Comparison of methods for calculating decay lifetimes

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A simple scattering model is used to test alternative methods for calculating decay lifetimes, or equivalently, resonance widths. We consider the scattering of s-wave particles by a square well with a square barrier. Exact values for resonance energies and resonance widths are compared with values calculated from Wigner-Weisskopf perturbation theory and from the Garside-MacDonald projection operator formalism. The Garside-MacDonald formalism gives essentially exact results while the predictions of the Wigner-Weisskopf formalism are fairly poor.

[RADIOACTIVITY Methods for calculating lifetime for decay by barrier penetration tested on a soluble model.]

I. INTRODUCTION

There has been a long standing discrepancy between the calculated values of α-decay lifetimes and the measured values notwithstanding the fact that the relative values of the lifetimes for decays to levels of the same nucleus agree rather well with the calculated ratios.[1] Fliessbach[2] has suggested that this discrepancy is due to the failure of the theory to correctly include exchange between the nucleons in the α and the nucleons in the daughter nucleus. He has proposed a modification of the Wigner-Weisskopf expression[3] for the decay lifetime to account for nucleon exchange. An alternative approach for including exchange effects in the theory of radioactivity has been given by the author[4] and is based on the Garside-MacDonald projection operator formalism.[5]

In light of the complexities of the many-body versions of the decay formalisms and the drastic approximations required for their implementation, we felt that it would be worthwhile to check the capability of the conventional theory to treat barrier penetration and to see if there is any reason to prefer the Wigner-Weisskopf (WW) method over the Garside-MacDonald (GM) formalism. We have analyzed the scattering of s-wave particles by a square well inside a square barrier. By fitting a Breit-Wigner resonance form to the energy dependence of the exact phase shift we have determined the exact resonance energy and exact resonance width for a number of cases. The decay lifetime is just $\hbar$ divided by the resonance width. These were then compared to values calculated by means of the WW method, the GM method, and two approximate versions of the GM method.

Most methods of calculating resonance energies and resonance widths are based on either the WW method or the GM method. A recent review of several such methods is provided by Jackson and Rhoades-Brown.[6] Some examples of work based on the GM method are listed in Ref. 7. Some examples, of work based on the WW method are given in Ref. 8. Reference 9 is one of the few treatments not closely related to either the WW method or the GM method.

The GM method was found to give consistently better results for both the resonance width and the resonance energy. This is perhaps to be expected inasmuch as the WW method does seem to require rather drastic approximations in its derivation while the GM method is essentially exact. The two approximate versions of the GM method that were tested were found to give good results for the resonance widths.

In Sec. II the scattering model is presented and the method for calculating the exact resonance energy and resonance width is described. The WW method is given in Sec. III, and the GM method is given in Sec. IV. The results of the calculation are presented in Sec. V, and the conclusions are outlined in Sec. VI.

II. RESONANCES OF A SQUARE WELL WITH A SQUARE BARRIER

Consider the scattering of a particle of zero angular momentum by a square potential well with a square barrier. The potential energy is taken to be

$$\begin{aligned} V &= -V_W, \quad 0<r<R_W \\ &= V_B, \quad R_W<r<R_B \\ &= 0, \quad R_B<r. \end{aligned} \tag{1}$$

The scattering phase shift is

$$\delta = -kR_B - \tan^{-1}\mathfrak{K}, \tag{2a}$$

$$\mathcal{K} = -\frac{k[\kappa \tan KR_W + K \tanh\kappa(R_B - R_W)]}{\kappa[K + \kappa \tan(KR_W)\tanh\kappa(R_B - R_W)]}\ , \tag{2b}$$

$$K^2 = k^2 + 2m\hbar^{-2}V_W, \tag{2c}$$

$$\kappa^2 = 2m\hbar^{-2}V_B - k^2, \tag{2d}$$

where

$$E = \hbar^2 k^2/2m \tag{3}$$

is the energy of the particle. The collision function is defined by

$$\mathcal{S} = e^{2i\delta} = \mathcal{S}_a(1 - i\mathcal{K})/(1 + i\mathcal{K}), \tag{4a}$$

$$\mathcal{S}_a = e^{2i\delta_a}, \tag{4b}$$

$$\delta_a = -kR_B. \tag{4c}$$

The transition amplitude is then given by

$$\mathcal{T} = (1 - \mathcal{S})/2i$$
$$= \mathcal{T}_a + \mathcal{S}_a\mathcal{K}/(1 + i\mathcal{K}), \tag{5a}$$

where

$$\mathcal{T}_a = (1 - \mathcal{S}_a)/2i = -e^{i\delta_a}\sin\delta_a, \tag{5b}$$

$$\mathcal{K} = -\tan(\delta - \delta_a). \tag{5c}$$

For the energy E sufficiently near a pole Ξ_0 of the reactance $\mathcal{K}$, the reactance can be approximated by the sum of a pole term and a constant background term.

$$\mathcal{K} \approx \bar{\mathcal{K}} + \tfrac{1}{2}\Gamma_0/(E - \Xi_0). \tag{6a}$$

