The energy and lifetime of resonant states with real basis sets

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Abstract
Using a probabilistic interpretation of resonant states and square-integrable real basis set
expansion techniques, we propose a formula useful to calculate the lifetime of a resonance.
Our approach does not require an estimation of the density of states. The method is illustrated
with calculations of s- and p-resonant state energies and lifetimes.

(Some figures may appear in colour only in the online journal)

1. Introduction

Since the pioneering work of Gamow modeling the α decay in radiative nuclei [1], resonant states have become of great importance in quantum physics. Resonant states appear in nuclear physics [1, 2], atomic and molecular physics [3, 4] and, more recently, in nanophysics [5–7].

In a series of papers Hatano and collaborators [8–10] presented a probabilistic interpretation of resonant states. In these works, a resonance is defined as an eigenfunction of a Hamiltonian with Siegert boundary conditions, that is, when the potential goes to zero, the wave function is only an outgoing wave [11]. Due to Siegert conditions, the problem is not Hermitian; the eigenvalues are complex, the wave functions are not square-integrable and the particle number around a central volume exponentially decays in time because of momentum leaks from the volume.

Many methods were developed in order to calculate the complex eigenvalues of resonant states. The most widely used methods are based in complex scaling transformations that turn the resonance state into a square-integrable function [12, 13]. In particular, a modification called exterior complex scaling [14] was used recently in many photoionization problems [15, 16].

However, due to its simplicity, there also exist several techniques to calculate the real part of a resonance eigenvalue using the Ritz-variational method with a square-integrable real basis set. These methods, generally called stabilization methods [17], use the abrupt change of a physical quantity when a variable is 'crossing' a resonance. In particular

different authors used the variational energies [18, 19], the von Neumann entropy [7] or properties such as the double-orthogonality condition [20] to obtain the real part of the energy. In order to calculate the imaginary part of the resonant energy, all these methods use an approximation of the density of states fitting the numerical data using a Lorentzian function [17, 19, 21].

In this paper we use the formalism of Hatano [8–10] to obtain an expression of the imaginary part of the energy useful to calculate it only using a stabilization method, without an extra fitting or approximation.

The paper is organized as follows. In section 2 we use the Hatano formalism to obtain a relation between the real and imaginary part of the energy and the density of probability in the central region. In section 3 we apply the results of the preceding section together with real basis set expansions to calculate the complex energy of a resonance. Finally, section 4 contains the conclusions with a discussion of the most relevant points of our findings.

2. Definition and properties of resonances

Here and elsewhere we use atomic units, $\hbar = 1; m = 1$. A general solution of the time-dependent Schrödinger equation

$$H\psi(\vec{x}, t) = i\frac{\partial}{\partial t}\psi(\vec{x}, t), \qquad (1)$$

obeys a continuity equation

$$\frac{\partial \rho(\vec{x}, t)}{\partial t} + \nabla \cdot \vec{J}(\vec{x}, t) = 0, \qquad (2)$$

where ρ and J are the standard density and current of the probability [22]

$$\rho(\vec{x}, t) = |\psi(\vec{x}, t)|^2;$$
$$\vec{J}(\vec{x}, t) = \frac{1}{2i} [\psi^*(\vec{x}, t) \nabla \psi(\vec{x}, t) - \psi(\vec{x}, t) \nabla \psi^*(\vec{x}, t)]. \quad (3)$$

Equation (2) could be written in integral form

$$\frac{\partial}{\partial t} \int_\Omega \rho(\vec{x}, t) \, d^d x = - \int_{\partial \Omega} \vec{J}(\vec{x}, t) \cdot d\vec{S}, \quad (4)$$

where d is the spatial dimension, Ω an arbitrary volume and $\partial\Omega$ its frontier. Following Hatano [8–10], we define N_Ω, the number of particles inside a volume Ω

$$N_\Omega(t) = \int_\Omega \rho(\vec{x}, t) \, d^d x. \quad (5)$$

From the definition of J [22], equation (5) takes the form

$$\frac{\partial}{\partial t} N_\Omega(t) = -\text{Re} \left(\int_{\partial \Omega(t)} \psi^*(\vec{x}, t) \, \vec{p} \, \psi(\vec{x}, t) \cdot d\vec{S} \right). \quad (6)$$

This equation, that expresses the particle-number conservation inside the volume Ω, corresponds to equation (15) of reference [9]. If the wave function goes to zero faster than $r^{-(d-1)}$ for large values of r the right-hand side of equation (6) goes to zero, expressing the conservation of the normalization, as happens for bound states. Resonant eigenstates are not Hermitian solutions of the Schrödinger equation and the wave functions have exponential divergences, equation (6) describes a flux of particles outside any volume Ω, even in the limit $\Omega \to \mathbb{R}^d$ and the particle-number is not conserved.

