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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, $\psi(\beta,x)$ 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 $\psi(\beta,x)$ 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,

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

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$>\lambda>$0.65 A (0.005 ev$<E<$0.2 ev) has been measured using a crystal

spectrometer. This spectrometer was of novel design, in that it utilized a beam of neutrons derived from the 2-ft thick, D_2O bottom reflector of the MIT reactor and directed vertically downward through the port of the medical therapy room. The results of such measurements were felt to be essential to the proper use of the medical therapy facility.

The beam was brought onto the crystal by a stainless steel collimator with an angular divergence of 7.8 minutes of arc. The detector used was a 12in. × 1in. BF_3 tube, using enriched gas at 120 cm pressure. Measurements were made using the (111) planes of Ge, Cu, and LiF in reflection. All the crystals were between ⅛in. and ¼in. thick. The data thus obtained was analyzed by use of the IBM-709 computer at MIT. Corrections were made for the following energy-dependent effects: Contamination of the beam by higher order crystal reflections; crystal reflectivity; instrumental resolution; counter efficiency; transmission of the collimator (total reflection); instrumental geometry; absorption by aluminum in the beam path. These effects are discussed in detail elsewhere (1, 2). The data were fitted by trial-and error to a Maxwellian distribution, which has been shown to give a good representation of the spectrum of a D_2O reactor by Larsson et al. (3) and Johansson et al. (4). The results were insensitive to the wavelength limits used in the fitting process, provided both sides of the thermal peak were included.

Figure 1 shows the corrected experimental data obtained with Ge(111) and the fitted Maxwellian distribution, in terms of a flux spectrum as a function of wavelength. The fitted curve is adjusted to give the same area over the region covered by the experimental points. The neutron temperature was found to be (63 ± 10)°C. with a moderator temperature of 35°C. Results for Ge(111) and Cu(111) were in good agreement. The Maxwellian provided a reasonable fit to the data at wavelengths shorter than 2 A. At longer wavelengths, the data fell off as $\lambda^{-5.9}$ rather than as λ^{-5} as would be predicted by a Maxwellian. This deviation has been tentatively attributed to the effect of possible inaccuracies in the large correction for higher order contamination at long wavelengths. Even in the most favorable case, Ge(111), higher orders contributed 75% of the total count rate at 0.005 ev. In all cases it appeared that the higher order contamination was overestimated by the calculation. It should be realized that the measurements were extended to wavelengths well beyond those usually considered appropriate for crystal spectrometry. A part of this additional factor of $\lambda^{-0.9}$ is due to hardening of the spectrum by preferential fast leakage. Larsson et al. (3) have reported a factor of $\lambda^{-.075}$ due to this effect.

A number of physical constants for the crystal, collimator, and detector were needed for the calculation. Of these, the ones most subject to uncertainty were the crysta mosaic spread and the length of inactive gas at the fron
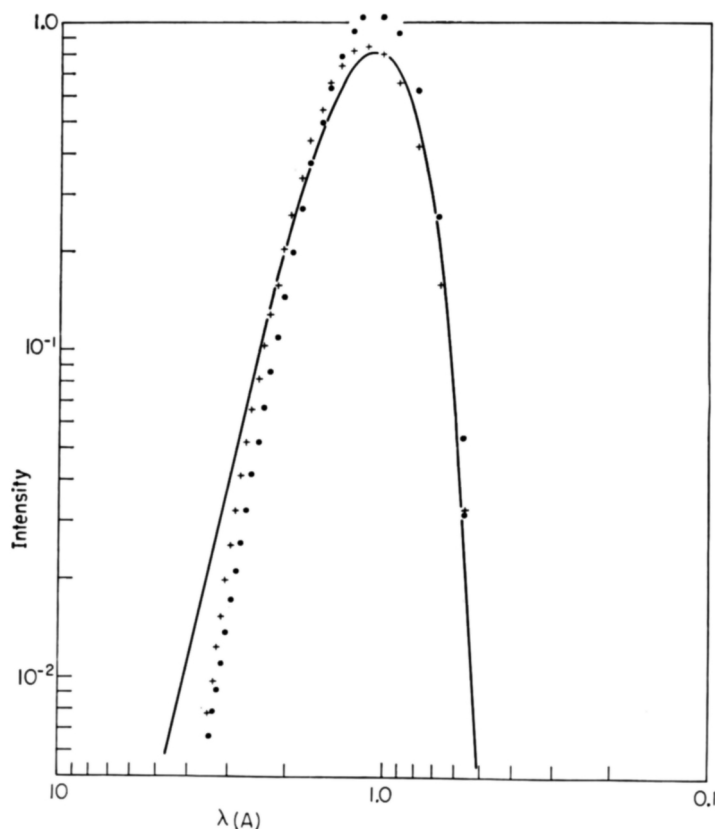

