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ORIGINAL RESEARCH ARTICLE

Resonant-State Expansion Applied to Non-Relativistic Wave Equation in One-Dimension

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ABSTRACT
The resonant-state expansion (RSE), a rigorous perturbation theory recently developed in electrodynamics, is here applied to the non-relativistic wave equation in one-dimension. The resonant states (RSs) wave numbers for the double well system are analytically calculated and used as the unperturbed basis for calculating the RSE. We demonstrate the efficiency of the RSE by verifying its convergence to the exact solution for a triple well potential. We show that for the chosen perturbations (i.e., for $b = 0$ and $b \neq 0$), the method is particularly suitable for calculating all the RSs within the spectrum.

INTRODUCTION

The resonant-state expansion (RSE) is a rigorous perturbation method in electrodynamics recently invented in Cardiff (Muljarov et al, 2010). The method has been successfully applied to 1, 2, and 3-dimensional open optical systems (Armitage et al., 2014; Doost et al., 2012; Muljarov et al., 2010). It uses the solution of the non-relativistic wave equation (the Schrödinger equation) in one dimension for an unperturbed basis of resonant states (RSs) for calculating the RSE. RSs have been studied for quite a long time (Siegert, 1939; Gamow, 1928). In quantum mechanics, they are referred to as the stationary states solution to the Schrödinger equation with purely boundary conditions of only outgoing waves (Hatano, 2008; Tanimu and Muljarov, 2018; Tanimu and Bagudo, 2020). These boundary conditions strictly define RSs. They appear, in the form of resonances, in almost every field of Physics, from classical mechanics and electrodynamics to quantum physics and gravity. In spite of this fact, however, many fundamental aspects are still to be investigated. Also, resonant phenomena are of increasing importance in quantum mechanics, especially in view of the rapid progress in the physics of semiconductor nanostructures, which various types of quantum potentials can describe. In a quantum system, RSs wave function leaks out of the system, which then causes exponential growth at the tail of the function.

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 (Siegert, 1939 and Gamow, 1928). Due to this exponential growth, the RSs wave function cannot be normalized by the usual normalization condition. As such, a special normalization condition (Muljarov et al., 2010; Siegert, 1939) is used. In this work, we study the convergence of the RSE by applying it to the non-relativistic wave equation in one dimension. We first calculated the RSs wave numbers for a double well system and used them as unperturbed basis for calculating the RSE (Tanimu and Muljarov, 2018). We test the accuracy and study the convergence of the RSE for both symmetric and anti-symmetric triple well potential for different perturbations. Here, the potential with positions $b = 0$ or $b \neq 0$ serves as a perturbation.

THEORETICAL BACKGROUND AND METHOD

Resonant state expansion (RSE) requires a potential with known analytical solution (in this case double well system composed of a delta functions) and uses it as a basis for calculating the RSE. RSE requires that the wave functions be normalized (Muljarov et al., 2010), so an appropriate normalization condition is required. Once this is achieved, the RSE could be investigated and used on different quantum mechanical problems.

Normalization of Resonant states in 1D

In one-dimensional quantum systems, it requires that the solutions to the wave functions for both even and odd

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states have to be normalized but care has to be taken during the calculations. For bound states, this is an easy task, but for the resonant states, which have exponentially increasing tails, an additional term must be considered to normalize them correctly. An outer limit is required for their normalization and is given by R. It is found that the value of R can be taken arbitrarily, and thus, for convenience, we are free to choose the boundaries of the well as the limits of this normalization. The orthonormality condition is given by (Muljarov et al., 2010):

$$\delta_{nm} = \int_{-a}^{a} dx\psi_n(x)\psi_m(x) - \frac{\psi_n(a)\psi_m(a) + \psi_n(-a)\psi_m(-a)}{i(k_n + k_m)} \tag{1}$$

It can be shown that this equation is suitable for the usual normalization of bound states as it reduces to the standard normalization condition as R tends to infinity the condition tends towards $\delta_{nm} = \int_{-\infty}^{\infty} dx\psi_n(x)\psi_m(x)$ which is the standard approach to normalizing the bound states. Utilizing the normalization condition, the constants are found as:

$$A_n = \left(4a + \frac{2}{k_n}\sin(2k_n a) - \frac{4}{ik_n}cos^2(k_n a)\right)^{-\frac{1}{2}} \tag{2}$$

and

$$B_n = \left(-4a + \frac{2}{k_n}\sin(2k_n a) + \frac{4}{ik_n}sin^2(k_n a)\right)^{-\frac{1}{2}} \tag{3}$$

Resonant State Expansion (RSE)