Hatano suggested how to maintain the probabilistic interpretation of the wave function for resonant states [8–10]. The resonance is interpreted as a metastable state, which is localized inside a volume Ω_0 at $t = 0$. Hatano defined a time-dependent volume $\Omega(t)$ by the condition

$$\frac{d}{dt} N_{\Omega(t)}(t) = 0. \quad (7)$$

The reasonable initial condition for this equation is $N_{\Omega(0)}(0) = 1$. This condition together with equation (7) imply that $N_{\Omega(t)}(t) = 1 \; \forall t \geqslant 0$. The expectation value of an operator $\hat{\mathcal{O}}$ is calculated inside the volume $\Omega(t)$ as

$$\langle \hat{\mathcal{O}} \rangle_{\Omega(t)} \equiv \frac{\langle \psi | \hat{\mathcal{O}} | \psi \rangle_{\Omega(t)}}{\langle \psi | \psi \rangle_{\Omega(t)}}, \quad (8)$$

which is well-defined for all times.

Equations (5)–(7) give an equation for $\partial\Omega(t)$

$$\text{Re} \left(\left\langle \psi \left| \left(\frac{\partial \vec{x}}{\partial t} - \vec{p} \right) \right| \psi \right\rangle_{\partial \Omega(t)} \right) = 0. \quad (9)$$

In order to obtain solutions of equation (9), we have to particularize the system. We restricted our study to solutions of the time-dependent Schrödinger equation with fixed energy

$$\psi(\vec{x}, t) = e^{-iEt} \psi_E(\vec{x}), \quad (10)$$

where E and $\psi_E(\vec{x})$ are the eigenvalue and eigenfunction of the time-independent Schrödinger equation. We assume one-particle Hamiltonians with central potentials that tend to zero at infinity. Then, for central potentials we can use the reduced radial Schrödinger equation for l-waves

$$H_l u_{E,l}(r) = E u_{E,l}(r), \quad (11)$$

where

$$H_l = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + \mathcal{V}(r) \quad \text{and}$$
$$\psi_E(\vec{x}) = \frac{u_{E,l}(r)}{r} Y_{l,m}(\Omega), \quad (12)$$

where $Y_{l,m}(\Omega)$ are the spherical harmonics [22].

Resonant states obey non-Hermitian Siegert boundary conditions [11], $u_{E,l}(r) \sim e^{ikr}$ for $r \to \infty$, where $k = \sqrt{2E}$. Siegert states are non normalizable, so they do not belong to the Hilbert space and their complex eigenvalues $E = \mathcal{E} - i\Gamma/2$ are interpreted as energies $\mathcal{E}$ and inverse lifetimes Γ of metastable resonant states.

By symmetry, the solution of equation (7) for the volume $\Omega(t)$ is a sphere of radius $R(t)$, $\Omega(t) = B(R(t))$, with the initial condition $R_0 = R(t = 0)$. In this case, equation (9) gives the evolution of $R(t)$

$$\dot{R}(t) = \text{Im} \left(\frac{\partial_r u_{E,l}(r)}{u_{E,l}(r)} \right) \bigg|_{r=R(t)}. \quad (13)$$

The right-hand side of this equation does not depend explicitly on t and the formal solution is

$$t = \int_{R(0)}^{R(t)} \frac{dr}{\text{Im} \left(\frac{\partial_r u_{E,l}(r)}{u_{E,l}(r)} \right)}. \quad (14)$$

Even the resonant-state functions are not square-integrable; the initial conditions for N_B fix the arbitrary normalization constant

$$N_{B(R_0)}(0) = \int |\psi(\vec{x}, 0)|^2 \, d^3 x = \int_0^{R_0} |u_{E,l}(r)|^2 \, dr = 1. \quad (15)$$