Substituting Eq. (6a) into Eq. (5a) gives the Breit-Wigner expression for the transition amplitude,

$$\mathcal{T} = \bar{\mathcal{T}} + \frac{\bar{\mathcal{S}}\,\tfrac{1}{2}\Gamma}{E - \Xi + i\,\tfrac{1}{2}\Gamma}\ , \tag{6b}$$

where

$$\bar{\mathcal{S}} = \mathcal{S}_a(1 - i\bar{\mathcal{K}})/(1 + i\bar{\mathcal{K}}), \tag{6c}$$

$$\bar{\mathcal{T}} = \mathcal{T}_a + \mathcal{S}_a\bar{\mathcal{K}}/(1 + i\bar{\mathcal{K}}), \tag{6d}$$

$$\Gamma = \Gamma_0/(1 + \bar{\mathcal{K}}^2), \tag{6e}$$

$$\Xi = \Xi_0 - \tfrac{1}{2}\bar{\mathcal{K}}\Gamma_0/(1 + \bar{\mathcal{K}}^2). \tag{6f}$$

Equations (6e) and (6f) relate the resonance energy Ξ and resonance width Γ to the pole energy Ξ_0 and pole residue $\frac{1}{2}\,I_0$. By superposing scattering states with energies in the vicinity of Ξ one can form a wave packet corresponding to a metastable state of mean life $\tau = \hbar/\Gamma$.

The pole and residue of the reactance were found by searching for the zero of $1/\mathcal{K}$ and then finding the slope of $1/\mathcal{K}$ at the zero:

$$(1/\mathcal{K})_{E=\Xi_0} = 0, \tag{7a}$$

$$\left[\frac{d}{dE}(1/\mathcal{K})\right]_{E=\Xi_0} = 2/\Gamma_0. \tag{7b}$$

The background reactance was deduced from the second derivative of $1/\mathcal{K}$:

$$\left[\frac{d^2}{dE^2}(1/\mathcal{K})\right]_{E=\Xi_0} = -8\bar{\mathcal{K}}/\Gamma_0^2. \tag{7c}$$

The widths Γ and energies Ξ calculated by means of Eqs. (6), (7), and (2) will be referred to as the "exact" resonance widths and energies.

III. THE WIGNER-WEISSKOPF (WW) METHOD

We seek an expression for the wave packet representing a metastable state. The wave packet ψ is the solution of the time dependent Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V\right)\psi = H\psi. \tag{8}$$

Initially, at $t = 0$, ψ is equal to Φ, the "resonant state." The wave function Φ is taken to be a bound state eigenfunction of H_0, where

$$H_0 = H - U, \tag{9a}$$

$$U = V_B, \quad 0 < r < R_B$$
$$= 0, \quad R_B < r. \tag{9b}$$

H_0 is identical to H except for the fact that a constant potential energy equal to the barrier height has been subtracted from H in the interior region, $r < R_B$. Thus Φ has the same shape in the interior region as does the scattering eigenfunction ψ_Ξ of H at resonance.

We express the wave packet ψ as a superposition of the eigenstates of H_0,

$$\psi = a(t)\Phi + \int dE\, b_E(t)\phi_E, \tag{10a}$$

$$H_0\Phi = E_0\Phi, \quad (E_0 < 0), \tag{10b}$$

$$H_0\phi_E = E\phi_E, \quad (E > 0). \tag{10c}$$

The initial condition requires that

$$a(t = 0) = 1, \quad b_E(t = 0) = 0. \tag{11}$$

Let the normalization factors be chosen such that

$$\langle\Phi\,|\Phi\rangle = 1, \tag{12a}$$

$$\langle\phi_E\,|\phi_{E'}\rangle = \delta(E - E'). \tag{12b}$$

We note that

$$\langle\phi_E\,|\Phi\rangle = 0. \tag{12c}$$

In Eq. (10) we are ignoring the contribution of any bound state of H_0 other than Φ.

Substitution of the wave packet ψ into the Schrödinger equation gives

$$i\hbar\dot{a} = a\langle\Phi\,|H\,|\Phi\rangle + \int dE' b_{E'}\langle\Phi\,|H\,|\phi_{E'}\rangle\,, \tag{13a}$$

$$i\hbar\dot{b}_E = a\langle\phi_E|H|\Phi\rangle + \int dE' b_{E'}\langle\phi_E|H|\phi_{E'}\rangle . \quad (13b)$$

Now let us set

$$\langle\Phi|H|\Phi\rangle = E_0 + \langle\Phi|U|\Phi\rangle = E_1, \quad (14a)$$

$$\langle\phi_E|H|\phi_{E'}\rangle = E\delta(E - E'), \quad (14b)$$

so that Eq. (13) becomes

$$i\hbar\dot{a} = aE_1 + \int dE' b_{E'}\langle\Phi|U|\phi_{E'}\rangle , \quad (15a)$$

$$i\hbar\dot{b}_E = a\langle\phi_E|U|\Phi\rangle + Eb_E . \quad (15b)$$

In Eq. (14b) the continuum-continuum transition amplitudes $\langle\phi_{E'}|U|\phi_E\rangle$, $E' \neq E$ have been neglected.

