used in all calculations are given in Appendix-II. Tables-I and II respectively give the zero temperature resonance integrals in a homogeneous mixture of and hydrogen when the nuclear concentrations are such that N_u:N_h = 1 and 5.

The last column in the tables gives resonance integrals obtained through a numerical solution of equation (2.2). The numerical scheme is the same as that employed by Horner and Keane [57,58]. The integral appearing on the RHS of equation (2.2) is approximated by Simpson's formula. This enables one to evaluate $f(x)$ at equidistant points through a recursion formula if it is assumed to be known for very large values of x. In obtaining the results we assumed that $f(x) = 1$ for $x \geq 1000$. Once $f(x)$ is known at many equidistant points, they can be used to evaluate the resonance integral numerically.

The resonances chosen are typical in the sense that the first three are usually categorized as wide resonances where as the last two are said to be narrow resonances. The resonances at energies 102 and 192 *eV* ae usually labeled as intermediate resonances because the resonance integrals calculated in the narrow resonance and wide resonance approximations differ considerably.

From this table it is seen that the improvements on narrow resonance and wide resonance approximations introduced by Spiney and Chernic and Vernon are good only for those resonance belonging to the respective classes. For the resonance belonging to the intermediate class, the narrow resonance and wide resonance approximations give results which differ approximately by a factor of 2. The intermediate resonance approximation of Goldstein gives good results for all the resonance. The analytical expression for the resonance integral obtained by the WKB method is found to give accurate results. It is found to be applicable to resonance belonging to narrow, wide and intermediate classes. Thus we have been able to bridge the gap between the limiting narrow resonance and wide resonance approximations through this analytical expression.

C. Temperature Dependent Resonance Integrals:

In this section we shall give a method for solving the integral equation (2.17).

(i) Solution of the integral equation for $\theta(k,\xi)$

The kernel of the integral equation for $\theta(k,\xi)$ contains a factor $exp[- k^2 /\xi^2]$ and it suggests the use of Gauss-Hermite quadrature formulae for approximating the integral terms [61]. The quadrature formula may be written as

(2.68) $$\int_{-\infty}^{\infty} f(k)\exp(-k^2)\,dk \;\approx\; \sum_{j=1}^{N} W_j\, f(k_j)$$

where k_j are the roots of the Hermite polynomials of order N and W_j are the corresponding weights [60]. The above equation is exact if *f(k)* is any arbitrary polynomial of degree *2N-1*. For other functions it gives an approximation to the integral in the sense of approximating *f(k)* to a polynomial degree *2N-1* [60].

We notice that in the zero temperature limit $\xi \to \infty$ and the quadrature formulae can not be employed at all. Therefore we separate the zero temperature part of the solution and write [62].

(2.69) $$\theta(k,\xi) = \exp\left(-\frac{k^2}{\xi^2}\right)\left[\theta(k,\infty) + \varphi(k,\xi)\right]$$

The quadrature formula will be used to determine $\varphi(k,\xi)$ alone. Thus for small values of ξ which corresponds to higher temperatures the quadrature formula gives a good approximation to $\varphi(k,\xi)$. When ξ large $\varphi(k,\xi)$ is quite small and contributes very little to the resonance integral although the method of evaluating it may be inaccurate. Using (2.69) in equation (2.17) we get

(2.70) $$\varphi(k,\xi) + \frac{1}{2}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - 2k'^2/\xi^2 + 2kk'/\xi^2\right] g(k',\varepsilon)\, \varphi(k',\xi)\, dk' = S(k)$$

where

(2.71) $$S(k) = \frac{1}{2}\exp\left[-|k|\right] - \theta(k,\infty)$$
$$-\frac{1}{2}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - 2k'^2/\xi^2 + 2kk'/\xi^2\right] g(k',\varepsilon)\, \theta(k',\infty)\, dk'$$

The WKB solution for $\theta(k,\infty)$ obtained in the previous section is somewhat complicated and its calculation for values of $k \neq 0$ would involve a lot numerical work. Therefore in evaluating *S(k)*, we use the approximate form for $\theta_{WKB}(k,\infty)$ given by equation (2.66). That is,

(2.72) $$S(k) = \frac{1}{2}\exp\left[-|k|\right] - \frac{1}{2\beta_{eff}}\exp\left[-\beta_{eff}|k|\right]$$
$$-\frac{1}{4\beta_{eff}}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - 2k'^2/\xi^2 + 2kk'/\xi^2 - \beta_{eff}|k'|\right] g(k',\varepsilon)\, dk'$$

Now we define the transformation

(2.73) $$\Phi(k,\xi) = g(k,\varepsilon)\varphi(k,\xi)$$

and rewrite equation (2.70) as

$$(2.74)\quad \Phi(k,\xi)g(k,\varepsilon)^{-1}+\frac{1}{2}\int_{-\infty}^{\infty}\exp\left[-|k-k'|-2k'^2/\xi^2+2kk'/\xi^2\right]\Phi(k',\xi)\,dk'=S(k)$$

Equations (2.69) and (2.73) show that the resonance integral is given by

$$(2.75)\qquad I_{eff}(\xi)\ =2I_0\left[\frac{1}{\beta_{eff}}+\frac{\Phi(0,\xi)}{g(0,\varepsilon)}\right]$$

The integral term on the R.H.S. of equation (2.74) is now approximated as

$$(2.76)\qquad \int_{-\infty}^{\infty}\exp\left[-2k'^2/\xi^2\right]\exp\left[-|k-k'|+2k\,k'/\xi^2\right]\Phi(k',\xi)\,dk'=$$

$$\xi^*\sum_{j=1}^{N}W_j\ \exp\left[-\left|k-\xi^*k_j\right|-k\ k_j/\xi^*\right]\Phi(\xi^*k_j,\xi)$$

where $\xi^*=\xi/\sqrt{2}$. However, for better accuracy we introduce a convergence parameter ω and rewrite the above equation as

$$(2.77)\quad \int_{-\infty}^{\infty}\exp\left[-2k'^2/\xi^2\right]\exp\left[-|k-k'|+2k\,k'/\xi^2\right]\Phi(k',\xi)\,dk'$$

$$=\int_{-\infty}^{\infty}\exp\left[-\omega^2k'^2/\xi^2\right]\exp\left[-|k-k'|+\left(\omega^2-2\right)k'^2/\xi^2+2k\,k'/\xi^2\right]\Phi(k',\xi)\,dk'$$

$$=\bar{\xi}\sum_{j=1}^{N}W_j\ \exp\left[-\left|k-\bar{\xi}k_j\right|-(\omega^2-2)\,k_j^{\,2}/\omega^2+(2/\omega^2)k\ k_j/\bar{\xi}\right]\Phi(\bar{\xi}k_j,\xi)$$

where $\bar{\xi}=\xi/\omega$. The choice of parameter ω will be given in the next sub-section. Using (2.77) the integral equation (2.74) becomes

$$(2.78)\qquad \Phi(k,\xi)g(k,\varepsilon)^{-1}+\frac{\bar{\xi}}{2}\sum_{j=1}^{N}\exp\left[-\left|k-\bar{\xi}k_j\right|-(\omega^2-2)\,k_j^{\,2}/\omega^2\right]\times$$

$$\times\ \exp\left[(2/\omega^2)k\ k_j/\bar{\xi}\right]\Phi(\bar{\xi}k_j,\xi)=S(k)$$

Putting *k*= $\bar{\xi}$ *k*$_i$,for *1≤i≤ N*, we get *N* algebraic equations for the unknown $\Phi(\bar{\xi}k_i,\xi)$ which can be written in matrix notation

$$(2.79)\qquad \mathbf{B}\vec{\mathbf{\Phi}}=\vec{S}$$

The elements of the square matrix ***B*** and the vectors $\vec{\mathbf{\Phi}}$ and $\vec{S}$ are given by

$$(2.78)\qquad B_{i\,j}=\frac{\delta_{i\,j}}{g_i}+W_j\frac{\bar{\xi}}{2}\exp\left[-\bar{\xi}\left|k_i-k_j\right|-(\omega^2-2)\,k_j^{\,2}/\omega^2+(2/\omega^2)k_ik_j\right]$$

$$\Phi_i = \Phi(\bar{\xi}\, k_i)\ ,\ \ S_i = S(\bar{\xi}\, k_i)\ \ ,\ 1 \le i \le N\ ,\ 1 \le j \le N$$

To obtain S_i the integral appearing in equation (2.72) is to be evaluated numerically. It has been found that Simpson's rule evaluation, to an accuracy of 10^{-4}, is quite fast.

It is seen from equation (2.75) that to obtain the resonance integral it is sufficient to know $\Phi(0,\xi)$. Therefore we choose the order of the qadrature formula to be an odd number so that one of its roots, say, k_1 is zero. Thus, when Φ_1 is evaluated it gives the resonance integral directly.

Since $g(k, \varepsilon)$ is a complex valued function, the unknown function $\Phi(k,\xi)$ also is a complex function. Therefore the system of equations (2.79) is equivalent to *2N* real equations. It is our aim to show that these equations can be reduced to *(N+1)/2* real equations.

The roots of the Hermite polynomials occur in conjugate pairs, that is, the roots to be used in an odd order quadrature formula can be arranged as

$$0 \quad k_2 \quad k_3 \quad k_4 \quad .... \quad k_{(N+1)/2} \quad -k_2 \quad -k_3 \quad -k_4 \quad .... \quad -k_{(N+1)/2}$$

We separate the real and imaginary parts of the square matrix ***B*** and the vectors $\vec{\mathbf{\Phi}}$ and $\vec{S}$ by writing them as

(2.81)
$$\mathbf{B} = \mathbf{B}^R + i\,\mathbf{B}^I$$
$$\vec{\Phi} = \vec{\Phi}^{\,R} + i\,\vec{\Phi}^{\,I}$$
$$\vec{S} = \vec{S}^{\,R} + i\,\vec{S}^{\,I}$$

Substituting in equation (2.79), we get

(2.82)
$$\mathbf{B}^R\,\vec{\mathbf{\Phi}}^R - \mathbf{B}^I\,\vec{\mathbf{\Phi}}^I = \vec{S}^R$$
$$\mathbf{B}^I\,\vec{\mathbf{\Phi}}^R + \mathbf{B}^R\,\vec{\mathbf{\Phi}}^I = \vec{S}^I$$

From the definition we know that the real and imaginary parts of *g(k, ε)* are respectively even and odd functions. Therefore, the integral equation (2.74) shows that the real and imaginary parts of $\Phi(k,\xi)$ are also even and odd functions. Thus with the ordering of the roots as indicated earlier, we have

(2.83)
$$\Phi_i^R = +\ \Phi_{i+(N-1)/2}^R\ \ ,\ 2 \le i \le (N+1)/2$$
$$\Phi_i^I = -\ \Phi_{i+(N-1)/2}^R\ \ ,\ 2 \le i \le (N+1)/2$$
$$\Phi_1^I = 0$$

Exactly similar relations hold between the elements of the source vector $\vec{S}$. The matrix elements B_{ij} have the property

(2.84)
$$\begin{aligned}
&\mathbf{B}^R_{1,\ i} = \mathbf{B}^R_{1,\ i+(N-1)/2} \\
&\mathbf{B}^R_{i,\ 1} = \mathbf{B}^R_{i+(N-1)/2,\ 1} \\
&\mathbf{B}^R_{i,\ 1} = \mathbf{B}^R_{i+(N-1)/2,\ 1} \\
&\mathbf{B}^R_{i,\ j+(N-1)/2} = \mathbf{B}^R_{i+(N-1)/2,\ j} \\
&\mathbf{B}^R_{i,\ j} = \mathbf{B}^R_{i+(N-1)/2,\ j+(N-1)/2} \\
&2 \le i \le (N+1)/2\ ,\ 2 \le i \le (N+1)/2
\end{aligned}$$

The matrix $\boldsymbol{B}^{\mathrm{I}}$ is diagonal with the property that

(2.85)
$$\begin{aligned}
&\mathbf{B}^I_{i,\ j} = -\mathbf{B}^I_{i+(N-1)/2,\ j+(N-1)/2} \\
&\mathbf{B}^I_{1,\ 1} = 0 \quad , \quad 2 \le i \le (N+1)/2
\end{aligned}$$

Therefore, the matrix equations (2.82) can be partitioned as

(2.86)
$$\begin{bmatrix} B^R_{11} & \vec{B}^R_r & \vec{B}^R_r \\ \vec{B}^R_c & B^R_1 & B^R_2 \\ \vec{B}^R_c & B^R_2 & B^R_1 \end{bmatrix} \begin{bmatrix} \Phi^R_1 \\ \vec{\Phi}^R \\ \vec{\Phi}^R \end{bmatrix} - \begin{bmatrix} 0 & \vec{O}_r & \vec{O}_r \\ \vec{O}_c & B^I_1 & O \\ \vec{O}_c & O & -B^I_1 \end{bmatrix} \begin{bmatrix} 0 \\ \vec{\Phi}^I \\ -\vec{\Phi}^I \end{bmatrix} = \begin{bmatrix} S^R_1 \\ \vec{S}^R \\ \vec{S}^R \end{bmatrix}$$

$$\begin{bmatrix} 0 & \vec{O}_r & \vec{O}_r \\ \vec{O}_c & B^I_1 & O \\ \vec{O}_c & O & -B^I_1 \end{bmatrix} \begin{bmatrix} \Phi^R_1 \\ \vec{\Phi}^R \\ \vec{\Phi}^R \end{bmatrix} + \begin{bmatrix} B^R_{11} & \vec{B}^R_r & \vec{B}^R_r \\ \vec{B}^R_c & B^R_1 & B^R_2 \\ \vec{B}^R_c & B^R_2 & B^R_1 \end{bmatrix} \begin{bmatrix} 0 \\ \vec{\Phi}^I \\ -\vec{\Phi}^I \end{bmatrix} = \begin{bmatrix} 0 \\ \vec{S}^I \\ -\vec{S}^I \end{bmatrix}$$

where $\vec{B}^R_r$ and $\vec{B}^R_c$, $\vec{\Phi}^R$, $\vec{\Phi}^I$, $\vec{S}^R$, $\vec{S}^I$ are, respectively, *(N-1)/2* dimensional row and column vectors and B^R_1 , B^R_2 and $B^{I\ \mathrm{I}}_1$ are square matrices of order *(N-1)/2*. Expanding the above equations we get

(2.87)
$$\begin{aligned}
&\mathbf{B}^R_{11}\Phi^R_1 + 2\vec{\mathbf{B}}^R_r\vec{\Phi}^R = S^R_1 \\
&\vec{\mathbf{B}}^R_c\Phi^R_1 + \left(\mathbf{B}^R_1 + \mathbf{B}^R_2\right)\vec{\Phi}^R - \mathbf{B}^I_1\vec{\Phi}^I = \vec{S}^R \\
&\mathbf{B}^I_1\vec{\Phi}^R + \left(\mathbf{B}^R_1 - \mathbf{B}^R_2\right)\vec{\Phi}^I = \vec{S}^I
\end{aligned}$$

$\mathbf{B}^I_1$ being a diagonal matrix, it’s inverse can be obtained very easily. Therefore we can solve for $\vec{\Phi}^I$ from the second of the above equations:

(2.88)
$$\vec{\Phi}^I = \left[\mathbf{B}^R_1\right]^{-1}\left[\vec{\mathbf{B}}^R_c\Phi^R_1 + \left(\mathbf{B}^R_1 + \mathbf{B}^R_2\right)\vec{\Phi}^R - \vec{S}^R\right]$$

Substituting in the third of equation (2.87) we get the following *(N+1)/2* real equations

(2.89) $$\mathbf{B}_{11}^{R}\Phi_{1}^{R} + 2\vec{\mathbf{B}}_{r}^{R}\vec{\Phi}^{R} = S_{1}^{R}$$

$$(\mathbf{B}_{1}^{R} - \mathbf{B}_{2}^{R})[\mathbf{B}_{1}^{I}]^{-1}\vec{\mathbf{B}}_{c}^{R}\Phi_{1}^{R} + \left[\mathbf{B}_{1}^{I} + (\mathbf{B}_{1}^{R} - \mathbf{B}_{2}^{R})[\mathbf{B}_{1}^{I}]^{-1}\left(\mathbf{B}_{1}^{R} + \mathbf{B}_{2}^{R}\right)\right]\vec{\Phi}^{R}$$
$$= \vec{S}^{I} + (\mathbf{B}_{1}^{R} - \mathbf{B}_{2}^{R})[\mathbf{B}_{1}^{I}]^{-1}\vec{S}^{R}$$

Φ_1^R can be obtained from these equations using Cramer's rule. Thus the effort involved in obtaining the resonance integral by this method is the evaluation of two determinates of order (N-1)/2. It may be noted that this reduction in the order of the determinants has been possible because the matrix $\mathbf{B}_1^I$ is diagonal. The transformation defined by equation (2.73) was introduced to accomplish this reduction in numerical work.

To estimate the accuracy of this method we shall apply it to the evaluation of resonance integral in the intermediate resonance approximation (narrow resonance and wide resonance approximations are included). In Chapter-I it was shown that $I_{eff}^{IR}(\xi)$ is proportional to the *J(ξ,β)* function. The following sub-section essentially gives a method for evaluating this function [46]. By comparing the *J(ξ,β)* function calculated by this method with the tabulations of Adler and Nordheim [62] we shall obtain a good estimate of the accuracy of this method.

(ii) <u>Evaluation of the *J(ξ,β)* function</u>

In the intermediate resonance approximation *g(k,ε)* is replaced by a constant γ_λ^2 and equation (2.17) becomes

(2.90) $$\theta_{IR}(k,\xi) + \frac{\gamma_\lambda^2}{2}\int_{-\infty}^{\infty}\exp\left[-|k-k'| - (k-k')^2/\xi^2\right]\,\theta_{IR}(k',\xi)\,dk' = \frac{1}{2}\exp\left[-|k| - k^2/\xi^2\right]$$

Since the kernel of this integral equation is of the displacement type its solution can be obtained by Fourier transformation [54]. Let *F(x,ξ)* be defined as

(2.91) $$F(x,\xi) = \int_{-\infty}^{\infty}\theta_{IR}(k,\xi)\exp(-ik\,x)\;dk$$

Taking the inverse transform of equation (2.90) we get

(2.92) $$F(x,\xi) = \frac{\psi(x,\xi)}{1+\gamma_\lambda^2\;\psi(x,\xi)}$$

Therefore $\theta_{IR}(k,\xi)$ becomes

$$\theta_{IR}(k,\xi) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(ik\,x)\,F(x,\xi)\,dx \tag{2.93}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(ik\,x)\frac{\psi(x,\xi)}{1+\gamma_\lambda^2\;\psi(x,\xi)}\,dx$$

From the definition of the J-function given in equation (1.76) we find that

$$J(\xi, 1/\gamma_\lambda^2) = \pi\,\gamma_\lambda^2\,\theta_{IR}(0,\xi) \tag{2.94}$$

$\theta_{IR}(k,\xi)$ can not be analytically evaluated from equation (2.93). Our aim is to obtain $\theta_{IR}(0,\xi)$ from the integral equation (2.90) using the quadrature formula. Separating the zero temperature part of the solution we write [61]

$$\theta_{IR}(k,\xi) = \left[\theta_{IR}(k,\infty) + \varphi_{IR}(k,\xi)\right]\exp(-k^2/\xi^2) \tag{2.95}$$

Substituting for $\theta_{IR}(k,\xi)$ in equation (2.90) we get

$$\varphi_{IR}(k,\xi) + \frac{\gamma_\lambda^2}{2}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - 2k'^2/\xi^2 + 2kk'/\xi^2\right]\varphi_{IR}(k',\xi)\,dk' = S(k) \tag{2.96}$$

where *S(k)* is given by

$$S(k) = \frac{1}{2}\exp(-|k|) - \theta(k,\infty) \tag{2.97}$$

$$-\frac{1}{2}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - 2k'^2/\xi^2 + 2kk'/\xi^2\right] g(k',\varepsilon)\;\theta(k',\infty)\,dk'$$

Substituting for $\theta_{IR}(k,\infty)$ from equation (2.44) we get

$$S(k) = \frac{1}{2}\exp\left[-|k|/\xi^2\right] - \frac{1}{2\beta_\lambda}\exp\left[-\beta_\lambda|k|\right] \tag{2.98}$$

$$-\frac{\gamma_\lambda^2}{4\beta_\lambda}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - 2k'^2/\xi^2 + 2kk'/\xi^2 - \beta_\lambda|k'|\right]\,dk'$$

and

$$\theta_{IR}(0,\xi) \;= \frac{1}{2\beta_\lambda} + \varphi_{IR}(0,\xi) \tag{2.99}$$

Applying the quadrature formula, equation (2.96) can be reduced to the system of algebraic equations

$$B\,\vec{X} = \vec{S} \tag{2.100}$$

where the elements of the matrix ***B*** and the vectors $\vec{X}$ and $\vec{S}$ are given by

$$B_{i\,j} = \delta_{i\,j} + W_j\,\gamma_\lambda^2\,\frac{\overline{\xi}}{2}\;\exp\left[-\overline{\xi}\;\left|k_i - k_j\right| - (\omega^2-2)\,k_j^{\,2}\big/\omega^2 + (2/\omega^2)k_i k_j\;\right] \tag{2.101}$$

$$X_j = \varphi_{IR}(\bar{\xi}\, k_j, \xi)$$

$$S_j = S(\bar{\xi}\, k_j) \quad , \quad 1 \le i \le N, 1 \le j \le N$$

Here also we choose and odd order quadrature formula so that $\varphi_{IR}(0, \xi) = X_1$. The integral equation (2.96) shows that $\varphi_{IR}(k, \xi)$ is an even function of *k*. Using this fact and arranging the roots of the quadrature formula as indicated in the previous sub-section the matrix equation (2.100) can be partitioned and the algebraic system can be reduced to *(N+1)/2* equations. For $k=k_i \ge 0$, the integral appearing in the expression for *S(k)* can be written as

(2.102)
$$\int_{-\infty}^{\infty} \exp\left[-|k_i - k'| - 2k'^2/\xi^2 + 2k_i\, k'/\xi^2 - \beta_\lambda |k'|\right]\, dk'$$

$$= \int_{0}^{\infty} \exp\left[-(k_i + k') - 2k'^2/\xi^2 - 2k_i\, k'/\xi^2 - \beta_\lambda k'\right]\, dk'$$

$$+ \int_{0}^{k_i} \exp\left[-(k_i - k') - 2k'^2/\xi^2 + 2k_i\, k'/\xi^2 - \beta_\lambda k'\right]\, dk'$$

$$- \int_{k_i}^{\infty} \exp\left[-(k_i - k') - 2k'^2/\xi^2 + 2k_i\, k'/\xi^2 - \beta_\lambda k'\right]\, dk'$$

It is clear that S_i can be expressed in terms of error functions. However, a direct Simpson's rule evaluation of these integrals, to an accuracy of 10^{-4}, was also found to be equally fast.

