A MULTILEVEL FORMALISM FOR NEUTRON ELASTIC SCATTERING CROSS SECTIONS

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Abstract

An extension of the Feshbach, Porter, and Weisskopf formalism has been developed for neutron elastic scattering. The emphasis in this paper is on resonance–resonance interference and explicit use of the background R matrix. The results of this formulation are compared with experimental data in the resonance region for the nuclides ^{238}U, ^{197}Au, and ^{23}Na.

I. Introduction

Reaction matrix theory has provided a convenient method of displaying a great deal of the physics of nuclear reactions. The theory of this method has been presented in review articles by Lane and Thomas (1958) and Vogt (1962). The present paper is an extension of the Feshbach, Porter, and Weisskopf (1954) formalism, which has previously been applied by Sailor (1955) and Cook (1967) in work on fissile nuclides. In Section II, Cook's formulation is extended to the derivation of a multilevel scattering formalism. The evaluation of relevant parameters is contained in Section III and the results obtained are compared with experimental values in Section IV.

II. A Multilevel Scattering Formula

Considering the elastic scattering of a neutron with orbital angular momentum l, the cross section may be written as (Schmidt 1966)

$$\sigma_{\mathrm{n}}(E) = (\pi/k^2)\sum_{Jlj} g_J\left(|1-U^J_{njl,njl}|^2 + \sum_{\substack{l'\neq l\\ j'\neq j}} |U^J_{nj'l',njl}|^2\right), \tag{1}$$

where

$$g_J = (2J+1)/2(2I+1),$$

j is the channel spin, J the spin of the compound nucleus, k the wavenumber, E the neutron energy, $U^J_{nj'l',njl}$ the collision matrix, and g_J the spin statistical factor, I being the spin of the target nucleus.

Ignoring spin-flip scattering, equation (1) reduces to

$$\sigma_{\mathrm{n}}(E) = (\pi/k^2)\sum_{Jlj} g_J\,|1-U^J_{n,n}|^2, \tag{2}$$

where n represents the channel numbers $\{njl\}$ and the collision matrix component for

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this channel is given by

$$U^J_{n,n} = \exp(-2\mathrm{i}\phi_l) + \sum_\lambda 2\mathrm{i}\{\Gamma^{(l)}_{\mathrm{n}\lambda}\exp(-2\mathrm{i}\phi_l)/\Gamma^{(l)}_\lambda(x^{(l)}_\lambda - \mathrm{i})\}\,, \tag{3}$$

where

$$x^{(l)}_\lambda = 2(E_\lambda - E)/\Gamma^{(l)}_\lambda\,,$$

$\Gamma^{(l)}_{\mathrm{n}\lambda}$ is the neutron width for level λ and orbital angular momentum l, $\Gamma^{(l)}_\lambda$ the total width for level λ, E_λ the resonance energy for level λ, and ϕ_l a background phase which is considered in Section III.

Suppressing the l superscript and substituting (3) into (2) gives

$$\begin{aligned}\sigma_{\mathrm{n}}(E) &= \frac{4\pi}{k^2}\sum_{Jlj} g_J \left|\frac{\exp(2\mathrm{i}\phi_l)-1}{2\mathrm{i}} - \sum_\lambda \frac{\Gamma_{\mathrm{n}\lambda}}{\Gamma_\lambda(x_\lambda - \mathrm{i})}\right|^2 \\ &= \frac{4\pi}{k^2}\sum_{Jlj} g_J\left[\left|\frac{\exp(2\mathrm{i}\phi_l)-1}{2\mathrm{i}}\right|^2 + \left|\sum_\lambda \frac{\Gamma_{\mathrm{n}\lambda}}{\Gamma_\lambda(x_\lambda - \mathrm{i})}\right|^2\right. \\ &\qquad \left. -2\,\mathrm{Re}\left\{\frac{\exp(2\mathrm{i}\phi_l)-1}{2\mathrm{i}}\left(\sum_\lambda \frac{\Gamma_{\mathrm{n}\lambda}}{\Gamma_\lambda(x_\lambda - \mathrm{i})}\right)^*\right\}\right]\,,\end{aligned} \tag{4}$$

where the asterisk denotes complex conjugation and $\mathrm{Re}\,f$ indicates the real part of the function f.

