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RESONANT-STATE EXPANSION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION

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Abstract
The resonant-state expansion (RSE), is a rigorous perturbative method recently developed in electrodynamics. This paper presents the RSE method applied to the one-dimensional Schrödinger equation. The method is used here to find the new spectrum of Eigen wavenumbers in a double-well system described by delta function potentials. The convergence of the RSE is tested with the available analytical solution for the triple well. RSE results are compared with the exact solutions for triple well. The method was demonstrated to be particularly suitable for calculating high-quality resonant states (RSs) and calculating their perturbations.
Keywords: Resonant-states expansion, Resonant-states, Schrödinger equation, Eigen wave numbers, Convergence.

INTRODUCTION

The resonant-state expansion (RSE) is a rigorous perturbation method recently developed in electrodynamics (Muljarov, 2010). The RSE has been applied and tested to various one-dimensional (1D), 2D, and 3D open optical systems (Armitage et al., 2014, Doos et al., 2012, Muljarov, 2010, Tanimu and Muljarov, 2018). The RSE uses the solution of the Schrödinger equation for an unperturbed system as a basis for calculating the resonant states (RSs) of the perturbed system. RSs have been studied for almost a decade (Siegert, 1939 and Gamow, 1928). In an open quantum system, RSs are referred to as the eigensolutions of the stationary Schrödinger equation with outgoing wave boundary conditions (Hatano, 2008; Tanimu and Muljarov, 2018, Tanimu and Bagudo, 2020). These boundary conditions strictly define RSs. These states have complex energy eigenvalues with negative imaginary parts as the inverse of lifetime, causing them to decay exponentially in time, leaking out of the system (such as a quantum well) (Siegert, 1939 and Gamow, 1928). Thus explaining the exponential decay law in quantum mechanics. Due to the system leakage, the RSs wave function has exponentially increasing tails outside the system and cannot be normalized by the usual normalization condition. Thus a special normalization and orthogonality condition is proposed and used in (Garcia, 1976, Siegert, 1939). The presence of a continuum in the spectrum of a system is a significant problem for any perturbation theory. In open quantum systems, such a continuum is often the dominating, if not the only part of the spectrum. However, going away from the real axis to the complex frequency plane, the continuum can, in many cases, be effectively replaced by a countable number of discrete RSs which form a complete basis. Therefore, the RSs of a perturbed system can be expanded into the unperturbed RSs. The expansion coefficients and perturbed wavenumbers can be found by diagonalizing a complex symmetric matrix which consists of a diagonal matrix representing the bare spectrum and the perturbation (Muljarov, 2010).

In this work, solutions of the Schrödinger equation with one-dimensional potentials composed of delta functions generate an analytic basis of RSs for their use in the RSE. Recently, the RSE has been applied to one-dimensional quantum systems (Tanimu and Muljarov, 2018), showing very good convergence. However, poor convergence was achieved when applied to a square quantum well in the work of Lind (1993).

This work aims to re-apply with this method and study its convergence to the one-dimensional Schrödinger equation. Firstly, we calculate the RSs in a symmetric double quantum well (Tanimu and Muljarov, 2018) structure modeled by δ-function potential. The RSs of this system are then taken as an unperturbed basis for the RSE. Once this is established, the RSE will be discussed and tested.

Triple quantum wells are chosen such that while they can be solved numerically, they can also be solved analytically. This is necessary as a means to test the accuracy and compare the results of the RSE against known analytic solutions.

BACKGROUND OF THE STUDY AND METHOD

Resonant state expansion (RSE) is the use of perturbation theory to calculate a new spectrum of resonant states that arise from adding a perturbation to the system. This method is ideal for determining the RSs that would exist in a complex system without having to consider it analytically which will normally require non-trivial solutions. Physically, RSs can be used to describe decaying systems due to their lifetime qualities, such as nuclear decay, and so RSE can be used to describe more elaborate decaying systems that originate from a trivial system. It is key to note that RSE deals with open systems that allow wave functions to leak outside of the potentials. This arises from the method's use of complex eigenvalues.

The formalism of the RSE

In this section, we present the formalism of the RSE that has already been developed (Muljarov, 2010). We consider the one-dimensional, time-independent Schrödinger equation:

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi_n(x)=\varepsilon_n\psi_n(x) \qquad (1)$$

where $\varepsilon_n=\frac{\hbar^2k_n^2}{2m}$ is the energy of RSs. For convenience, we use the following $2m=1$ and $\hbar^2=1$, so that $\varepsilon_n=k_n^2$, where k_n is the Eigen wave number of the particle, $\hbar$ is the Planck's constant, m is the effective mass of the particle. The perturbed potential is given by $\tilde{V}(x)=V(x)+\Delta V(x)$, where $V(x)$ is the unperturbed potential is given by (Tanimu and Muljarov, 2018).