In order to determine the accuracy of this method, we evaluated the J-function for a range of ξ and β values and compared them with the tabulations of Adler and Nordheim [62]. Without the introduction of the convergence parameter ω, that is, with the equations obtained by putting $\omega^2 = 2$, and a 19th order quadrature, the J-functions calculated were accurate to about 0.6%; see table-III. With several sets of numerical calculations, it was found that by varying the parameter ω as a function of ξ according to the empirical relation

(2.103) $\omega = 2.2 + 2\, \xi$

the accuracy can be improved to about 0.15%; see table-IV.

It should be pointed out that the effort involved in this method of obtaining the J-function is the evaluation of two determinants of order nine. A direct numerical evaluation of this function is very time consuming [62,63]. This has given rise to several approximate methods of evaluation [63]. The method given here is quite fast and accurate and is a bri-product of our method of solving the integral equation of slowing down theory.

(iii) Doppler coefficients of U-238 resonances

We shall apply the method outlined in sub-section (i) to calculate the temperature dependent resonance integrals and Doppler coefficients of the first few resonances of U_{238} in a mixture of U^{238} and hydrogen. Tables-V and VI give the results when the nuclear concentrations are such that $N_u:N_u=1$ and 5. For the sake of comparison we also give the results obtained by the intermediate resonance approximation. In obtaining the temperature dependent interpolation parameter, the transcendental equation given by Goldstein [21]

$$(2.104) \qquad \lambda = 1 - \frac{1}{z}\tan^{-1}(z)$$

$$z = \frac{\pi\varepsilon\left[\gamma_1^2 J(\xi, 1/\gamma_\lambda^2) - \gamma_\lambda^2 J(\xi, 1/\gamma_1^2)\right]}{2(\gamma_1^2 - \gamma_\lambda^2)\, J(\xi, \gamma_\lambda^2)\, J(\xi, \gamma_1^2)}$$

was solved using as iterative procedure. The J-functions appearing in this equation were_evaluated by the method given earlier.

Table-V shows that the Doppler coefficients calculated by the present method compare well with those obtained by the intermediate resonance approximation. However, some differences are found for the resonances at energies 6.68, 36.8 and 192 eV. The zero temperature resonance integrals obtained by the intermediate resonance approximation are overestimates for the resonances at 36.8 and 192 eV and hence their Dopper coefficients are found to be lower than that obtained by the present method. In view of the assumption of the intermediate resonance approximation, we feel that our results for the resonance at 192 eV are more accurate. Table-VI shows that the Doppler coefficients calculated by the present method are within the statistical uncertainty of Monte Carlo calculations [19] except for the resonance at energy 6.68 eV. The reason is that in our calculations the moderator collision integral is treated in the narrow resonance approximation where as in Monte Carlo calculations it is treated explicitly. Further, it is seen that there is good agreement between the results of intermediate resonance approximation and the present method for larger values of σ_m.

It may be worth pointing out one important difference in our method of calculating the Doppler coefficients. Since the change in the resonance integral due to an increase of temperature is rather small, round off errors get introduced in the Doppler coefficient when it is obtained from two independent calculations. In our method, the major contribution coming from the zero temperature part appear explicitly and therefore differences of large numbers do not occur in Doppler coefficient computations.

D. Summary

In this Chapter, using Fourier transforms we converted the slowing down equation to a Fredholm integral equation of second kind. In the zero temperature limit, it was shown that the integral equation can be reduced to a second order differential equation. The classical approximations, viz., the narrow resonance, wide resonance and intermediate resonance approximations were found to correspond to approximating the function $g(k,\varepsilon)$ by various constant values. The differential equation was solved in the WKB approximation and thus a new expression for the zero temperature resonance integral was obtained. It was found that after separating the zero temperature part of the solution, the Fredholm integral equation can be solved with the use of Gauss-Hermite quadrature formulae. As a bi-product of this method we obtained an accurate and fast method for evaluating the $J(\xi,\beta)$ function. The method was applied to evaluate resonance integrals and Doppler coefficients of some of the resonances of U^{238}.

Table-I

Zero Temperature Resonance integrals of U^{238} Resonances

Resonance Energy (eV)	Resonance Integrals (barns)						
	I_{eff}^{NR}	I_{eff}^{WRR}	I_{eff}^{SPR}	I_{eff}^{CV}	I_{eff}^{IR}	I_{eff}^{WKB}	$I_{eff}^{Numerical}$
6.68	4.795	4.038	-	4.043	4.043	4.062	4.045
21.0	1.853	1.765	1.536	1.768	1.768	1.772	1.770
36.8	1.184	1.487	1.989	1.477	1.463	1.438	1.448
66.3	0.4169	0.4471	0.4429	0.4340	0.4360	0.4350	0.4351
81.1	0.1289	0.1098	0.1244	0.2842	0.1246	0.1246	0.1246
102.8	0.2849	0.4464	0.4027	0.4006	0.3745	0.3683	0.3675
116.8	0.1650	0.1685	0.1661	0.1571	0.1660	0.1660	0.1660
192.0	0.1209	0.2529	0.1705	0.1730	0.1647	0.1632	0.1622
209.0	0.0967	0.1454	0.1085	0.0087	0.1079	0.1079	0.1079
238.0	0.0687	0.0818	0.0707	-	0.0707	0.0707	0.0707

Notes:

1. Nuclear concentrations are such that $N_u:N_h=1:1$
2. Resonance parameters used are given in Appendix-II
3. Resonance potential interference scattering is neglected.

Table-II

Zero Temperature Resonance integrals of U^{238} Resonances

Resonance Energy (eV)	Resonance Integrals (barns)						
	I_{eff}^{NR}	I_{eff}^{WRR}	I_{eff}^{SPR}	I_{eff}^{CV}	I_{eff}^{IR}	I_{eff}^{WKB}	$I_{eff}^{Numerical}$
6.68	9.176	9.012	8.368	9.017	9.017	9.018	9.017
21.0	3.548	3.940	4.344	3.887	3.883	3.887	3.876
36.8	2.267	3.317	3.860	3.170	3.065	3.038	3.026
66.3	0.7974	0.9956	0.8944	0.6268	0.8756	0.8760	0.8754
81.1	0.2431	0.2411	0.2429	0.3247	0.2429	0.2429	0.2428
102.8	0.5449	0.9902	0.7334	0.4624	0.6967	0.6982	0.6953
116.8	0.3147	0.3738	0.3259	-	0.3250	0.3252	0.3250
192.0	0.2310	0.5531	0.3032	-	0.2939	0.2954	0.2942
209.0	0.1845	0.3203	0.2037	-	0.2024	0.2028	0.2026
238.0	0.1310	0.1802	0.1352	-	0.1350	0.1351	0.1350

Notes:

1. Nuclear concentrations are such that N_u:N_h=1:5
2. Resonance parameters used are given in Appendix-II
3. Resonance potential interference scattering is neglected.

Table-III

Percentage Eror in *J(ξ,β)* Function Calculations:

k	ξ=0.1	ξ=0.2	ξ=0.3	ξ=0.4	ξ=0.5
4	0.53	0.41	0.24	0.15	0.12
5	0.48	0.50	0.39	0.29	0.21
6	0.43	0.55	0.49	0.41	0.33
7	0.43	0.52	0.56	0.51	0.46
8	0.27	0.46	0.54	0.56	0.52
9	0.18	0.39	0.49	0.52	0.50
10	0.09	0.31	0.35	0.49	0.49
11	0.01	0.26	0.36	0.36	0.46
12	0.01	0.14	0.30	0.32	0.36
13	-0.04	0.12	0.18	0.23	0.28

Notes:

1. β is given by the relation $\beta=2^k \text{x } 10^{-5}$
2. Order of the quadrature formula, N=19
3. Convergence parameter $\omega^2=2$
4. Comparison with tabulations of Adler and Nordheim [63]

Table-IV

Percentage Eror in *J(ξ,β)* Function Calculations:

k	ξ=0.1	ξ=0.2	ξ=0.3	ξ=0.4	ξ=0.5
4	0.16	0.16	0.09	0.06	0.07
5	0.11	0.16	0.13	0.12	0.09
6	0.09	0.15	0.13	0.12	0.10
7	0.14	0.13	0.14	0.12	0.12
8	0.04	0.12	0.13	0.11	0.09
9	0.01	0.10	0.02	0.10	0.10
10	-0.03	0.08	0.12	0.11	0.06
11	-0.07	0.08	0.10	0.03	0.09
12	-0.05	0.02	0.10	0.06	0.06
13	-0.07	0.04	0.05	0.05	0.05

Notes:

5. β is given by the relation $\beta=2^k \times 10^{-5}$
6. Order of the quadrature formula, N=19
7. Convergence parameter $\omega^2=2.2+2 \times \xi$
8. Comparison with tabulations of Adler and Nordheim [63]

Table-V

Doppler Coefficients of U^{238} Resonances

Resonance Energy (eV)	Doppler Coefficients $10^4\ \Delta I_{eff} / \Delta T$ (barns/°K)					
	T= 0 - 300°K		T= 300 - 600°K		T= 600 - 900°K	
	IR	FTM	IR	FTM	IR	FTM
6.68	1.40	1.02	1.58	1.48	1.57	1.56
21.0	1.09	1.06	1.17	1.16	1.18	1.17
36.8	0.656	0.845	0.720	0.778	0.724	0.735
66.3	1.20	1.20	1.13	1.12	1.04	1.05
81.1	2.72	2.66	1.33	1.30	0.931	0.898
102.8	0.459	0.498	0.462	0.461	0.456	0.418
116.8	1.52	1.53	1.11	1.11	0.897	0.899
192.0	0.187	0.245	0.189	0.204	0.186	0.159
209.0	0.447	0.501	0.390	0.401	0.356	0.354
238.0	0.891	0.928	0.600	0.602	0.471	0.470

Notes:

1. IR -Intermediate Resonance Approximation
2. FTM – Fourier Transform Method (present)
3. Nuclear concentrations are such that N_u:N_h=1:1
4. Resonance parameters used are given in Appendix-II
5. Resonance potential interference scattering is neglected.

Table-VI

Doppler Coefficients of U^{238} Resonances

Resonance Energy (eV)	Doppler Coefficients $10^4\ \Delta I_{eff} / \Delta T$ (barns/°K)				
	T= 0 - 300°K			T= 300 - 600°K	
	IR	MC	FTM	IR	FTM
6.68	14.42	12.9±0.57	14.44	13.83	13.77
21.0	10.08	9.7±0.62	10.13	9.28	9.50
36.8	5.61	5.71±0.64	5.23	5.43	5.30
66.3	5.81	5.78±0.47	5.96	4.80	5.03
81.1	7.83	7.8±0.41	7.83	2.64	2.64
102.8	2.49	2.57±0.33	2.59	2.24	2.18
116.8	6.27	6.08±0.35	6.35	3.50	3.54
192.0	0.906	0.93±0.08	1.03	0.812	0.740
209.0	2.17	2.07±0.20	2.27	1.48	1.48
238.0	3.00	2.9±0.35	3.06	1.55	1.55

Notes:

1. IR -Intermediate Resonance Approximation
2. MC – Monte Carlo Method [Ref.19]
3. FTM – Fourier Transform Method (present)
4. Nuclear concentrations are such that N_u:N_h=1:1
5. Resonance parameters used are taken from Ref.19
6. Resonance potential interference scattering is neglected.

CHAPTER-III

FOURIER TRANSFORM METHOD FOR EVALUATING RESONANCE INTEGRALS – PART-II

In this Chapter we shall extent the Fourier transform method to include resonance potential interference scattering. This is important whenever the scattering width Γ_n of the resonances becomes comparable to the absorption width Γ_r [14,24]. In Chapter-I we mentioned that in this situation certain problems arise in the intermediate resonance approximation. We also pointed out the difficulties encountered in solving the transcendental equations of intermediate resonance approximation.

In the previous Chapter resonance potential interference scattering was neglected for the sake of simplicity in presenting the ideas. However as we shall see the main ideas of the Fourier transform method are applicable here though some important modifications occur when this generalization is attempted. In the zero temperature limit we again get a second order differential equation in the transform space, but now it contains a first derivative term. The Fredholm integral equation resulting in the temperature dependent case is somewhat different from that obtained in the previous Chapter. The kernel of this integral equation contains the Heavisdie unit function and therefore the Gauss-Hermite quadrature formulae is not directly applicable for obtaining its solution. But we shall show that Hermite polynomials can be employed to obtain the resonance integral from this equation with minimum effort.

A: Derivation of the Freedom Integral Equation:

The equation to be treated here is (1.37). Substituting for the resonance cross-sections we get

$$\left[1+\gamma_1^2\,\psi(x,\xi)+\eta_1\,\chi(x,\xi)\right]f(x) = (1-A)+\frac{A}{\varepsilon}\int_x^{x+\varepsilon}\left[1+\gamma_\infty^2\,\psi(y,\xi)+\eta_\infty\,\chi(y,\xi)\right]f(y)\,dy \tag{3.1}$$

Introducing the discontinuity factor $H(x,y,\varepsilon)$ this equation can be written as

$$\left[1+\gamma_1^2\,\psi(x,\xi)+\eta_1\,\chi(x,\xi)\right]f(x)=(1-A) + A\int_{-\infty}^{\infty} dk'\,\nu(k',\varepsilon)e^{-ikx}\,\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ik'y}\left[1+\gamma_\infty^2\,\psi(y,\xi)+\gamma_\infty^2\,\chi(y,\xi)\right]f(y)\,dy \tag{3.2}$$

On Fourier transformation we get

(3.3) $$F(k)+\gamma_1^2\,\theta(k,\xi)+\eta_1\,G(k,\xi)=$$
$$=(1-A)\delta(k)+A\nu(k,\varepsilon)\left[F(k)+\gamma_\infty^2\theta(k,\xi)+\eta_\infty\,G(k,\xi)\right]$$

F(k), $\theta(k,\xi)$ and $\nu(k,\varepsilon)$ have been defined in equations (2.9) (2.8) and (2.6), $G(k,\xi)$ is defined as

(3.4) $$G(x,\xi)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{ikx}f(x)\,\chi(x,\xi)\,dx$$

It may be noted that $G(k,\xi)$ is proportional to the rate of scattering collisions contributed by the resonance potential interference.

Equation (3.3) can be rewritten as

(3.5) $$F(k)+g(k,\varepsilon)\,\theta(k,\xi)+h(k,\varepsilon)\,\chi(k,\xi)=\frac{(1-A)}{1-A\nu(k,\varepsilon)}\delta(k)\equiv\delta(k)$$

where $g(k,\varepsilon)$ is defined in equation (2.18) and $h(k,\varepsilon)$ is given by

(3.6) $$h(k,\varepsilon)=\frac{\eta_1-A\eta_\infty\,\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}$$

From the definition of the quantities η_1, η_∞ and *A*, it is found that

(3.7) $$h(0,\varepsilon)=\frac{\eta_1-A\eta_\infty}{1-A}=0$$

Now we have to eliminate *F(k)* and *G(k)* from equation (3.5). The equation (2.14) relating *F(k)* and $\theta(k,\xi)$ provides one of the relations for this purpose. Another relation between *F(k)* and $G(k,\xi)$ can be obtained from equation (3.4) and the convolution theorem, viz;

(3.8) $$G(k,\xi)=\int_{-\infty}^{\infty}F(k')\,\overline{\chi}(k-k',\xi)\,dk'$$

Here, $\overline{\chi}(k,\xi)$ is the Fourier transform of the $\chi(x,\xi)$ function. Now changing the variable in equation (3.5) to k' multiplying by $\overline{\psi}\,(k-k',\xi)$ and integrating we get

(3.9) $$\theta(k,\xi)+\int_{-\infty}^{\infty}\overline{\psi}(k-k',\xi)\,\left[g(k',\varepsilon)\,\theta(k',\xi)+h(k',\varepsilon)\,G(k',\xi)\right]dk'=\overline{\psi}(k,\xi)$$

Similarly, using $\overline{\chi}(k-k',\xi)$ we find

(3.10) $$G(k,\xi)+\int_{-\infty}^{\infty}\overline{\chi}\,(k-k',\xi)\,\left[g(k',\varepsilon)\,\theta(k',\xi)+h(k',\varepsilon)\,G(k',\xi)\right]dk'=\overline{\chi}(k,\xi)$$

Thus the slowing down equation has been transformed to two coupled Fredholm integral equations. These coupled integral equations can be rewritten in terms of a single function the following way. Multiplying equations (3.9) and (3.10) respectively by $g(k,\varepsilon)$ and $h(k,\varepsilon)$, and adding the resulting equations we get

$$\Phi(k,\xi) + \int_{-\infty}^{\infty} \left[g(k,\varepsilon)\overline{\psi}(k-k',\xi) + h(k,\varepsilon)\overline{\chi}(k-k',\xi) \right]\Phi(k',\xi)dk' = \left[g(k,\varepsilon)\overline{\psi}(k,\xi) + h(k,\varepsilon)\overline{\chi}(k,\xi) \right] \tag{3.11}$$

where $\Phi(k,\xi)$ is defined as

$$\Phi(k,\xi) = \left[g(k,\varepsilon)\ \theta(k,\xi)\ + h(k,\varepsilon)G(k,\xi) \right] \tag{3.12}$$

From equations (3.7) and (3.12) we notice that $\Phi(0,\xi)$ is proportional to $\theta(0,\xi)$. Therefore we get

$$I_{eff}(\xi) = 2I_0\theta(0,\xi) = \frac{2I_0}{g(0,\varepsilon)}\Phi(0,\xi) \tag{3.13}$$

To complete the derivation, we have to obtain $\overline{\chi}(k,\xi)$. Using equation (1.13) and the inverse of the convolution theorem we get

$$\overline{\chi}(k,\xi) = \imath H^*(k)\exp(-|k|)\exp(-k^2/\xi^2) \tag{3.14}$$

Here $H^*(k)$ is the Heaviside unit function defined as

$$H^*(k) = \begin{aligned} &1\ ,\ k > 0 \\ = \ &0\ ,\ k = 0 \\ = -&1\ ,\ k < 0 \end{aligned} \tag{3.15}$$

$\imath H^*(k)\exp(-|k|)$ is the Fourier transform of $x/(1+x^2)$. Using the expression (2.16) for $\overline{\psi}(k,\xi)$, the function $\overline{\chi}(k,\xi)$ can be written as

$$\overline{\chi}(k,\xi) = 2\ \imath H^*(k)\ \overline{\psi}(k,\xi) \tag{3.16}$$

Therefore, the integral equation (3.11) takes the form

$$\Phi(k,\xi) + \frac{1}{2}\int_{-\infty}^{\infty} \exp\left[-|k-k'| - (k-k')^2/\xi^2\right] \times \times \left[g(k,\varepsilon) + 2\imath H^*(k-k')h(k,\varepsilon)\right]\Phi(k',\xi)dk' = \frac{1}{2}\exp\left[-|k| - k^2/\xi^2\right]\left[g(k,\varepsilon) + 2\imath H^*(k)h(k,\varepsilon)\right] \tag{3.17}$$

This integral equation is slightly more complicated than the one obtained in the previous Chapter. Nevertheless, the problems associated with the Doppler broadened resonance cross-sections and the discontinuous nature of the slowing down kernel have been removed in this formulation.