It can be seen from inspection of equation (4) that the first term may be written as

$$(4\pi/k^2)\sum_{Jlj} g_J \sin^2\phi_l\,, \tag{4a}$$

and the third term may be evaluated as

$$-\sum_{Jlj} g_J \sum_\lambda \sigma_{0\lambda}\{2\sin^2\phi_l/(1+x^2_\lambda) + x_\lambda \sin 2\phi_l/(1+x^2_\lambda)\}\,, \tag{5}$$

where

$$\sigma_{0\lambda} = 4\pi g_J \Gamma_{\mathrm{n}\lambda}/k^2\Gamma_\lambda\,.$$

The method of expanding the second term in (4) is that used by Cook (1967).†

Contributions from many resonances may be expressed in a form resembling the single-level approximation, that is,

$$\sum_{Jlj}\sum_\lambda\left(\frac{\sigma_{0\lambda}\Gamma_{\mathrm{n}\lambda}}{\Gamma_\lambda(1+x^2_\lambda)} + \frac{a_\lambda + b_\lambda x_\lambda}{1+x^2_\lambda}\right)\,, \tag{6}$$

with

$$a_\lambda = \sum_{\mu\neq\lambda}\left(\frac{\sigma_{0\mu}\sigma_{0\lambda}\Gamma_{\mathrm{n}\mu}\Gamma_{\mathrm{n}\lambda}}{\Gamma_\lambda\Gamma_\mu}\right)^{\frac{1}{2}}\tfrac{1}{2}\Gamma_\mu\left(\frac{\Gamma_\lambda + \Gamma_\mu}{(E_\lambda - E_\mu)^2 + \frac{1}{4}(\Gamma_\lambda + \Gamma_\mu)^2}\right)$$

† Two misprints appeared in this paper. The last factor on the right-hand side of the first equation in Section III should be $1/(x_2 - \mathrm{i})$ and $E_2 - E_1$ should be substituted for $E_1 - E_2$ in equation (6). These misprints have no effect on the final result for fissile nuclides, but are important in a scattering calculation.

and

$$b_\lambda = \sum_{\mu\neq\lambda} \left(\frac{\sigma_{0\mu}\sigma_{0\lambda}\Gamma_{n\mu}\Gamma_{n\lambda}}{\Gamma_\lambda \Gamma_\mu}\right)^{\frac{1}{2}} \Gamma_\mu \left(\frac{E_\mu - E_\lambda}{(E_\lambda - E_\mu)^2 + \frac{1}{4}(\Gamma_\lambda + \Gamma_\mu)^2}\right),$$

where the μ summations are over resonances of the same spin and parity.

Gathering results (4a), (5), and (6) and using

$$\sum_{Jj} g_J = \sum_{J=|l-j|}^{l+j} \sum_{j=|I-\frac{1}{2}|}^{I+\frac{1}{2}} g_J = 2l+1,$$

one finally obtains

$$\sigma_n(E) = (4\pi/k^2) \sum_{l=0}^{\infty} (2l+1)\sin^2\phi_l$$

$$+ \sum_{l=0}^{\infty} \sum_{J=|l-j|}^{l+j} \sum_{j=|I-\frac{1}{2}|}^{I+\frac{1}{2}} \sum_\lambda \left(\frac{\sigma_{0\lambda}\Gamma_{n\lambda}}{\Gamma_\lambda(1+x_\lambda^2)} + \frac{a_\lambda + b_\lambda x_\lambda}{1+x_\lambda^2} - \frac{2\sigma_{0\lambda}\sin^2\phi_l + \sigma_{0\lambda}x_\lambda \sin 2\phi_l}{1+x_\lambda^2}\right). \tag{7}$$

The first term gives background scattering, the second and third terms represent resonance and resonance–resonance interference scattering, and the final term represents resonance–background interference scattering.

Cook (1967) shows that it is possible to Doppler-broaden result (7) by making the substitutions

$$1/(1+x_\lambda^2) = \psi(\xi_\lambda, x_\lambda), \qquad x_\lambda/(1+x_\lambda^2) = \phi(\xi_\lambda, x_\lambda),$$

where

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

and

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

are the standard Voigt profiles with

$$\xi_\lambda = 4E_\lambda BT/A\Gamma_\lambda^2,$$

B being Boltzmann's constant, A the atomic mass of the target, and T the temperature in degrees Kelvin.

Owing to the large number of open channels the reaction cross sections have been calculated as a sum of single-level contributions of the form

$$\sigma_{n,y} = \sum_\lambda \{\sigma_{0\lambda}\Gamma_{y\lambda}/\Gamma_\lambda(1+x_\lambda^2)\},$$

where $\Gamma_{y\lambda}$ is the partial width for reaction y.

III. Concerning ϕ_l

The previous method of fitting the thermal cross section consisted of inserting a negative energy resonance with parameters calculated to fit the discrepancy. The method outlined below achieves an equivalent fit using the background term of the R matrix.

