Cross section and resonance calculations: algorithms and numerical aspects

P. Fanto[1], G. F. Bertsch[2], and Y. Alhassid[1]

[1] *Center for Theoretical Physics, Sloane Physics Laboratory,*
Yale University, New Haven, CT 06520

[2] *Department of Physics and Institute for Nuclear Theory, Box 351560*
University of Washington, Seattle, WA 98915

I. HAMILTONIAN

The Hamiltonian describing the neutron channel and compound nucleus system can be written in matrix form as

$$\mathbf{H} = \begin{pmatrix} \mathbf{H_n} & \mathbf{V} \\ \mathbf{V}^T & \mathbf{H_c} \end{pmatrix} , \tag{1}$$

where $\mathbf{H_n}$ is the neutron channel Hamiltonian, $\mathbf{H_c}$ is the compound nucleus Hamiltonian, and $\mathbf{V}$ is the coupling matrix. $\mathbf{H_n}$ is derived by discretizing the radial Schrödinger equation on a spatial mesh and is given by

$$\mathbf{H}_{\mathbf{n},ij} = [2t + V(r_i)]\delta_{ij} - t\delta_{i,j+1} - t\delta_{i,j-1} . \tag{2}$$

where $i,j = (1,..,N_n)$. Here N_n is the number of sites on the channel mesh, $t = \hbar^2/2m\Delta r^2$ with Δr is the mesh spacing, and $r_i = i\Delta r$. $V(r_i)$ is the central Woods-Saxon potential given by

$$V(r) = \frac{V_0}{1 + e^{(r-R)/a}} , \tag{3}$$

where $R = r_0 A^{1/3}$ (A is the mass number of the target nucleus) and a is the surface thickness parameter.

The internal state Hamiltonian $\mathbf{H_c}$ is given by

$$\mathbf{H}_{\mathbf{c},\mu\nu} = (\mathcal{E}_\mu - i\Gamma_\gamma/2)\delta_{\mu\nu} , \tag{4}$$

where the spacings between nearest-neighbor energies $\mathcal{E}_\mu$ are given by the spacings between neighboring eigenvalues of the middle third of the spectrum of a GOE random matrix. The spacings are scaled to match the neutron resonance mean level spacing D on average. In practice, we choose lower and upper energies $\mathcal{E}_1$ and $\mathcal{E}_{N_c} = \mathcal{E}_1 + N_c D$ (N_c is the number of internal compound nucleus states). We then diagonalize a GOE random matrix of dimension $3N_c \times 3N_c$ and obtain the middle third of its eigenvalue spectrum $\eta_1, ..., \eta_{N_c}$. These eigenvalues have the average spacing d, which we determine using $\eta_{N_c} - \eta_1 \approx N_c d$. The internal state energies $\mathcal{E}_\mu$ ($\mu = (1, ..., N_n)$) are then take to be

$$\mathcal{E}_\mu = \frac{D}{d}(\eta_\mu - \eta_1) + \mathcal{E}_1 . \tag{5}$$

Γ_γ in Eq. (4) is the total gamma decay width and is taken to be the same for all internal states.

The coupling matrix $\mathbf{V}$ is given by

$$\mathbf{V}_{i,\mu} = \delta_{i,i_e}(v_0\Delta r^{-1/2})s_\mu , \tag{6}$$

where i_e is a fixed interaction point, v_0 is a coupling parameter, and s_μ is drawn from the normal distribution with zero mean and unit variance. s_μ accounts for the fluctuations of the GOE eigenvectors and is given by

$$s_\mu = \sum_{\alpha=1}^{N_c} \langle\phi_\alpha|\psi_\mu\rangle \tag{7}$$

In Eq. (7), $|\phi_\alpha\rangle$ describe a fixed basis in the compound-nucleus space, and $|\psi_\mu\rangle$ are the GOE eigenvectors. The projection $\langle\phi_\alpha|\psi_\mu\rangle$ of a GOE eigenvector $|\psi_\mu\rangle$ onto a fixed state $|\phi_\alpha\rangle$ is a Gaussian random variable with mean zero and variance $1/N$, where N is the dimension of the GOE matrix. In the limit of large N, the N components $\langle\phi_\alpha|\psi_\mu\rangle$ of an fixed eigenvector $|\psi_\mu\rangle$ can be treated as independent Gaussian variables and their sum in Eq. (7) is a Gaussian random variable with zero mean and unit variance. The Δr dependence of the average coupling strength in Eq. (6) is introduced to guarantee that the calculated physical observables are independent of Δr in the continuum limit $\Delta r \to 0$ (see below).