B. <u>Resonance Integrals in the Zero Temperature Limit:</u>

In the zero temperature limit it is easier to consider equation (3.9) instead of (3.17). Taking the limit ξ→∞ it takes the form

$$(3.18)\quad \theta(k,\infty)+\frac{1}{2}\int_{-\infty}^{\infty}\exp\left(-\left|k-k'\right|\right)\left[g(k')\,\theta(k',\infty)\ +h(k')\,G(k',\infty)\right]\,dk'=\frac{1}{2}\exp\left(-\left|k\right|\right)$$

As was done earlier, we reduce this equation to a second order differential equation in $\theta(k,\infty)$

(i) Derivation of a differential equation for θ

We have already seen that the kernel of the above integral equation $(1/2)\exp\left(-\left|k-k'\right|\right)$ is the Green's function of the second order differential operator: $\left(d^2/dk^2-1\right)$. Applying this operator we get

$$(3.19)\qquad \left(\frac{d^2}{dk^2}-1\right)\theta(k,\infty)-\left[g(k,\varepsilon)\,\theta(k,\infty)+h(k,\varepsilon)\,G(k,\infty)\right]=-\,\delta(k)$$

Using the zero temperature limiting form of the $\chi(x,\xi)$ function we find that

$$(3.20)\qquad G(k,\infty)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{\imath k x}\ f(x)\frac{2\,x}{1+x^2}\,dx$$

Similarly we have

$$(3.21)\qquad \theta(k,\infty)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{\imath k x}\ f(x)\frac{1}{1+x^2}\,dx$$

These equations show that

$$(3.22)\qquad G(k,\infty)=-2\,\imath\,\frac{d}{dk}\theta(k,\infty)$$

Such a simple relation between $\theta(k,\ \xi)$ and $G(k,\xi)$ does not exist for other values of ξ. Now equation (3.19) can be written as

$$(3.23)\qquad \frac{d^2\theta}{dk^2}+2\,\imath\,h(k,\varepsilon)\frac{d\,\theta}{dk}-\left[1+g(k,\varepsilon)\right]\theta(k,\infty)=-\,\delta(k)$$

Thus the evaluation of the zero temperature resonance integral including the resonance potential interference scattering effects has been reduced to the solution of this differential equation. A comparison with equation (2.23) shows that the inclusion of resonance potential interference scattering gives rise to the first derivative term $d\,\theta/dk$. The delta function appearing on the RHS of the above equation can be replaced by the discontinuity condition on $d\,\theta/dk$ at $k=0$. From equations (3.18) and (3.21) we find that the boundary conditions (2.27) and (2.28) on $\theta(k,\infty)$ apply here also.

(iii) WKB approximation for $\theta(k,\infty)$

The function *h(k,ε)* can be written as

(3.24)
$$h(k,\varepsilon) = \eta_1 + (\eta_1 - \eta_\infty)\frac{A\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)}$$

The homogenous part of equation (3.23) can be written as

(3.25)
$$\frac{d^2\theta}{dk^2} + 2\iota\left[\eta_1 + (\eta_1 - \eta_\infty)\frac{A\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)}\right]\frac{d\,\theta}{dk}$$
$$-\left[\beta_1^2 + (\gamma_1^2 - \gamma_\infty^2)\frac{A\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)}\right]\theta(k,\infty) = 0$$

Taking the limit ε→0, we obtain the narrow resonance approximation,

(3.26)
$$\frac{d^2\theta_{NR}}{dk^2} + 2\iota\eta_1\frac{d\theta_{NR}}{dk} - \beta_1^2\,\theta_{NR}(k,\infty) = 0$$

We also know that equation (3.25) reduces to the above form in the asymptotic range. To solve equation (3.26), we make the substitution

(3.27)
$$\theta_{NR}(k,\infty) = \theta_{NR}^*(k,\infty)\,e^{-\iota\,\eta_1\,k}$$

and obtain

(3.28)
$$\frac{d^2\theta_{NR}^*}{dk^2} - \left(\beta_1^2 - \eta_1^2\right)\theta_{NR}^*(k,\infty) = 0$$

It is seen that all the boundary conditions satisfied by θ_{NR} are also satisfied by θ_{NR}^*. Therefore, we have

(3.29)
$$\theta_{NR}^*(k,\infty) = \frac{1}{\sqrt{\beta_1^2 - \eta_1^2}}\exp\left[-\sqrt{\beta_1^2 - \eta_1^2}\;|k|\right]$$

and

(3.30)
$$\theta_{NR}\,(k,\infty) = \frac{1}{\sqrt{\beta_1^2 - \eta_1^2}}\exp\left[-\sqrt{\beta_1^2 - \eta_1^2}\;|k| - i\eta_1 k\right]$$

when $\beta_1^2 > \eta_1^2$. The resonance integral in the narrow resonance approximation becomes

(3.31)
$$I_{eff}\,(\infty) = 2I_0\,\theta_{NR}\,(0,\infty) = \frac{I_0}{\sqrt{\beta_1^2 - \eta_1^2}}$$

and is the same as given in equation (1.67). To obtain the WKB solution, we utilize the asymptotic form of *θ(k,∞)* and write

(3.32)
$$\theta(k,\infty) = C_+\,\exp\left[-\beta_1^*\,|k| - i\eta_1 k + \int_k^\infty S^+(k')dk'\right],\; k > 0$$
$$= C_-\,\exp\left[\beta_1^*\,|k| - i\eta_1 k + \int_{-\infty}^k S^-(k')dk'\right],\; k < 0$$

where

(3.33) $$\beta_1^* = \sqrt{\beta_1^2 - \eta_1^2}$$

and C_+ and C_- are arbitrary constants to be determined. As was done in the previous Chapter using the boundary conditions (2.28) and (2.29), $\theta(k,\infty)$ can be expressed as

(3.34)
$$\theta(k,\infty) = \frac{1}{2\beta_1^* + S^+(0) + S^-(0)} \exp\left[-\beta_1^* k - i\,\eta_1 k - \int_0^k S^+(k')dk' \right] \quad , \quad k > 0$$

$$= \frac{1}{2\beta_1^* + S^+(0) + S^-(0)} \exp\left[+\beta_1 k - i\,\eta_1 k - \int_k^0 S^-(k')dk' \right] \quad , \quad k < 0$$

The boundary conditions on $S^\pm(k)$ are given by

(3.35) $$S^\pm(k) \to 0 \quad as \quad k \to \pm\infty$$

Substituting for $\theta(k,\infty)$ in equation (3.25) we get

(3.36)
$$\mp \frac{dS^\pm}{dk} + 2\left[\beta_1^* - i(\eta_1 - \eta_\infty) \frac{A\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)} \right] S^\pm(k)$$
$$+ [S^\pm(k)]^2 = (a + i\,b) \frac{A\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)}$$

The upper sign stands for $k>0$ and the lower sign for $k<0$. The constants a and b are given by

(3.37) $$a = \gamma_1^2 - \gamma_\infty^2 - 2\eta_1(\eta_1 - \eta_\infty)$$
$$b = 2\,\beta_1^*(\eta_1 - \eta_\infty)$$

The above equations for $S^\pm(k)$ are quite similar to these obtained in the previous Chapter and can be solved by the iterative method. We consider the term:

$$2\,i\,(\eta_1 - \eta_\infty) \frac{A\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)} S^\pm(k) + [S^\pm(k)]^2$$

as perturbation terms. In the second order approximation we get

(3.38)
$$S_2^+(0) = (a + i\,b) \int_0^\infty \exp[-2\beta_1^*\,k] \frac{A\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)} dk$$

$$+ (a + ib)\,2\,(\eta_1 - \eta_\infty) \int_0^\infty \frac{A\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)} dk \int_k^\infty \exp[-2\beta_1^*\,k'] \frac{A\,\nu(k',\varepsilon)}{1 - A\,\nu(k',\varepsilon)} dk'$$

$$-(a + ib)^2 \int_0^\infty \exp[-2\beta_1^*\,k] dk \left[\int_k^\infty \exp[-2\beta_1^*\,k'] \frac{A\,\nu(k',\varepsilon)}{1 - A\,\nu(k',\varepsilon)} dk' \right]^2$$

and

(3.39)
$$S_2^-(0) = (a+i\,b)\int_{-\infty}^{0} \exp[2\beta_1^*\,k]\frac{A\,\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}dk$$
$$+(a+ib)\,2\,(\eta_1-\eta_\infty)\int_{-\infty}^{0}\frac{A\,\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}dk\int_{-\infty}^{k}\exp[2\beta_1^*\,k']\frac{A\,\nu(k',\varepsilon)}{1-A\,\nu(k',\varepsilon)}dk'$$
$$-(a+ib)^2\int_{-\infty}^{0}\exp[2\beta_1^*\,k]dk\left[\int_{-\infty}^{k}\exp[2\beta_1^*\,k']\frac{A\,\nu(k',\varepsilon)}{1-A\,\nu(k',\varepsilon)}dk'\right]^2$$

Here also we find that the real and imaginary parts of $S_2^{\pm}(0)$ have the property

$$S_{2R}^+(0) = +\,S_{2R}^-(0)$$

$$S_{2I}^+(0) = -\,S_{2I}^-(0)$$

Therefore the resonance integral is found to be

(3.40)
$$I_{eff}^{WKB}(\infty) \;=\frac{I_0}{\beta_1^* + S_{2R}^+(0)}$$

To evaluate the integrals is equation (3.38) we expand the integrands as power series in *A*. Keeping terms up to A^3 we obtain $S_{2R}^+(0)$ as

(3.41)
$$S_{2R}^+(0) = \frac{1}{2\beta_1^*}\sum_{n=1}^{3} A^n\left[a\times RI_n(c^*) + b\times II_n(c^*)\right]$$
$$+\frac{2(\eta_1-\eta_\infty)}{4\beta_1^{*2}}A^2\;\left[a\times IV_{11}(c^*) - b\times RI_{11}(c^*)\right]$$
$$+\frac{2(\eta_1-\eta_\infty)}{4\beta_1^{*2}}A^3\;\left[a\times(IV_{12}+IV_{21}) - b\times(RV_{12}+RV_{21})\right]$$
$$+\frac{A^2}{8\beta_1^{*3}}\;\left[(a^2-b^2)\times(RI_1^2 - II_1^2 - 2RV_{11}) + 4ab\times(RI_1\,RI_2 - IV_{11})\right]$$
$$+\frac{2A^3}{8\beta_1^{*3}}\;(a^2-b^2)\times\left[RI_1\,RI_2 - II_1\,II_2 - RV_{12} - RV_{21}\right]$$
$$+\frac{2A^3}{8\beta_1^{*3}}2ab\times(RI_1\,II_2 + RI_2\,II_1 - IV_{12} - IV_{21})$$

where $c^* = \varepsilon/2\beta_1^*$. Further, RI_n and II_n stand for the real and imaginary parts of the integrals in given in equal (2.64). Similarly, RV_{nm} and IV_{nm} denote the real and imaginary parts of the double integrals.

C. The Intermediate Resonance Approximation:

In this section, we shall apply the technique of intermediate resonance approximation to obtain an approximate solution to the differential equation. We shall develop the formulae in a slightly general way and obtain the results of Goldstein [23, 28] as a particular case. We shall also see that the new formulation circumvents some of the difficulties present in the intermediate resonance approximation.

Multiplying by $[1-A\,\nu(k,\varepsilon)]$ equation (3.25) can be written as

$$\frac{d^2\theta}{dk^2}+2\iota\eta_1\frac{d\,\theta}{dk}-\beta_1^2\ \theta(k,\infty)=A\nu(k,\varepsilon)\left[\frac{d^2\theta}{dk^2}+2\iota\eta_\infty\frac{d\,\theta}{dk}-\beta_\infty^2\ \theta(k,\infty)\right] \tag*{(3.42)}$$

where β_∞^2 = (1+γ_∞^2). Now, we add to both sides of the above equation the term:

$$2\iota\eta_\lambda\frac{d\,\theta}{dk}-\beta_\pi^2\ \theta(k,\infty)$$

and rewrite it as

$$\begin{aligned}\frac{d^2\theta}{dk^2}+2\iota\eta_\lambda\frac{d\,\theta}{dk}-\beta_\lambda^2\ \theta(k,\infty)&=\left(\beta_1^2-\beta_\lambda^2\right)\theta(k,\infty)-2\iota\left(\eta_1-\eta_\lambda\right)\frac{d\,\theta}{dk}\\&\quad+A\nu(k,\varepsilon)\left[\frac{d^2\theta}{dk^2}+2\iota\eta_\infty\frac{d\,\theta}{dk}-\beta_\infty^2\ \theta(k,\infty)\right]\end{aligned} \tag*{(3.43)}$$

Here, the quantities β_λ and η_λ are as yet unspecified and are to be determined from certain conditions to be imposed on $\theta(k,\infty)$. In the present formulation, these constants are considered as two independent parameters.

The method of intermediate resonance approximation can be developed in the following manner. A first order approximation $\theta_1(k,\infty)$ is obtained by neglecting all the terms on the RHS of equation (3.43). That is

$$\frac{d^2\theta_1}{dk^2}+2\iota\eta_\lambda\frac{d\,\theta_1}{dk}-\beta_\lambda^2\ \theta_1(k,\infty)=0 \tag*{(3.44)}$$

The solution of this equation satisfying the three boundary conditions is given by

$$\theta_1(k,\infty)=\frac{1}{2\beta_\lambda^*}\exp\left[-\iota\eta_\lambda\,k-\beta_\lambda^*\,|k|\,\right] \tag*{(3.45}$$

when $\beta_\lambda^2>\eta_\lambda^2$. Further

$$\beta_\lambda^*=\sqrt{\beta_\lambda^2-\eta_\lambda^2}\ . \tag*{(3.46)}$$

A second order approximation is obtained by substituting $\theta_1(k,\infty)$ on the RHS of equation (3.43). That is

(3.47)
$$\frac{d^2\theta_2}{dk^2}+2\iota\eta_\lambda\frac{d\,\theta_2}{dk}-\beta_\lambda^2\;\theta_2(k,\infty)$$
$$=\left[\beta_1^2-\beta_\lambda^2+2i\left(\eta_1-\eta_\lambda\right)\left(\pm\beta_\lambda^*-i\eta_\lambda\right)\right]\frac{1}{2\beta_\lambda^*}\exp\left[-\iota\eta_\lambda\,k-\beta_\lambda^*\,|k|\,\right]$$
$$+A\nu(k,\varepsilon)\left[\beta_\lambda^{*\,2}-\beta_\infty^2-\eta_\lambda^{\;2}+2\eta_\lambda\,\eta_\infty\pm2i\,\beta_\lambda^*(\eta_\lambda-\eta\infty)\right]\frac{1}{2\beta_\lambda^*}\exp\left[-\iota\eta_\lambda\,k-\beta_\lambda^*\,|k|\,\right]$$

On the RHS the ± signs refer respectively to the cases k>0 and k<0. To solve this equation, we make the substitution

(3.48)
$$\theta_2(k,\infty)=\theta_2^*(k,\infty)\,e^{-\iota\,\eta_\lambda\,k}$$

and obtain

(3.49)
$$\frac{d^2\theta_2^*}{dk^2}-\beta_\lambda^{*\,2}\;\theta_2^*(k,\infty)=\left(\beta_1^2-\beta_\lambda^2\;\right)\frac{1}{2\beta_\lambda^*}\exp\left[-\beta_\lambda^*\,|k|\,\right]+$$
$$+\left[2i\left(\eta_1-\eta_\infty\right)\left(\pm\beta_\lambda^*-i\eta_\lambda\right)+A\nu(k,\varepsilon)\,(X\pm iY)\right]\frac{1}{2\beta_\lambda^*}\exp\left[-\beta_\lambda^*\,|k|\,\right]$$

where the constants X and Y are given by

(3.50)
$$X=\beta_\lambda^{*2}-\beta_\infty^2-\eta_\lambda^{\;2}+2\eta_\lambda\,\eta_\infty$$
$$Y=2\,\beta_\lambda^*\,(\eta_\lambda-\eta_\infty)$$

We notice that the boundary conditions on $\theta_2^*(k,\infty)$ are same as those on $\theta_2(k,\infty)$. $\theta_2^*(k,\infty)$, which vanishes at $\pm\infty$ is given by

(3.51)
$$\theta_2^*(k,\infty)=C_+\exp\left[-\beta_\lambda^*\,k\right]$$
$$-k\left[\beta_1^2-\beta_\lambda^2+2\left(\eta_1-\eta_\infty\right)\left(+i\beta_\lambda^*-\eta_\lambda\right)\right]\frac{1}{4\beta_\lambda^{*2}}\;\exp\left[-\beta_\lambda^*\,|k|\,\right]$$
$$+A(X+iY)\frac{1}{2\beta_\lambda^*}\exp\left[-\beta_\lambda^*\,k\,\right]\int_k^\infty dk'\int_{k'}^\infty e^{-2\beta_\lambda^*(k''-k')}\,\nu(k'',\varepsilon)\;dk''\;,\quad k>0$$

and

(3.52)
$$\theta_2^*(k,\infty)=C_-\exp\left[\;\beta_\lambda^*\,k\;\right]$$
$$+k\left[\beta_1^2-\beta_\lambda^2+2\left(\eta_1-\eta_\infty\right)\left(-i\beta_\lambda^*-\eta_\lambda\right)\right]\frac{1}{4\beta_\lambda^{*2}}\;\exp\left[-\beta_\lambda^*\,|k|\,\right]$$
$$+A(X-iY)\frac{1}{2\beta_\lambda^*}\exp\left[\beta_\lambda^*\,k\,\right]\;\int_{-\infty}^{k}dk'\int_{-\infty}^{k'}e^{2\beta_\lambda^*(k''-k')}\,\nu(k'',\varepsilon)\;dk''\;,\quad k<0$$

The continuity condition on $\theta_2^*(k,\infty)$ gives

$$\theta_2^*(0,\infty) = C_+ + \frac{A(X+iY}{2\beta_\lambda^*}) \int_0^\infty dk' \int_{k'}^\infty e^{-2\beta_\lambda^*(k''-k')}\, \nu(k'',\varepsilon)\; dk'' \tag{3.53}$$

$$= C_- + \frac{A(X-iY}{2\beta_\lambda^*}) \int_{-\infty}^0 dk' \int_{-\infty}^{k'} e^{2\beta_\lambda^*(k''-k')}\, \nu(k'',\varepsilon)\; dk''$$

Differentiating equations (3.51) and (3.52) we get

$$\left.\frac{d\theta_2^*}{dk}\right|_{0+} = -\beta_\lambda^*\, \theta_2^*(0,\infty) \tag{3.54}$$

$$-\left[\beta_1^2 - \beta_\lambda^2 + 2\left(\eta_1 - \eta_\infty\right)\left(+i\beta_\lambda^* - \eta_\lambda\right)\right]\frac{1}{4\beta_\lambda^{*2}} - A\frac{X+iY}{2\beta_\lambda^*}(Z_1 - iZ_2)$$

and

$$\left.\frac{d\theta_2^*}{dk}\right|_{0-} = \beta_\lambda^*\, \theta_2^*(0,\infty) \tag{3.55}$$

$$+\left[\beta_1^2 - \beta_\lambda^2 + 2\left(\eta_1 - \eta_\infty\right)\left(-i\beta_\lambda^* - \eta_\lambda\right)\right]\frac{1}{4\beta_\lambda^{*2}} + A\frac{X-iY}{2\beta_\lambda^*}(Z_1 + iZ_2)$$

The quantities Z_1 and Z_2 are given by

$$Z_1 = \int_0^\infty e^{-2\beta_\lambda^* k}\, \frac{\sin(\varepsilon k)}{\varepsilon k}\, dk = \frac{2\beta_\lambda^*}{\varepsilon} \tan^{-1}\left(\frac{\varepsilon}{2\beta_\lambda^*}\right) \tag{3.56}$$

$$Z_2 = \int_0^\infty e^{-2\beta_\lambda^* k}\, \frac{1-\cos(\varepsilon k)}{\varepsilon k}\, dk = \frac{1}{2}\frac{2\beta_\lambda^*}{\varepsilon} Ln\left(1 + \frac{\varepsilon^2}{4\beta_\lambda^{*2}}\right) \tag{3.57}$$