Following the usual procedure the R matrix has been split into contributions from resonances in a restricted energy range and those from distant or background levels $R^0_{n,n}$. This gives rise to a corresponding division in the collision matrix with the contribution from the background U matrix being given by

$$U^0_{n,n} = \Omega^2(1-R^0_{n,n}L^{0*}_n)(1-R^0_{n,n}L^0_n)^{-1} = \exp(-2i\phi_l), \tag{8}$$

where the hard sphere scattering phase shift θ_l enters through

$$\Omega = \exp(-i\theta_l)$$

and

$$\begin{aligned}\phi_l &= \theta_l+\arg(1-R^0_{n,n}L^0_n)\\ &= \theta_l-\tan^{-1}[R^0_{n,n}P_l/\{1-R^0_{n,n}(S_l-B_l)\}].\end{aligned} \tag{9}$$

By suitably choosing the boundary conditions B_l one may set S_l-B_l equal to zero. In equation (9) S_l and P_l are the shift factor and penetration factor for which a table of values is given by Preston (1962).

The recurrence relation

$$\theta_l = \theta_{l-1}-\tan^{-1}[P_{l-1}/(l-S_{l-1})]$$

given by Lane and Thomas (1958, p. 350) is used to generate θ_l and one now has only to determine $\xi = \tan^{-1}(R^0_{n,n}P)$. The background R matrix is approximately independent of energy, so that one may write (Lane and Thomas 1958, p. 325)

$$R^0_{n,n} = (Ka)^{-1}$$

where $K \sim 10^{13}\ \mathrm{cm}^{-1}$ and a is the channel radius. Hence, once K is obtained ξ can be calculated.

The thermal cross section is calculated setting $R^0_{n,n}$ equal to zero. One then assumes that any discrepancy between this result and the exact cross section is due to the fact that the s-wave background scattering and the asymmetric resonance-background interference terms have no contribution from $R^0_{n,n}$. For $l = 0$,

$$\theta_0 = P_0 = ka,$$

where the channel radius a has been taken as the nuclear radius given by the relation

$$a = r_0 A^{\frac{1}{3}}\ \ \mathrm{fm}.$$

The value of r_0 chosen was $1\cdot47$. At thermal energies $ka \ll 1$ and one may make the approximations

$$\sin\phi_0 = \phi_0 \qquad \text{and} \qquad \xi = k/K = kd,$$

where $d = K^{-1}$.

Hence

$$\sigma_{\text{exact}}-\sigma_{\text{calc}} = \Delta = (4\pi/k^2)(ka-kd)^2-4\pi a^2 - \sum_\lambda \{\sigma_{0\lambda}\, x_\lambda/(1+x_\lambda^2)\}\, 2(ka-kd)-2ka\,. \tag{10}$$

Defining

$$I = \sum_\lambda \{\sigma_{0\lambda}\, x_\lambda\, 2ka/(1+x_\lambda^2)\}a^{-1},$$

leads to a quadratic equation in d. The solution used in this work is given by

$$K^{-1} = d = a-(I/8\pi a)-\tfrac{1}{2}\{(2a-I/4\pi a)^2+\Delta/\pi\}^{\frac{1}{2}}\,. \tag{11}$$

In the numerical calculation of the thermal cross sections described in the following section, the absorption cross section has been treated as a known quantity, as it is difficult to calculate the exact absorption cross section and any discrepancies in this result would give rise to a miscalculation of the value of ξ.

IV. Analysis of Results

Calculations of non-Doppler broadened cross sections were programmed for the A.A.E.C. IBM 360/50 computer. As results over a wide range of target mass numbers are desirable the nuclides ^{197}Au, ^{238}U, and ^{23}Na were chosen, with the following results:

(a) ^{197}Au

The resolved resonance parameters to an energy of 293 eV were taken from Schmidt (1968). A comparison of the calculated total cross section with the experimental points from Hughes and Schwartz (1958) is shown in Figure 1. The calculation has produced the interference dips quite well, but a comparison of the resonance peak heights has not been possible owing to the poor resolution width of the experimental data. A factor of importance is the result for the calculation of K used to determine the background R matrix. The value obtained was

$$K = -1\cdot 197\times 10^{13},$$

the negative value of K indicating that the background matrix arose from nearby negative energy resonances.

One expects the R matrix formalism to be independent of the channel radius a. This was tested by changing the value of r_0 from $1\cdot 47$ to $1\cdot 50$. The average variation in the cross section was $0\cdot 009\%$, showing that the expected channel-radius independence is correct to a high degree of precision.