With this condition, the expression for $N_{B(R(t))}(t)$ takes the form

$$N_{B(R(t))}(t) = e^{-\Gamma t} \int_0^{R(t)} dr |u_{E,l}(r)|^2 = 1 \quad (16)$$

and the derivative with respect to t gives

$$\Gamma = \frac{|u_{E,l}(R(t))|^2}{\int_0^{R(t)} dr |u_{E,l}(r)|^2} \dot{R}(t). \quad (17)$$

Combining this equation with equation (13) we obtain

$$\Gamma = \frac{\text{Im}(u_{E,l}^*(R(t)) \partial_r u_{E,l}(r)|_{r=R(t)})}{\int_0^{R(t)} dr |u_{E,l}(r)|^2}. \quad (18)$$

This simple expression for Γ is not convenient for numerical calculation with real basis sets. With this in view, we write the explicit expression for the asymptotic behavior of the wave function

$$u_{E,l}(r) = C e^{ikr} v_l(k, r), \quad (19)$$

where C is a normalization constant given by equation (15). Equation (19) in equation (18) gives

$$\Gamma = \left(\text{Im} \left\{ ik + \frac{\partial_r v_l(k, r)}{v_l(k, r)} \bigg|_{r=R(t)} \right\} \right) \frac{|u_{E,l}(R(t))|^2}{\int_0^{R(t)} dr |u_{E,l}(r)|^2}. \quad (20)$$

By definition $k^2 = 2E = 2\mathcal{E} - i\Gamma$, which gives

$$\text{Im}(ik) = \text{Re}(k) = \left[\sqrt{\mathcal{E}^2 + \left(\frac{\Gamma}{2}\right)^2} + \mathcal{E}\right]^{1/2}. \quad (21)$$

Finally, using equation (21) in equation (20), we arrive at the expression

$$\Gamma = \left(\left[\mathcal{E} + \sqrt{\mathcal{E}^2 + \left(\frac{\Gamma}{2}\right)^2}\right]^{\frac{1}{2}} + \text{Im}\left(\frac{\frac{d}{dr}v_l(k,r)}{v_l(k,r)}\right)\Bigg|_{r=R(t)}\right)$$
$$\times \frac{|u_{E,l}(R(t))|^2}{\int_0^{R(t)} dr |u_{E,l}(r)|^2}. \quad (22)$$

For the important case treated in [8, 9] of potentials with a finite support,

$$\mathcal{V}(r) = \begin{cases} V(r) & \text{if } r < r_0 \\ 0 & \text{if } r > r_0 \end{cases}, \quad (23)$$

we have an explicit expression of v for l-waves, valid for $r > r_0$

$$v_l(k,r) = \sum_{j=0}^{l} (-1)^j \frac{(l+j)!}{j!(l-j)!} \frac{1}{(2ikr)^j}. \quad (24)$$

In particular, for s-waves $l = 0$, $v_0(k,r) = 1$; then equation (22) reduces to a linear relation for Γ^2, which gives

$$\Gamma = \left[2\mathcal{E} + \left(\frac{|u_{E,0}(R(t))|^2}{2\int_0^{R(t)} dr |u_{E,0}(r)|^2}\right)^2\right]^{1/2}$$
$$\times \frac{|u_{E,0}(R(t))|^2}{\int_0^{R(t)} dr |u_{E,0}(r)|^2}. \quad (25)$$

Equation (22) and, for $l = 0$, equation (25) relate Γ with real magnitudes, $\mathcal{E}$ and $|u_{E,l}(R)|^2$. This fact makes these equations useful tools to calculate Γ using square-integrable real basis sets, as we show in the next section.

3. The Ritz-variational method and resonances: numerical expansions

In this section we use equations (22) and (25) to calculate the imaginary part of the energy of a resonant state, applying the Ritz-variational method with real square-integrable basis sets.

We exploit three facts of the variational expansion.

(i) There are several accurate methods to calculate the real part of the eigenvalue, or energy, $\mathcal{E}$, of a resonant state.
(ii) The variational method gives good approximations to the exact (non-normalizable) densities $\rho(r)$ where the resonant states are localized (see figure 1).
(iii) Equation (22) involves just real quantities that could be evaluated with Ritz-variational wave functions.