Applying the discontinuity condition on $d\theta_2^*/dk$ and using equation (3.53), we get

$$\theta_2^*(0,\infty) = \frac{1}{2\beta_\lambda^*} - \frac{1}{4\beta_\lambda^{*3}}\left[\beta_1^2 - \beta_\lambda^2 - 2\eta_\lambda\left(\eta_1 - \eta_\infty\right)\right] - \frac{A}{2\beta_\lambda^{*2}}\left(X \times Z_1 + Y \times Z_2\right) \tag{3.58}$$

In the first and second order approximations we have two unknowns, β_λ and η_λ. We get one relation between them on imposing the condition that at $k=0$ the two approximations are equal. That is,

$$\theta_1(0,\infty) = \theta_2(0,\infty) \equiv \theta_2^*(0,\infty) \tag{3.59}$$

In the intermediate resonance formulation, Goldstein employed the condition that the resonance integrals are same in the two orders of approximation. Since $\theta(0,\infty)$ is proportional to the resonance integral, we see that (3.59) is same as Goldstein's condition. Thus we get

$$\beta_\lambda^2 = \beta_1^2 - 2\eta_\lambda\left(\eta_1 - \eta_\infty\right) + 2A\beta_\lambda^*\left(X \times Z_1 + Y \times Z_2\right) \tag{3.60}$$

The next condition to be imposed on $\theta_1(k,\infty)$ and $\theta_2(k,\infty)$ can be on their derivatives at *k=0*. This becomes quite natural because on matching the derivative of $\theta_1(k,\infty)$ also it can become a better approximation. $d\theta/dk$ at *k=0* is proportional to *G(0,∞)*. Therefore the two conditions together impose a further restriction that the resonance scattering rate is same in the two approximations. Equations (3.45), (3.54) and (3.55) show that if (3.60) is satisfied, we also have

(3.61) $$RP\left[\frac{d\theta_1}{dk}\right]_{0\pm} = RP\left[\frac{d\theta_2}{dk}\right]_{0\pm}$$

We use *RP* and *IP* to denote the real part of the quantities in the respective brackets. Therefore, we impose the condition

(3.62) $$IP\left[\frac{d\theta_1}{dk}\right]_{0\pm} = IP\left[\frac{d\theta_2}{dk}\right]_{0\pm}$$

In terms of $\theta_2^*(k,\infty)$, this condition becomes

(3.63) $$IP\left[\frac{d\theta_1}{dk}\right]_{0\pm} = -\eta_\lambda\,\theta_2^*(0,\infty) + IP\left[\frac{d\theta_2^*}{dk}\right]_{0\pm}$$

Substituting for the derivatives at 0_+ we get

(3.64) $$-\frac{\eta_\lambda}{2\beta_\lambda^*} = -\eta_\lambda\,\theta_2^*(0,\infty) - \frac{\eta_1-\eta_\lambda}{2\beta_\lambda^*} - \frac{A}{2\beta_\lambda^*}\left(Y\times Z_1 - X\times Z_2\right)$$

The same result can be obtained by equating the derivatives at $0\_$. Using equation (3.59), we get

(3.65) $$\eta_\lambda = \eta_1 + A\left(Y\times Z_1 - X\times Z_2\right)$$

Thus we have the transcendental equations (3.60) and (3.65) to be solved to determine β_λ and η_λ. Once they are obtained, the resonance integral is given by

(3.66) $$I_{eff}^{IR}(\infty) \;= 2I_0\theta_1(0,\infty) = 2I_0\theta_2(0,\infty) = \frac{I_0}{\beta_\lambda^*}$$

The condition imposed on the derivative of $\theta_1(k,\infty)$ is the factor which makes the present formulation different from that of Goldstein.

(i). Goldstein’s Method [23,28]:

Golddstein’s transcendental equation (1.72) for the interpolation parameter λ can be obtained from equation (3.60). In the narrow resonance approximation, we know that equation (3.25) reduces to (3.26). In the wide resonance limit we have

$$\frac{d^2\theta_{WR}}{dk^2}+2\imath\frac{\eta_1-A\eta_\infty}{1-A}\frac{d\,\theta_{WR}}{dk}-\frac{\beta_1^2-A\beta_\infty^2}{1-A}\theta_{WR}(k,\infty)=0 \tag{3.67}$$

From equation (3.7) we notice that the coefficient of the first derivative term is identically zero. That is, in the wide resonance approximation inclusion of resonance potential interference scattering does not modify the equations. Introducing the interpolation parameter λ through the definitions

$$\beta_\lambda^2=\frac{\beta_1^2-A\beta_\infty^2(1-\lambda)}{1-A(1-\lambda)} \tag{3.68}$$

and

$$\eta_\lambda=\frac{\lambda\,\eta_1}{1-A(1-\lambda)} \tag{3.69}$$

we find that the narrow resonance and wide resonance approximations are obtained when λ is taken as 1 and 0 respectively. In fact, Goldstein had introduced the parameter by writing the slowing down operator as a linear combination of the approximate operators obtained in these approximations. But this leads to the same expressions for β_λ^2 and η_λ. The equations (3.68) and (3.69) take the place of our second equation (3.65). Using the identities,

$$\beta_\lambda^2-\beta_1^2=\frac{A(1-\lambda)\left(\beta_1^2-\beta_\infty^2\right)}{1-A(1-\lambda)} \tag{3.70}$$

$$\beta_\lambda^2-\beta_\infty^2=\frac{\left(\beta_1^2-\beta_\infty^2\right)}{1-A(1-\lambda)} \tag{3.71}$$

and equation (3.60) it can be shown that λ is given by

$$\lambda=1-Z_1-\frac{2\sqrt{\beta_\lambda^2-\eta_\lambda^2}\,(\eta_1-\eta_\infty)\,Z_2}{\beta_1^2-\beta_\infty^2-2\eta_\lambda(\eta_1-\eta_\infty)} \tag{3.72}$$

which is same as equation (1.72) except for notational differences. When resonance potential interference scattering is neglected, our method does not reduce to that of Goldstein. The second transcendental equation (3.65) remains and a non-zero value of would be obtained. Then the method becomes similar to that of Pomraning and Dyos [31] with two interpolation parameters.

(ii). New Transcendental Equations:

Since the quantity of interest in the evaluation of resonance integrals is β_λ^* the equations (3.60) and (3.65) can be rewritten as

(3.73) $$\beta_\lambda^* = \beta_1^* + (\eta_\lambda - \eta_1)^2 + A\left[\beta_\lambda^{*2} - \beta_\infty^{*2} - (\eta_\lambda - \eta_\infty)^2\right]Z_1 + 2A\beta_\lambda^*(\eta_\lambda - \eta_\infty)Z_2$$

and

(3.74) $$\eta_\lambda = \eta_1 + A(\eta_\lambda - \eta_\infty)Z_1 - \frac{A}{2\beta_\lambda^*}\left[\beta_\lambda^{*2} - \beta_\infty^{*2} - (\eta_\lambda - \eta_\infty)^2\right]Z_2$$

Here $\beta_\infty^{*2} = \beta_\infty^2 - \eta_\infty^2$. When ε→∞, we have $Z_1 \to 0$ and $Z_2 \to 0$. Hence

(3.75) $$\beta_{NR}^{*2} = \beta_1^{*2} \quad , \quad \eta_{NR} = \eta_1$$

When ε→0, we have $Z_1 \to 1$ and $Z_2 \to 0$. Therefore

(3.76) $$\beta_{WR}^{*2} = \beta_1^{*2} + (\eta_{WR} - \eta_1)^2 + A\left[\beta_{WR}^{*2} - \beta_\infty^{*2} - (\eta_{WR} - \eta_\infty)^2\right]$$

$$\eta_{WR} = \eta_1 + A(\eta_{WR} - \eta_\infty)$$

Equation (3.7) shows that η_{WR} =0. Thus we get

(3.77) $$\beta_{WR}^{*2} = \frac{\beta_1^{*2} - A\beta_\infty^{*2}}{1 - A}$$

Thus the new equations give the limiting narrow resonance and wide resonance approximations.

For a given value of β_λ^* equation (3.74) is quadratic in η_λ. Therefore it can be solved in terms of β_λ^* to obtain

(3.78) $$\eta_\lambda^\pm = \frac{1}{AZ_2}\left[A\eta_\infty Z_2 + \beta_\lambda^*(1 - AZ_1)\right]$$

$$\pm \frac{1}{AZ_2}\left[\left\{A\eta_\infty Z_2 + \beta_\lambda^*(1 - AZ_1)\right\}^2 - AZ_2\left\{2\beta_\lambda^*(\eta_1 - \eta_\infty Z_1)\right\} - A\left\{\beta_\lambda^{*2} - \beta_\infty^2\right\}Z_2\right]^{1/2}$$

The positive root η_λ^+ will be a very large quantity and is to be rejected. The transcendental equations (3.73) and (3.78) can be solved easily by the iterative method. Setting $\eta_\lambda = \eta_1$ in equation (3.73), β_λ^* can be found by iteration. Having obtained it, the negative root in equation (3.78) gives the new value of η_λ. This process can be repeated till their magnitudes converge to the required accuracy. η_λ^- has been found to be positive number in all numerical calculations for U-238 resonances except for the one at 6.68 e.V.

(iii) Comparison of Resonance Integrals:

Here we give a comparison of the zero temperature resonance integrals calculated by the Fourier transform method and intermediate resonance approximation.

Tables VII and VIII give the results for the resonances of U^{238} in a homogenous mixture with hydrogen. The nuclear concentrations are such that N_u:N_h = 1 and 5. Tables also contain resonance integrals obtained by the numerical solution of equation (3.1). It is seen that the resonance integ4rals obtained by the WKB solution compares well with the numerical results. As seen from table VII, maximum difference is about 4% for the resonance at 36.8% eV. For the resonances at energies 102 eV and 192 eV belonging to the intermediate class also the agreement is quite good.

Tables also show that the agreement between the numerical results and those obtained by the new transcendental equations is fairly good. The major advantage of the new equations is that they can be solved easily by the iterative method. This does not happen to be the case with Goldstein's equation (27). Further, the two roots are sufficiently separated and we are able to pick up the required root easily. In Goldstein's method also equation (3.72) gives two values of λ. But they are very closely spaced and it becomes necessary to choose the criterion that its value of which gives the larger resonance integral must be chosen [27].

D. Solution of the integral equation for $\Phi(k,\xi)$

In this section we shall outline a procedure to solve the integral equation (3.11). We notice that the kernel of this integral equation contains the Heaviside unit function. The quadrature formulae for approximating any integral are applicable only when the integrand can be approximated by a polynomial. Hence it is not appropriate to use the quadrature formulae for its solution. Therefore, we attempt to expand $\Phi(k,\xi)$ in a series of suitable functions. In this series expansion, it would be advantageous to factorize the known behavior of the function $\Phi(k,\xi)$. For instance, we know that there is an exponential dependence in the zero temperature part of $\Phi(k,\xi)$. That is

$$(3.79) \qquad \Phi(k,\infty) \propto \exp\left[-\beta|k|\right]$$

where β is given by

$$(3.80) \qquad \beta = \beta_1^* + S_{2R}^+(0)$$

The source term on the RHS of equation (3.11) shows that $\Phi(k,\xi)$ would have a dependence given by $exp(-k^2/\xi^2)$. Further, the integral equation (3.11) shows that the real and imaginary parts of $\Phi(k,\xi)$ are respectively even and odd functions. Incorporating all these facts, we write

$$\Phi(k,\xi) \; = \; \exp\left(-\beta|k| - k^2/\xi^2\right)\left[\sum_{n=0}^{N} C_n\, H_{2n}^*(k) + i\sum_{n=0}^{N-1} D_n\, H_{2n+1}^*(k)\right] \tag{3.81}$$

where $H_n^*(k)$ are related to the Hermite polynomials $H_n(k)$ through the definition,

$$\begin{aligned} &H_0^*(k) = H_0(k) \\ &H_{2n+1}^*(k) = H_{2n+1}(k)\;,\; n \geq 0 \\ &H_{2n}^*(k) = H_{2n}(k) - H_{2n}(0)\;,\; n \geq 1 \end{aligned} \tag{3.82}$$

The expansion in terms of $H_n^*(k)$ shows that $\Phi(0,\xi)$ given by

$$\Phi(0,\xi) \; = C_0 \tag{3.83}$$

In fact the expansion (3.81) can be in terms of any polynomials. The use of $H_n^*(k)$, rather than $H_n(k)$, makes $\Phi(0,\xi)$ to be given by C_o. Later on, we shall show that with the above expansion it is possible to obtain the matrix elements of the system of algebraic equations determining C_n and D_n by suitable recursion formulae. Substituting for $\Phi(k,\xi)$ in equation (3.11), we get

$$\begin{aligned} &\sum_{n=0}^{N}\left[\exp(-\beta\,|\,k\,|)H_{2n}^*(k) + Y_{2n}(k)\right]C_n \\ &+ i\sum_{n=0}^{N}\left[\exp(-\beta\,|\,k\,|)H_{2n+1}^*(k) + Y_{2n+1}(k)\right]D_n = S(k) \end{aligned} \tag{3.84}$$

where

$$S(k) = \exp(-\beta\,|\,k\,|)\;\left[g(k,\varepsilon) + 2iH^*(k)\,h(k,\varepsilon)\right] \tag{3.85}$$

and

$$\begin{aligned} Y_{2n}(k) = \frac{1}{2}\int_{-\infty}^{\aleph} &H_n^*(k')\exp\left(-\beta|k'| - |k-k'| - 2k'^2/\xi^2 + 2k\,k'/\xi^2\right)\times \\ &\left[g(k,\varepsilon) + 2i\,H^*(k-k')\,h(k,\varepsilon)\right]dk' \end{aligned} \tag{3.86}$$

Thus we have a relation between the *(2N+1)* expansion coefficients C_n and D_n. One possible way of obtaining *(2N+1)* equations to determine C_n and D_n is by writing equation (3.84) for *(2N+1)* values of k [49]. We choose these k values as the roots of $H_{2N+1}(k)$ which is proportional to the first term neglected from the series expansion (3.81). Thus the present choice eliminates the error contributed to the equations by the neglecting this term. One of the roots, say k_o of $H_{2N+1}(k)$ is zero and the remaining *2N* roots occur as pairs with opposite sign. Writing equation (3.84) for these values of *k*, we get

$$(3.87)\qquad \sum_{n=0}^{N}\left[\exp\left(-\beta\,|\,k_j\,|\right)H^{*}_{2n}(k_j)+Y_{2n}(k_j)\right]C_n$$

$$+\,i\sum_{n=0}^{N-1}\left[\exp\left(-\beta\,|\,k_j\,|\right)H^{*}_{2n+1}(k_j)+Y_{2n+1}(k_j)\right]D_n=S(k_j)\ ,\ 0\le j\le 2N$$

Another reason for choosing Hermite polynomials for the expansion (3.81) may be pointed out here. It is clear from equation (3.87) that all the *k* values have to be distinct so that there are *(2N+1)* independent equations for determining all the constants C_n and D_n. The orthogonal polynomials $H_{2N}(k)$ have simple zeros distributed on the real axis and therefore we get *(2N+1)* independent equations.

From equation (3.85) we notice that the real and imaginary parts of *S(k)* are respectively even and odd functions. Similarly, equation (3.86) shows that the real and imaginary parts of $Y_{2n}(k)$ are even and odd functions whereas that of $Y_{2n+1}(k)$ are odd and even functions respectively. Therefore, for the positive values of k_j, we have

$$(3.88)\qquad \sum_{n=0}^{N}\left[\exp\left(-\beta\,k_j\right)H^{*}_{2n}(k_j)+Y^{R}_{2n}(k_j)+i\,Y^{I}_{2n}(k_j)\right]C_n$$

$$+\,i\sum_{n=0}^{N-1}\left[\exp\left(-\beta\,k_j\right)H^{*}_{2n+1}(k_j)+Y^{R}_{2n+1}(k_j)+i\,Y^{I}_{2n+1}(k_j)\right]D_n$$

$$=S^{R}(k_j)+S^{I}(k_j)\ ,\ 1\le j\le N$$

Here the super scripts *R* and *I* on $Y_n(k)$ and *S(k)* denote the real and imaginary parts. For the negative values of k_j, we have

$$(3.89)\qquad \sum_{n=0}^{N}\left[\exp\left(-\beta\,k_j\right)H^{*}_{2n}(k_j)+Y^{R}_{2n}(k_j)-i\,Y^{I}_{2n}(k_j)\right]C_n$$

$$+\,i\sum_{n=0}^{N-1}\left[\exp\left(-\beta\,k_j\right)H^{*}_{2n+1}(k_j)+Y^{R}_{2n+1}(k_j)-i\,Y^{I}_{2n+1}(k_j)\right]D_n$$

$$=S^{R}(k_j)-S^{I}(k_j)\ ,\ 1\le j\le N$$

Adding and subtracting equations (3.88) and (3.89), we get

$$(3.90)\qquad \sum_{n=0}^{N}\left[\exp\left(-\beta\,k_j\right)H^{*}_{2n}(k_j)+Y^{R}_{2n}(k_j)\ \right]C_n$$

$$-\sum_{n=0}^{N-1}Y^{I}_{2n+1}(k_j)\,D_n=S^{R}(k_j),\ 1\le j\le N$$

and

(3.91)
$$\sum_{n=0}^{N} Y_{2n}^{I}(k_j)\,C_n-\sum_{n=0}^{N-1}\Big[\exp\big(-\beta k_j\big)\,H_{2n+1}^{*}(k_j)+Y_{2n+1}^{R}(k_j)\,\Big]D_n$$
$$=S^{I}(k_j),\ 1\le j\le N$$

For the zero root, we get

(3.92)
$$\sum_{n=0}^{N}\Big[H_{2n}^{*}(0)+Y_{2n}^{R}(0)\,\Big]C_n-\sum_{n=0}^{N-1}Y_{2n+1}^{I}(0)\,D_n=S^{R}(0)$$

Thus we have *(2N+1)* unknowns and the same number of equations. The k_j values appearing in equations (3.90) and (3.91) are the N positive roots of $H_{2N+1}(k)$.

As has been pointed out in Ref.[49] this method becomes attractive if the quantities $Y_n(k_j)$ can be evaluated using recursion relations. This possibility will certainly depend on the kernel of the integral equation. We shall now show that this is indeed the case with equation (3.11). Splitting the integral in equation (3.86) for positive values of k_j, we get

(3.93)
$$\begin{aligned}Y_n(k_j)\ &=e^{-k_j}\,J_n^{1}(k_j)\,\big[g(k_j,\varepsilon)+2i\ h(k_j,\varepsilon)\big]\\&+e^{k_j}\,J_n^{2}(k_j)\,\big[g(k_j,\varepsilon)-2i\ h(k_j,\varepsilon)\big]\\&+(-1)^n\,e^{-k_j}\,J_n^{3}(k_j)\,\big[g(k_j,\varepsilon)+2i\ h(k_j,\varepsilon)\big]\end{aligned}$$

where

(3.94)
$$J_n^{1}(k_j)=\int_{0}^{k_j}H_n^{*}(k)\exp\big(-\beta k+k-2k^2/\xi^2+2k_j\,k/\xi^2\big)\,dk$$

(3.95)
$$J_n^{2}(k_j)=\int_{k_j}^{\infty}H_n^{*}(k)\exp\big(-\beta k-k-2k^2/\xi^2+2k_j\,k/\xi^2\big)\,dk$$

and

(3.96)
$$J_n^{3}(k_j)=\int_{0}^{\infty}H_n^{*}(k)\exp\big(-\beta k-k-2k^2/\xi^2-2k_j\,k/\xi^2\big)\,dk$$

Therefore, it is sufficient to have recursion relations for $J_n^{l}\,(l=1,2,3)$. Subsituting for $H_n^{*}(k)$, we get

(3.97)
$$J_{2n+1}^{l}(k_j)=I_{2n+1}^{l}(k_j)\ ,\ n\ge 0$$

(3.98)
$$J_{2n}^{l}(k_j)=I_{2n}^{l}(k_j)-I_{0}^{l}(k_j)\,H_{2n}(0)\ ,\ n\ge 1$$

and

(3.99) $$J_0^l(k_j) = I_0^l(k_j)$$

where $I_n^l(k_j)$ are given by the same equations defining $J_n^l(k_j)$ but with the difference that $H_n^*(k)$ is replaced by $H_n(k)$. For instance, $I_n^1(k_j)$ is given by

(3.100) $$I_n^1(k_j) = \int_0^{k_j} H_n(k)\exp\left(-\beta k + k - 2k^2/\xi^2 + 2k_j k/\xi^2\right) dk$$

Performing integration by parts, we get

(3.101) $$I_n^1(k_j) = \frac{1}{2k_j/\xi^2 - \beta + 1}\left[H_n(k_j)\exp\left(-\beta k_j + k_j\right) - H_n(0)\right]$$

$$-\int_0^{k_j} H_n(k)\exp\left(-\beta k + k - 2k^2/\xi^2 + 2k_j k/\xi^2\right)\left[H_n{}'(k) - 4kH_n(k)/\xi^2\right]dk$$

Using the recursion formulae for Hermite polynomials [66] we get

(3.102) $$\left(2/\xi^2\right)I_n^1(k_j) = H_n(0) - H_n(k_j)\exp\left(-\beta k_j + k_j\right)$$
$$+ 2n\,I_{n-1}^1\,(k_j)\left(1 - 2/\xi^2\right) + \left(k_j\,2/\xi^2 - \beta + 1\right)I_n^1(k_j)$$

Thus all the $I_n^1(k_j)$ can be evaluated if $I_0^1(k_j)$ and $I_1^1(k_j)$ are known. Equation (3.100) clearly shows that these can be expressed in terms of error functions. The recursion formulae for $I_n^2(k_j)$ and $I_n^3(k_j)$ can be obtained exactly in the same way. They are given by

(3.103) $$\left(2/\xi^2\right)I_n^2(k_j) = H_n(k_j)\exp\left(-\beta k_j - k_j\right)$$
$$+ 2n\,I_{n-1}^2\,(k_j)\left(1 - 2/\xi^2\right) + \left(k_j\,2/\xi^2 - \beta - 1\right)I_n^2(k_j)$$

and

(3.104) $$\left(2/\xi^2\right)I_n^3(k_j) = H_n(0) + 2n\,I_{n-1}^3(k_j)\left(1 - 2/\xi^2\right) - \left(k_j\,2/\xi^2 - \beta + 1\right)I_n^3(k_j)$$

Once the quantities $Y_n(k_j)$ are evaluated, C_o can be obtained from the system of algebraic equations using Cramer's rule. Thus in this method, the effort involved in obtained $\Phi(0,\xi)$ and hence the resonance integral would be the evaluation of two determinants of order $(2N+1)$.