(b) ^{238}U

The resolved resonance parameters to $846\cdot 6$ eV were taken from Schmidt (1966), and the resulting cross section is compared with the evaluated data of Langner, Schmidt, and Woll (1968) in Figure 2. The discrepancy between 12 and 18 eV could be due to interference between the $11\cdot 32$ and $19\cdot 6$ eV levels. Overall the results

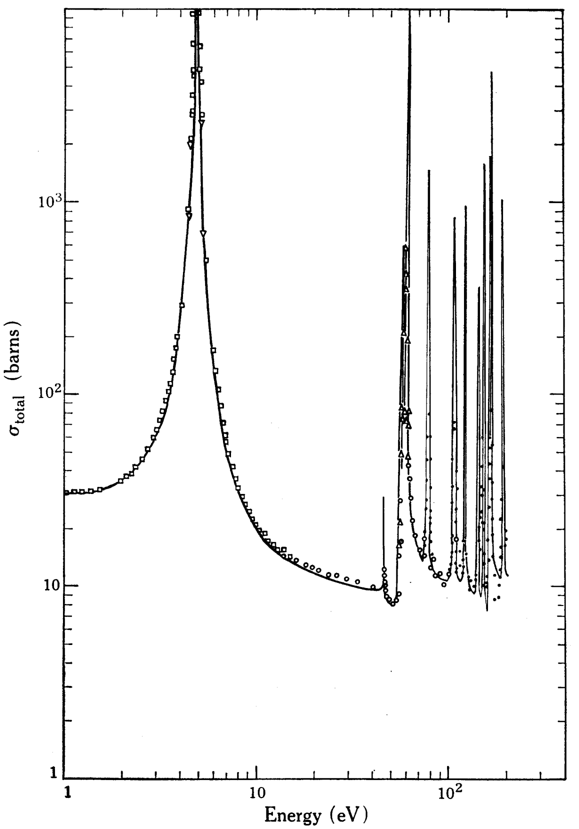

Fig. 1.—Comparison of experimental points and calculated total cross section for ^{197}Au from 1 to 200 eV.

obtained are in excellent agreement with the experimental evaluation. The value of K obtained was

$$K = -3\cdot959\times10^{13},$$

again indicating the presence of nearby negative energy resonances.

(c) ^{23}Na

At first sight the $2\cdot85$ keV level in sodium appears to be an unusual resonance to investigate with a multilevel formulation, as it is over 30 keV from the nearest resolved resonance. There has been a great deal of controversy about this level however, arising from the difficulty of fitting the experimental data (see Schmidt 1966). Stephenson (1966) succeeded by assuming spin-dependent scattering radii. One must also consider the possibility that the unusual shape of the $2\cdot85$ keV level is due to interference with other levels. Most experimental measurements on sodium have aluminium in the target, and the presence of the 35 keV resonance in aluminium would tend to mask the effect of a sodium resonance in that region. Transmission measurements by Ribon *et al.* (1966) without aluminium showed a resonance at

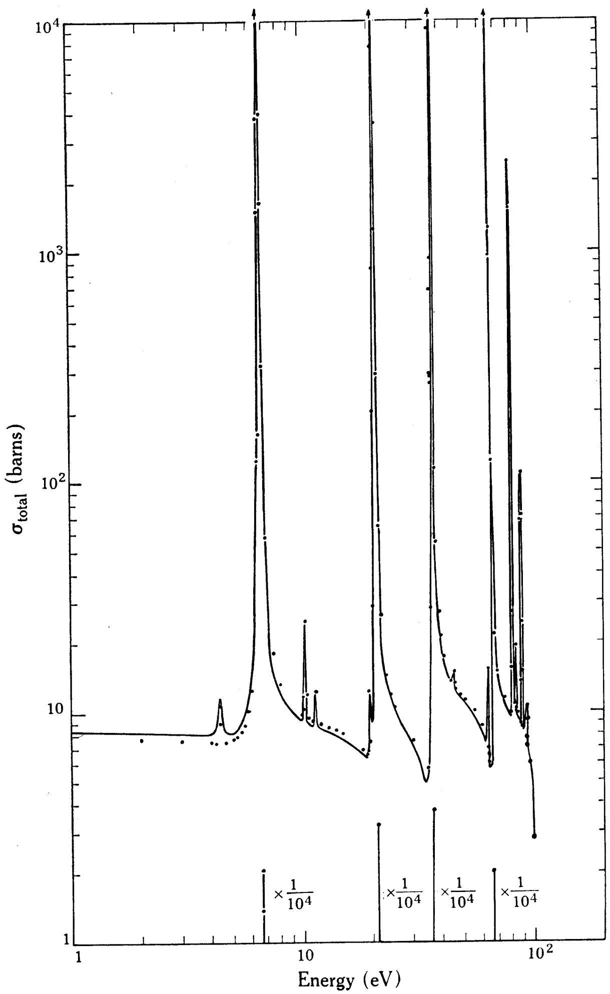

Fig. 2.—Comparison of experimental points and calculated total cross section for ^{238}U from 1 to 100 eV.

about 35 keV. Accordingly, calculations were performed inserting a resonance at that energy. Its parameters, together with those of the 2·85 keV level, were as follows.

