FISSION INTERFERENCE WITH DOPPLER BROADENING

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Summary

The multilevel interference term between two resonances of the same spin and parity is examined and transformed to an expression that allows the evaluation of the Doppler-broadened cross section in terms of known functions.

I. Introduction

One of the difficulties underlying the use of the Breit–Wigner single-level approximation (Breit and Wigner 1936) for fissile nuclides is that considerable interference may occur in the fission cross section between resonances of the same spin and parity states. Doherty (1965) has remarked that some formulations of the multilevel problem do not allow the use of the standard resonance contour functions. In the present paper it is shown that in those cases of practical interest the fission interference correction can be expressed in terms of these standard contour functions, within the experimental error, and that Doppler broadening is accounted for analytically.

II. Multilevel Formulae

The full two-level approximation for the fission cross section in the vicinity of two levels that lie close together in energy, and are of the same spin and parity, has been evaluated by Lane and Thomas (1958*b*). It has the form

$$\sigma_{\mathrm{n,f}}(E)=\frac{\pi g_j}{k^2}\sum_{s,s'}\frac{\left\{(E_2-E)\,\Gamma_{1c}^{\frac{1}{2}}\Gamma_{1c'}^{\frac{1}{2}}+(E_1-E)\,\Gamma_{2c}^{\frac{1}{2}}\Gamma_{2c'}^{\frac{1}{2}}\right\}^2+\frac{1}{2}\left\{\sum_{c''}\pi_{c''c}\pi_{c''c'}\right\}^2}{\{(E_1-E)(E_2-E)+\frac{1}{4}(\Gamma_{12}^2-\Gamma_1\Gamma_2)\}^2+\frac{1}{4}\{\Gamma_1(E_2-E)+\Gamma_2(E_1-E)\}^2},\tag{1†}$$

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† This quoted formula is open to ambiguity. The summation over "c" could be interpreted as that over types of channels, instead of over all subchannels. The former interpretation is contradicted by the authors' statement that $\Gamma_{11}=\Gamma_1$. Although the latter interpretation was chosen in this work, the essential features of the Doppler-broadened formula are unaffected by the choice.

where E_1, E_2 are the two resonance energies,

E = neutron energy,

k = neutron momentum,

g_J = spin weight statistical factor,

Γ_{1c}, Γ_{2c} are the partial widths in levels 1 and 2 respectively for transitions via a channel c,

Γ_1, Γ_2 are the total widths of resonances 1 and 2,

$\pi_{c''c} = \Gamma_{1c''}^{\frac{1}{2}}\Gamma_{2c}^{\frac{1}{2}} - \Gamma_{2c''}^{\frac{1}{2}}\Gamma_{1c}^{\frac{1}{2}}$,

$\Gamma_1 \equiv \Gamma_{11}$, and Γ_{12} is a cross term (partial width) related to the reduced widths γ_{1c} and γ_{2c} by

$$\Gamma_{12} = \sum_{c''} P_{c''}\gamma_{1c''}\gamma_{2c''},$$

where P_c is the "penetration factor" defined by Lane and Thomas (1958*a*).

The sum in equation (1) extends over all orbital angular momentum states l and pairs of resonances. In order to compare with the single-level approximation, we express equation (1) in the form

$$\sigma_{\mathrm{n,f}}(E) = \frac{4\pi g_J}{k^2}\sum \frac{K(x_1,x_2)+f(\Gamma_{12})}{H(x_1,x_2)+g(\Gamma_{12})}, \tag{2}$$

where $K(x_1,x_2) = \alpha_1^2(1+x_1^2)+\alpha_2^2(1+x_2^2)+2(1+x_1x_2)\alpha_1\alpha_2$,

$$H(x_1,x_2) = (1+x_1^2)(1+x_2^2),$$

$$\alpha_i^2 = \Gamma_{\mathrm{n}}^l(i)\,\Gamma_{\mathrm{f}i}/\Gamma_i^2,$$

$\Gamma_{\mathrm{n}}^l(i)$ = neutron width for level i and orbital angular momentum l,

$\Gamma_{\mathrm{f}i}$ = fission width for level i,

$$x_i = 2(E_i-E)/\Gamma_i.$$

Also, by evaluation of the product terms in (1) we arrive at the results for a given l of

$$\left.\begin{aligned} f(\Gamma_{12}) &= 2(\alpha_1+\alpha_2)(\Gamma_{12}B-\Gamma_{12}^{\frac{1}{2}}A)+(\Gamma_{12}B-\Gamma_{12}^{\frac{1}{2}}A)^2,\\ g(\Gamma_{12}) &= \frac{2\Gamma_{12}^2}{\Gamma_1\Gamma_2}(x_1x_2-1)+\left(\frac{\Gamma_{12}^2}{\Gamma_1\Gamma_2}\right)^2, \end{aligned}\right\} \tag{3}$$