Fig. 1. Flux spectrum as a function of wavelength. Solid points were derived by treating data obtained using Ge(111). Crosses are the same data, treated without correcting for mirror reflection in the collimator. Solid curve is the best-fitting Maxwellian.

end of the counter. It was found that the predicted temperature was highly insensitive to large changes in these parameters. Of the 10% standard deviation given for the neutron temperature, 9% was due to counting statistics, while only 1% was due to an assumed factor of two uncertainty in the mosaic spread.

The effect of total reflection at the collimator walls is very large at low energies. For example, the beam intensity from our collimator was raised by a factor of 5 at 0.005 ev due to this effect. Taylor (5) neglected total reflection in analyzing his data, and reported that a Maxwellian with a neutron temperature equal to the moderator temperature provided a good fit at wavelengths shorter than 2 A. Similar results were obtained here, as shown by the crosses in Fig. 1, representing data analyzed without correction for mirror reflection. This result must be regarded as fortuitous, since the presence of totally reflected neutrons in our beam was definitely established by the following experiment. The counter aperture was stopped down with a cadmium slit, an angular scan of the direct beam was made, and the total cross section of indium was measured as a function of the scanning angle. The beam was considerably wider than would be predicted by line-of-sight calculations, and the indium cross section rose rapidly in the "wings," indicating the presence of neutrons of increasingly lower energy at larger angular divergencies.

The observed count rate spectrum showed sharp intensity variations, which have been ascribed to secondary, or multiple, Bragg scattering in the crystal (6). The effect of these deviations upon the predicted spectrum were studied by analyzing the data in three ways: (1) a smooth curve was drawn through the peaks of the original data, and points at equally spaced angles were chosen to be analyzed; (2) the data were first analyzed, after which the smooth curve was drawn through the peaks and representative points chosen to be fit; (3) the complete set of unsmoothed data was analyzed and fit. It was found that the temperatures predicted by the three methods were identical to within the quoted experimental uncertainty.

The presence of secondary scattering precludes the observation of spectral details. Since the process is a purely geometrical one, crystals of similar structure will exhibit the effect at equal Bragg angles but not at equal wavelengths. It had been hoped that the results obtained using several crystals could be superimposed in order to "wash out" this effect, but it was found that there was enough deviation between the various crystals used so that this could not be done with any accuracy.

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Total Cross Sections of Hydrocarbons and Tissue*

The total neutron cross section of several organic materials has been measured in the energy region 0.015 ev $<E<$ 0.2 ev. The object of these measurements was to obtain data which would assist in the application of the medical therapy facility at the MIT Research Reactor. Neutron penetration into organic material is of critical importance in the medical application of neutrons. Substances whose neutron cross section were studied include formic, acetic, propionic, and butyric acids, ethyl, propyl, and butyl alcohols, methyl-ethyl ketone, and human muscle, brain, and bone.

The measurements were made using the transmission method with the crystal spectrometer described in the preceding letter, with Ge(111) as a monochromator. Liquid samples were contained in an aluminum cell with aluminum foil windows. The cell was calibrated by measuring the
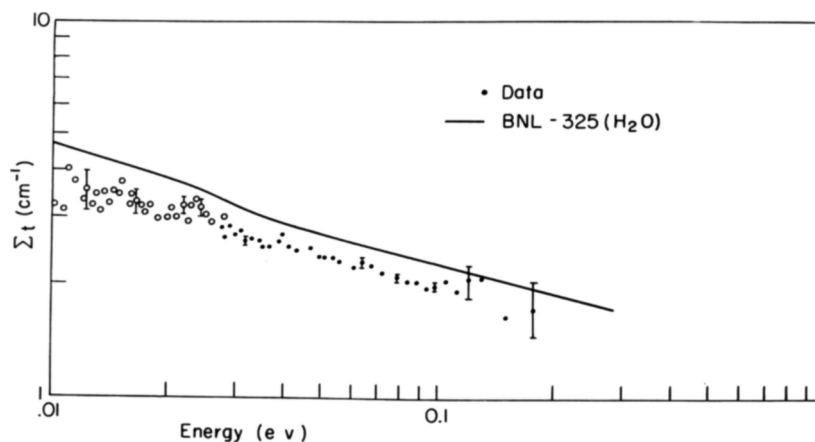
FIG. 1. Total macroscopic cross section of n-Butyl alcohol, compared to that for water.