Even equations (22) and (25) are valid for $R \geqslant r_0$ because (see item (ii)) in the numerical calculations we take $R = R_0 = r_0$ and then $\int_0^{R_0} dr |u_{E,l}(r)|^2 = 1$.

3.1. $l = 0$

We begin with the simple case of s-waves, $l = 0$.

For a clear notation, we will omit the subindexes E and $l = 0$, then $u(r)$ for an arbitrary potential $V(r)$ has the form

$$u(r) = \begin{cases} u^<(r) & \text{if } r < r_0 \\ u^<(r_0) e^{ik(r-r_0)} & \text{if } r > r_0 \end{cases}. \quad (26)$$

Then, in this case equation (25) takes the form

$$\Gamma = \left[2\mathcal{E} + \left(\frac{|u^<(r_0)|^2}{2}\right)^2\right]^{1/2} |u^<(r_0)|^2. \quad (27)$$

Equation (27) involves two real quantities, $|u^<(r_0)|^2$ and $\mathcal{E}$, both quantities are well-approximated by applying the Ritz method using a real square-integrable basis set truncated at order N, $\{\Phi_i\}_1^N$. In this approximation, the Hamiltonian H_l is replaced by a $N \times N$ Hermitian matrix $[H_l]_{i,j} = \langle \Phi_i | H_l | \Phi_j \rangle$ and we obtain N eigenvalues E_n and eigenvectors $\vec{a}^{(n)}$. The corresponding orthonormal eigenfunctions are

$$\psi_n^{(N)}(r) = \sum_{i=1}^{N} a_i^{(n)} \Phi_i(r);$$
$$\sum_{i=1}^{N} \left(a_i^{(n)}\right)^2 = 1 ; \; n = 1, \dots, N. \quad (28)$$

In particular, we have used the double-orthogonality method (DO) [20] in order to calculate the real part of the resonant energy $\mathcal{E}^{(N)}$ and the variational square-integrable approximation for the resonant wave function $u^{(N)}(r)$. This method assumes that the potential depends on a parameter λ, and when λ is varied on an interval $[\lambda_L, \lambda_R]$ a given eigenvalue n_0 crosses the resonant energy value at λ_{n_0}, as illustrated in figure 2. The method uses the fact that in both sides of the interval, λ_L and λ_R, the n_0 eigenvalues and eigenvectors in the left and in the right of the avoiding-crossing zone correspond to different states of the quasi-continuum and the resonant state is orthogonal to both of them. We define the double-orthogonality function

$$D_n(\lambda) = |\langle \psi_n(\lambda_L), \psi_n(\lambda) \rangle|^2$$
$$+ |\langle \psi_n(\lambda_R), \psi_n(\lambda) \rangle|^2, \quad \text{for } \lambda_L < \lambda < \lambda_R. \quad (29)$$

Because the eigenfunctions are normalized, $0 \leqslant D_n(\lambda) \leqslant 2$. For a given eigenvalue n_0, we define the localization of the resonance λ_{n_0} as the value of λ where $D_{n_0}(\lambda)$ reaches its minimum, that is, where the eigenfunction has a minimum projection onto the quasi-continuum states, as shown in figures 3 and 6. This method has the advantage over other stabilization methods in that we only have to solve the variational problem once. The price we pay is that λ_n is also an output of the method and we cannot choose it arbitrarily. The best approximation of the resonance is defined as

$$\lambda_{n_0} = \min_{\lambda \in [\lambda_L, \lambda_R]} D_{n_0}(\lambda); \; \mathcal{E}(\lambda_{n_0}) = E_{n_0}(\lambda_{n_0}). \quad (30)$$