The total dimension of the Hamiltonian (1) is $N_n + N_c$. The wavefunction $\vec{u}$ describing the system is a $(N_n + N_c)$-dimensional column vector, where the top N_n components correspond to the sites of the neutron channel mesh and the bottom N_c components correspond to the internal states.

II. SCATTERING AMPLITUDE AND CROSS SECTIONS

We may use the Hamiltonian of Eq. (1) together with appropriate boundary conditions on the wavefunction $\vec{u}$ to calculate the neutron scattering amplitude. As discussed in the main text, we impose $u(0) = 0$ so that the wavefunction is regular at the origin. The asymptotic behavior at large r for a scattering solution with a real and positive wavenumber k is

$$u(r) \to A(k) \left[e^{-ikr} - S_{nn}(k)e^{ikr} \right] \ , \tag{8}$$

where $S_{nn}(k)$ is the elastic neutron scattering amplitude [1] and $A(k)$ is an overall normalization factor. Using Eq. (8) at the points N_n and $N_n + 1$, we find

$$\frac{u(N_n)}{u(N_n + 1)} = \frac{1 - S_{nn}e^{ik(2N_n)\Delta r}}{e^{-ik\Delta r} - S_{nn}e^{ik(2N_n+1)\Delta r}} \ , \tag{9}$$

where $x \equiv u(N_n)/u(N_n + 1)$. In writing Schrödinger equation for the last mesh point N_n in the neutron channel, we have to consider the non-vanishing term $-tu(N_n + 1)$. Since the point $N_n + 1$ is not in the vector space of the channel, it leads to an inhomogeneous equation for the scattering solution at energy $E = \hbar^2 k^2/2m$ of the form

$$(E - \mathbf{H})\vec{u} = \vec{h} \ , \tag{10}$$

where $h(i) = -tu(N_n + 1)\delta_{i,N_n}$. Inverting (10) we find

$$\frac{u(N_n)}{u(N_n + 1)} = -tG(E)_{N_n,N_n} \tag{11}$$

where $G(E) = (E - \mathbf{H})^{-1}$ is the Green's function matrix at energy E. Using Eq. (9), we obtain an expression for the scattering amplitude

$$S_{nn} = e^{-ik(2N_n)\Delta r} \left[\frac{1 + tG(E)_{N_n,N_n}e^{-ik\Delta r}}{1 + tG(E)_{N_n,N_n}e^{ik\Delta r}} \right] \ . \tag{12}$$

The elastic and reaction cross sections are calculated from S_{nn} using

$$\begin{aligned}
\sigma_{\text{el}} &= \frac{\pi}{k^2} \left| 1 - S_{nn} \right|^2 \ , \\
\sigma_{\text{r}} &= \frac{\pi}{k^2} \left(1 - \left| S_{nn} \right|^2 \right) \ .
\end{aligned} \tag{13}$$

In our model, the reaction cross section is the neutron capture cross section, i.e., $\sigma_{\text{r}} = \sigma_{\text{capture}}$.

III. NUMERICAL METHOD FOR FINDING THE RESONANCES

In addition to the elastic and capture cross sections, we are interested in finding the energies and widths of the compound nucleus resonances. The complex resonance wavenumbers k_r are poles of the S matrix. Thus, in principle, we could find the resonance solutions by finding the wavenumbers at which the denominator on the r.h.s. of Eq. (12) is zero, i.e., by solving the equation

$$1 + tG(E)_{N_n,N_n}e^{ik\Delta r} = 0 \tag{14}$$

However, near a resonance the Green's function $G(E)$ becomes singular and, in practice, the numerical solution of Eq. (14) is challenging.

As discussed in the main text, we use a mathematically equivalent method to find the resonances that is easier to implement in practice. We impose the outgoing wave boundary condition for a resonance, $u(r) \to B(k)e^{ikr}$ at large r when k is complex. This leads to the condition

$$u(N_n + 1) = u(N_n)e^{ik\Delta r} \ . \tag{15}$$

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[1] In general we are interested in the S matrix but in the present model this matrix contains only a single number S_{nn} (since the gamma decay is treated by assigning an imaginary part to the internal state energies).

Combining this boundary condition with the regularity condition $u(0) = 0$ and with the Schrödinger equation yields the nonlinear eigenvalue problem

$$\mathbf{M}(k)\vec{u} = \left(\mathbf{H} - te^{ik\Delta r}\mathbf{C} - E\right)\vec{u} = 0 \tag{16}$$

where $\mathbf{C}_{ij} = \delta_{i,j}\delta_{i,N_n}$ and k is assumed to be complex (in contrast to the S-matrix calculation in which k is assumed real and positive).