with $$A = \frac{1}{\Gamma_1\Gamma_2}\left\{(\Gamma_1\Gamma_{\mathrm{n}2}\Gamma_{\mathrm{f}1})^{\frac{1}{2}}+(\Gamma_1\Gamma_{\mathrm{n}2}\Gamma_{\mathrm{f}2})^{\frac{1}{2}}+(\Gamma_2\Gamma_{\mathrm{n}2}\Gamma_{\mathrm{f}1})^{\frac{1}{2}}+(\Gamma_2\Gamma_{\mathrm{n}1}\Gamma_{\mathrm{f}2})^{\frac{1}{2}}\right\},$$

$$B = \frac{1}{\Gamma_1\Gamma_2}\left\{(\Gamma_{\mathrm{n}1}\Gamma_{\mathrm{f}1})^{\frac{1}{2}}+(\Gamma_{\mathrm{n}2}\Gamma_{\mathrm{f}2})^{\frac{1}{2}}\right\},$$

where $\Gamma_{\mathrm{n}i}$ is the neutron width with the l suppressed. Note that $f(0) = 0$, $g(0) = 0$.

It is plausible to assume that cancellations between terms usually make Γ_{12} small when compared with $E_1 - E_2$, so we carry out a binomial expansion of (1) to obtain the two-level result for a given l of

$$\sigma_{n,f}(E) = \frac{K(x_1,x_2)}{H(x_1,x_2)} + \frac{H(x_1,x_2)\,f(\Gamma_{12}) - \{K(x_1,x_2)+f(\Gamma_{12})\}g(\Gamma_{12})}{H^2(x_1,x_2)} + O(\Gamma_{12}^2/H^2). \quad (4)$$

The energy region in the wings of *either* resonance corresponds to large values of x_1 or x_2, while from (3) and (4) it can be seen that the constant term $f(\Gamma_{12})$ becomes of lesser importance as either x_1 or x_2 increases and that $g(\Gamma_{12})$ does not increase nearly as fast as $H(x_1,x_2)$. This is borne out by numerical applications, where it has been found that the second term in (4) becomes appreciable only if $E_1 - E_2 < \Gamma_{12}$, a circumstance that should occur only rarely. No physical case is known to the author where the second term cannot be neglected to within the experimental error.

Finally, the combination of equations (2) and (4) leads to the interference formula given by Sailor (1955) of

$$\sigma_{n,f}(E) = K(x_1,x_2)/H(x_1,x_2),$$

which may be reduced to

$$\sigma_{n,f}(E) = \frac{\Gamma_{f1}}{\Gamma_1}\left(\frac{\sigma_{01}}{1+x_1^2}\right) + \frac{\Gamma_{f2}}{\Gamma_2}\left(\frac{\sigma_{02}}{1+x_2^2}\right) + \frac{4\pi g_j}{k^2}\sum\frac{\alpha_1\,\alpha_2\,(1+x_1x_2)}{(1+x_1^2)(1+x_2^2)}, \quad (5)$$

where
$$\sigma_{0i} = \left(\frac{4\pi g_j}{k^2}\right)\frac{\Gamma_{ni}}{\Gamma_i}.$$

III. Doppler Broadening

The effect of atomic motion upon the shape of the interference contour will now be evaluated. The expression (5) may be written

$$\sigma_{n,f}(E) = \left|\left(\frac{\sigma_{01}\Gamma_{f1}}{\Gamma_1}\right)^{\frac{1}{2}}\left(\frac{1}{x_1-\mathrm{i}}\right) \pm \left(\frac{\sigma_{02}\Gamma_{f2}}{\Gamma_2}\right)^{\frac{1}{2}}\left(\frac{1}{x_2+\mathrm{i}}\right)\right|^2,$$

$$= \sigma_{01}\frac{\Gamma_{f1}}{\Gamma_1}\left(\frac{1}{1+x_1^2}\right) + \sigma_{02}\frac{\Gamma_{f2}}{\Gamma_2}\left(\frac{1}{1+x_2^2}\right) \pm 2\,\mathrm{Re}\left\{\left(\frac{\sigma_{01}\,\sigma_{02}\,\Gamma_{f1}\,\Gamma_{f2}}{\Gamma_1\Gamma_2}\right)^{\frac{1}{2}}\left(\frac{1}{x_1-\mathrm{i}}\right)\left(\frac{1}{x_2+\mathrm{i}}\right)\right\},$$

which is the same as equation (5). Now,

$$\mathrm{Re}\left(\frac{1}{x_1-\mathrm{i}}\times\frac{1}{x_2+\mathrm{i}}\right) = \frac{\Gamma_1\Gamma_2}{4}\mathrm{Re}\left(\frac{1}{E-z_1}\times\frac{1}{E-z_2^*}\right),$$

where $z_i = E_i + \frac{1}{2}\mathrm{i}\Gamma_i$.