Once we determine the optimal λ_{n_0}, its eigenfunction $\psi_{n_0}^{(N)}(r)$ [20] together with the normalization condition equation (15) give
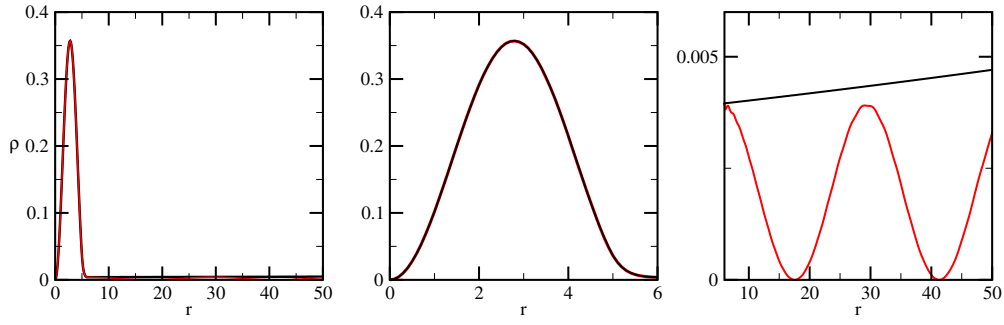
Figure 1. $\rho(r)$ for a $l = 0$ resonant state; exact (black line) and Ritz-DO approximations with $N = 100$ (red line) of the potential from equation (34). (a) Global view, (b) region $0 \leqslant r \leqslant r_0 = 6$, where the resonant state is localized and (c) the exterior region $r \geqslant r_0 = 6$, where the resonance diverges and the variational expansion is a stationary wave.
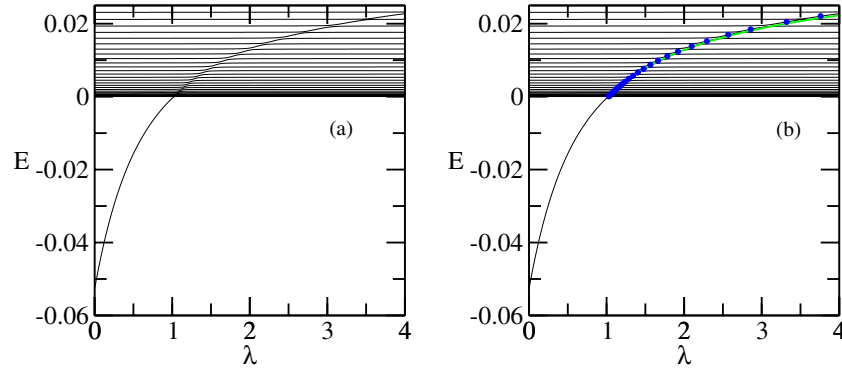

Figure 2. (a) The first 30 eigenvalues of the $N = 100$ Hamiltonian matrix of the $l = 0$ block of the potential equation (34) as a function of the barrier height λ. (b) Same as (a) with exact (green line) and approximate (blue dots) energies of the resonant state.

$$u^{(N)}(r) = \frac{\psi_{n_0}^{(N)}(r)}{\int_0^{r_0} \left| \psi_{n_0}^{(N)}(r) \right|^2 \, \mathrm{d}r}$$

$$= \frac{\sum_{i=1}^{N} a_i^{(N)} \Phi_i(r)}{\sqrt{\sum_{i,j=1}^{N} a_i^{(N)} a_j^{(N)} I_{i,j}(r_0)}}, \tag{31}$$

where

$$I_{i,j}(R) = \int_0^R \Phi_m(r) \Phi_n(r) \, \mathrm{d}r. \tag{32}$$

Then, from equation (27) we obtain for $\Gamma^{(N)}$

$$\Gamma^{(N)} = \frac{\left(\psi_{n_0}^{(N)}(r_0) \right)^2}{\sum_{i,j=1}^{N} a_i^{(N)} a_j^{(N)} I_{i,j}(r_0)}$$

$$\times \left[\left(\frac{\left(\psi_{n_0}^{(N)}(r_0) \right)^2}{2 \sum_{i,j=1}^{N} a_i^{(N)} a_j^{(N)} I_{i,j}(r_0)} \right)^2 + 2\mathcal{E} \right]^{1/2}. \tag{33}$$

