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A Differential Equation for Calculating Doppler Broadened Resonances

A Doppler-broadened Breit-Wigner resonance is commonly approximated(1) as the unbroadened value at the resonance energy multiplied by

$$\psi(\beta, x) = \frac{1}{\beta\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\exp -[(x - y)/\beta]^2}{1 + y^2}\, dy, \qquad (1)$$

where

$$\beta = (4/\Gamma)\sqrt{E_R kT/A} \quad \text{and} \quad x = 2(E - E_R)/\Gamma. \qquad (2)$$

E_R and Γ are the resonance energy and half-width; E is the laboratory-system energy of the incident neutron; kT is the energy of thermal motion of the absorber, and A is its mass number.

For the calculation of resonance integrals or detailed neutron flux, ψ (β,x) is required for many values of x but only one value of β for each resonance. Thus while the well-known formula,

$$\frac{\partial^2\psi}{\partial x^2} = \frac{2}{\beta}\frac{\partial\psi}{\partial\beta} \quad \text{with} \quad \psi(0, x) = \frac{1}{1 + x^2}, \qquad (3)$$

provides an alternative to numerically integrating the expression in Eq. (1), it suffers from the fact that $\psi(\beta,x)$ can be obtained for a given β only after the complete x-dependence has been determined for all smaller values. Therefore, for most programs requiring values of ψ without recourse to tables, it would be very desirable to have a differential equation for each resonance only in the variable x, with the parameter β held constant. Such an equation would enable one to calculate ψ entirely from those adjacent values that are needed anyway.

One can verify, after considerable manipulation, that ψ (β,x) in Eq. (1) satisfies the simple linear second order differential equation,

$$\tfrac{1}{4}\beta^4 \psi'' + \beta^2 x\, \psi' + (1 + \tfrac{1}{2}\beta^2 + x^2)\, \psi = 1, \qquad (4)$$

where the primes denote total derivatives with respect to x. To make the definition complete, there are the boundary conditions,

$$\psi(\beta,0) = (\sqrt{\pi}/\beta)\exp(\beta^{-2})\,[1 - \operatorname{erf}(\beta^{-1})]$$
$$\text{and} \quad \psi'(\beta,0) = 0 \qquad (5)$$

for starting at the resonance energy, and $\psi(\beta,x) \simeq (1 + x^2)^{-1}$ or other asymptotic expressions for starting at energies far from E_R. The present author and K. W. Morton at Harwell have both derived Eqs. (4) and (5) independently a few years ago as incidental subjects in larger technical reports. These formulas have been found very useful in a variety of codes using several of the usual numerical methods for solving second order differential equations.

If $\psi(\beta,x)$ is desired for a range of values of β as well as x, substituting the left side of Eq. (3) for ψ'' in Eq. (4) will result in a more useful expression than Eq. (3) alone, since no derivatives higher than the first appear. By differentiating Eq. (4) twice with respect to x, eliminating the third derivative terms between the third and fourth order differential equations, and substituting the first derivative term of the resulting expression into Eq. (4), one can obtain a fourth order differential equation in x with only even derivatives present. Eq. (3) can then be applied to get a second order total differential equation only in the variable β (3). Sometimes the quantity

$$\varphi(\beta, x) = \frac{1}{\beta\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{y \exp -[(x - y)/\beta]^2}{1 + y^2}\, dy, \qquad (6)$$

is desired to account for Doppler broadening the interference term in resonance scattering. This quantity can be evaluated conveniently in conjunction with Eq. (4) by means of the expression(2),

$$\varphi(\beta, x) = \frac{1}{2}\beta^2 \frac{\partial\psi(\beta, x)}{\partial x} + x\,\psi(\beta, x). \qquad (7)$$

It would seem that the mesh spacing in x should be small compared to β in forward or central difference schemes for solving Eq. (4), since both derivative terms vanish with β. The danger of an indeterminancy would be absent if Eq. (4) were applied at one mesh point with its derivatives calculated from previous mesh points.

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Crystal Spectrometer Measurement of the MITR Thermal Neutron Spectrum*

A neutron spectrum in the wavelength range 4 A>λ>0.65 A (0.005 ev<E<0.2 ev) has been measured using a crystal

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