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INTERMEDIATE RESONANCE ABSORPTION*

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INTRODUCTION

The difficulty of obtaining an exact analytical solution to the equations for the slowing down of neutrons has lead to a number of approximate solutions to the problem. Historically, the narrow resonance (NR) and wide resonance (WR) approximations were the initial attempts at approximate analytical solutions. Improvements to these first approximations were later made (1) by iterating them in the basic integral equation.

The choice between these limiting approximations has been to some extent arbitrary. In some cases a choice is actually difficult to make. To overcome these difficulties, the intermediate resonance (IR) approximation was born (2). Here, a parameter which characterizes all intermediate situations, including the limiting NR and WR extremes, is introduced. Analytic approximation techniques such as a variational principle or successive approximation are employed in order to determine the value of the parameter for each particular situation. Once the formulae for the intermediate parameter have been obtained, one need no longer guess as to whether a resonance is wide or narrow.

Just as the wide resonance approximation originally appeared to be the most appropriate to treat the important low energy resonances in heavy absorbers, the narrow resonance approximation has been most useful in treating the moderator scattering. However, for these same low energy wide resonances, it now appears that the NR approach is not always an accurate characterization of the moderator scattering.

The ultimate generalization of the IR approach is to introduce parameters for all scattering species present in the

system. One then solves a coupled set of equations for the parameters in terms of the characteristics of the system. This approach has yielded results for homogeneous systems which are in excellent agreement with numerical solutions to the equations (3,4).

The extension of the IR formulation to non-zero temperatures may be accomplished by the use of the zero temperature parameters in a temperature dependent resonance integral formulation. The validity of such an approach has been borne out by numerical calculations (4,5).

For nonhomogeneous systems, the spatial complications can be avoided by the use of certain "equivalence relationships" (6). However, accompanying these simplifications are additional approximations necessary for the equivalence to apply. The treatment of the scattering by the moderator outside the absorbing lump is slightly more complicated. Again the standard NR treatment may be inaccurate. Furthermore, for certain systems the removal of this approximation is quite important. A first approximation may be obtained by assuming spatially flat fluxes; the outside moderator scattering is then easily treated in the IR approach (7). But the resulting equations show that equivalence in the standard sense does not hold.

THE IR APPROXIMATION

Consider, initially, the case of a space- and time-dependent system consisting of a homogeneous mixture of a resonance absorber and a non-absorbing moderator at zero temperature. We neglect the interference between the resonance and potential scattering of the absorber and assume that the resonance is far enough below all sources and other resonances that the flux has achieved its asymptotic form before entering the resonance region of interest. The asymptotic flux per unit

lethargy above the resonance is normalized to unity.

$$\lim_{u \rightarrow -\infty} \Psi(u) = 1 \quad (1)$$

If we characterize the slowing down due to the moderator in an NR approximation, then the major contribution to the resonance flux from moderator scatterings comes from off-resonance, where Ψ is unity. Let K_m denote the moderator slowing down operator; then in the NR approximation

$$K_m \sigma_m \Psi = \sigma_m \int_{u-\Delta_m}^u du' \frac{e^{-(u-u')}}{1-\alpha_m} \Psi(u') \xrightarrow{\text{NR}} \sigma_m, \quad (2)$$

where σ_m is the constant moderator scattering per absorber atom.

We write the balance equation between removals due to absorptions and scatterings out of a lethargy interval and sources due to scattering into the interval. The result is an inhomogeneous integral equation in which σ_m acts like a source.

$$(\sigma_m + \sigma) \Psi = \sigma_m + K \sigma_s \Psi \quad (3)$$

or

$$H \Psi = \sigma_m, \text{ where } H = \sigma_m + \sigma - K \sigma_s \quad (4)$$

Here, K is the absorber slowing down operator, σ_s is the total scattering (resonance plus potential) of the absorber and $\sigma = \sigma_a + \sigma_s$.

If one is primarily interested in a weighted average of the unknown flux, such as a resonance integral, then a variational principle is a particularly convenient method for obtaining such an average.