As a particular case, we calculated the resonant states for a problem with an exact solution, the well+barrier potential [23]

$$\mathcal{V}(r) = \begin{cases} -V_0 & \text{if } r < \Delta \\ +\lambda & \text{if } \Delta < r < r_0 \end{cases}, \tag{34}$$

where all the parameters are positive. The exact wave functions are different combinations of exponential functions in each sector, with continuous logarithm derivatives at $r = \Delta$ and $r = r_0$. The exact energies for bound, virtual and resonant
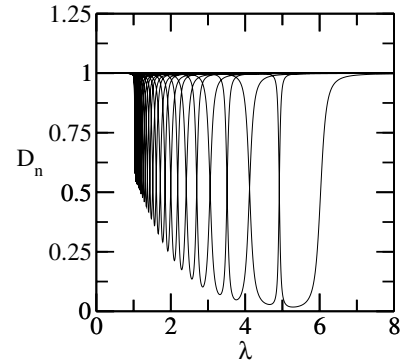

Figure 3. D_n for the $l = 0$ block of the potential equation (34) as a function of the barrier height λ for $N = 100$ and $n = 2, \ldots, 30$. The minimum of each curve is defined as the localization of the resonant state.

states are given as solutions of three different transcendental algebraic equations, which are obtained by applying the corresponding boundary condition at $r = r_0$ [23].

The calculations were done as a function of the barrier height λ, with fixed values of $V_0 = 0.15$, $\Delta = 5$ and $r_0 = 6$. A convenient orthonormal basis set is given by

$$\Phi_i(r) = \frac{1}{\sqrt{(i+1)(i+2)}} \, \mathrm{e}^{-r/2} L_i^{(2)}(r); \; i = 1, \ldots, N, \tag{35}$$

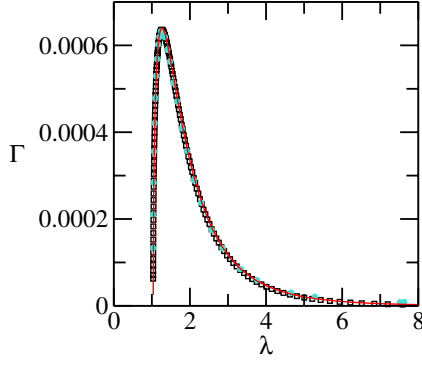where $L_i^{(2)}(r)$ is the Laguerre polynomial of degree i and order 2 [24].

Figure 4. Exact (red line), $N = 100$ (turquoise dots) and $N = 500$ (black squares) values of Γ against the barrier height λ for the $l = 0$ block of the potential equation (34).
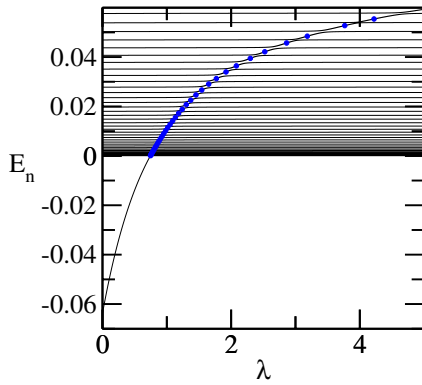

Figure 5. The first 30 eigenvalues of the $N = 100$ Hamiltonian matrix of the $l = 1$ block of the potential equation (34) as a function of the barrier height λ. The approximate energies of the resonant state calculated with DO are also shown (blue dots).

Figure 6. D_n for the $l = 1$ block of the potential equation (34) as a function of the barrier height λ for $N = 100$ and $n = 2, \ldots, 30$. The minimum of each curve is defined as the localization of the resonant state.

Figure 7. Exact (red line), $N = 100$ (turquoise dots) and $N = 500$ (black squares) values of Γ against the barrier height λ for the $l = 1$ block of the potential equation (34).

In figure 2(a) we show the first 30 eigenvalues given by the Ritz method with $N = 100$. In figure 2(b) we add the exact resonant energy curve and the values calculated with the DO_n functions, which are shown in figure 3 for $N = 100$ and $n = 2, \ldots, 30$. Once the energy was obtained, the width Γ of the resonance is calculated using equation (33). In figure 4 we show $\Gamma(\lambda_n)$ for two different sizes of the basis set: $N = 100$, for $n = 2, \ldots, 30$ and $N = 500$, for $n = 2, \ldots, 140$. Our data show an excellent agreement with the exact curve $\Gamma(\lambda)$, that is also included in the figure.