Next we set

$$a = \exp(-i\mathcal{E}t/\hbar), \quad (16a)$$

$$\mathcal{E} = \Lambda + \Delta - i\tfrac{1}{2}\Gamma = \Xi - i\tfrac{1}{2}\Gamma, \quad (16b)$$

$$\Lambda = E_0 + V_B, \quad (16c)$$

where the level shift Δ, the approximate resonance energy Λ, and the resonance width Γ are real. Substitution into Eq. (15) gives

$$\Delta - i\tfrac{1}{2}\Gamma = e^{i\mathcal{E}t/\hbar}\int dE' b_{E'}\langle\Phi|U|\phi_{E'}\rangle + \langle\Phi|U|\Phi\rangle - V_B , \quad (17a)$$

$$i\hbar\dot{b}_E = Eb_E + e^{-i\mathcal{E}t/\hbar}\langle\phi_E|U|\Phi\rangle . \quad (17b)$$

The solution of Eq. (17b) is

$$b_E = \frac{\langle\phi_E|U|\Phi\rangle}{\mathcal{E} - E}(e^{-i\mathcal{E}t/\hbar} - e^{-iEt/\hbar}) . \quad (18)$$

Combining this with Eq. (17a) gives

$$\Delta - i\tfrac{1}{2}\Gamma = \int dE' \frac{|\langle\Phi|U|\phi_{E'}\rangle|^2}{\mathcal{E} - E'}(1 - e^{i(\mathcal{E}-E')t/\hbar}) + \langle\Phi|U|\Phi\rangle - V_B . \quad (19)$$

Now the assumption that Δ and Γ are much smaller than Λ is made. Then in the limit as t becomes very large,

$$\frac{1 - e^{i(\mathcal{E}-E)t/\hbar}}{\mathcal{E} - E} \approx \frac{\mathcal{P}}{\Lambda - E} - i\pi\delta(\Lambda - E) \quad (20)$$

so that

$$\Xi = E_0 + \mathcal{P}\int dE' \frac{|\langle\Phi|U|\phi_{E'}\rangle|^2}{\Lambda - E'} + \langle\Phi|U|\Phi\rangle , \quad (21a)$$

$$\Gamma = 2\pi|\langle\Phi|U|\phi_\Lambda\rangle|^2, \quad (21b)$$

where $\mathcal{P}$ denotes principal value. For sufficiently large values of $R_B - R_W$ and V_B it is a good approximation to set $\langle\Phi|U|\Phi\rangle$ equal to V_B.

For our model Φ and ϕ_E are the wave functions for an s-wave particle interacting with a square well W,

$$W = -V_W - V_B, \quad 0 < r < R_W$$
$$= 0, \quad R_W < r. \quad (22)$$

The required transition amplitude is easily evaluated.

$$\langle\Phi|U|\phi_E\rangle = V_B\int_0^{R_B} dr\,\Phi\phi_E$$
$$= -V_B\int_{R_B}^{\infty} dr\,\Phi\phi_E$$
$$= \frac{AV_B e^{-\kappa_0(R_B - R_W)}}{(\kappa_0^2 + k^2)}(\kappa_0\sin\theta + k\cos\theta) , \quad (23a)$$

$$\theta = kR_B + \delta_0, \quad (23b)$$

$$\delta_0 = -kR_W + \tan^{-1}\left(\frac{k}{K_0}\tan K_0 R_W\right) , \quad (23c)$$

$$A = \left[\frac{4m}{\pi\hbar^2 kR_W}\Big/\left(1 + \frac{1}{\kappa_0 R_W} + \frac{\kappa_0^2}{K_0^2} + \frac{\kappa_0}{K_0^2 R_W}\right)\right]^{1/2} , \quad (23d)$$

$$k = (2mE/\hbar^2)^{1/2}, \quad (23e)$$

$$\kappa_0 = (-2mE_0/\hbar^2)^{1/2}, \quad (23f)$$

$$K_0 = [2m(V_W + V_B + E_0)/\hbar^2]^{1/2} . \quad (23g)$$

An alternative version of the WW theory was tested. This version is in fact very similar to what is often done in practice. The alternative version of the WW theory consists in replacing the square well scattering function ϕ_E that appears in Eq. (21) and Eq. (23) by a scattering eigenfunction $\tilde{\psi}_E$ of the Hamiltonian $\tilde{H}$. $\tilde{H}$ is identical to H as given in Eqs. (8) and (1) except that the depth V_W of the square well is increased by a small amount which we arbitrarily chose to be 0.0201 $(V_W + E_0)$. This choice increases the wavenumber inside the well by one percent. Thus $\tilde{\psi}_E$ is essentially what the exact scattering wave function ψ_E would be "off resonance." To calculate the alternative version of the WW transition amplitudes we use Eq. (23a) with the square well phase shift δ_0 [Eq. (23c)] replaced by the off resonance value of the well plus barrier phase shift δ [Eq. (2a)].

The alternative version of the WW theory is hard to justify in the context of the WW formalism since the assumed orthogonality between the resonant state Φ and the newly chosen continuum state $\tilde{\psi}_E$ is lost. Nevertheless, we find that the alternative

version of the theory gives better results. Some justification for the alternative version will be provided by the GM formalism result.

IV. GARSIDE-MacDONALD (GM) METHOD

It has been noted that the transition amplitude is approximated by the Breit-Wigner expression shown in Eq. (6b) in the vicinity of a resonance. It is seen that the scattering amplitude is the sum of a resonant term and a nonresonant term. The resonant term is very small off resonance if the width of the resonance is very small. The GM method constructs an expression for the transition amplitude in which the resonant term is isolated and identified.