We solve (16) by iterations, following a method described in Ref. [1]. We start from an initial guess k_g that is close to the resonance solution k_r. Taking $\vec{u}$ to belong to the kernel of $\mathbf{M}(k_r)$ and linearizing $\mathbf{M}(k_r)$ about k_g, we obtain

$$\mathbf{M}(k_g)\vec{u} = (k_g - k_r)\frac{d\mathbf{M}}{dk}\bigg|_{k=k_g}\vec{u}\,, \tag{17}$$

where $\mathbf{M}'(k_g) = \frac{d\mathbf{M}}{dk}\big|_{k=k_g}$ is the derivative matrix. Eq. (17) defines a generalized eigenvalue problem that can be easily solved since the derivative of $\mathbf{M}(k)$ is diagonal

$$\mathbf{M}'(k_g) = -i\Delta rte^{ik\Delta r}\mathbf{C} - \hbar^2 k/m\,. \tag{18}$$

The complex eigenvalues λ of the matrix $[\mathbf{M}'(k_g)]^{-1}\mathbf{M}(k_g)$ correspond to solutions for $k_g - k_r$. We choose the minimal modulus eigenvalue $\bar{\lambda}$ and obtain the iterative condition

$$k_{g+1} = k_g - \bar{\lambda}\,. \tag{19}$$

We repeat this procedure until Eq. (16) is satisfied or until a preset maximal number of iterative steps is taken. Our condition that (16) is satisfied is that $\mathbf{M}(k_r)$ has an eigenvalue with absolute value less than a numerical tolerance $\epsilon = 10^{-12}$.

To use the iterative method, we must find initial guesses $\{k_g\}$ that are sufficiently close to the resonance solutions. We note that the real and imaginary parts of $k\Delta r$ are small for the compound nucleus resonances. Therefore, we may well approximate the resonance solutions of (16) by expanding the exponential $e^{ik\Delta r}$ to quadratic order in $k\Delta r$. Doing this expansion yields the quadratic eigenvalue problem

$$\left(\mathbf{U_0} - k\mathbf{U_1} - k^2\mathbf{U_2}\right)\vec{u} = 0\,, \tag{20}$$

where $\mathbf{U_0} = \mathbf{H} - t\mathbf{C}$, $\mathbf{U_2} = it\Delta r\mathbf{C}$, and $\mathbf{U_3} = (\hbar^2/2m) - (t\Delta r^2/2)\mathbf{C}$. Eq. (20) can be solved by linearization [2]. We impose the additional condition

$$\vec{v} = k\vec{u}\,, \tag{21}$$

and rewrite (20) as

$$\mathbf{U_0}\vec{u} - \mathbf{U_1}\vec{v} - k\mathbf{U_2}\vec{v} = 0\,. \tag{22}$$

Combining conditions (21) and (22) yields a generalized eigenvalue problem

$$\begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{U_0} & -\mathbf{U_1} \end{pmatrix}\begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} - k\begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{U_2} \end{pmatrix}\begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} = 0 \tag{23}$$

Thus, we have simplified the problem by doubling the size of the matrices involved. It is straightforward to solve Eq. (23) because the matrix in the second term on the l.h.s. is invertible and diagonal. Therefore, we obtain $2N$ possible guesses $\{k_g\}$ (where N is the dimension of $\mathbf{M}(k)$) as the solutions of the standard eigenvalue problem

$$\left[\begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{U_2}^{-1}\mathbf{U_0} & -\mathbf{U_2}^{-1}\mathbf{U_1} \end{pmatrix} - k\right]\begin{pmatrix} \vec{u} \\ \vec{v} \end{pmatrix} = 0\,. \tag{24}$$

We select guesses that correspond to the middle of the resonance spectrum. In practice, we decompose the total number of internal states $N_c = N_{\text{int}} + 2N_{\text{buf}}$, where N_{int} is the number of resonances that we take as data from each realization and N_{buf} is the number of "buffer" internal states placed at either end of the spectrum and not taken as data. For example, in the results shown in the paper, we have $N_c = 240$ total internal states, with $N_{\text{int}} = 160$ and $N_{\text{buf}} = 40$. Thus, we choose the N_{int} initial guesses that solve Eq. (24) in the middle of the internal state spectrum, disregarding the $2N_{\text{buf}}$ resonances at the upper and lower ends. These initial guesses converge to resonances in the middle of the resonance spectrum. This selection method allows us to avoid the numerical artifacts that originate in the finite band of internal states (see below).