Also,

$$\mathrm{Re}\left(\frac{1}{E-z_1}\times\frac{1}{E-z_2^*}\right) = \frac{1}{(E_1-E_2)^2+\frac{1}{4}(\Gamma_1+\Gamma_2)^2}\left[(E_1-E_2)\left\{\frac{2}{\Gamma_1}\left(\frac{x_1}{1+x_1^2}\right)-\frac{2}{\Gamma_2}\left(\frac{x_2}{1+x_2^2}\right)\right\}\right.$$
$$\left.+\frac{\Gamma_1+\Gamma_2}{2}\left\{\frac{2}{\Gamma_1}\left(\frac{1}{1+x_1^2}\right)+\frac{2}{\Gamma_2}\left(\frac{1}{1+x_2^2}\right)\right\}\right]. \tag{6}$$

Solbrig (1961) and Melkonian, Havens, and Rainwater (1953) have shown that in order to average (6) over atomic speeds one must multiply each term by the appropriate weight factor

$$\frac{\exp\{-(x_i-y_i)^2/4\theta_i\}}{(2\pi\theta_i)^{\frac{1}{2}}}$$

and integrate the formula with x_i replaced by y_i over the ranges $-\infty < y_i < \infty$, where

$\theta_i = 4E_iKT/A\Gamma^2$, K = Boltzmann's constant,

A = atomic mass of absorber, T = temperature in degrees Kelvin.

This procedure yields

$$\sigma_{\mathrm{n,f}}(E) = \frac{\sigma_{01}\Gamma_{\mathrm{f}1}}{\Gamma_1}\psi(\theta_1,x_1)+\frac{\sigma_{02}\Gamma_{\mathrm{f}2}}{\Gamma_2}\psi(\theta_2,x_2)$$
$$\pm 2\left(\frac{\sigma_{01}\sigma_{02}\Gamma_{\mathrm{f}1}\Gamma_{\mathrm{f}2}}{\Gamma_1\Gamma_2}\right)^{\frac{1}{2}}\frac{\Gamma_1\Gamma_2}{4}\left\{\frac{I_1+I_2}{(E_1-E_2)^2+\frac{1}{4}(\Gamma_1+\Gamma_2)^2}\right\}, \tag{7}$$

where $I_1 = (E_1-E_2)\left\{\frac{2}{\Gamma_1}\phi(\theta_1,x_1)-\frac{2}{\Gamma_2}\phi(\theta_2,x_2)\right\}$,

$$I_2 = \frac{\Gamma_1+\Gamma_2}{2}\left\{\frac{2}{\Gamma_1}\psi(\theta_1,x_1)+\frac{2}{\Gamma_2}\psi(\theta_2,x_2)\right\};$$

and, furthermore,

$$\psi(\theta,x) = \frac{1}{2(\pi\theta)^{\frac{1}{2}}}\int_{-\infty}^{\infty}\exp\{-(x-y)^2/4\theta\}\frac{dy}{1+y^2},$$

$$\phi(\theta,x) = \frac{1}{2(\pi\theta)^{\frac{1}{2}}}\int_{-\infty}^{\infty}\exp\{-(x-y)^2/4\theta\}\frac{y\,dy}{1+y^2}$$

are the usual standard Voigt profiles. Equation (7) has the form of a direct sum of two Doppler-broadened single levels plus an interference term which is expressed by a combination of the standard contour functions $\psi(\theta,x)$ and $\phi(\theta,x)$. Therefore, the Doppler broadening of the fission interference term has been determined analytically.

Equation (7) is readily generalized to the sums over contributions from many resonances, in which case it may be written in a form that resembles the single-level approximation, that is,

$$\sigma_{\mathrm{n,f}}(E) = \sum_i \left\{a_i \psi(\theta_i, x_i) + b_i \phi(\theta_i, x_i)\right\},$$

where

$$a_i = \sigma_{0i}\frac{\Gamma_{\mathrm{f}i}}{\Gamma_i} + \sum_{j\neq i} s_j \left(\frac{\sigma_{0i}\,\sigma_{0j}\,\Gamma_{\mathrm{f}i}\,\Gamma_{\mathrm{f}j}}{\Gamma_i\,\Gamma_j}\right)^{\frac{1}{2}} \frac{\Gamma_j}{2}\left\{\frac{1}{(E_i-E_j)^2+\frac{1}{4}(\Gamma_i+\Gamma_j)^2}\right\}(\Gamma_i+\Gamma_j),$$

$$b_i = \sum_{j\neq i} s_j \left(\frac{\sigma_{0i}\,\sigma_{0j}\,\Gamma_{\mathrm{f}i}\,\Gamma_{\mathrm{f}j}}{\Gamma_i\,\Gamma_j}\right)^{\frac{1}{2}} \Gamma_j \frac{E_i-E_j}{(E_i-E_j)^2+\frac{1}{4}(\Gamma_i+\Gamma_j)^2},$$

and $s_j = \pm 1$, the sign of which must be determined from experiment.

IV. Conclusions

An expression for the multilevel interference term between two resonances of the same spin and parity has been derived and the Doppler-broadened form determined. In all applications to date, the approximate version has been found to differ from the Lane–Thomas version by less than the experimental error (Musgrove, personal communication 1966).

The formula (7) involves only constants and the usual two profile functions, so applications to all neutron cross-section calculations on digital computers now involve the computation of these two functions only. It is of great practical interest to determine the effect of such asymmetric interference terms in the standard resonance theory of reactor physics, and we are currently undertaking such a project.

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