Consider the adjoint problem

$$H^+ \phi = \sigma_a \quad (5)$$

and define the scalar product

$$(\sigma_a, \Psi) = \int \sigma_a \Psi \, du \quad (6)$$

The functional F below (among others) has the property of being stationary about the resonance integral (6) of interest.

$$F(\Psi, \phi) = (\sigma_a, \Psi) + (\phi, \sigma_m) - (\phi, H\Psi) \quad (7)$$

In practical terms this means that calculations of the resonance integral will be accurate to second order when the solutions to Eqs. (4) and (5) are known only to first order. Of course, the better the trial functions that are used in (7) represent the real solution, the better will be the results for the resonance integral. The remaining question then is to determine appropriate trial functions.

For this purpose we examine the basic equation (4) (in particular, the absorber slowing down integral) in some limiting cases. In the absorber NR limit the assumption is that the resonance is so narrow that the main contribution to the resonance integral comes from slowing down from far above the resonance. Here, $\sigma_s = \sigma_p$ (σ_p is the constant potential scattering of the absorber) and $\Psi = 1$. Thus, if in the absorber slowing down term

$$K\sigma_s \Psi = \int_{u-\Delta}^u du' \frac{e^{-(u-u')}}{1-\alpha} \sigma_s(u') \Psi(u') ; \quad \Delta = \ln \frac{1}{\alpha} \quad (8)$$

we replace $\sigma_s \Psi$ by σ_p , the result is $K\sigma_{s \text{ NR}} \Psi \rightarrow \sigma_p$, since the remaining integral is unity. In the WR limit, the resonance

is taken to be so wide that $\sigma_s \Psi$ is assumed to be slowly varying with respect to $e^{-(u-u')}$ over the integration range Δ . Therefore, we may remove $\sigma_s \Psi$ from the integration to obtain $K\sigma_s \Psi \rightarrow \sigma_s(u) \Psi(u)$. We write, consequently,

$$K\sigma_s \Psi = \lambda \sigma_p + (1-\lambda) \sigma_s \Psi. \quad (9)$$

The parameter λ characterizes the slowing down operator K for the absorber. In the one extreme, $\lambda = 0$, we have the WR result, and in the other extreme, $\lambda = 1$, we have the NR result. Substituting (9) into (3), we obtain

$$\Psi_\lambda = \frac{\sigma_m + \lambda \sigma_p}{\sigma_m + \sigma_a + \lambda \sigma_s} \quad (10)$$

as the trial function which gives the correct limiting solutions to the basic equation (3) for $\lambda = 0$ or 1.

Using a similar approach for the adjoint problem, one may then proceed to use the variational principle to determine the intermediate parameters and thence the resonance integrals of interest. The solutions for the parameters thus characterize all situations intermediate between the narrow and wide resonance extremes.

Another convenient method for finding approximate solutions to Eq. (3) is the iterative approach. By iterating on lower order solutions, one obtains higher order solutions to the integral equation

$$\Psi^{(n+1)} = \frac{1}{\sigma_m + \sigma} \left(\sigma_m + K\sigma_s \Psi^{(n)} \right). \quad (11)$$

The convergence of this equation means that the result is eventually independent of the initial trial function. However,

as the iterated integrals in Eq. (11) become increasingly complex, the formal approach of continued iteration is not necessarily the most practical. We avoid this problem by using the trial function (10) in Eq. (11) to calculate the iterate $\psi_\lambda^{(2)}$. Then by evaluating the first and second order resonance integrals as functions of λ , we determine λ by requiring that these successive iterates be equal. The basis for this approximation is that it is a necessary (though, of course, not sufficient) condition for an exact solution to Eq. (11). Once one has the λ from this successive approximation approach, the resonance integral may be calculated directly from Eq. (6).

It turns out that the successive approximation approach gives analytic results which are somewhat simpler in form than the variational results; yet the numerical results of the two methods seem to agree quite well. One of the reasons for the good numerical agreement between the iterative procedure and the perhaps more mathematically sound variational principle, is the good choice of initial trial functions that was made. This is borne out by the mathematical investigation given in reference (8).