According to the Gell-Mann and Goldberger two potentials formula[10]

$$\mathcal{T} = \mathcal{T}_0 + \mathcal{S}_0\pi\langle\phi_E|T_E|\phi_E\rangle, \tag{24a}$$

$$\mathcal{S}_0 = e^{2i\delta_0} = 1 - 2i\mathcal{T}_0, \tag{24b}$$

$$T_E = U + UG_E T_E, \tag{25}$$

$$G_E = (E - H_0 + i\epsilon)^{-1}. \tag{26}$$

Here T is the transition operator and Eq. (25) is the Lippmann-Schwinger equation.[11] A projection operator method will be used to separate off the nonresonant part of T. This nonresonant part is defined by

$$\hat{T}_E = U + UPG_E\hat{T}_E, \tag{27a}$$

$$P = 1 - Q, \tag{27b}$$

$$Q = |\Phi\rangle\langle\Phi|, \tag{27c}$$

where the projection operator P acts to eliminate the resonant state contribution from the Green's function operator G_E. Now using Eq. (27a) to eliminate U from Eq. (25) gives the relationship we seek:

$$\begin{aligned} T_E &= \hat{T}_E + \hat{T}_E Q(E - H_0 - \hat{T}_E Q)^{-1}\hat{T}_E \\ &= \hat{T}_E + \hat{T}_E|\Phi\rangle(E - E_0 - \langle\Phi|\hat{T}_E|\Phi\rangle)^{-1}\langle\Phi|\hat{T}_E. \end{aligned} \tag{28}$$

Upon substitution of this result into Eq. (24) one finds

$$\mathcal{T} = \overline{\mathcal{T}} + \frac{\mathcal{S}_0\pi\langle\Phi|\hat{T}_E|\phi_E\rangle\langle\phi_E|\hat{T}_E|\Phi\rangle}{E - E_0 - \langle\Phi|\hat{T}_E|\Phi\rangle}, \tag{29a}$$

$$\overline{\mathcal{T}} = \mathcal{T}_0 + \mathcal{S}_0\pi\langle\phi_E|\hat{T}_E|\phi_E\rangle. \tag{29b}$$

This provides a separation of the transition operator into a nonresonant part and a resonant part. Equation (29) is exact while Eq. (6b) is valid only in the immediate vicinity of a resonance. Comparison of these two equations indicates that in the vicinity of a resonance

$$\pi\mathcal{S}_0\langle\Phi|\hat{T}_\Xi|\phi_\Xi\rangle\langle\phi_\Xi|\hat{T}_\Xi|\Phi\rangle \approx \mathcal{S}\tfrac{1}{2}\Gamma, \tag{30a}$$

$$E_0 + \langle\Phi|\hat{T}_\Xi|\Phi\rangle \approx \Xi - i\tfrac{1}{2}\Gamma. \tag{30b}$$

The above equations provide two alternative expressions for the resonance width. Consistency then requires

$$\overline{\mathcal{S}}^{-1}\mathcal{S}_0\langle\Phi|\hat{T}_\Xi|\phi_\Xi\rangle\langle\phi_\Xi|\hat{T}_\Xi|\Phi\rangle = -\mathrm{Im}\langle\Phi|\hat{T}_\Xi|\Phi\rangle. \tag{31}$$

We will show that this consistency relation is valid as a consequence of the unitarity requirement. If we set

$$\mathcal{T} = \overline{\mathcal{T}} + \overline{\mathcal{S}}\mathfrak{M}, \tag{32}$$

then the unitarity requirements,

$$\mathrm{Im}\mathcal{T} = -\mathcal{T}\mathcal{T}^* \quad \text{and} \quad \mathrm{Im}\overline{\mathcal{T}} = -\overline{\mathcal{T}}\,\overline{\mathcal{T}}^*, \tag{33}$$

imply

$$\mathrm{Im}\mathfrak{M} = -\mathfrak{M}\mathfrak{M}^*. \tag{34}$$

Thus,

$$\mathfrak{M} = Q/(1 + iQ), \quad \text{where } Q = Q^*. \tag{35}$$

As a matter of fact,

$$Q = (\mathcal{K} - \overline{\mathcal{K}})/(1 + \mathcal{K}\overline{\mathcal{K}}). \tag{36}$$

Comparison of Eq. (29a) with Eqs. (32) and (35) then leads to Eq. (31).

Equation (30b) provides us with the GM theory expressions for the resonance energy and the decay width:

$$\Xi = E_0 + \mathrm{Re}\langle\Phi|\hat{T}_\Lambda|\Phi\rangle, \tag{37a}$$

$$\Gamma = -2\,\mathrm{Im}\langle\Phi|\hat{T}_\Lambda|\Phi\rangle, \tag{37b}$$

where Ξ has been replaced by Λ on the right on the assumption that Δ is small. To evaluate these expressions one must solve the integral equation for the nonresonant scattering operator, Eq. (27). Such calculations were done and were found to give satisfactory results.