E. Summary

In this Chapter we extended the Fourier transform method to include resonance potential interference scattering. We derived a Fredholm integral equation for a function related to $\theta(k,\xi)$. In the zero temperature limit, in the integral equation was reduced to a second order differential equation. The inclusion of resonance potential interference scattering introduced a first derivative term in the equation. The WKB method was extended to solve this equation. Further analysis of the differential equation led to a new formulation of the intermediate resonance approximation. Finally we have given a method to solve the Fredholm integral equation resulting in the temperature dependent case.

Table-VII

Zero Temperature Resonance integrals of U^{238} Resonances

Resonance Energy (eV)	Resonance Integrals (barns)				
	I_{eff}^{NR}	$I_{eff(1)}^{IR}$	$I_{eff(2)}^{IR}$	I_{eff}^{WKB}	$I_{eff}^{Numerical}$
6.68	4.840	4.088	4.091	4.103	4.090
21.0	1.939	1.839	1.884	1.858	1.873
36.8	1.316	1.672	1.663	1.566	1.621
66.3	0.4491	0.5002	0.5178	0.5104	0.5124
81.1	0.1305	0.1301	0.1310	0.1308	0.1309
102.8	0.3269	0.4794	0.4645	0.4702	0.4676
116.8	0.1757	0.1826	0.1921	0.1933	0.1935
192.0	0.1425	0.2175	0.2086	0.2246	0.2192
209.0	0.1104	0.1348	0.1352	0.1403	0.1399
238.0	0.0756	0.0806	0.0835	0.0848	0.0849

Notes:

1. Nuclear concentrations are such that N_u:N_h=1:1
2. Resonance parameters used are given in Appendix-II
3. Resonance potential interference scattering is included.
4. $I_{eff(1)}^{IR}$ refers to Goldstein’s intermediate resonance approximation
5. $I_{eff(2)}^{IR}$ refers to intermediate resonance approximation of Chapter-III

Table-VIII

Zero Temperature Resonance integrals of U^{238} Resonances

Resonance Energy (eV)	Resonance Integrals (barns)				
	I_{eff}^{NR}	$I_{eff(1)}^{IR}$	$I_{eff(2)}^{IR}$	I_{eff}^{WKB}	$I_{eff}^{Numerical}$
6.68	9.119	9.106	9.116	9.114	9.115
21.0	3.591	4.080	4.076	4.062	4.062
36.8	2.328	3.358	3.306	3.307	3.285
66.3	0.8127	0.9520	0.9472	0.9561	0.9547
81.1	0.2439	0.2467	0.2475	0.2477	0.2477
102.8	0.5636	0.7843	0.7649	0.7960	0.7880
116.8	0.3198	0.3451	0.3447	0.3465	0.3463
192.0	0.2403	0.3335	0.3239	0.3410	0.3380
209.0	0.1905	0.2229	0.2211	0.2251	0.2248
238.0	0.1341	0.1438	0.1435	0.1443	0.1443

Notes:

1. Nuclear concentrations are such that N_u:N_h=1:5
2. Resonance parameters used are given in Appendix-II
3. Resonance potential interference scattering is included.
4. $I_{eff(1)}^{IR}$ refers to Goldstein's intermediate resonance approximation
5. $I_{eff(2)}^{IR}$ refers to intermediate resonance approximation of Chapter-III

CHAPTER-IV

FOURIER TRANSFORM FOR EVALUATING RESONANCE INTERACTION EFFECTS

In earlier chapters the Fourier transform method for evaluating resonance integrals of isolated resonances was developed. When resonances are isolated it is possible to use the unperturbed flux distribution, viz., the *1/e* distribution above the resonance under consideration. Thus one is able to calculate the absorption rate in each resonance independently. When resonances of the absorber are closely spaced the above assumption breaks down.

For fissile nuclides the overlapping of the resonances is important in calculating the neutron absorption rate [1]. This effect is generally important for fertile nuclides in the higher energy range and hence it can be analyzed in narrow resonance approximation. However, there are other resonances such as the two low energy resonances of Th^{232} which overlap to a certain extent. For these resonances the absorption rate in the first resonance perturbs the flux distribution in the second resonance with the result that the overall absorption is reduced in comparison to that obtained in the isolated resonance approximation. The overlap effect would also lead to a modification of the Doppler coefficient of resonance absorption.

The problem of overlapping resonances was first analyzed by Corngold and Schermer [35] using the variational approach to the slowing down equation. Later, using the narrow resonance approximation to evaluate the collision integrals, Hwang [51,65], Haggblom [66] and Jawas [67] estimated interaction effects. Our aim is to extend the Fourier transform method to treat this problem [50].

A. Derivation Of The Fourier Transformed Equations:

We consider a homogenous mixture of a moderator and absorber which has two overlapping resonances. With the narrow resonance approximation for the moderator collision integral the slowing down equation (1.15) becomes

$$(4.1) \qquad \left[\sigma_a(e)+\sigma_s(e)+\sigma_m\right]\Phi(e)=\frac{\sigma_m}{e}+\int_e^{e/\alpha}\frac{\sigma_s\Phi(e')}{(1-\alpha)}\,\frac{de'}{e'}$$

The microscopic scattering and absorption cross-sections are given by the superposition of the Breit-Wigner cross-sections for individual resonances.

(4.2) $$\sigma_s(e)=\sum_{j=1}^{2}\left[\sigma_{0j}\frac{\Gamma_{nj}}{\Gamma_j}\psi\left(2\frac{e-e_{rj}}{\Gamma_j},\xi_j\right)+\sigma_{0pj}\,\chi\left(2\frac{e-e_{rj}}{\Gamma_j},\xi_j\right)\right]+\sigma_p$$

(4.3) $$\sigma_a(e)=\sum_{j=1}^{2}\sigma_{0j}\frac{\Gamma_{rj}}{\Gamma_j}\psi\left(2\frac{e-e_{rj}}{\Gamma_j},\xi_j\right)$$

Let us assume that we are interested in calculating the absorption rate in the resonance denoted by the subscript 1. Now, the variable e equation (4.1) can be changed to x defined by (2.2)

(4.4) $$x=2\frac{e-e_{r1}}{\Gamma_1}$$

The equation (4.1) becomes

(4.5) $$\left[1+\sum_{j=1}^{2}\gamma_j^2\,\psi_j(x,\xi_j)+\eta_j\,\chi(x,\xi_j)\right]f(x)$$
$$=(1-A)+\frac{A}{\varepsilon}\int_{x}^{x+\varepsilon}\left[1+\sum_{j=3}^{4}\gamma_j^2\,\psi_j(y,\xi_j)+\eta_j\,\chi(y,\xi_j)\right]f(y)\,dy$$

γ_j^2, η_j and ε are defined by

(4.6) $$\gamma_j^2=\frac{\sigma_{0j}}{\sigma_P+\sigma_m}\ ,\ \eta_j=\frac{\sigma_{0Pj}}{\sigma_P+\sigma_m}\ ,\ j=1,2$$

$$\gamma_j^2=\frac{\sigma_{0j}}{\sigma_P}\frac{\Gamma_{nj}}{\Gamma_j}\ ,\ \eta_j=\frac{\sigma_{0Pj}}{\sigma_P}\ ,\ j=3,4$$

$$\varepsilon=2e_{rj}\frac{1-\alpha}{\Gamma_1}$$

Resonance integral of the first resonance is given by

(4.7) $$I_{eff}^{(1)}(\xi)=\frac{I_0^{(1)}}{\pi}\int_{-\infty}^{\infty}f(x)\,\psi_1(x,\xi_1)\,dx$$

The quantities ψ_j and χ_j and are given by

(4.8) $$\psi_1(x,\xi_1)=\psi(x,\xi_1)\ ,\ \chi_1(x,\xi_1)=\chi(x,\xi_1)$$
$$\psi_2(x,\xi_2)=\psi\left(\frac{x-\mu}{\nu^*},\ \xi_2\right)\ ,\ \chi_2(x,\xi_2)=\chi\left(\frac{x-\mu}{\nu^*},\ \xi_2\right)$$

where

(4.9) $$\mu=\frac{e_{r2}-e_{r1}}{\Gamma_1}\ ,\ \nu^*=\frac{\Gamma_2}{\Gamma_1}$$

The parameter μ_j determines the magnitude of the overlap effect. If it is very large, equations (4.5) and (4.7) show that the presence of the second resonance will not affect the nature of *f(x)* near the origin and hence the resonance integral, $I_{eff}^{(1)}(\xi)$.

We define the quantities

$$\theta_j(k,\xi_j) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx} f(x)\psi_j(x,\xi_j)\,dx \tag{4.10}$$

$$G_j(k,\xi_j) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx} f(x)\chi_j(x,\xi_j)\,dx\ ,\ j=1,2 \tag{4.11}$$

On Fourier transformation of equation (4.5) we get

$$\begin{aligned} F(k) + \sum_{n=1}^{2}\gamma_n^2\,\theta_n(k,\xi_n) + \eta_n\,G_n(k,\xi_n) &= \\ = (1-A)\delta(k) + A\nu(k,\varepsilon)&\left[F(k) + \sum_{n=3}^{4}\gamma_n^2\theta_n(k,\xi_n) + \eta_n\,G_n(k,\xi_n)\right] \end{aligned} \tag{4.12}$$

This equation is now rewritten as

$$F(k) + \sum_{n=1}^{2} g_n(k,\varepsilon)\,\theta_n(k,\xi_n) + h_n(k,\varepsilon)\,\chi_n(k,\xi_n) = \delta(k) \tag{4.13}$$

where

$$\begin{aligned} g_n(k,\varepsilon) &= \frac{\gamma_n^2 - A\gamma_{n+2}^2\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)} \\ h_n(k,\varepsilon) &= \frac{\eta_n - A\eta_{n+2}\,\nu(k,\varepsilon)}{1 - A\,\nu(k,\varepsilon)}\ ,\ n=1,2 \end{aligned} \tag{4.14}$$

In order to eliminate *F(k)* from this equation further relations between *F(k)*, $\theta_j(k,\xi_j)$ and $G_j(k,\xi_j)$ are to be obtained. On applying the convolution theorem to equations (4.10) and (4.11), we obtain

$$\theta_j(k,\xi_j) = \int_{-\infty}^{\infty} F(k')\,\overline{\psi}_j(k-k',\xi_j)\,dk' \tag{4.15}$$

$$G_j(k,\xi_j) = \int_{-\infty}^{\infty} F(k')\,\overline{\chi}_j(k-k',\xi_j)\,dk'\ ,\ j=1,2 \tag{4.16}$$

Here $\overline{\psi}_j(k,\xi_j)$ and $\overline{\chi}_j(k,\xi_j)$ are respectively the Fourier transforms of $\psi_j(x,\xi_j)$ and $\chi_j(x,\xi_j)$. The transform $\overline{\psi}_1(k,\xi_1)$ is same as $\overline{\psi}(k,\xi_1)$. To obtain $\overline{\psi}_2(k,\xi_2)$ we use equation (4.8) and the integral representation of the $\psi(x,\xi)$ function. Applying the inverse of the convolution theorem, we get

(4.17) $$\overline{\psi}_2(k,\xi_2) = \frac{\nu^*}{2}\exp\left[-\nu^*|k| + i\,\mu\,k - \nu^*\,k^2/\xi^2\right]$$

The transforms $\overline{\chi}_j(k,\xi_j)$ are obtained as in equation (3.14)

(4.18) $$\overline{\chi}_j(k,\xi_j) = \imath\,H^*(k)\,\overline{\psi}_j(k,\xi_j) \quad , \quad j = 1,2$$

where *H*(k)* is the Heaviside unit function.

Now changing the variable to *k'* in equation (4.13), then multiplying it by $\overline{\psi}_j(k-k',\xi_j)$ and integrating over *k'* we get

(4.20) $$\theta_j(k,\xi_j) + \int_{-\infty}^{\infty} dk'\;\overline{\psi}_j(k-k',\xi_j)\times$$
$$\sum_{n=1}^{2} g_n(k',\varepsilon)\,\theta_n(k',\xi_n) + h_n(k',\varepsilon)\,G_n(k',\xi_n) = \overline{\psi}_j(k,\xi_j) \quad , \quad j = 1,2$$

Similarly multiplying by $\overline{\chi}_j(k-k',\xi_j)$ we get

(4.21) $$G_j(k,\xi_j) + \int_{-\infty}^{\infty} dk'\;\overline{\chi}_j(k-k',\xi_j)\times$$
$$\sum_{n=1}^{2} g_n(k',\varepsilon)\,\theta_n(k',\xi_n) + h_n(k',\varepsilon)\,G_n(k',\xi_n) = \overline{\chi}_j(k,\xi_j) \quad , \quad j = 1,2$$

Thus we have transformed the slowing down equation to the above coupled Fredholm integral equations. The temperature dependent resonance integral including the interaction effect is given by

(4.22) $$I_{eff}^{(1)}(\xi_1) = 2I_0^{(1)}\,\theta_1(0,\xi_1)$$

$\theta_1(0,\xi_1)$ can be obtained as the solution of the coupled Fredholm integral equations (4.20) and (4.21). These equations can be arranged to contain one unknown function defined by

(4.23) $$\Phi(k,\xi_1,\xi_2) = \sum_{n=1}^{2} g_n(k,\varepsilon)\;\theta_n(k,\xi_n)\; + h_n(k,\varepsilon)\,G_n(k,\xi_n)$$

Multiplying equation (4.20) by *g*$g_j(k,\varepsilon\,)$ and equation (4.21) by $h_j(k,\varepsilon\,)$ and adding the resulting equations and summing over the values of *j*, we get

(4.24) $$\Phi(k,\xi_1,\xi_2) + \int_{-\infty}^{\infty} dk'\;\Phi(k',\xi_1,\xi_2)\times$$
$$\sum_{j=1}^{2} g_j(k,\varepsilon)\,\overline{\psi}_j\,(k-k',\xi_j)\; + h_j(k,\varepsilon)\,\overline{\chi}_j\,(k-k',\xi_j)$$

$$= \sum_{j=1}^{2} g_j(k,\varepsilon)\overline{\psi}_j(k,\xi_j) + h_j(k,\varepsilon)\,\overline{\chi}_j(k,\xi_j)$$

Using the explicit expression for $\overline{\psi}_1(k,\xi_1)$ and equation (4.20) we find

(4.25) $$\theta_1(0,\,\xi_1) = \frac{1}{2} - \frac{1}{2}\int_{-\infty}^{\infty} \Phi(k)\exp[-|k| - k^2/\xi^2]\,dk$$

Thus, $\theta_1(0,\,\xi_1)$ is obtained from the solution of the coupled integral equations or using equations (4.24) and (4.25).

B. Resonance Interaction Effect in the Zero Temperature Limit:

In this section we show that in the zero temperature limit the integral equations can be reduced to coupled second order differential equations. Taking the limit $\xi_j \to \infty$ in equations (4.20) we get

(4.26) $$\theta_j(k,\infty) + \int_{-\infty}^{\infty} dk'\,\overline{\psi}_j(k-k',\infty)\times \sum_{n=1}^{2} g_n(k',\varepsilon)\,\theta_n(k',\xi_n) + h_n(k',\varepsilon)\,G_n(k',\xi_n) = \overline{\psi}_j(k,\infty) \quad , \quad j = 1,2$$

$\overline{\psi}_j(k-k',\infty)$ are given by

(4.27) $$\overline{\psi}_1(k-k',\infty) = \frac{1}{2}\exp\left(-|k-k'|\right)$$

(4.28) $$\overline{\psi}_2(k-k',\infty) = \frac{\nu^*}{2}\exp\left[-\nu^*\,|k-k'| + i\,\mu\left(k-k'\right)\right]$$

(i) Reduction to coupled differential equations:

We already know that $\overline{\psi}_1(k-k',\infty)$ is the Green’s function of the operator

(4.29) $$\widehat{O}_1 = \frac{d^2}{dk^2} - 1$$

Similarly $\overline{\psi}_2(k-k',\infty)$ can be identified as the Green’s function of the operator: $\widehat{O}_2$

(4.30) $$\widehat{O}_2 = \frac{1}{\nu^{*2}}\left[\frac{d^2}{dk^2} - 2i\,\mu\frac{d}{dk} - \left(\mu^2 + \nu^{*2}\right)\right]$$

These Green’s functions satisfy the boundary conditions

(4.31) $$\overline{\psi}_j(k-k',\infty)\Big|_{k=\pm\infty} = 0 \quad , \quad j = 1,2$$

Applying the operators $\widehat{O}_1$ and $\widehat{O}_2$ respectively to equation (4.26) for *j=1* and *2*, we get

(4.32) $$\left(\frac{d^2}{dk^2} - 1\right)\theta_1(k,\infty) - \left[g_n(k,\varepsilon)\,\theta_n(k,\infty) + h_n(k,\varepsilon)\,G_n(k,\infty)\right] = -\,\delta(k)$$

and

$$\left(\frac{d^2}{dk^2}-\left(\mu^2+\nu^{*2}\right)\right)\theta_2(k,\infty)-2i\,\mu\frac{d}{dk}\theta_2 \\ -\nu^{*2}\left[g_n(k,\varepsilon)\,\theta_n(k,\infty)+h_n(k,\varepsilon)\,G_n(k,\infty)\right]=-\nu^{*2}\delta(k) \tag{4.33}$$

From the previous Chapter we know that

$$G_1(k,\infty)=-2i\frac{d}{dk}\theta_1 \tag{4.34}$$

When $\xi_2\to\infty$, we have

$$\theta_2(k,\infty)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{\imath kx}\,f(x)\frac{\nu^{*2}}{\nu^{*2}+(x-\mu)^2}\,dx \tag{4.35}$$

and

$$G_2(k,\infty)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{\imath kx}\,f(x)\frac{2\nu^{*2}(x-\mu)}{\nu^{*2}+(x-\mu)^2}\,dx \tag{4.36}$$

From the above two equations we get

$$G_2(k,\infty)=-\frac{2i}{\nu^*}\left[\frac{d}{dk}\theta_2-i\,\mu\,\theta_2(k,\infty)\right] \tag{4.37}$$