$$V(x)=-\gamma\delta(x-a)-\gamma\delta(x+a) \qquad (2)$$

Which describe a double quantum well (or barrier) system, $\Delta V(x)$ is a perturbation taken in the form of

$$\Delta V(x)=-\sum_{K=2}^{N-1}\beta_k\delta(x-b_k) \qquad (3)$$

Here N is the total number of wells/barriers and $b_k=-a+\Delta(k-1)$, where $\Delta=\frac{2a}{N-1}$. For the unperturbed and triple well system, $N=2$ and $N=3$, respectively. For a periodic quantum lattice (Tanimu and Muljarov, 2018), $N\geq 2$ and $\beta_k=\gamma$, where γ is the strength of the potential.

The wave function $\psi_n(x)$ is continuous across the delta function while its first derivative has a discontinuity. Outside the system

$$\psi_n(x)=\pm B_n e^{ik_n|x|} \qquad (4)$$

Where B's are the amplitude of the outgoing waves, RSs are normalized according to the following orthonormality condition (Garcia, 1976, Muljarov, 2010, Siegert, 1939).

$$\int_{-a}^{a}dx\psi_n(x)\psi_m(x)-\frac{\psi_n(a)\psi_m(a)+\psi_n(-a)\psi_m(-a)}{i(k_n+k_m)}=\delta_{nm} \qquad (5)$$

Where $x=\pm a$ are the boundaries of the system. The perturbed states are expanded into the complete set of normalized unperturbed RSs.

$$\tilde{\psi}_v(x)=\sum_n\frac{C_{nv}}{\sqrt{k_n}}\psi_n(x) \qquad (6)$$

Resulting in a linear symmetric eigenvalue problem (the RSE equation)

$$\sum_m\left(k_n\delta_{nm}+\frac{\Delta V_{nm}}{\sqrt[2]{k_nk_m}}\right)C_{mv}=\kappa_v C_{nv} \qquad (7)$$

κ_v and $\tilde{\psi}_v$ are referred to as a perturbed system, and the perturbation matrix

$$\Delta V_{nm}=\int_{-a}^{a}\Delta V(x)\psi_n(x)\psi_m(x)dx. \qquad (8)$$

is determined by the unperturbed wave functions $\psi_n(x)$ and the perturbation $\Delta V(x)$.

The perturbed wave numbers κ_v and expansion coefficient C_{nv} can be obtained by diagonalizing the complex symmetric matrix, equation (7).

Unperturbed Basis of Resonant states

In this work, we have chosen as unperturbed RSs, the solution of the one-dimensional Schrödinger equation with a double-well superimposed by a double delta-function potential. The unperturbed potential is thus given by equation (2). Whereas a is the distance between the wells and γ is the strength of the potential, The unperturbed basis of RSs is thus given by

$$\psi_n(x) = \begin{cases} B_n e^{ik_n x}, & x > a, \\ C_n(e^{ik_n x} \pm e^{-ik_n x}) & -a < x < a, \\ B_n e^{-ik_n x} & x < -a \end{cases} \quad (9)$$

Applying the outgoing wave boundary conditions (BCs) obtained

$$e^{2ik_n x} = 1 \pm \frac{2ik_n}{\gamma} \quad (10)$$

with upper and lower signs corresponding to even and odd states respectively.

Note that equation (10) cannot be solved analytically. However, in this work, we employ the use of the Newton-Raphson procedure in MATLAB, which is typically fast to converge for their complex roots, which gives rise to all types of states, including bound, antibound, and normal RSs, which are discussed in detail in (Hatano, 2008, Tanimu and Muljarov, 2018).

Triple quantum well: verification of the RSE

So far, we have developed a system in which we could find its exact solutions in sub-sec. (2.2). However, within quantum mechanics, the vast majority of the systems cannot be solved exactly, and we need to develop appropriate tools to deal with them. Perturbation theory is extremely successful in dealing with those cases that can be modeled as a small change in a system that is solved exactly. Once the small change was made to the system, the new eigenvalues and eigenvectors of the perturbed system were calculated. Formulating a simple and accurate perturbation theory is essential within the context of quantum mechanics, as the vast majority of problems in quantum mechanics don't have a known analytic solution, thus there is a need to develop a strong numerical method. In this case, the RSE method in sub-sec. (2.2) is considered. Since the RSE method was already formulated, we need to define a perturbed well to be used for the verification of this method. A triple well is chosen as it is of a form similar to the double-well but with a third well (barrier) positioned at x = b, somewhere between the two equal wells (barriers): −a < b < a. The form of this potential is given by

$$V(x) = -\gamma\delta(x-a) - \gamma\delta(x+a) - \beta\delta(x-b) \quad (11)$$

where β is an additional well (barrier) different from the two other wells, with $\beta > 0$ ($\beta < 0$) corresponding to an additional well (barrier).