An alternative form of Eq. (37) is found by replacing $\hat{T}$ by the formal solution of Eq. (27):

$$\begin{aligned} \langle\Phi|\hat{T}_E|\Phi\rangle &= \langle\Phi|U + UP(E - H_0 - PUP + i\epsilon)^{-1}PU|\Phi\rangle \\ &= \langle\Phi|U + \sum\!\!\!\!\!\!\int dE' \frac{UP|\hat{\phi}_{E'}\rangle\langle\hat{\phi}_{E'}|PU|\Phi\rangle}{E - E' + i\epsilon} \\ &= \langle\Phi|U + \mathcal{P}\sum\!\!\!\!\!\!\int dE' \frac{UP|\hat{\phi}_{E'}\rangle\langle\hat{\phi}_{E'}|PU|\Phi\rangle}{E - E'} \\ &\quad - i\pi\langle\Phi|UP|\hat{\phi}_E\rangle\langle\hat{\phi}_E|PU|\Phi\rangle. \end{aligned} \tag{38}$$

Here $\hat{\phi}_E$ is the solution of

$$(E - H_0 - PUP)\hat{\phi}_E = 0 \tag{39}$$

and $\sum\!\!\!\!\!\!\int dE'$ means a sum over discrete spectrum eigenstates as well as an integral over the contin-

uum. Next substitute Eq. (38) into Eq. (37):

$$\Xi = E_0 + \langle\Phi|U|\Phi\rangle + \mathcal{P}\int dE' \frac{\langle\Phi|UP|\hat{\phi}_{E'}\rangle\langle\hat{\phi}_{E'}|PU|\Phi\rangle}{\Lambda - E'}, \tag{40a}$$

$$\Gamma = 2\pi\langle\Phi|UP|\hat{\phi}_\Lambda\rangle\langle\hat{\phi}_\Lambda|PU|\Phi\rangle. \tag{40b}$$

Inasmuch as P commutes with H_0, it will be true that $P\hat{\phi}_E$ equals $\hat{\phi}_E$ except if there is a bound state with $E = E_0$. If such an eigenstate $\hat{\phi}_{E_0}$ exists, then $\hat{\phi}_{E_0} + A\Phi$ with A an arbitrary constant is also an eigenstate with eigenvalue E_0. Let A be chosen so that the resultant state is orthogonal to Φ. Then the projection operator P may be deleted from Eq. (40):

$$\Xi = E_0 + \langle\Phi|U|\Phi\rangle + \mathcal{P}\int dE' \frac{|\langle\Phi|U|\hat{\phi}_{E'}\rangle|^2}{\Lambda - E'}, \tag{41a}$$

$$\Gamma = 2\pi|\langle\Phi|U|\hat{\phi}_\Lambda\rangle|^2. \tag{41b}$$

This form of the GM theory result is very similar to the WW theory result shown in Eq. (21). In the GM result the contribution to the resonance energy of possible bound eigenstates of the nonresonant Hamiltonian are included. The principle differ-

TABLE I. Level shifts and resonance widths for s-wave resonances of a square well with a square barrier. The shifts and widths for a series of barrier thicknesses calculated by several methods are compared. The methods are the exact method (EX), the Wigner-Weisskopf method (WW), the alternative Wigner-Weisskopf method (AW), the Garside-MacDonald method (GM), and the alternative Garside-MacDonald method (AG). The mass of the incident particle is $m = 1.0$ u. The well radius is $R_W = 3.5$ fm. The barrier height is $V_B = 40.0$ MeV. The other parameters are V_W = well depth, $R_B - R_W$ = well thickness, N = number of nodes in the resonant state wave function and Λ = approximate resonance energy. The quantities calculated are $\Delta = \Xi - \Lambda$ = level shift, and Γ = resonance width. Energies are in MeV and lengths are in fm. The notation $A - n$ means $A \times 10^{-n}$.