Thus the coupled differential equations (4.32) and (4.33) can be written in terms of $\theta_j(k,\infty)$ alone. The boundary conditions on $\theta_j(k,\infty)$ can be obtained from equation (4.26) by putting $k=\pm\infty$:

$$\theta_j(k,\,\infty)\Big|_{k=\pm\infty}=0\ ,\ \ j=1,2 \tag{4.38}$$

Using the explicit expressions for $g_j(k,\varepsilon)$ and $h_j(k,\varepsilon)$ the differential equations for $\theta_j(k,\infty)$ can be written in the matrix notation

$$\frac{d^2\vec{\theta}}{dk^2}+2\imath\left[\mathcal{D}_1+\mathcal{D}_2\frac{A\nu(k,\varepsilon)}{1-A\nu(k,\varepsilon)}\right]\frac{d\,\vec{\theta}}{dk}-\left[\mathcal{M}_1+\mathcal{M}_2\frac{A\nu(k,\varepsilon)}{1-A\nu(k,\varepsilon)}\right]\vec{\theta}(k,\infty)=-\vec{e}\,\delta(k) \tag{4.39}$$

where $\vec{\theta}$ and $\vec{e}$ are two dimensional vectors given by

$$\vec{\theta}=\begin{bmatrix}\theta_1\\ \theta_2\end{bmatrix} \tag{4.40}$$

and

$$\vec{e}=\begin{bmatrix}1\\ \nu^{*2}\end{bmatrix} \tag{4.41}$$

The quantities $\mathcal{D}_1$, $\mathcal{D}_2$, $\mathcal{M}_1$ and $\mathcal{M}_2$ are square matrices of order two defined by

$$(4.42)\qquad \mathcal{D}_1 = \begin{bmatrix} \eta_1 & \eta_2 / \nu^* \\ \nu^* \eta_1 & \nu^* \eta_2 - \mu \end{bmatrix}$$

$$(4.43)\qquad \mathcal{D}_2 = \begin{bmatrix} \eta_1 - \eta_3 & (\eta_2 - \eta_4)/\nu^* \\ \nu^* (\eta_1 - \eta_3) & \nu^* (\eta_2 - \eta_4) \end{bmatrix}$$

$$(4.44)\qquad \mathcal{M}_1 = \begin{bmatrix} 1 + \gamma_1^2 & (\gamma_2^2 + 2\,\mu\,\eta_2 / \nu^*) \\ \nu^* \gamma_1^2 & \nu^{*2} (1 + \gamma_2^2) + \mu^2 + 2\nu^* \mu\,\eta_2 \end{bmatrix}$$

$$(4.45)\qquad \mathcal{M}_2 = \begin{bmatrix} \gamma_1^2 - \gamma_3^2 & \gamma_1^2 - \gamma_3^2 + 2\mu(\eta_2 - \eta_4)/\nu^* \\ \nu^{*2} (\gamma_1^2 - \gamma_3^2) & \nu^{*2} (\gamma_2^2 - \gamma_4^2) + 2\nu^* \mu (\eta_2 - \eta_4) \end{bmatrix}$$

From the definition of the transforms $\theta_j(k,\infty)$ we know that they are continues at *k=0*. Further, the delta function on the RHS of equation (4.39) can be replaced by the discontinuity condition on $d\vec{\theta}/dk$. Thus we have to solve the homogenous system of second order differential equations.

$$(4.46)\qquad \frac{d^2\vec{\theta}}{dk^2} + 2\imath \left[\mathcal{D}_1 + \mathcal{D}_2 \frac{A\nu(k,\varepsilon)}{1 - A\nu(k,\varepsilon)} \right] \frac{d\vec{\theta}}{dk} - \left[\mathcal{M}_1 + \mathcal{M}_2 \frac{A\nu(k,\varepsilon)}{1 - A\nu(k,\varepsilon)} \right] \vec{\theta}(k,\infty) = \vec{0}$$

subject to the boundary conditions

$$(4.47)\qquad (a)\quad \vec{\theta}(k,\infty) \to \vec{0} \ \ as\ \ k \to \pm\infty$$

$$(4.48)\qquad (b)\quad \vec{\theta}(k,\infty)\Big|_{0+} = \vec{\theta}(k,\infty)\Big|_{0-}$$

$$(4.49)\qquad (c)\quad \frac{d}{dk}\vec{\theta}(k,\infty)\Big|_{0+} - \frac{d}{dk}\vec{\theta}(k,\infty)\Big|_{0-} = \vec{e}$$

In equation (4.46), $\vec{0}$ denotes a two dimensional null vector. Before attempting to solve this equation by WKB method we consider the narrow resonance approximation.

(ii) Solution in the narrow resonance approximation:

The narrow resonance approximation is obtained by taking the limit $\varepsilon \to \infty$. Then the function $\nu(k, \varepsilon) \to 0$ and we get

$$(4.50)\qquad \frac{d^2\vec{\theta}^{NR}}{dk^2} + 2\imath\,\mathcal{D}_1 \frac{d\vec{\theta}^{NR}}{dk} - \mathcal{M}_1 \vec{\theta}^{NR}(k,\infty) = \vec{0}$$

Since for large value of k the function $\nu(k, \varepsilon) \to 0$, the above equation represents the asymptotic form of equation (4.46) also. Now, we try a solution of the form

$$(4.51)\qquad \vec{\theta}^{NR}(k,\infty) = \vec{\theta}_0(w) \exp(i\,w\,k)$$

Substituting in equation (4.50), we get

(4.52) $$\left(w^2 E + 2\,wD_1 + M_1\right)\vec{\theta}_0(w) = \vec{0}$$

Here E denotes a unit matrix of order two. For a non-trivial solution $\vec{\theta}_0(w)$, *w* would be chosen as the roots of the secular equation

(4.53) $$\det\left(w^2 E + 2\,wD_1 + M_1\right) = 0$$

Substituting for D_1 and M_1 we get a fourth order polynomial equation for *w*.

(4.54) $$\begin{aligned} & w^4 + 2w^3\left(\nu^*\eta_2 + 2\eta_1 - \mu\right) + w^2\left[\nu^{*2}(1+\gamma_2^2) + 1 + \gamma_1^2 + \mu^2 + 2\mu(\nu^*\eta_2 - 2\eta_1)\right] \\ & + w\left[\eta_1\eta_2\,\mu\,(\nu^* - 1) + \eta_1(\nu^{*2} + \mu^2) + 2(\nu^*\eta_2 - \mu) - 2\gamma_1^2\mu\right] \\ & + \left[\nu^*(1+\gamma_2^2) + \gamma_1^2(\nu^{*2} + \mu^2) + 2\,\nu^*\mu\eta_2 + \mu^2\right] = 0 \end{aligned}$$

Since the coefficients of various powers of *w* are real, the four roots will occur as conjugate pairs. Let them be denoted by

(4.55) $$w_j^{\pm} = a_j \pm i\,b_j \quad , \quad 1 \le j \le 2$$

where the imaginary parts b_j are positive quantities. Therefore, the general solution $\vec{\theta}^{NR}(k,\infty)$ vanishing at $\pm\infty$ are given by

(4.56) $$\begin{aligned} \vec{\theta}^{NR}(k,\infty) &= \sum_{j=1}^{2} C_j^+\,\vec{\theta}_0\,(w_j^+)\exp\left(i\,w_j^+\,k\right) \ , \ k > 0 \\ &= \sum_{j=1}^{2} C_j^-\,\vec{\theta}_0\,(w_j^-)\exp\left(i\,w_j^-\,k\right) \ , \ k < 0 \end{aligned}$$

Here $\vec{\theta}_0\,(w_j^{\pm})$ are the eigenvectors of the system (4.52). It can be seen that

(4.57) $$\vec{\theta}_0\,(w_j^{\pm}) = \begin{bmatrix} 1 \\ l_j + i\,d_j \end{bmatrix}$$

Here l_j and d_j respectively denote the real and imaginary parts of the second component of the vector: $\vec{\theta}_0\,(w_j^{\pm})$. They are defined by

(4.57a) $$l_j + i\,d_j = \frac{2w_j^{\pm}\eta_2/\nu^* + \gamma_2^2 + 2\mu\eta_2/\nu^*}{w_j^{\pm\,2} + 2w_j^{\pm}\,\eta_1 + 1 + \gamma_1^2}$$

The boundary conditions (4.48) and (4.49) give

(4.58) $$\sum_{j=1}^{2} C_j^+\,\vec{\theta}_0\,(w_j^+) = \sum_{j=1}^{2} C_j^-\,\vec{\theta}_0\,(w_j^-)$$

and

(4.59) $$i\sum_{j=1}^{2}\left[C_j^-\, w_j^-\, \vec{\theta}_0\,(w_j^-) - C_j^+\, w_j^+\, \vec{\theta}_0\,(w_j^+)\right] = \vec{e}$$

The fact that $\vec{\theta}^{NR}(0,\infty)$ is real demands that C_j^+ and C_j^- should occur as conjugate pairs. Separating $C_j^{\pm}$ into real and imaginary parts, we get

(4.60) $$C_j^{\pm} = C_j^R \pm i\, C_j^I \;\;,\;\; 1 \le j \le 2$$

and using equations (4.55), (4.57), (4.58) and (4.59) we get

(4.61) $$b_1\, C_1^R + a_1\, C_1^I + b_2\, C_2^R + a_2\, C_2^I = \frac{1}{2}$$

$$C_1^I + C_2^I = 0$$

$$d_1\, C_1^R + l_1\, C_1^I + d_2\, C_2^R + l_2\, C_2^I = 0$$

$$(b_1 l_1 + a_1 d_1)\, C_1^R + (a_1 l_1 - b_1 d_1)\, C_1^I + (b_2 l_2 + a_2 d_2)\, C_2^R + (a_2 l_2 - b_2 d_2)\, C_2^I = \frac{\nu^{*2}}{2}$$

Eliminating C_1^I and C_2^I from the last two equations we get

(4.62) $$\left[b_1 + d_1\,\frac{a_1 - a_2}{l_2 - l_1}\right] C_1^R + \left[b_2 + d_2\,\frac{a_1 - a_2}{l_2 - l_1}\right] C_2^R = \frac{1}{2}$$

$$\left[b_1 l_1 + a_1 d_1 + d_1\,\frac{a_1 l_1 - b_1 d_1 - a_2 l_2 + b_2 d_2}{l_2 - l_1}\right] C_1^R +$$

$$\left[b_2 l_2 + a_2 d_2 + d_2\,\frac{a_1 l_1 - b_1 d_1 - a_2 l_2 + b_2 d_2}{l_2 - l_1}\right] C_2^R = \frac{\nu^{*2}}{2}$$

and

(4.63) $$C_1^I = -C_2^I = \frac{d_1 C_1^R + d_2 C_2^R}{l_2 - l_1}$$

Equation (4.56) shows that

(4.64) $$I_{eff-NR}^{(1)}\,(\infty) = 2 I_0^{(1)} \left[C_1^R + C_2^R\right]$$

Thus we find that once the roots of the polynomial equation (4.54) are obtained, the resonance integral in the narrow resonance approximation can be easily evaluated.

(iii) WKB approximation to system of differential equations

For obtaining the solution of the system of equations (4.46), we write as before

(4.65) $$\vec{\theta}(k,\infty) = \sum_{j=1}^{2} C_j^+\, \vec{\theta}_0\,(w_j^+) \exp\left(i\, w_j^+\, k - \int_0^k S_j^+(k')\, dk'\right) \;\;,\;\; k > 0$$

$$= \sum_{j=1}^{2} C_j^- \, \vec{\theta}_0\,(w_j^-) \exp\left(i\, w_j^-\, k - \int_k^0 S_j^-(k')\, dk' \right) \;,\; k < 0$$

Here $\vec{\theta}_0\,(w_j^\pm)$ are the eigenvectors of the system (4.52) and are given by equation (4.57). The constants $C_j^\pm$ are to be determined. In writing $\vec{\theta}(k,\infty)$ in this form, we have incorporated the asymptotic part of the solution (same as the solution in the narrow resonance approximation). To ensure the boundary condition (4.47) on $\vec{\theta}(k,\infty)$, we have

(4.66) $$S_j^\pm(k) \to 0 \;\; as \;\; k \to \pm\infty \;\;,\;\; j = 1,2$$

Substituting for $\vec{\theta}(k,\infty)$ in equation (4.46) we get

(4.67) $$\left[\mp \frac{dS_j^\pm}{dk} E - 2i \left\{ w_j^+ E - D_1 - D_2 \frac{A\,\nu(k,\varepsilon)}{1 - A\;\nu(k,\varepsilon)} \right\} S_j^\pm(k) + [S^\pm(k)]^2 E \right] \theta_0(w_j^\pm)$$

$$= \frac{A\,\nu(k,\varepsilon)}{1 - A\;\nu(k,\varepsilon)} M_2\, g \vec{\theta}_0(w_j^\pm) \;\;,\;\; 1 \le j \le 2$$

The upper sign stands for *k > 0* and the lower sign for *k<0*. Applying the boundary conditions (4.48) and (4.49) we get

(4.68) $$\sum_{j=1}^{2} C_j^+ \, \vec{\theta}_0\,(w_j^+) = \sum_{j=1}^{2} C_j^- \, \vec{\theta}_0\,(w_j^-)$$

$$i \sum_{j=1}^{2} \left[C_j^- \left\{ w_j^- + S_j^-(0) \right\} \vec{\theta}_0\,(w_j^-) - C_j^+ \left\{ w_j^+ + S_j^+(0) \right\} \vec{\theta}_0\,(w_j^+) \right] = \vec{e}$$

When equations (4.67) and solved by the interactive method, $S_j^+(k)$ and $S_j^-(k)$ would occur as conjugate functions. Therefore we can separate $S_j^\pm(0)$ into real and imaginary parts:

(4.69) $$S_j^\pm(0) = S_j^R(0) \pm i\, S_j^I(0) \;\;,\;\; 1 \le j \le 2$$

Now, the requirement that $\vec{\theta}(0,\infty)$ should be real demands that C_j^+ and C_j^- to be conjugate pairs. Using equations (4.60), (4.68) and (4.69), we get exactly similar relations (4.62) between C_1^R and C_2^R. The differences are the replacements of a_j and b_j in these equations by

(4.70) $$a_j \;\Rightarrow\; a_j + S_j^I(0) \;\;,\;\; 1 \le j \le 2$$

$$b_j \;\Rightarrow\; b_j + S_j^R(0) \;\;,\;\; 1 \le j \le 2$$

Once $S_j^R(0)$ and $S_j^I(0)$ are obtained, $\theta_1(0,\infty)$ and thereafter $I_{eff}^{(1)}(\infty)$ can be evaluated. Equation (4.67) is a vector equation for $S_j^+(k)$ and can be reduced to a scalar equation by taking dot product with the vector $\vec{\theta}_0\,(w_j^+)$. Thus we have

(4.67)
$$-\frac{dS_j^+}{dk}-2i\left\{w_j^+-p_j^+-q_j^+\,\frac{A\,\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}\right\}S_j^+(k)+S_j^{+\,2}(k)$$
$$=\frac{A\,\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}r_j^+\ \ ,\ 1\le j\le 2$$

where

(4.72)
$$p_j^+=\frac{\left\langle\vec{\theta}_0\,|\,D_1\,|\,\vec{\theta}_0\right\rangle}{\left\langle\vec{\theta}_0\,|\,\theta_0\right\rangle}$$

$$q_j^+=\frac{\left\langle\vec{\theta}_0\,|\,D_2\,|\,\vec{\theta}_0\right\rangle}{\left\langle\vec{\theta}_0\,|\,\theta_0\right\rangle}$$

$$r_j^+=\frac{\left\langle\vec{\theta}_0\,|\,M_2\,|\,\vec{\theta}_0\right\rangle}{\left\langle\vec{\theta}_0\,|\,\theta_0\right\rangle}$$

Another possibility is to take the first component of the vector equation (4.67). The resulting equation would be exactly similar to (4.71) but now the quantities p_j^+, q_j^+, and r_j^+ are given by

(4.73)
$$p_j^+=\eta_1+\eta_2\,\frac{\left(l_j+i\,d_j\right)}{\nu^*}$$

$$q_j^+=\left(\eta_1-\eta_3\right)+\left(\eta_2-\eta_4\right)\frac{\left(l_j+i\,d_j\right)}{\nu^*}$$

$$r_j^+=\left(\gamma_1^2-\gamma_3^2\right)+\left[\left(\gamma_2^2-\gamma_4^2\right)+2\frac{\mu}{\nu^*}\left(\eta_2-\eta_4\right)\left(l_j+i\,d_j\right)\right]\ ,\ 1\le j\le 2$$

In any case we find that the equations to be solved to determine $S_j^R(0)$ and $S_j^I(0)$ are very much similar to the types encountered in earlier chapters. The first order approximation to $S_j^+(0)$ gives

(4.74)
$$S_j^+(0)=r_j^+\int_0^\infty \exp\left[2\,i\left(w_j^+-p_j^+\right)k\right]\frac{A\,\nu(k,\varepsilon)}{1-A\,\nu(k,\varepsilon)}\,dk$$

Although the integral can be expanded as a power series in A, the resulting integrals are complicated for analytical evaluation. The results given below for the two overlapping resonances of Th^{232} were obtained in the first order approximation by a numerical evaluation of the integrals (4.74).

(iv) Interaction effect on zero-temperature resonance integrals -Th^{232} resonances

The two low energy resonances of Th^{232} at energies 21.8 and 23.47 eV are somewhat close together. The resonance parameters given in Appendix-I show that the scattering widths are much smaller than the total widths. Therefore resonance potential interference scattering can be neglected. In table-X we give the zero temperature resonance integrals with and without the interaction effect for various values of σ_m. When interaction between the resonances is neglected, the resonance integrals calculated in the first and second order perturbation approximations match well. Therefore the results obtained in the first order perturbation approximation showing the effect of interaction are of the correct magnitude. The table also contains resonance integrals calculated in the narrow resonance approximation.

The general observation is that the interaction effect decreases as the moderator scattering cross-section σ_m increases. This happens because as σ_m increases, the value of the resonance integral approaches the infinite dilution limit which corresponds to the unperturbed *1/e* energy distribution. Further it is found that the magnitude of the interaction effect calculated in the narrow resonance approximation is of appropriate magnitude.

C. Resonance Interaction Effect At Non-Zero Temperature:

Having solved the problem of resonance interaction in the rigorous way for the zero temperature-limit, we now turn our attention to the temperature dependent problem. We mentioned that for fertile nuclides the overlap effect is significant in the higher energy range. Therefore they can be studied in the narrow resonance approximation. In the zero temperature limit we have seen that for the low energy resonances of Th^{232} the narrow resonance approximation can be applied to obtain the interaction effect. Hence we shall discuss this problem further in this approximation only.

ϕ(e) can be obtained in the narrow resonance approximation from equation (4.1) by replacing *ϕ(e')* and *σ(e')* in the collision integral by their asymptotic values. This is equivalent to replacing the integrand in equation (4.5) by 1. Therefore we get

(4.75) $$f_{NR}(x)=\frac{1}{\left[1+\sum_{j=1}^{2}\left\{\gamma_j^2\psi_j+\eta_j\chi_j\right\}\right]}$$

and the resonance integral becomes

(4.76) $$I_{eff}^{(1)}(\xi_1)=2\frac{I_0^{(1)}}{\pi}J^*$$

where *J** is the generalized J-function defined as [66,67]

(4.77) $$J^*=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\psi_1(x,\xi_1)}{1+\sum_{j=1}^{2}\gamma_j^2\psi_j+\eta_j\chi_j}dx$$

Thus the problem reduces to the evaluation of this complicated function. Haggblom [65] and Jawas [67] assume that the interaction term $\gamma_2^2\psi_2+\eta_2\chi_2$ is small and therefore *J** can be expanded in a series. Neglecting higher order terms, they approximate *J** as

(4.78) $$J^*\approx J-\frac{1}{2}\int_{-\infty}^{\infty}\frac{\psi_1\left\{\gamma_2^2\psi_2+\eta_2\chi_2\right\}}{\left\{1+\gamma_1^2\psi_1+\eta_1\chi_1\right\}\left\{\gamma_1^2\psi_1+\eta_1\chi_1\right\}}dx$$

Here the first term *J* is the ordinary J-function. In evaluating *J**, Hwang [51] has avoided the series expansion by rewriting it as

(4.79) $$J^*=J-\frac{1}{2}\int_{-\infty}^{\infty}\frac{\psi_1\left\{\gamma_2^2\psi_2+\eta_2\chi_2\right\}}{\left\{1+\gamma_1^2\psi_1+\eta_1\chi_1\right\}\left\{1+\sum_{j=1}^{2}\gamma_j^2\psi_j+\eta_j\chi_j\right\}}dx$$

An accurate evaluation of *J** from equation (4.77) will be quite difficult and is the reason for separating the overlap part as given in equations (4.78) and (4.79). He then evaluates the integrals using Jacobi quadrature formulae. In any case it is clear that the calculation of *J** function leads to the evaluation of very complicated integrals.