E_r (keV)	Γ_n (eV)	Γ_γ (eV)	J	l
2·85	410	0·36	1	0
35·0	500	0·6	1	0

The spin and parity of the 35 keV level are different from the measurements by Ribon *et al.* (1966) of $g_J \approx 7/8$, $l \geqslant 2$. However, its spin and parity must be the same as the 2·85 keV level for mutual interference to occur. The parameters listed above give a calculated thermal (n, γ) cross section of 526 mb in fairly good agreement with the presently recommended value of 534±5 mb (Stehn *et al.* 1964). The K

value obtained was

$$K = -0\cdot 423 \times 10^{13}.$$

As resonances in sodium are resolved to $857\cdot 5$ keV, the value of ξ calculated at thermal energies and denoted by ξ_0 would not give an accurate background over the whole of the range. An energy-dependent background of the form

$$\xi(E) = \xi_0 - 5\xi_0 E \times 10^{-6} + \xi_0 E^2 \times 10^{-11}$$

was used and calculations were made to 50 keV. The resonance parameters above

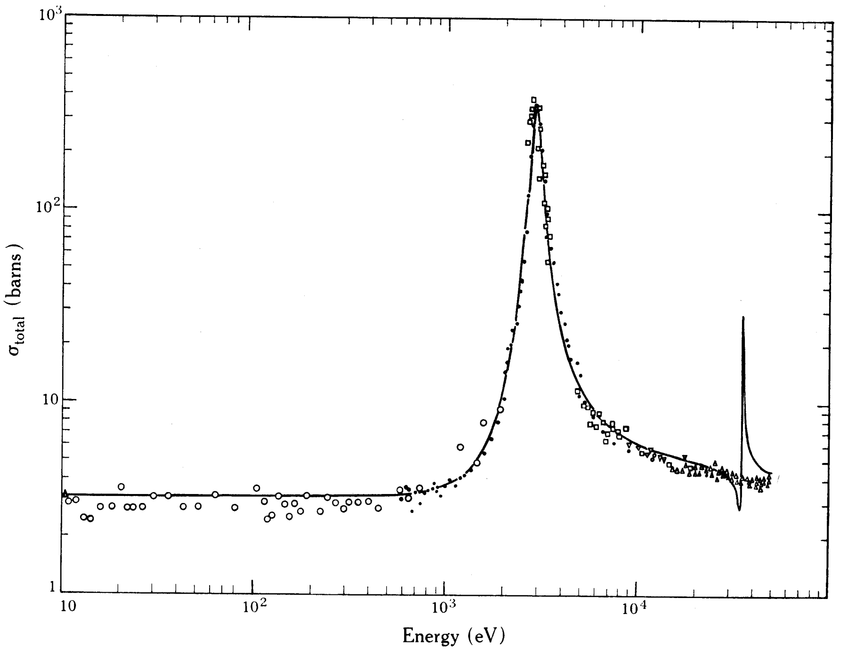

Fig. 3.—Comparison of experimental points and calculated total cross section for ^{23}Na from 10 eV to 50 keV.

$2\cdot 85$ keV were taken from Schmidt (1966) to an energy of $397\cdot 9$ keV. These parameters are from the experimental work of Hibdon (1960, 1961) and were used after a consideration of Schmidt's analysis of Hibdon's experimental technique and method of determination of the parameters.

Below 10 keV the results are compared in Figure 3 with the values from Hughes and Schwartz (1958) and between 10 and 50 keV with Hibdon (1960). The cross section appears slightly high at low energies, but from 600 eV the shape of the $2\cdot 85$ keV resonance has been faithfully reproduced. The range 30–50 keV is difficult to comment on as Ribon *et al.* gave no experimental cross section for comparison. Between 50 and 200 keV an attempt was made to fit the differential energy measurements using the parameters obtained by Hibdon's area analysis. The resolution of the experimental data was too poor, however, for a meaningful comparison.

V. Conclusions

This paper has described the development of a multilevel scattering formalism that is easily amenable to Doppler broadening. It has been tested over a wide range of target mass numbers with reasonable success, particularly with regard to the shape of the $2 \cdot 85$ keV resonance in ^{23}Na.

VI. Acknowledgments

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