Analytic solution

Employing the same approach and boundary conditions as in the previous sub-sec. (2.2), with the additional boundary conditions that the wave function be continuous at x = b, leads to the following wave functions:

$$\psi_n(x) = \begin{cases} A_1 e^{ik_n x}, & x > a, \\ B_1 e^{ik_n x} + B_2 e^{-ik_n x} & b < x < a, \\ C_1 e^{ik_n x} + C_2 e^{-ik_n x} & -a < x < b, \\ D_2 e^{-ik_n x} & x < -a, \end{cases} \quad (12)$$

Considering the continuity of the wave function at the boundaries without derivation leads to the following secular transcendental equation.

$$1 + \frac{2ik_n}{\gamma} = \frac{1 - 2ik_n}{1 + \frac{2ik_n}{\beta}} e^{2ik_n a} \quad (13)$$

This equation is solved numerically using the Newton-Raphson procedure to find the exact solutions. The exact solutions, RSE, and unperturbed RSs for even and odd states are presented in Figs. 1-2.

RESULTS AND DISCUSSION

a. RSE for a symmetric triple well

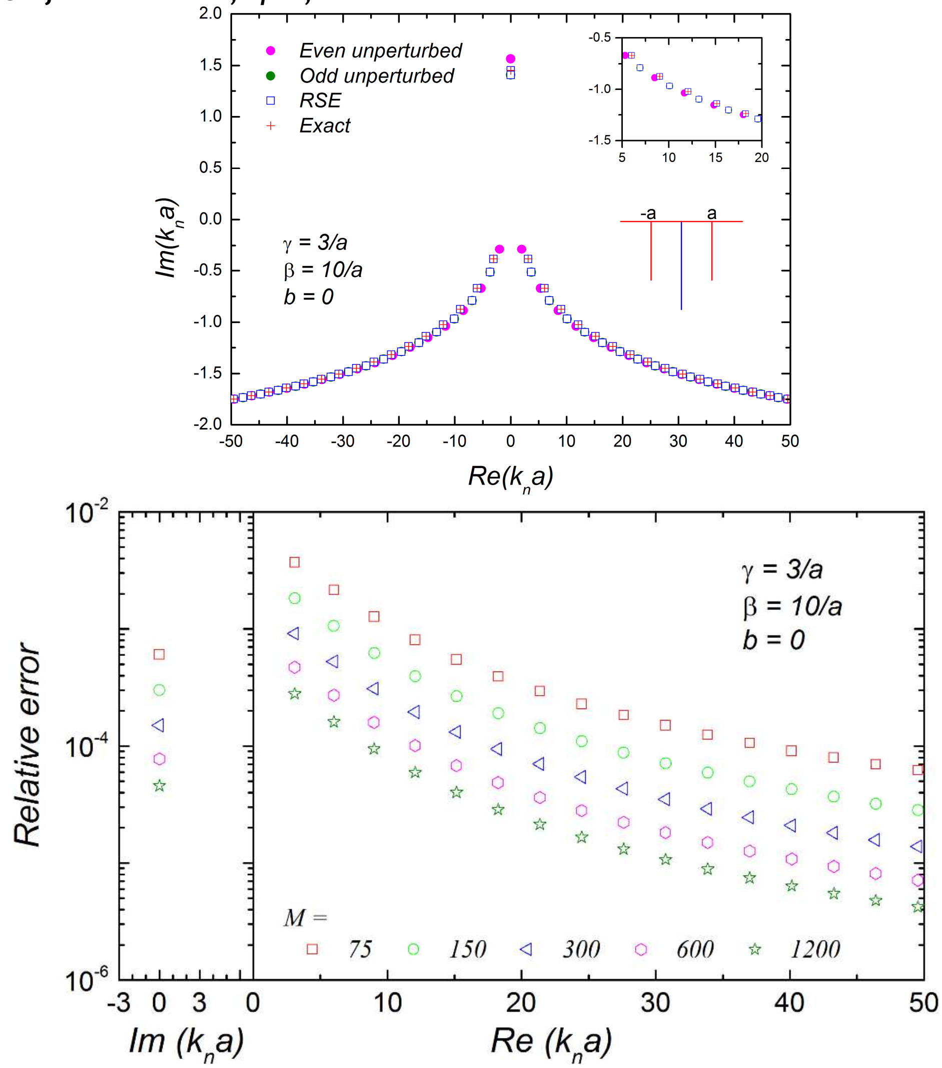

Figure 1: (a) Complex spectrum of perturbed wave numbers for a triple symmetric (b = 0, γ =3/a, β = 10/a) quantum well structures with an even and odd unperturbed RSs wave numbers for a double quantum well structure calculated via Equation (10) (solid symbols) with the help of Newton-Raphson procedure in Matlab. The RSE results are calculated via Equation (7) (blue square), while the exact solutions are calculated by solving the analytic secular transcendental equation for a triple symmetric quantum well in Equation (13) (red cross) and (b) relative error between the RSE results and exact solutions for different basis size M.