IV. Δr DEPENDENCE OF THE AVERAGE COUPLING

Here we discuss the explicit Δr dependence introduced in the coupling matrix (6). This scaling is necessary to obtain convergence of the scattering amplitude S_{nn} in the continuum limit $\Delta r \to 0$. Table I shows the results for the real and imaginary parts of S_{nn} as a function of Δr at neutron energy of 8 keV, averaged over 20 runs of the code for a fixed Woods-Saxon depth $V_0 = -44.54$ MeV and average coupling $v_0 = 11$ keV-fm$^{1/2}$. We observe some weak Δr dependence, but the changes in $\bar{S}_{nn}$ are much smaller compared to the changes in Δr.

Δr (fm)	Re $\bar{S}_{nn}$	Im $\bar{S}_{nn}$
0.5	0.91	-0.39
0.2	0.88	-0.43
0.1	0.88	-0.44
0.05	0.87	-0.44

TABLE I: Real and imaginary parts of the average scattering amplitude $\bar{S}_{nn}$ at 8 keV neutron energy. The average is taken over 20 runs of the code. We use the baseline values $V_0 = -44.54$ MeV and $v_0 = 11$ keV-fm$^{1/2}$. The length of the neutron channel mesh is $N_n \Delta r = 30$ fm.
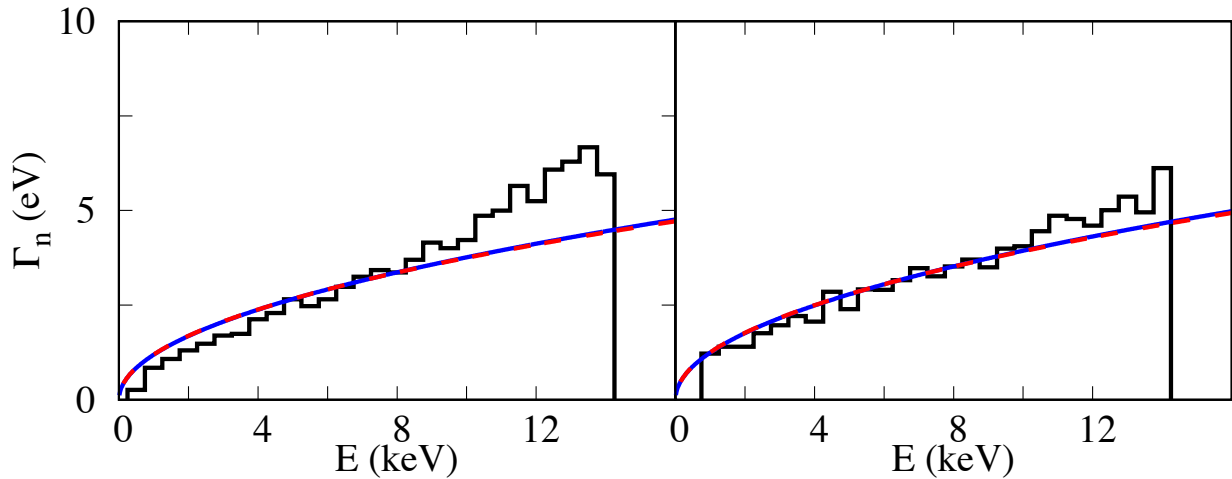
V. FINITE BANDWIDTH EFFECTS

FIG. 1: The average neutron resonance width $\bar{\Gamma}_n$ as a function of energy (solid black histograms) is compared with the $\sqrt{E}$ behavior (blue solid lines) and the neutron probability density $u_E^2(r_e)$ (red dashed line) for 240 (left panel) and 560 (right panel) internal states.

Here, we discuss the apparent deviation of the calculated average neutron width $\bar{\Gamma}_n$ from the neutron probability density $u_E^2(r_e)$ and from the $\sqrt{E}$ form in model M3 as shown in the bottom left panel of Fig. 2 in the main text. In our model, the internal states have a finite band width. As the average coupling strength increases, the strength is concentrated more in the edge of the band, distorting the shape of the function $\bar{\Gamma}_n(E)$. In a physical compound nucleus, there are additional states above our band edge. In Fig. 1, we compare $\bar{\Gamma}_n$ with the $\sqrt{E}$ behavior and the neutron probability density for 240 internal states (which corresponds to model M3 shown in the paper), and for 560 internal states. With more internal states, the apparent deviation essentially disappears. The reduced chi-squared value for the case of 560 internal states for reduction B is $\chi_r^2 = 1.1$, indicating that the PTD fits well the reduced widths extracted with the $\sqrt{E}$ assumption. We conclude that the apparent deviation of the average neutron width

from $\sqrt{E}$ in model M3 is a purely numerical effect.

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