$N=1$	$V_W=10.8$		$\Lambda=1.07$						
R_B-R_W	Δ(EX)	Δ(WW)	Δ(AW)	Δ(GM)	Γ(EX)	Γ(WW)	Γ(AW)	Γ(GM)	Γ(AG)
2.0	−0.255 − 1	−0.630 − 2	−0.690 − 2	−0.248 − 1	0.171 − 1	0.353 − 1	0.141 − 1	0.164 − 1	0.161 − 1
3.0	−0.166 − 2	−0.364 − 3	−0.451 − 3	−0.166 − 2	0.113 − 2	0.456 − 2	0.112 − 2	0.113 − 2	0.112 − 2
4.0	−0.109 − 3	−0.196 − 4	−0.294 − 4	−0.106 − 3	0.740 − 4	0.457 − 3	0.740 − 4	0.753 − 4	0.745 − 4
5.0	−0.750 − 5	−0.937 − 6	−0.192 − 5	−0.429 − 5	0.483 − 5	0.389 − 4	0.483 − 5	0.482 − 5	0.486 − 5
6.0	−0.879 − 6	−0.351 − 7	−0.890 − 8		0.316 − 6	0.292 − 5	0.316 − 6	0.304 − 6	0.307 − 6
7.0					0.206 − 7	0.197 − 6	0.206 − 7	0.214 − 7	0.207 − 7
8.0					0.135 − 8	0.120 − 7	0.135 − 8	0.127 − 8	0.131 − 8
9.0					0.874 − 10	0.655 − 9	0.879 − 10	0.883 − 10	0.839 − 10
10.0					0.527 − 11	0.312 − 10	0.574 − 11	0.556 − 11	0.561 − 11
$N=1$	$V_W=8.0$		$\Lambda=3.75$						
R_B-R_W	Δ(EX)	Δ(WW)	Δ(AW)	Δ(GM)	Γ(EX)	Γ(WW)	Γ(AW)	Γ(GM)	Γ(AG)
2.0	−0.266 − 1	−0.872 − 2	−0.902 − 2	−0.265 − 1	0.380 − 1	0.688 − 1	0.304 − 1	0.359 − 1	0.347 − 1
3.0	−0.191 − 2	−0.596 − 3	−0.648 − 3	−0.189 − 2	0.274 − 2	0.757 − 2	0.270 − 2	0.265 − 2	0.265 − 2
4.0	−0.137 − 3	0.398 − 4	−0.466 − 4	−0.137 − 3	0.197 − 3	0.561 − 3	0.197 − 3	0.199 − 3	0.196 − 3
5.0	−0.963 − 5	0.259 − 5	−0.335 − 5	−0.954 − 5	0.142 − 4	0.283 − 4	0.142 − 4	0.140 − 4	0.142 − 4
6.0	−0.507 − 6	0.163 − 6	−0.228 − 6	0.000	0.102 − 5	0.809 − 6	0.102 − 5	0.948 − 6	0.101 − 5
7.0					0.731 − 7	0.326 − 8	0.731 − 7	0.766 − 7	0.746 − 7
8.0					0.525 − 8	0.135 − 8	0.525 − 8	0.485 − 8	0.505 − 8
9.0					0.377 − 9	0.487 − 9	0.377 − 9	0.388 − 9	0.377 − 9
10.0					0.270 − 10	0.663 − 10	0.271 − 10	0.249 − 10	0.258 − 10
$N=2$	$V_W=40.0$		$\Lambda=9.40$						
R_B-R_W	Δ(EX)	Δ(WW)	Δ(AW)	Δ(GM)	Γ(EX)	Γ(WW)	Γ(AW)	Γ(GM)	Γ(AG)
2.0	−0.622 − 1	0.348 − 1	−0.374 − 1	−0.283 − 1	0.192 − 0	0.157 − 0	0.167 − 0	0.194 − 0	0.192 − 0
3.0	−0.541 − 2	0.294 − 2	−0.332 − 2	−0.217 − 2	0.172 − 1	0.911 − 3	0.170 − 0	0.170 − 1	0.172 − 1
4.0	−0.478 − 3	−0.246 − 3	−0.296 − 3	−0.201 − 3	0.154 − 2	0.445 − 3	0.153 − 2	0.152 − 2	0.152 − 2
5.0	−0.405 − 4	−0.202 − 4	−0.263 − 4	−0.148 − 4	0.137 − 3	0.158 − 3	0.137 − 3	0.142 − 3	0.138 − 3
6.0	−0.167 − 5	0.165 − 5	−0.230 − 5	−0.477 − 6	0.122 − 4	0.159 − 4	0.122 − 4	0.116 − 4	0.121 − 4
7.0					0.108 − 5	0.560 − 6	0.108 − 5	0.106 − 5	0.106 − 5
8.0					0.963 − 7	0.271 − 10	0.963 − 7	0.967 − 7	0.966 − 7
9.0					0.857 − 8	0.476 − 8	0.857 − 8	0.834 − 8	0.798 − 8
10.0					0.759 − 9	0.101 − 8	0.762 − 9	0.765 − 9	0.760 − 9

ence between the two formalisms is that in the WW theory continuum eigenstates of H_0 are used whereas in the GM theory the continuum eigenstates of $\hat{H}=H_0+PUP$ are used. In both cases the continuum eigenstates are orthogonal to the resonant state Φ. However, for energies slightly off resonance, the eigenstate of $\hat{H}$ will be very nearly identical to the eigenstate of the exact Hamiltonian H while the eigenstate of H_0 will be quite different. If being similar to the exact continuum wave function off resonance is more important in this analysis than maintaining strict orthogonality to the resonant state, then the GM formalism provides some justification for what we have called the alternative version of the WW theory.

The transition amplitude appearing in Eq. (41) can be evaluated in the same way as the WW theory amplitudes were evaluated. The result is given by Eq. (23) with the H_0 phase shift δ_0 replaced by a phase shift calculated from $\hat{H}=H_0+PUP$. There is an approximation involved in doing this. In getting the expression shown in Eq. (23a) it was assumed that the asymptotic form of ϕ_E is valid down to a radius of R_B. This is true for ϕ_E but only approximately true for $\hat{\phi}_E$ because the range of PUP extends slightly beyond R_B.

The GM theory resonance energy and resonance width were evaluated by first solving the integral equation for the nonresonant transition operator. For evaluation of Eq. (37) the following expressions were used

$$\langle\Phi|\hat{T}_\Lambda|\Phi\rangle=\hat{t}_0, \tag{42a}$$

$$\hat{t}_0=\langle\Phi|U|\Phi\rangle+\sum\!\!\!\!\!\!\int dE'\,\frac{\langle\Phi|UP|\phi_{E'}\rangle\hat{t}_{E'}}{\Lambda-E'+i\epsilon}, \tag{42b}$$

$$\hat{t}_E=\langle\phi_E|U|\Phi\rangle+\sum\!\!\!\!\!\!\int dE'\,\frac{\langle\phi_E|UP|\phi_{E'}\rangle\hat{t}_{E'}}{\Lambda-E'+i\epsilon}, \tag{42c}$$

$$(E-H_0)\phi_E=0. \tag{42d}$$

We will refer to this as the GM theory method. To evaluate Eq. (41) we used Eq. (23) with the phase shift δ_0 replaced by $\hat{\delta}$, where

$$\hat{\delta}=\tan^{-1}\left(\frac{\mathrm{Im}\hat{\tau}_\Lambda}{\mathrm{Re}\hat{\tau}_\Lambda}\right)+\delta_0, \tag{43a}$$

$$\hat{\tau}_E=\langle\phi_E|U|\phi_\Lambda\rangle+\sum\!\!\!\!\!\!\int dE'\,\frac{\langle\phi_E|UP|\phi_{E'}\rangle}{\Lambda-E'+i\epsilon}\hat{\tau}_{E'} \tag{43b}$$