Figure 1 compares the RSE results with the exact solutions for even perturbed systems (b = 0, γ =3/a, β = 10/a). In Figure 1 (a), it has been shown that the RSE is reproducing the exact values to the required accuracy, which is quantified by the relative errors shown in Figure 1 (b). The graphs show that accuracy is maintained for almost all the states considered within the spectrum, with inaccuracies only occurring at the extreme ends of the real axis. This is due to the size of the matrix. It is found that increasing the matrix size M would lead to very high accuracy for the RSE. It has been shown that the spectrum of the RSE results and exact solutions are almost similar to that of the double quantum well, indicating simple perturbation into the system. This is unlike what we will see later for the case of ($b \neq 0$) which shows a stronger deviation due to a differ perturbation into the system.

We can see the unperturbed RSs for even states shifted from the perturbed states, indicating the effect of the perturbation. In this case, only the even states are perturbed, while the odd states are not. This is because odd RSs are unaffected by the perturbation at the position of the delta function, hence we can just use the unperturbed solution from the two delta problems without change. Figure 1 (b) shows that there is a uniform change in the relative error with an increase in the number of basis size M. It has been shown that, with an increase in the number of M, the numerical results eventually converge to the exact solutions. It has also been shown that as you get close to the origin, the relative error goes up.

b. RSE for a non-symmetric triple well

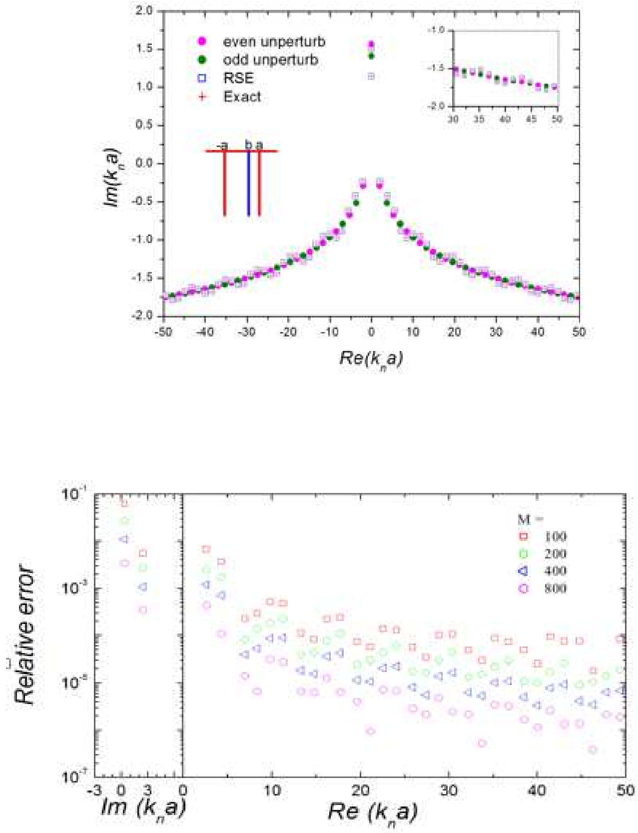

Figure 2. As in Figure 1, but for b = a/4, $\gamma = \beta$ = 4/a

Here we apply strong (non-symmetric) perturbations into the system of two quantum well potentials. Unlike in Figure 1 where we placed our perturbation exactly at the middle of the two quantum well system (i.e. b = 0), here, the perturbations was chosen to have a different position b ($\text{i.e.}, b \neq 0$). Note that we fixed the parameter γ = β = 4/a and vary b for clear observations and comparison with our RSE results. It is found that, unlike the previous calculation for (b = 0), here, the spectrum is quite unusual to the normal RSs for the two delta well system. This is due to stronger perturbations into the system. As such it mixes both even and odd RSs.

CONCLUSION

The RSE has been implemented and shown to be an accurate method for calculating the RSs of a one-dimensional Schrödinger equation. The convergence of the RSE to the exact solutions has been studied. A single perturbation was introduced at b = 0 for a symmetric triple well and $b \neq 0$ for a non-symmetric triple well and the RSE was calculated. It was found that for b = 0, the symmetric RSs were perturbed and shifted closer in wavenumbers. However, this does not affect any of the anti-symmetric RSs wave numbers due to the system symmetry. For $b \neq 0$, the spectrum is quite different from the unperturbed RSs due to the strong perturbation in the system. The accuracy of the perturbation is tested by comparing the RSE results to the exact solutions. It was observed that there is a constant change in the relative error with an increase in the number of basis size

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