3.2. $l = 1$

From equation (24), the function $v_l(k, r)$ for p-waves takes the form

$$v_1(k, r_0) = 1 + \frac{i}{kr_0}. \tag{36}$$

In this case, it is convenient to re-write equation (22) as a function of $x \equiv \mathrm{Im}(k)$:

$$x^3 + \left(\frac{1}{r_0} + \frac{|u(r_0)|^2}{2} \right) x^2 + \left(\mathcal{E} + \frac{1}{2r_0^2} + \frac{|u(r_0)|^2}{2r_0} \right) x$$

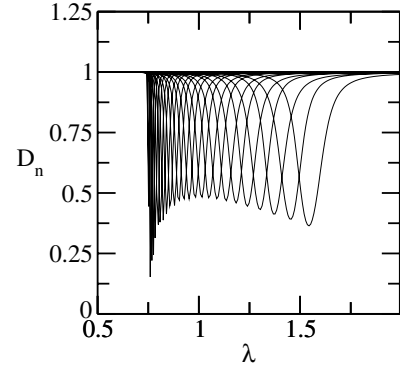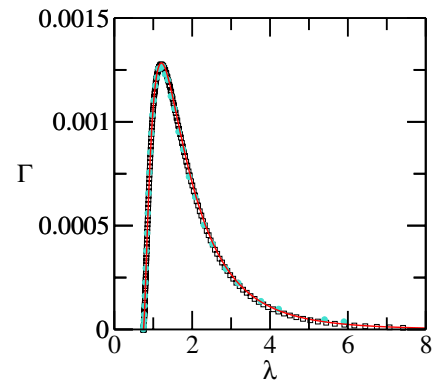$$+ \mathcal{E} \frac{|u(r_0)|^2}{2} = 0. \tag{37}$$

The definition of resonance establishes that $\mathrm{Im}(k) > 0$ and we have already proved for each case that we have studied that equation (37) has a unique positive root. Finally Γ is obtained from the definition of k as

$$\Gamma = -2x_p \sqrt{2\mathcal{E} + x_p^2}, \tag{38}$$

where x_p is the positive root of equation (37).

We calculated the inverse lifetime Γ for a $l = 1$ resonant state of the potential equation (34) as a function of the barrier height λ, with fixed values of $V_0 = 0.3$, $\Delta = 5$ and $r_0 = 6$. In figure 5 we show the first 30 eigenvalues of the $N = 100$ p-block of the Hamiltonian matrix and the resonant energies $\mathcal{E}$ calculated with the DO method. The curves $D_n(\lambda)$ for $n = 2, \ldots, 30$ are shown in figure 6. Note the qualitative differences between the DO curves for $l = 0$ and $l = 1$ in figures 3 and 6 respectively. These differences are due to the existence of a virtual state between the bound and the resonant states for the $l = 0$ case, which is absent in the $l = 1$ case, where the bound state is continued directly in a resonant state.

In figure 7 we show the exact curve Γ versus λ and the approximate values obtained with two different basis set sizes: $N = 100$, for $n = 2, \ldots, 40$ and $N = 500$, for $n = 2, \ldots, 200$. As in the case with zero angular momentum, we obtain an excellent agreement between exact and approximate results.

4. Conclusions

In this work we used a probabilistic interpretation of resonant (Siegert) states based on the conservation of the number of particles inside a time-dependent volume [8–10]. The advantage of the probabilistic interpretation of resonant states is that it is possible to work with Siegert states in a similar way to bound states, by calculating probabilities, expectation values, etc.

In particular, we obtain the exact equation (22), which reduces to equation (25) and equation (37) for $l = 0$ and $l = 1$ respectively. These equations relate the inverse lifetime with other real magnitudes, the energy and the density of a resonance. In previous papers, once the energy of a resonance has been obtained by applying a real algebra stabilization-like method, the resonance width is calculated by performing a fitting of the density of states ([19] and references therein, [20]). In the present work equation (22) gives a value for Γ with the same degree of accuracy that we obtain for the energy of the resonance $\mathcal{E}$.

We emphasize the simplicity of the calculations compared to other methods that use complex algebra to study resonant states. We present our results for potentials with finite support, but equation (22) is valid in general, and the calculation of Γ could be corrected by a systematic perturbative expansion.

An open question is how equation (22) could be generalized for few-particle systems, where many channels are present. We are working in this direction.

Acknowledgments

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