Equation (43a) is derived by setting

$$\overline{\tau}=-e^{i\hat{\delta}}\sin\hat{\delta} \tag{44}$$

in Eq. (29b) and finding that

$$\langle\phi_E|\hat{T}_E|\phi_E\rangle=-e^{i(\hat{\delta}-\delta_0)}\sin(\hat{\delta}-\delta_0)/\pi=\hat{\tau}_E. \tag{45}$$

This second method of doing the GM theory calculation will be called the alternative GM theory method. The alternative GM theory method and the alternative WW theory method are both approximate versions of the GM theory.

V. RESULTS OF THE CALCULATION

The results of three series of calculations are reported here. The three series are distinguished by the value of the approximate resonance energy $\Lambda=E_0+V_B$, the values being 1.07 MeV for series a, 3.75 MeV for series b, and 9.40 MeV for series c. The mass of the incident particle was taken to be 1.0 u. The cases within each series are disting-

TABLE II. Level shifts and resonance widths for s-wave resonances of a square well with a square barrier. Comparison is made of the shifts and widths calculated from transition operators evaluated using several choices for NMP = the number of Gaussian points used to discretize the integral equation. The methods used are the Garside-MacDonald method (GM) and the alternative Garside-MacDonald method (AG). The mass of the indident particle is $m=1.0$ u. The well radius is $R_W=3.5$ fm. The barrier height is $V_B=40.0$ MeV. The other parameters are V_W = well depth, R_B-R_W = well thickness, N = number of nodes in the resonant state wave function, and Λ = approximate resonance energy. The quantities calculated are $\Delta=\Xi-\Lambda$ = level shift and Γ = resonance width. Energies are in MeV and lengths are in fm. The notation $A-n$ means $A\times10^{-n}$

$N=2$		$V_W=40.0$			$\Lambda=9.4$				
		$R_B-R_W=2$			$R_B-R_W=5$			$R_B-R_W=8$	
NMP	Δ(GM)	Γ(GM)	Γ(AG)	Δ(GM)	Γ(GM)	Γ(AG)	Γ(GM)	Γ(AG)
20	−0.262 − 1	0.190 − 0	0.191 − 0	−0.114 − 4	0.138 − 3	0.138 − 3	0.927 − 7	0.920 − 7
28	−0.283 − 1	0.190 − 0	0.192 − 0	−0.148 − 4	0.142 − 3	0.138 − 3	0.967 − 7	0.966 − 7
36	−0.280 − 1	0.191 − 0	0.191 − 0	−0.143 − 4	0.138 − 3	0.136 − 3	0.987 − 7	0.959 − 7
44	−0.272 − 1	0.188 − 0	0.190 − 0	−0.148 − 4	0.140 − 3	0.137 − 3	0.962 − 7	0.954 − 7
56	−0.301 − 1	0.194 − 0	0.191 − 0	−0.119 − 4	0.133 − 3	0.136 − 3	0.958 − 7	0.966 − 7
68	−0.285 − 1	0.191 − 0	0.191 − 0	−0.114 − 4	0.134 − 3	0.136 − 3	0.970 − 7	0.966 − 7
80	−0.292 − 1	0.190 − 0	0.190 − 0	−0.114 − 4	0.135 − 3	0.136 − 3	0.961 − 7	0.965 − 7
		Δ(EX) = 0.622 − 1			Δ(EX) = −0.405 − 4			Γ(EX) = 0.963 − 7	
		Γ(EX) = 0.192 − 0			Γ(EX) = 0.137 − 3				

uished by the choice of the barrier thickness $T_B = R_B - R_W$ which ranged between 2 and 10 fm. This produced for each series a range of values for resonance widths that went from about 0.1 to about 10^{-11} MeV. The calculated values for the level shifts proved erratic for values less than about 10^{-5} MeV and so are shown for the smaller barrier thicknesses only. The results are displayed on Table I.

The widths given by the WW theory are generally in poor agreement with the exact widths. The widths given by the other three methods—the alternative WW theory, the GM theory, and the alternative GM theory—are in good agreement with each other and in good agreement with the exact widths. No very striking improvement is observed for the smaller widths as compared with the larger widths. The alternative WW theory widths seem to be slightly better than the GM theory widths except for the smallest value of the barrier thickness.