In the narrow resonance approximation equations (4.20) for *j=1* gives

(4.80) $$\theta_1(k,\xi_1)+\int_{-\infty}^{\infty}\sum_{n=1}^{2}\left[\gamma_n^2\,\theta_n(k',\xi_n)+\eta_n\,G_n(k',\xi_n)\right]\times$$

$$\overline{\psi}_1(k-k',\xi_1)dk'=\overline{\psi}_1(k,\xi_1)$$

This equation is obtained by replacing $g_n(k,\varepsilon)$ and $h_n(k,\varepsilon)$ by the constant γ_n^2 and η_n . It is possible to eliminate $\theta_2(k,\xi_2)$ and $G_2(k,\xi_2)$ from this equation and obtain a single equation for $\theta_1(k,\xi_1)$. Using equation (4.15), we have

$$\int_{-\infty}^{\infty}\overline{\psi}_1(k-k',\xi_1)\theta_2(k',\xi_2)\,dk' \tag{4.81}$$

$$=\int_{-\infty}^{\infty}\overline{\psi}_1(k-k',\xi_1)\,dk'\int_{-\infty}^{\infty}\overline{\psi}_2(k'-k'',\xi_2)F(k'')\,dk''$$

Interchanging the order of integration, we get

$$LHS=\int_{-\infty}^{\infty}F(k'')\,dk''\int_{-\infty}^{\infty}\overline{\psi}_1(k-k',\xi_1)\,\overline{\psi}_2(k'-k'',\xi_2)dk' \tag{4.82}$$

Changing the variable of integration *k'* in the second integral to *(k-k*+k”)*, we get

$$LHS=\int_{-\infty}^{\infty}F(k'')\,dk''\int_{-\infty}^{\infty}\overline{\psi}_1(k^*-k'',\xi_1)\,\overline{\psi}_2(k-k^*,\xi_2)dk^* \tag{4.83}$$

Interchanging the order of integration again and using equation (4.15), we get

$$LHS=\int_{-\infty}^{\infty}\overline{\psi}_2(k-k^*,\xi_2)dk^*\int_{-\infty}^{\infty}F(k'')\,\overline{\psi}_1(k^*-k'',\xi_1)dk'' \tag{4.84}$$

$$=\int_{-\infty}^{\infty}\overline{\psi}_2(k-k^*,\xi_2)\,\theta_1(k^*,\xi_1)dk^*$$

Similarly using equation (4.16) we can show that

$$\int_{-\infty}^{\infty}\overline{\psi}_1(k-k',\xi_1)G_n(k',\xi_n)\,dk' \tag{4.85}$$

$$=\int_{-\infty}^{\infty}\overline{\chi}_n(k-k',\xi_n)\,\theta_1(k',\xi_1)dk' \quad ,\; n=1,2$$

Using equations (4.84) and (4.85) in equation (4.80), we get

$$\theta_1(k,\xi_1)+\int_{-\infty}^{\infty}dk'\,\theta_1(k',\xi_1)\,\times \tag{4.86}$$

$$\sum_{n=1}^{2}\left[\gamma_n^2\,\overline{\psi}_n(k-k',\xi_n)+\eta_n\,\overline{\chi}_n(k-k',\xi_n)\right]dk'=\overline{\psi}_1(k,\xi_1)$$

The kernel of this integral equation is of the displacement type. Therefore on taking the inverse transform and using the convolution theorem we get

$$F(x,\xi_1)+F(x,\xi_1)\sum_{n=1}^{2}\gamma_n^2\,\psi_n+\eta_n\,\chi_n=\psi_1(x,\xi_1) \tag{4.87}$$

where $F(x,\xi_1)$ given by

(4.88) $$F_1(x,\xi_1)=\int_{-\infty}^{\infty} \exp(-i\,k\,x)\;\theta_1(k,\xi_1)\,dk$$

Solving for *F(x,*ξ_1*)* from equation (4.87) and again taking the Fourier transform we get

(4.89) $$\theta_1(k,\xi_1)=\frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(-i\,k\,x)\;\frac{\psi_1(x,\xi_1)}{1+\sum_{j=1}^{2}\gamma_j^2\psi_j+\eta_j\chi_j}\,dx$$

On comparison with equation (4.77) we find that the *J** function is given by

(4.90) $$J^*=\pi\,\theta_1(0,\xi_1)$$

Now our aim is to solve the integral equation (4.86) using the quadrature method. Neglecting terms arising from resonance potential interference scattering, we get

(4.91) $$\theta_1(k,\xi_1)+\int_{-\infty}^{\infty} dk'\;\theta_1(k',\xi_1)\Big[\gamma_1^2\exp\big\{-|\,k-k'|-(k-k')^2/\xi_1^2\big\}+$$
$$+\nu^*\,\gamma_2^2\exp\big\{-\nu^*\,|\,k-k'|-\nu^*(k-k')^2/\xi_2^2+i\mu(k-k')\big\}\Big]=\frac{1}{2}\exp\big(-|\,k\,|-k/\xi_1^2\big)$$

From the definition of ν^* and ξ_2 we find that

(4.92) $$\frac{\nu^*}{\xi_2^2}=\frac{1}{\xi_1^2}\left(1+\frac{e_{r2}-e_{r1}}{e_{r1}}\right)=\frac{1}{\xi_1^2}(1+t)$$

To apply the quadrature method we write

(4.93) $$\theta_1(k,\xi_1)=\left[\theta_1(k,\infty)+\phi(k,\xi_1)\right]\exp\left\{-k^2/\xi_1^2\right\}$$

where $\theta_1(k,\infty)$ is the zero temperature part of the solution and is given by equation (4.56). Substituting from equations (4.92) and (4.93) and applying the quadrature formula, equation (4.91) can be converted to the system of algebraic equations.

(4.94) $$\phi(\xi^*k_i)+\frac{\xi^*}{2}\sum_{j=1}^{N}W_j\phi(\xi^*k_j)Z\left\{\xi^*(k_i-k_j)\right\}\times$$
$$\exp\Big[(M^2-2)k_j^2/M^2+2k_i\,k_j/M^2\Big]=S(\xi^*k_i)\,,\;1\le i\le N$$

Here k_i and W_i are the roots and weights of the quadrature formula of order N and $\xi^*=\xi_1/M$. Further, $Z(\xi^*k_i)$ and $S(\xi^*k_i)$ are given by

(4.95) $$Z(\xi^*k_i)=\gamma_1^2\exp\left\{-\xi^*\,|\,k_i\,|\right\}+\nu^*\,\gamma_2^2\exp\left\{-\nu^*\xi^*\,|\,k_i\,|+i\mu\,\xi^*\,k_i-tk_i^2/M^2\right\}$$

and

(4.96) $$S(\xi^*k_i)=\frac{1}{2}\exp\left\{-\xi^*k_i\right\}-\theta_1(\xi^*k_i,\infty)$$
$$-\xi^*\int_{-\infty}^{\infty}dk\,\theta_1(\xi^*k,\infty)Z\left\{\xi^*(k_i-k)\right\}\exp\left\{-\left(2k^2+2k_ik\right)/M^2\right\}$$

From the integral equation (4.91) we know that the real and imaginary parts of $\theta_1(k,\xi_1)$ and hence that of $\phi_1(k,\xi_1)$ are respectively even and odd functions. Using this fact and arranging the order of the roots and weights of the quadrature formula as indicated in Chapter-II, it is possible to reduce (4.94) to a system of N real equations. Choice of the parameter $M= 2.2 +2\xi_1$ and other details which make $\phi_1(\xi^* k_i)$ to give the J^* function directly are exactly as discussed earlier and hence will not be repeated here.

Using this method we estimated the effect of interaction on the Doppler coefficients of the Th^{232} resonances. Results in Table-XI show that the interaction effect is destructive and leads to a reduction in Doppler coefficient for low temperature. This is expected because when resonances overlap broadening of the resonances introduces lesser changes in the neutron cross-sections and hence in the neutron absorption rate. Once again we note that the effect of interaction decreases as a moderator scattering cross-section increases.

D. Summary

In this Chapter we extended the Fourier transform method to treat the problem of interacting resonances of an absorber. For the case of two closely spaced resonances the slowing down equation was converted to a Fredholm integral equation. In the zero temperature limit the problem was reduced to the solution of two coupled second order differential equations. The WKB method was extended to solve these equations. The temperature dependent problem was analyzed in the narrow resonance approximation only. Solution of the Fredholm integral equation using the quadrature formulae gave us a new method to evaluate the generalized J-function. Finally the method of this Chapter was applied to evaluate the effect of interaction of the two low energy resonances of Th^{232}.

Table-X

Zero Temperature Resonance integrals of Th^{232} Resonances

Resonance Energy 21.8 eV

σ_m (barns)	NR Approximation		WKB Approximation		
	Without interaction	With interaction	Without interaction 1-order	Without interaction 2-order	With interaction
20	0.9373	0.9001	0.8206	0.8229	0.7785
30	1.082	1.048	0.9982	0.9988	0.9635
40	1.209	1.178	1.147	1.147	1.116
50	1.324	1.295	1.277	1.277	1.248

Resonance Energy 22.47 eV

σ_m (barns)	NR Approximation		WKB Approximation		
	Without interaction	With interaction	Without interaction 1-order	Without interaction 2-order	With interaction
20	1.119	1.084	1.002	1.005	0.9644
30	1.292	1.260	1.221	1.221	1.129
40	1.444	1.415	1.403	1.403	1.374
50	1.582	1.555	1.563	1.563	1.536

Notes:

1. Resonance parameters used are given in Appendix-II
2. Resonance potential interference scattering is neglected.

Table-XI

Doppler Coefficient ($10^4\ \Delta I_{eff} / \Delta T$) of Th^{232} Resonances

σ_m (barns)	T (°K)	21.8 eV		22.47 eV	
		Without interaction	With interaction	Without interaction	With interaction
20	0-300	3.367	0.9782	2.413	1.166
	300-600	2.881	4.261	2.395	2.462
	600-900	2.551	3.013	2.112	2.352
30	0-300	4.802	1.600	3.581	1.936
	300-600	4.056	6.087	3.329	3.965
	600-900	3.493	3.955	3.026	3.106
40	0-300	6.351	2.320	4.830	2.783
	300-600	5.143	7.765	4.329	5.518
	600-900	4.339	5.023	3.851	3.783
50	0-300	7.931	3.033	6.217	3.668
	300-600	6.192	9.529	5.249	7.066
	600-900	5.140	5.941	4.653	4.469

Notes:

1. Resonance parameters used are given in Appendix-II
2. Calculations have been done using NR approximation.

CHAPTER-V

FOURIER TRANSFORM METHOD FOR TREATING THE MODERATOR AND ABSORBER COLLISION INTEGRALS EXACTLY

In all the previous chapters we were working under the approximation that the moderator collision integral can be treated in the narrow resonance approximation. In most of the situations this approximation is adequate, however, from a mathematical standpoint the implications of this approximation are to be analyzed. The present Chapter will be devoted for this purpose.

The basic problem in resonance absorption theory is the solution of the initial value problem posed by the slowing down equation and the normalization condition on $\phi(e)$ viz., $\phi(e)\sim 1/e$ when $e>>e_r$. In treating the moderator collision integral in the narrow resonance approximation, the asymptotic form of $\phi(e)$ is required and we were using the normalization condition explicitly in the asymptotic form. The resulting equation is an inhomogeneous equation. Thus we find that the basic structure of the problem is modified by the introduction of narrow resonance approximation for moderator collision integral in that a homogenous equation is converted into an inhomogeneous equation. The main aim of this Chapter is to study the mathematical properties of the original homogenous equation and the initial value problem using Fourier transforms. In order to simplify the treatment we shall assume that resonance potential interference scattering can be neglected.

A: <u>Derivation of the Freedom Integral Equation</u>:

The equation to be treated in this situation is (1.23). Substituting the resonance cross-sections, equation (1.23) becomes

$$(5.1)\qquad \left[1+\gamma_1^2\,\psi(x,\xi)\right]f(x)=\frac{1-A}{\varepsilon_m}\int_x^{x+\varepsilon_m} f(y)\,dy+\frac{A}{\varepsilon}\int_x^{x+\varepsilon}\left[1+\gamma_\infty^2\,\psi(y,\xi)\right]f(y)\,dy$$

This equation shows that for large values of x when, $\psi(y,\xi)\approx 0$ for $x\le y\le x+\varepsilon$, f(x) = c, a constant, is a solution. This constant is to be normalized to unity so that resonance integral is given by equation (1.32). Introducing the discontinuity factors $H(x,y,\varepsilon)$ and $H(x,y,\varepsilon_m)$, we get

$$(5.2)\qquad \left(1+\gamma_1^2\,\psi\right)f(x)=(1-A)\int_{-\infty}^{\infty}dk'\,\nu(k',\varepsilon_m)e^{-ik'x}\,\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{iky}\;f(y)\,dy$$

$$+A\int_{-\infty}^{\infty} dk'\nu(k',\varepsilon)e^{-ik'x}\,\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{iky}\left(1+\gamma_{\infty}^{2}\,\psi\right)f(y)\,dy$$

Here, $\nu(k,\varepsilon_m)$ is defined as

$$\nu(k,\varepsilon_m)=\frac{(1-e^{-ik\varepsilon_m})}{ik\varepsilon_m} \tag{5.3}$$

In terms of *F(k)* and *θ(k,ξ)*, equation (5.3) can be rewritten as

$$\left[1+\gamma_1^2\,\psi(x,\xi)\right]f(x)=(1-A)\int_{-\infty}^{\infty} dk'\;\nu(k',\varepsilon_m)\,e^{-ik'x}\,F(k') \tag{5.4}$$

$$+A\int_{-\infty}^{\infty} dk'\;\nu(k',\varepsilon)\;e^{-ik'x}\left[F(k')+\gamma_{\infty}^{2}\,\theta(k',\xi)\right]$$

On Fourier transformation we get

$$\left[1-A\nu(k,\varepsilon)\;-\left(1-A\right)\nu(k,\varepsilon_m)\;\right]F(k)\,\theta(k,\xi)+\left[\gamma_1^2-\gamma_{\infty}^{2}\,\nu(k,\varepsilon)\;\right]\theta(k,\xi)=0 \tag{5.5}$$

Our aim is to convert this relation between *F(k)* and *θ(k,ξ)* into an equation in *θ(k,ξ)*. But we notice that

$$\left[1-A\nu(k,\varepsilon)\;-\left(1-A\right)\nu(k,\varepsilon_m)\;\right]=0\;\;at\;\;k=0 \tag{5.6}$$

The zero of this function at *k=0* is of first order. Therefore *F(k)* can be a distribution [52] and is given by

$$F(k)+P\left[\frac{\left(\gamma_1^2-\gamma_{\infty}^2\nu(k,\varepsilon)\right)\theta(k,\xi)}{1-A\nu(k,\varepsilon)-\left(1-A\right)\nu(k,\varepsilon_m)}\right]\equiv\lambda\,\delta(k) \tag{5.7}$$

The alphabet *P* in front of the square bracket denotes the principle value of the terms inside and *λ* is an arbitrary constant. The above equation can be rewritten as

$$F(k)+\gamma_1^2\,\theta(k,\xi)\;+\;P\left[\frac{R(k)}{k}\right]\theta(k,\xi)\;\equiv\;\lambda\;\delta(k) \tag{5.8}$$

where *R(k)* is regular at *k=0* and is given by

$$\frac{R(k)}{k}=\frac{A\left(\gamma_1^2-\gamma_{\infty}^2\right)\nu(k,\varepsilon)+\left(1-A\right)\gamma_1^2\,\nu(k,\varepsilon_m)}{1-A\nu(k,\varepsilon)-\left(1-A\right)\nu(k,\varepsilon_m)} \tag{5.9}$$

Changing the variable in equation (5.8) to *k'*, multiplying by $\overline{\psi}(k-k',\xi)$ and integrating over *k'* we get

$$\theta(k,\xi)+\gamma_1^2\int_{-\infty}^{\infty}\overline{\psi}(k-k',\xi)\;\theta(k',\xi)\,dk' \tag{5.10}$$

$$+P\int_{-\infty}^{\infty}\overline{\psi}(k-k',\xi)\,\frac{R(k')}{k'}\,\theta(k',\xi)\,dk'=\lambda\,\overline{\psi}(k,\xi)$$

In obtaining this equation we have made use of the relation (2.14). To complete the derivation of the Fredholm integral equation we have to evaluate the constant, *λ*. So far we have not made use of the normalization condition of *f(x)*. Thus it is clear that λ is to be obtained using this condition. Taking the inverse transform of equation (5.8) we get

$$f(x)+\gamma_1^2\, f(x)\,\psi(x,\xi)+P\int_{-\infty}^{\infty}\exp(-ikx)\frac{R(k)}{k}\theta(k,\xi)\,dk=\lambda \tag{5.11}$$

Substituting for $\theta(k,\xi)$ from equation (2.8) we find

$$f(x)+\gamma_1^2\, f(x)\,\psi(x,\xi)+\frac{1}{2\pi}\int_{-\infty}^{\infty} f(y)\,\psi(y,\xi)\,Z(x-y)\,dy=\lambda \tag{5.12}$$

where

$$Z(x-y)=P\int_{-\infty}^{\infty}\exp[-ik(x-y)]\,\frac{R(k)}{k}\,dk \tag{5.13}$$

Since *R(k)* is analytic in the lower half of the complex plane, *Z(x-y)* can be evaluated easily using the residue theorem when *(x-y)>0.* Thus we get [52]

$$\begin{aligned} Z(x-y) &= -\pi\, i\, R(0)\ ,\ (x-y)>0 \\ &= -2\pi\ \frac{\left(\gamma_1^2-A\gamma_\infty^2\right)}{A\varepsilon+(1-A)\varepsilon_m}\ \equiv Q \end{aligned} \tag{5.14}$$

When *(x-y)< 0,* the poles of *R(k)* in the upper half of the complex plane also contribute to the integral. For our purpose it is sufficient to obtain the result (5.14). Equation (5.12) can now be rewritten as

$$\begin{aligned} & f(x)+\gamma_1^2\, f(x)\,\psi(x,\xi) \\ & +\frac{1}{2\pi}\,P\int_{x}^{\infty} f(y)\,\psi(y,\xi)\,Z(x-y)\,dy-Q\int_{-\infty}^{x} f(y)\,\psi(y,\xi)\,dy=\lambda \end{aligned} \tag{5.15}$$

Taking the limit $x\to\infty$ and using the normalization condition on *f (x)* we get

$$\lambda=1-\frac{Q}{2\pi}\int_{-\infty}^{\infty} f(y)\,\psi(y,\xi)\,dy=1-Q\ \theta(0,\xi) \tag{5.16}$$

Therefore equation (5.10) becomes

$$\begin{aligned} & \theta(k,\xi)+\gamma_1^2\int_{-\infty}^{\infty}\overline{\psi}(k-k',\xi)\ \theta(k',\xi)\,dk' \\ & +P\int_{-\infty}^{\infty}\overline{\psi}(k-k',\xi)\frac{R(k')}{k'}\theta(k',\xi)\,dk'=\left[1-Q\,\theta(0,\xi)\right]\overline{\psi}(k,\xi) \end{aligned} \tag{5.17}$$

If $\theta(0,\xi)$ is obtained from this equation, $I_{eff}(\xi)$ equals $2\,I_0\,\theta(0,\xi)$

Introduction of the arbitrary constant λ and the above method of determining it did not arise in earlier chapters. This happened because in evaluating the moderator collision integral in the narrow resonance approximation, we used the normalization condition on *f(x)* explicitly. The central point in the above derivation is the realization that *F(k)* is a distribution [52]. The steps involved in going from equation (5.5) to (5.7) are similar to those encountered in Case's method of solving plane geometry transport problems [53].

In the narrow resonance approximation to moderator collision integral $\varepsilon_m \to \infty$ and we have

(5.18) $$Lim\left(\varepsilon_m \to \infty\right) Q = 0$$

$$Lim\left(\varepsilon_m \to \infty\right) \nu\left(k, \varepsilon_m\right) = 0$$

Therefore *R(k)/k* becomes regular at *k=0* and we get back equation (2.15) of Chapter-II.