Having established the IR method for the absorber scattering, the next logical step would be to apply the same procedure to the moderator scattering. By introducing a parameter κ to represent the moderator slowing down, we have

$$K_{m m} \psi = \kappa \sigma_m + (1-\kappa) \sigma_m \psi. \quad (12)$$

Using this as the moderator scattering source in Eq. (3), instead of σ_m , we obtain

$$\psi_{\kappa \lambda} = \frac{\kappa \sigma_m + \lambda \sigma_p}{\kappa \sigma_m + \sigma_a + \lambda \sigma_s} \quad (13)$$

By iterating on this first order solution one now obtains a pair of coupled equations for the IR parameters κ and λ in terms of the resonance characteristics. These equations may

be solved easily by numerical iteration (3). The method may be generalized to the case of several scatterers and absorbers.

The IR method may also be used for the temperature dependent case. Numerical calculations (4,5) have revealed that good results may be obtained with the use of the zero-temperature intermediate parameters. By use of these, the Doppler-broadened resonance integrals may be written in terms of tabulated J-functions as

$$I_{\kappa\lambda}(\theta) = \frac{\sigma_o \Gamma_\gamma}{E_r} \gamma_{\kappa\lambda} J(\theta, \gamma_{\kappa\lambda}) , \quad (14)$$

where

$$\gamma_{\kappa\lambda} = \frac{\kappa\sigma_m + \lambda\sigma_p}{\sigma_o} \frac{\Gamma}{\Gamma_\gamma + \lambda\Gamma_n} \quad (15)$$

In Eq. (14) the temperature dependent quantity θ and the integral J are as defined in reference (9), except that the β there (which equals our γ_{11} -the NR case) is to be replaced by the more general $\gamma_{\kappa\lambda}$ for the IR case.

Although good values for Doppler-broadened resonance integrals may be obtained in this fashion, the theory of temperature dependence used here is probably too simple to give very accurate values for the Doppler coefficients. A generally more rigorous approach would require the use of the temperature dependent intermediate parameters and this would probably entail a semi-analytic or numerical solution to the temperature dependent equations.

NONHOMOGENEOUS SYSTEMS

The extension of the IR formulation to nonhomogeneous systems requires the consideration of the spatially dependent slowing down equations. Consider the integral form of the transport equation under the assumption of isotropic scattering in the laboratory system:

$$\begin{aligned} \phi_o(\vec{r}, u) = & \int_{V_o} d\vec{r}' P(\vec{r}' \rightarrow \vec{r}; u) \int du' \phi_o(\vec{r}', u') \left[\Sigma_m K_m(u' \rightarrow u) + \Sigma_s(u') K_o(u' \rightarrow u) \right] \\ & + \int_{V_1} d\vec{r}' P(\vec{r}' \rightarrow \vec{r}; u) \int du' \phi_1(\vec{r}', u') \Sigma_1 K_1(u' \rightarrow u) , \quad (16) \end{aligned}$$

where $K(u' \rightarrow u)$ is the probability that a neutron with lethargy u' will be slowed down into lethargy u within du , $P(\vec{r}' \rightarrow \vec{r}; u)$ is the probability that a neutron which is scattered isotropically at $\vec{r}'$ into lethargy u will reach the point $\vec{r}$ without an intervening collision, and the subscripts $o, 1$ and m correspond to the absorbing lump, the non-absorbing moderator outside the lump and the moderator admixed with the absorber, respectively.