The relatively poor value of the alternative WW theory width at barrier thickness 2 fm is a consequence of the failure of our well depth alteration to get a completely nonresonant scattering wave function because the resonance width is very large. On the other hand, the fact that the GM theory and alternative GM theory do not do quite as well as the alternative WW theory for the other widths is a consequence of a certain amount of instability in the matrix inversion scheme used to solve the integral equation for the transition operator. This instability is demonstrated in Table II where some GM theory and alternative GM theory resonance widths and energy level shifts are given which were calculated from transition operators evaluated using different numbers of Gaussian points to discretize the integral equation. It is seen that as the number of Gaussian points assumes various values between 20 and 80 the calculated width oscillates back and forth around the correct value by as much as 6%. This instability may be related to the lack of smoothness of the square well and square potential barrier.

The level shifts that result from the GM theory calculation give good agreement with the exact level shifts for the cases in series a and series b while the WW theory and alternative WW theory level shifts do not. On the other hand, for the cases of series c the level shifts given by the three theories are in rough agreement with each other but are about half the exact value. We are at a loss to explain this outcome.

The alternative GM theory calculation of the level shift was not performed because it would have been too time consuming.

At this point we can make a remark about the approximation made in Eq. (37) of replacing the exact resonance energy Ξ by the approximate energy Λ. It is assumed that our expressions for the width Γ and level shift $\Delta = \Xi - \Lambda$ are essentially constant for variations of the energy of the order of magnitude of Δ about the value Λ. We have ver-

TABLE III. Resonance widths and resonance energies for s-wave resonances of a square well with a square barrier. Comparison is made of the resonances energies and widths calculated using several different choices for Λ = the approximate resonance energy. The values of Ξ = the resonance energy and Γ = the resonance width are calculated by the exact method (EX), the Garside-MacDonald method (GM), and the alternative Garside-MacDonald method (AG). The mass of the incident particle is 1.0 u. The well radius is $R_W = 3.5$ fm. The barrier height is $V_B = 40.0$ MeV. The other parameters are V_W = well depth, $R_B - R_W$ = well thickness, N = numbers of nodes in the resonant state wave function, and Λ = approximate resonance energy. Energies are in MeV and lengths are in fm. The notation $A-n$ means $A \times 10^{-n}$.

$N = 1 \quad V_W = 10.8 \quad R_B - R_W = 3.0$

Λ	Ξ(GM)	Γ(GM)	Γ(AG)
1.074 18	1.070 02	0.112 903 − 2	0.112 005 − 2
1.073 334	1.070 02	0.112 862 − 2	0.111 965 − 2
1.072 51	1.070 02	0.112 824 − 2	0.111 919 − 2
1.071 68	1.070 02	0.112 784 − 2	0.111 876 − 2
1.070 85	1.070 02	0.112 744 − 2	0.111 835 − 2
1.070 02	1.070 02	0.112 705 − 2	0.111 788 − 2
1.069 19	1.070 02	0.112 667 − 2	0.111 741 − 2
1.068 36	1.070 02	0.112 624 − 2	0.111 704 − 2
1.067 53	1.070 02	0.112 585 − 2	0.111 658 − 2

Ξ(EX) = 1.070 02 $\quad$ Γ(EX) = 0.113 239 − 2

$N = 2 \quad V_W = 40.0 \quad R_B - R_W = 2.0$

Λ	Ξ(GM)	Γ(GM)	Γ(AG)
9.460 83	9.370 90	0.193 655 − 0	0.192 611 − 0
9.429 73	9.370 60	0.193 971 − 0	0.192 411 − 0
9.398 63	9.370 28	0.194 270 − 0	0.192 263 − 0
9.367 52	9.369 96	0.194 566 − 0	0.192 080 − 0
9.336 42	9.369 64	0.194 853 − 0	0.191 893 − 0
9.305 32	9.369 32	0.195 128 − 0	0.191 697 − 0
9.274 22	9.369 00	0.195 389 − 0	0.191 496 − 0

Ξ(EX) = 9.336 42 $\quad$ Γ(EX) = 0.192 296 − 0

$N = 2 \quad V_W = 40.0 \quad R_B - R_W = 5.0$

Λ	Ξ(GM)	Γ(GM)	Γ(AG)
9.398 67	9.398 61	0.142 217 − 3	0.138 317 − 3
9.398 65	9.398 61	0.142 217 − 3	0.138 316 − 3
9.398 63	9.398 61	0.142 220 − 3	0.138 317 − 3
9.398 61	9.398 61	0.142 221 − 3	0.138 316 − 3
9.398 59	9.398.61	0.142 220 − 3	0.138 316 − 3
9.398 57	9.398 61	0.142 218 − 3	0.138 317 − 3
9.398 53	9.398 61	0.142 218 − 3	0.138 316 − 3

Ξ(EX) = 9.398 59 $\quad$ Γ(EX) = 0.136 624 − 3

ified this for all cases by evaluating our expressions for Γ and Δ for a range of energy values. This is illustrated for a couple of cases in Table III.

VI. CONCLUSIONS

For resonances in the scattering of a particle by a square well with a square barrier we find that the standard form of the Wigner-Weisskopf (WW) theory does poorly in predicting resonance widths and resonance level shifts. The resonance width predicted by WW theory is much improved if the continuum function used in the calculation is taken to be approximately equal to the exact scattering wave function off resonance. This is done in the alternative WW theory. The resulting resonance level shifts remain poor.

The only formalism that was found to do well for both widths and level shifts was the Garside-MacDonald formalism wherein the level shift and the width are taken to be the real part and $(-2\times)$ the imaginary part respectively of the expectation value of the off resonance elastic scattering operator with respect to the resonant state.

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