B Zero Temperature Limit:

In this limit equation (5.17) becomes

(5.19) $$\theta(k,\infty) + \frac{\gamma_1^2}{2}\int_{-\infty}^{\infty} \exp(-|k-k'|)\ \theta(k',\infty)\,dk'$$

$$+P\int_{-\infty}^{\infty} \exp(-|k-k'|)\ \frac{R(k')}{k'}\theta(k',\infty)\,dk' = \left[1 - Q\,\theta(0,\infty)\right]\frac{1}{2}\exp\left(-|k|\right)$$

In the following it will be shown that $\theta(k,\infty)$ satisfies a second order differential equation. Because of the presence of the principal value term we do not use the fact that *½ exp (-| k –k'|)* is the Green's function of the operator *(d^2/dk^2-1)*. For $k>\tau$, a small positive constant, equation (5.10) can be written as

(5.20) $$\theta(k,\infty) + \int_{-\infty}^{-\tau} \frac{1}{2}\ \frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk'$$

$$+P\int_{-\tau}^{+\tau} \frac{1}{2}\ \frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk'$$

$$+\int_{\tau}^{k} \frac{1}{2}\ \frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk'$$

$$+\int_{k}^{\infty} \frac{1}{2}\ \frac{R^*(k')}{k'}\exp(k-k')\ \theta(k',\infty)\,dk'$$

$$= \left[1 - Q\,\theta(0,\infty)\right]\frac{1}{2}\exp\left(-k\right)$$

For brevity we have used the notation,

(5.21) $$\frac{R^*(k)}{k} = \frac{R(k)}{k} + \gamma_1^2$$

Differentiating equation (5.20) with respect to *k* we get

$$
\begin{aligned}
(5.22)\qquad & \frac{d}{dk}\theta(k,\infty) - \int_{-\infty}^{-\tau} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk' \\
& - P\int_{-\tau}^{+\tau} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk' \\
& - \int_{\tau}^{k} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk' \\
& + \int_{k}^{\infty} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(k-k')\ \theta(k',\infty)\,dk' \\
& = -\left[1-Q\,\theta(0,\infty)\right]\frac{1}{2}\exp(-k)
\end{aligned}
$$

Differentiating with respect to k again and using equation (5.20) we get

$$
(5.23)\qquad \frac{d^2}{dk^2}\theta(k,\infty) - \left[\frac{R(k)}{k} + \beta_1^2\right]\theta(k,\infty) = 0\ ,\ \ k>0
$$

Here $\beta_1^2 = 1+\gamma_1^2$. When $k<-\tau$, equation (5.19) can be written as

$$
\begin{aligned}
(5.24)\qquad & \theta(k,\infty) + \int_{-\infty}^{k} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk' \\
& + \int_{k}^{-\tau} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(k-k')\ \theta(k',\infty)\,dk' \\
& + P\int_{-\tau}^{+\tau} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk' \\
& + \int_{\tau}^{\infty} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(k-k')\ \theta(k',\infty)\,dk' \\
& = \left[1-Q\,\theta(0,\infty)\right]\frac{1}{2}\exp(k)
\end{aligned}
$$

Differentiating with respect to k we get

$$
\begin{aligned}
(5.25)\qquad & \frac{d}{dk}\theta(k,\infty) - \int_{-\infty}^{k} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(-k+k')\ \theta(k',\infty)\,dk' \\
& + \int_{k}^{-\tau} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(k-k')\ \theta(k',\infty)\,dk' \\
& + P\int_{-\tau}^{+\tau} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(k-k')\ \theta(k',\infty)\,dk' \\
& + \int_{\tau}^{\infty} \frac{1}{2}\,\frac{R^*(k')}{k'}\exp(k-k')\ \theta(k',\infty)\,dk' \\
& = \left[1-Q\,\theta(0,\infty)\right]\frac{1}{2}\exp(k)
\end{aligned}
$$

Differentiating with respect to k again,

$$\frac{d^2}{dk^2}\theta(k,\infty)-\left[\frac{R(k)}{k}+\beta_1^2\right]\theta(k,\infty)=0\ ,\quad k<0 \tag{5.26}$$

Thus, $\theta(k,\infty)$ satisfies the same differential equation for the positive and negative halves of the real axis.

The boundary conditions (2.27) and (2.28) on $\theta(k,\infty)$ are applicable here also. In order to solve the above boundary value problem, one more condition on at *k=0* is required. Putting $k=+\tau$ and $-\tau$ respectively in equations (5.22) and (5.25) and subtracting the resulting equations we get

$$\begin{aligned}
&\left.\frac{d\theta}{dk}\right|_{-\tau}-\left.\frac{d\theta}{dk}\right|_{+\tau} \\
&-\int_{-\infty}^{-\tau}\frac{1}{k'}\left[R^*(-k')\,\theta(-k',\infty)-R^*(k')\,\theta(k',\infty)\right]\frac{1}{2}\exp(-\tau+k')\ dk' \\
&-\int_{-\tau}^{+\tau}\frac{1}{k'}\left[R^*(-k')\,\theta(-k',\infty)-R^*(k')\,\theta(k',\infty)\right]\frac{1}{2}\exp(-\tau+k')\ dk' \\
&-\int_{+\tau}^{\infty}\frac{1}{k'}\left[R^*(-k')\,\theta(-k',\infty)-R^*(k')\,\theta(k',\infty)\right]\frac{1}{2}\exp(\tau-k')\ dk' \\
&=\ \left[1-Q\,\theta(0,\infty)\right]\frac{1}{2}\exp(\tau)
\end{aligned} \tag{5.27}$$

In the limit $\tau\to 0$, the integral terms in the above equation cancel out and we get

$$\left.\frac{d\theta}{dk}\right|_{-\tau}-\left.\frac{d\theta}{dk}\right|_{+\tau}=\left[1-Q\,\theta(0,\infty)\right] \tag{5.28}$$

This completes the derivation of the differential equation and the boundary conditions. When $\varepsilon_m\to\infty$ equation (5.28) reduces to (2.29) obtained in Chapter-II.

The origin *k=0* is a regular singular point of the differential equations (5.23) and (5.26) [68]. Further, the singularity is of first order. Therefore both the independent solutions of the differential equations are regular at *k=0* [68]. Methods for solving these equations to evaluate the resonance integral have not been developed completely and will not be presented here.

D. Summary

In this Chapter we generalized the Fourier transform method relaxing the assumption of narrow resonance approximation to the moderator collision integral. The initial value problem posed by the homogenous equation (5.1) and the normalization condition on *f(x)* has been reduced to a boundary value problem in the Fourier transform space. This reduction removes the discontinuous nature of the kernel of the integral equation for *f(x)*. In this process we found it necessary to make use of elementary ideas from the theory of distributions [52]. In the zero temperature limit we reduced the problem to solving a second order differential equation.

Conclusions

The phenomenon of resonance absorption plays a crucial role in determining the criticality, conversion ratios and the reactivity coefficients of nuclear reactor systems. Thus it has been the subject of many investigations in the past. Essentially the problem involves the solution of the integral equation of neutron slowing down theory when the parameters of the equation, namely the cross-sections, are given by the Doppler broadened Breit-Wigner formulae. In these investigations the quantity of direct physical interest is not the detailed solution but an integral parameter called the resonance integral which determines the total absorption rate in the resonance.

Because of the doubly discontinuous nature of the kernel of the slowing down equation and the complicated form of the Doppler broadened cross-sections (only the integral representations being available) it is generally not possible to use the analytical methods for solving this problem. Recourse has therefore to be made to the numerical methods. However there are several questions for which numerical methods are inappropriate, for example, the assessment of the errors in Doppler coefficient computations due to the neglect ion of the overlapping of neighboring resonances. Further, the analytical methods throw greater light on the basic structure of the equation. Our aim in this thesis has been to study as to how far the standard techniques of applied Mathematics can be used to obtain the solution of this problem.

We have seen that by using the Fourier transforms the slowing down equation can be converted into an integral equation with continuous kernel – in fact a Fredholm integral equation over the interval $(-\infty,\infty)$. Further the cross-sections have simple analytical representations in the Fourier space. Lastly, the Fourier transform can be so defined as to directly give the resonance integral, being the value at the origin, thus avoiding the need of later evaluation of a linear functional of the solution vector. The use of Fourier transforms thus provides an opportunity to analytically solve some of the resonance absorption problems.

The three Chapters (Chapter-II to IV) of this thesis have been devoted to the evaluation of resonance integrals analytically as far as possible. Thus we have found that at zero temperature the problem can be reduced to the solution of a second order differential equation which can be solved by the WKB method. We have thus derived accurate expressions for the zero temperature resonance integrals. Various complications like resonance potential interference scattering or the overlap of neighboring resonances pose further difficulties, as in other methods, but are not insurmountable. At higher temperatures, for evaluating Doppler coefficients, we have to solve the Fourier transformed integral equation itself. Here we observed that the corrections due to higher temperatures, that is, those related to the Doppler coefficients, can be obtained by the use of Gauss-Hermite quadratures for solving the integral equation. Again various complications pose further problems but they can all be accounted for in a successful manner.

In the last Chapter we have studied the use of Fourier transforms for solving the homogenous form of the integral equation of slowing down theory. As is well known the integral transforms are generally used for solving inhomogeneous equations. However we have seen that in this case the Fourier transformed solution is a distribution in the sense of Schwarts and that the normalization condition determines the singular part of this distribution. The regular part of this distribution is thus determined by solving an inhomogeneous equation whose free term is determined by the singular part, that is, the normalization condition.

In conclusion, therefore, we have seen that the use of some standard techniques of applied Mathematics like Fourier transforms WKB method and Gauss-Hermite quadratures can be profitably used to analytically solve some resonance absorption problems. We believe that this is a common occurrence and that classical methods with slight modifications can profitably be used to study many useful problems of reactor physics and other practical subjects.

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APPENDIX–I

The integrals required for the evaluation of the zero temperature resonance integrals are

(I.1) $$I_n(c)=\int_0^\infty e^{-k}\,\nu^n\left(k,\varepsilon\right)dk \ \ , \ \ n=1,2,3$$

(I.2) $$V_{nm}(c)=\int_0^\infty \nu^n\left(k,\varepsilon\right)\int_k^\infty e^{-k'}\,\nu^n\left(k',\varepsilon\right)\,,\ (n,m)=(1,1),\ (1,2),\ (2,1)$$

The real and imaginary parts of $I_n(c)$ are given by

(I.3) $$RI_n(c)=\int_0^\infty e^{-k}\left[\frac{\sin(ck/2)}{ck/2}\right]^n\cos(nck/2)dk$$

(I.4) $$II_n(c)=\int_0^\infty e^{-k}\left[\frac{\sin(ck/2)}{ck/2}\right]^n\sin(nck/2)dk$$

These integrals can be evaluated analytically. For instance, consider $RI_1(c)$ given by

(I.5) $$c\,RI_1(c)=\int_0^\infty e^{-k}\ \frac{\sin(ck/2)}{k/2}\ \cos(ck/2)dk$$

$$=\int_0^\infty e^{-k}\,\frac{\sin(ck)}{k}\ dk$$

Differentiating with respect to c, we get

(I.6) $$\frac{d}{dc}\left[c\,RI_1(c)\right]=\int_0^\infty e^{-k}\ \cos(ck)dk\ =\frac{1}{1+c^2}$$

Now integrating with respect to c, and noting that $c\,RI_1(c)=0$ at $c=0$, we get

(I.7) $$c\,RI_1(c)=\int_0^c\frac{1}{1+c'^2}\,dc'=\ \tan^{-1}(c)$$

Thus we find

(I.8) $$RI_1(c)=\frac{1}{c}\tan^{-1}(c)$$

Proceeding exactly in the same way we find

(I.9) $$II_1(c)=\frac{1}{2c}\ln\left(1+c^2\right)$$

For $n=2$, one of the integrals to be evaluated is

(I.10) $$RI_2(c) = \int_0^\infty e^{-k} \left[\frac{\sin(ck/2)}{k/2}\right]^2 \left[2\cos(ck/2) - 1\right] dk$$

$$= \frac{2}{c^2} J_1(c) - \frac{1}{(c/2)^2} J_1(c/2)$$

where

(I.11) $$J_1(c) = \int_0^\infty e^{-k} \left[\frac{\sin(ck)}{k}\right]^2 dk$$

Differentiating with respect to c

(I.12) $$\frac{d}{dc} J_1(c) = \int_0^\infty e^{-k}\ 2\frac{\sin(ck)}{k}\ \cos(ck) dk = \tan^{-1}(2c)$$

where we have used equations (I.5) and (I.7). Integrating equation (I.12) with respect to c, and noting that $J_1(c) = 0$ at $c = 0$, we get

(I.13) $$J_1(c) = c\ \tan^{-1}(2c) - \frac{1}{4}\ln(1 + 4c^2)$$

Therefore $RI_2(c)$ becomes

(I.14) $$RI_2(c) = \frac{2}{c}\ \tan^{-1}\left[\frac{c}{1+2c^2}\right] = \frac{1}{2c^2}\ln\left[\frac{1+4c^2}{(1+c^2)^2}\right]$$

The other integral for $n=2$ is given by

(I.15) $$II_2(c) = \frac{1}{(c/2)^2}\ J_2(c/2)$$

where

(I.16) $$J_2(c) = \int_0^\infty e^{-k} \left[\frac{\sin(ck)}{k}\right]^2 \sin(2ck)\ dk$$

Differentiating with respect to c

(I.17) $$\frac{d}{dc} J_2(c) = 2\left[K_1(2c) - K_1(c)\right]$$

where $K_1(c)$ is given by

(I.18) $$K_1(c) = \int_0^\infty e^{-k}\ \frac{\sin^2(ck)}{k}\ dk$$

Now, dK_1/dc is found to be

(I.19) $$\frac{d}{dc} K_1(c) = 2\int_0^\infty e^{-k} \sin(ck)\ \cos(ck)\ dk = \frac{2c}{1+4c^2}$$

Since $K_1(c)=0$ at $c=0$, we get

$$K_1(c)=\frac{1}{4}\ln\left(1+4c^2\right) \tag{I.20}$$

Therefore equation (I.17) becomes

$$\frac{d}{dc}J_2(c)=\frac{1}{2}\ln\left(1+16c^2\right)-\frac{1}{2}\ln\left(1+4c^2\right) \tag{I.21}$$

Integrating with respect to c, using the result $J_2(c)=0$ at $c=0$ and equation (I.15) we get

$$II_2(c)=\frac{1}{c}\ln\left[\frac{1+4c^2}{1+c^2}\right]-\frac{1}{c^2}\tan^{-1}\left[\frac{2c^3}{1+3c^2}\right] \tag{I.22}$$

Proceeding along these lines $RI_3(c)$ and $II_3(c)$ can be evaluated. Final results are:

$$RI_3(c)=\frac{3}{2c^2}\left[\frac{\left(9c^2-1\right)}{3}\tan^{-1}(3c)-\left(4c^2-1\right)\tan^{-1}(2c)+\left(c^2-1\right)\tan^{-1}(c)\right]$$
$$+\frac{3}{2c^2}\ln\left[\frac{\left(1+4c^2\right)^2}{\left(1+9c^2\right)\left(1+c^2\right)}\right] \tag{I.23}$$

$$II_3(c)=\frac{3}{4c^2}\left[\frac{\left(9c^2-1\right)}{3}\ln\left(1+9c^2\right)-\left(4c^2-1\right)\ln\left(1+4c^2\right)+\left(c^2-1\right)\ln\left(1+c^2\right)\right]$$
$$\frac{3}{c^2}\left[\tan^{-1}(3c)-2\tan^{-1}(2c)+\tan^{-1}(c)\right] \tag{I.24}$$

Real part of the double integral $V_{11}(c)$ is

$$c^2\,RV_{11}(c)=\int_0^\infty\frac{\sin(ck)}{k}dk\int_k^\infty e^{-k'}\,\frac{\sin(ck')}{k'}\,dk'$$
$$-\int_0^\infty\frac{1-\cos(ck)}{k}dk\int_k^\infty e^{-k'}\,\frac{1-\cos(ck')}{k'}\,dk' \tag{I.25}$$

Now, consider the integral

$$J_1(c,k)=\int_k^\infty e^{-k'}\,\frac{\sin(ck')}{k'}\,dk' \tag{I.26}$$

Differentiating with respect to c we get

$$\frac{d}{dc}J_1(c,k)=\int_k^\infty e^{-k'}\,\cos(ck')\,dk' \tag{I.27}$$

On integration by parts we find

$$\frac{d}{dc}J_1(c,k)=e^{-k}\left[\cos(ck)-c\times\sin(ck)\right]-c^2\frac{d}{dc}J_1(c,k) \tag{I.28}$$

Since $J_1(c)=0$ at c$=0$, we get

$$J_1(c,k)= e^{-k}\int_0^c \frac{\cos(c'k)-c'\times\sin(c'k)}{1+c'^{\,2}} \tag{I.29}$$

Proceeding exactly in the same way we can show that

$$J_2(c,k)=\int_k^\infty e^{-k'}\,\frac{1-\cos(ck')}{k'}\,dk' \tag{I.30}$$

$$= e^{-k}\int_0^c \frac{\sin(c'k)-c'\times\cos(c'k)}{1+c'^{\,2}}$$

Therefore equation (I.25) becomes

$$c^2\,RV_{11}(c)= \int_0^c \frac{dc'}{1+c'^{\,2}}\left[\int_0^\infty e^{-k}\left\{\frac{\sin(c'+c)k}{k}-\frac{\sin(c'k)}{k}\right\}dk\right. \tag{I.31}$$

$$\left.-\;c'\int_0^\infty e^{-k}\left\{\frac{\sin(c'k)\,\sin(ck)}{k}+\frac{1-\cos(ck)}{k}\cos(c'k)\right\}dk\right]$$

The first integral in the square bracket can be evaluated using equations (I.5) and (I.7). The other integrals can be shown to be

$$K_1(c,c')\;=\int_0^\infty e^{-k}\,\frac{\sin(c'k)\,\sin(ck)}{k}\,dk \tag{I.32}$$

$$=\ln\left[\frac{1+(c+c')^2}{1+(c-c')^2}\right]$$

$$K_2(c,c')\;=\int_0^\infty e^{-k}\,\frac{1-\cos(ck)}{k}\;\;\cos(ck)dk \tag{I.33}$$

$$=\frac{1}{4}\ln\left[\left\{1+(c+c')^2\right\}\left\{1+(c-c')^2\right\}\right]-\frac{1}{2}\ln\left(1+c'^{\,2}\right)$$

The steps involved in getting these results are as given earlier. Therefore equation (I.31) becomes

$$c^2\,RV_{11}(c)= \int_0^c \frac{dc'}{1+c'^{\,2}}\left[\tan^{-1}(c+c')-\frac{c'}{2}\ln\left(1+c+c'^{\,2}\right)\right] \tag{I.34}$$

$$-\int_0^c \frac{dc'}{1+c'^{\,2}}\left[\tan^{-1}(c')+\frac{c'}{2}\ln\left(1+c'^{\,2}\right)\right]$$

The last integration can be performed and we get

(I.35)
$$RV_{11}(c)=\frac{1}{c^2}\left[\int_0^c \frac{dc'}{1+c'^2}\left\{\tan^{-1}(c+c')-\frac{c'}{2}\ln\left(1+c+c'^2\right)\right\}\right]$$
$$-\frac{1}{2c^2}\left[\left(\tan^{-1}c\right)^2-\left\{\frac{1}{2}\ln\left(1+c'^2\right)\right\}\right]$$

Thus we have reduced the double integral to a single integral. Imaginary part of $V_{11}(c)$ is given by

(I.36)
$$IV_{11}(c)=\int_0^\infty \frac{\sin(ck)}{k}dk\int_k^\infty e^{-k'}\frac{1-\cos(ck')}{c\,k'}dk'$$
$$+\int_0^\infty \frac{1-\cos(ck)}{k}dk\int_k^\infty e^{-k'}\frac{\sin(ck')}{k'}dk'$$

Proceeding along the lines given earlier, it can be reduced to the form

(I.37)
$$IV_{11}(c)=\frac{1}{c^2}\int_0^c \frac{dc'}{1+c'^2}\left[\frac{1}{2}\ln\left\{\frac{1+c+c'^2}{1+c'^2}\right\}+c'\tan^{-1}\left\{\frac{c}{1+c'(c+c')}\right\}\right]$$

The integrals in equations (I.35) and (I.37) have to be evaluated numerically. It was not possible to simplify $V_{12}(c)$ and $V_{21}(c)$. In the calculations they were evaluated using Simpson’s rule.

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APPENDIX–II

Parameters of U^{238} Resonances

E_r (eV)	Γ_n (eV)	Γ_r (eV)	σ_0 (barns)
6.68	0.0015	0.025	22058.9
21.0	0.0089	0.025	32545.1
36.8	0.034	0.025	40765.6
66.3	0.018	0.025	16436.3
81.1	0.002	0.025	2377.7
102.8	0.067	0.025	18442.0
116.8	0.014	0.025	8000.8
192.0	0.140	0.025	11600.0
209.0	0.060	0.025	8792.3
238.0	0.028	0.025	5778.6

1. Statistical spin factor = 1
2. Potential scattering cross-section = 10 barns
3. Scattering cross-section of hydrogen = 20.2 barns

Parameters of Th^{232} Resonances

E_r (eV)	Γ_n (eV)	Γ_r (eV)	σ_0 (barns)
21.8	0.0021	0.0245	9427.5
23.47	0.004	0.0245	15567.4

4. Statistical spin factor = 1
5. Potential scattering cross-section = 10 barns

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