There is a similar equation for the moderator flux and the fluxes are normalized to unity far above the resonance.

$$\lim_{u \rightarrow -\infty} \phi_{o,1} = 1 \quad (17)$$

Equation (16) simplifies considerably in the NR and WR limits. By writing the limiting equations in terms of the intermediate parameters κ , λ and $\bar{\mu}$ for the admixed moderator, absorber and outside moderator, respectively, we obtain

$$\begin{aligned}
\phi_o(\vec{r}, u) = & \bar{\mu} P_o(\vec{r}, u) + \frac{\kappa \Sigma_m + \lambda \Sigma_p}{\Sigma_o} (1 - P_o(\vec{r}, u)) \\
& + \left[(1 - \kappa) \Sigma_m + (1 - \lambda) \Sigma_s(u) \right] \int_{V_o} d\vec{r}' \phi_o(\vec{r}', u) P(\vec{r}' \rightarrow \vec{r}; u) + (1 - \bar{\mu}) \Sigma_1 \int_{V_1} d\vec{r}' \phi_1(\vec{r}', u) \cdot \\
& \cdot P(\vec{r}' \rightarrow \vec{r}; u), \quad (18)
\end{aligned}$$

where $P_o(\vec{r}, u)$ is the probability of escape from the lump for a unit isotropic source of lethargy u at the point $\vec{r}$, and $\Sigma_o = \Sigma_a + \Sigma_s + \Sigma_m$. Defining the volume averaged flux and escape probability for the lump as

$$\bar{\phi}_o(u) = \frac{1}{V_o} \int_{V_o} d\vec{r} \phi_o(\vec{r}, u) \quad \text{and} \quad \bar{P}_o(u) = \frac{1}{V_o} \int_{V_o} d\vec{r} P_o(\vec{r}, u) \quad (19)$$

and averaging Eq. (18) over the lump, we obtain

$$\begin{aligned}
\left[\sigma_a(u) + \kappa \sigma_m + \lambda \sigma_s(u) \right] \bar{\phi}_o = & \bar{\mu} \sigma_o \bar{P}_o + (\kappa \sigma_m + \lambda \sigma_p) (1 - \bar{P}_o) \\
& - \left[(1 - \kappa) \sigma_m + (1 - \lambda) \sigma_s \right] M_o + (1 - \bar{\mu}) \sigma_1 M_1, \quad (20)
\end{aligned}$$

where

$$\begin{aligned}
\sigma_m = \Sigma_m / N_o, \quad \sigma_1 = \Sigma_1 V_1 / N_o V_o \quad \text{and} \\
M_i = \frac{1}{V_i} \int_{V_i} d\vec{r} \phi_i(\vec{r}, u) P_i(\vec{r}, u) \quad \text{for } i \text{ equal to } o \text{ or } 1. \quad (21)
\end{aligned}$$

The corresponding equation for the volume averaged moderator flux $\bar{\phi}_1$ is

$$\begin{aligned}
\bar{\mu} \sigma_1 \bar{\phi}_1 - \bar{\mu} \sigma_1 (1 - \bar{P}_1) - (\kappa \sigma_m + \lambda \sigma_p) \frac{\sigma_1 \bar{P}_1}{\sigma_o} = \\
\left[(1 - \kappa) \sigma_m + (1 - \lambda) \sigma_s \right] M_o - (1 - \bar{\mu}) \sigma_1 M_1 \quad (22)
\end{aligned}$$

We substitute Eq. (22) into Eq. (20) to eliminate the integrals M_i and making use of the reciprocity theorem in the form

$$\Sigma_1 V_1 \bar{P}_1 = \Sigma_0 V_0 \bar{P}_0 \text{ or } \sigma_1 \bar{P}_1 = \sigma_0 \bar{P}_0, \text{ we obtain}$$

$$(\sigma_a + \kappa\sigma_m + \lambda\sigma_s) \bar{\phi}_0 = \kappa\sigma_m + \lambda\sigma_p + \bar{\mu}\sigma_1(1-\bar{\phi}_1) \quad (23)$$

Equations (20) and (23) now form our basic equations. Note that thus far no spatial approximation has been made.

If we assume that the flux in the lump and the moderator is spatially flat ($\phi_i = \bar{\phi}_i$), then the integrals M_i become $\bar{\phi}_i \bar{P}_i$ and the equations simplify. In addition we approximate the average escape probability $\bar{P}_0$ by the rational form

$$\bar{P}_0 = \frac{s}{s+\sigma_0}, \quad (24)$$

where $s = a(1-C)/N_0 \bar{l}_0$, C is the Dancoff factor for the lattice and $\bar{l}_0$ is the mean chord length of the lump, modified by the factor a to bring (24) in better agreement with the exact escape probability. With these approximations applied to Eqs. (20) and (23), the average lump flux becomes

$$\bar{\phi}_0(u) = \frac{\kappa\sigma_m + \lambda\sigma_p + \mu s}{\kappa\sigma_m + \sigma_a + \lambda\sigma_s + \mu s} = \frac{1 + x^2}{\beta_{\kappa\lambda\mu}^2 + x^2}; \quad x = \frac{2}{\Gamma} (E - E_r) \quad (25)$$

where

$$\beta_{\kappa\lambda\mu}^2 = 1 + \frac{\sigma_0}{\kappa\sigma_m + \lambda\sigma_p + \mu s} \frac{\Gamma_\gamma + \lambda\Gamma_n}{\Gamma} \quad \text{and} \quad (26)$$

$$\mu = \frac{\bar{\mu}}{\bar{\mu} + (1-\bar{\mu})s/\sigma_1}. \quad (27)$$

If one proceeds by equating successive orders of resonance integrals as a means of determining the IR parameters, then they are solutions to the following coupled set of equations:

$$\begin{aligned}
 \kappa &= 1 - X_{\kappa\lambda\mu}^{(m)} \\
 \lambda &= 1 - X_{\kappa\lambda\mu}^{(o)} \\
 \bar{\mu} &= 1 - X_{\kappa\lambda\mu}^{(1)}
 \end{aligned} \tag{28}$$

where

$$\begin{aligned}
 X_{\kappa\lambda\mu}^{(i)} &= \frac{1}{x_{\kappa\lambda\mu}^{(i)}} \tan^{-1} x_{\kappa\lambda\mu}^{(i)} \quad \text{and} \\
 x_{\kappa\lambda\mu}^{(i)} &= \frac{2E_r(1-\alpha_i)}{\Gamma(\beta_{111} + \beta_{\kappa\lambda\mu})}
 \end{aligned} \tag{29}$$

The superscript i in Eq. (29) stands for $o, 1$ or m and corresponds to the absorber, outside moderator or admixed moderator, respectively. Only the α_i in Eq. (29) changes and it should correspond to the appropriate scattering species.

The resonance integral is given by

$$I_{\kappa\lambda\mu} = \frac{I^{(o)}}{\beta_{\kappa\lambda\mu}} \tag{30}$$

where $I^{(o)}$ is the infinite dilution resonance integral.

To be consistent, the standard NR calculation of the Dancoff factor C should be modified to account for the fact that $\bar{\mu}\Sigma_1$ gives the effective scattering of the outside moderator. In order to keep the model simple, C is chosen as a function of the effective removal scattering of the outside moderator through the parameter μ .

The IR approximation has been applied to all scattering species in the system in Eqs. (28)-(30). Calculations have been carried out with these equations (7) and they are in good agreement with numerical methods. In a number of cases, the fact that the moderator is not treated in the NR approximation makes a considerable improvement in the results.

Note that the third equation in (28) for the outside moderator parameter is different from the other two equations, since $\bar{\mu}$ occurs in it. Only if s , which represents the "effective scattering of the lattice", equals σ_1 , which is the volume weighted outside moderator scattering, does $\bar{\mu} = \mu$, and then all three equations (28) have the same form. In this special case, admixing a fictitious moderator of cross section s homogeneously with an absorber (σ_a) and moderator (σ_m) would result in the same equations as (28). In this sense, there is an "equivalence" between the two systems. In general, however, equivalence does not exist.

The spatial aspects of the above problem have been treated only in a first approximation. If one removes the flat-flux assumption, the equations become more complicated. One might, for example, use a spatial expansion for the fluxes and then evaluate the moments of the escape probabilities contained in the M_i in Eq. (20). These higher order IR approximations would represent a truer characterization of the spatially dependent slowing down problem.

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