So far, we have developed a system in which we can find its exact solutions in sub-sections (2.3) and (2.4). However, within quantum mechanics, the majority of the systems cannot be solved exactly, and we need to develop appropriate models 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 we can solve exactly. Once this change was made to the system, the new eigenvalues and eigenvectors of the perturbed system were calculated. Let's consider the perturbed Hamiltonian as:

$$H = H_0 + V \tag{4}$$

whereH_0 is the Hamiltonian of the unperturbed system, and V is the perturbed potential. From Eq. (4) without derivation (Muljarov et al., 2010, Lind, 1992)

$$(H_0)_{nm} = k_n\delta_{nm} \tag{5}$$

$$H_{nm} = k_n\delta_{nm} + \frac{V_{nm}}{\sqrt[2]{k_n k_m}} \tag{6}$$

$$V_{nm} = \int_{-a}^{a} V(x)\psi_n(x)\psi_m(x)dx \tag{7}$$

Therefore,

$$H_{nm}\chi_v = \kappa_v\chi_v \tag{8}$$

The perturbed eigenvectors χ_v and eigenvalues κ_v can be determined by diagonalizing the Hamiltonian matrixH_{nm}. The simplicity of the method lies in the fact that the matrix contains terms based only on the unperturbed problem and the perturbation (Mostert, 2014). The eigenvalues and eigenvectors form a complete set, and thus, the perturbed wave function can be defined as:

$$\tilde{\psi}_v(x) = \sum_n B_{nv}\,\psi_{nv}(x) \tag{9}$$

Where

$$B_{nv} = \frac{\chi_v}{\sqrt{k_n}} \tag{10}$$

Unperturbed Resonant states

To apply the RSE to a one-dimensional non-relativistic wave equation, we need a known suitable basis for RSs. We choose here the RSs of a Schrödinger equation with a double well as:

$$V(x) = -\gamma\delta(x - a) - \gamma\delta(x + a) \tag{11}$$

which describes a double potential well (or barrier) system. Where *a* is the distance between the well and γ is the strength of the potential, which is the depth of the quantum well multiplied by its width. The solution to the Schrödinger equation for unperturbed basis RSs is thus given by (Tanimu and Muljarov, 2018, and Tanimu and Bagudo, 2022).

$$\psi_n(x) = \begin{cases} B_n e^{ik_n x}, & x > a, \\ C_n\left(e^{ik_n x} \pm e^{-ik_n x}\right) & -a < x < a, \\ \pm B_n e^{-ik_n x} & x < -a \end{cases} \quad (12)$$

After some algebra obtained, the secular equation

$$e^{2ik_n x} = 1 \pm \frac{2ik_n}{\gamma} \quad (13)$$

with upper and lower signs corresponding to even and odd states, respectively. This equation generates a complete set of spectra for unperturbed RSs. Eq. (13)is solved numerically with the help of the Newton-Raphson procedure in MATLAB (Tanimu and Muljarov, 2018; Tanimu and Bagudo, 2022).

Verification of the RSE for a Triple well system

In this section, we verify the convergence of the RSE for a triple well potential. The vast majority of the systems in quantum mechanics cannot be solved exactly unless employing the use of other models. Here, we make use of perturbation theory, which is extremely successful in dealing with those cases (Muljarov et al., 2010) with the formulation of the RSE method in sub-sec. (2.2), we need to have a well define perturbed potential to be used for the verification of the RSE and study its convergence. We first chose a simple perturbation so that the results could be tested and compared with the numerical results found through the RSE. This simple perturbation was added somewhere between the two existing well systems, see eq.(11), forming a triple well potential, and this perturbation was chosen to have the same strength as the two wells. *The form of this potential as given by (*Tanimu and Muljarov, 2018), is

$$V(x) = -\gamma\delta(x-a) - \gamma\delta(x+a) - \beta\delta(x-b) \quad (14)$$

whereβ is an additional well (barrier) depending on the position of the perturbation. With $\beta > 0$ ($\beta < 0$) corresponding to the well (barrier).

Exact solution

Here, the same approach is used as in the previous sub-sec. (2.3), but with the additional boundary conditions that the wave function be continuous at $x = b$, and obtain the secular equation for triple well potential. The secular equation of this perturbed system is given by

$$e^{2ik_n a} = \frac{(-2ik_n + \beta)(-2ik_n - \gamma)}{\gamma(-2ik_n - \beta)} \quad (15)$$

Eq. (15) shows a special case for $b = 0$ (symmetric). However, for the case of $b \neq 0$(anti-symmetric), we have the following transcendental equation:

$$\left((-2ik-\gamma)e^{ikb} + \gamma e^{2ika}e^{-ikb}\right)\left(\gamma e^{2ika}e^{ikb}\left(1+\frac{\beta}{ik}\right) - (-2ik-\gamma)\left(1-\frac{\beta}{ik}\right)e^{-ikb}\right) - \left((-2ik-\gamma)e^{ikb} - \gamma e^{2ika}e^{-ikb}\right)\left((-2ik-\gamma)e^{-ikb} + \gamma e^{2ika}e^{ikb}\right) = 0 \quad (16)$$

The resonant states with odd (anti-symmetric) wave functions are not affected by the delta-function potential at $x = 0$ since the wavefunctions vanish at $x = 0$. Hence we can use the solution from the double well system without change. Eqs. (13), (15), and (16)are solved numerically using the Newton-Raphson method in MATLAB to find the exact solutions for the unperturbed and perturbed RSs wave numbers for both even and odd states, respectively. These results are presented in Figures 1 - 2.

RESULT AND DISCUSSION

In this section, the resonant state expansion (RSE) is tested by comparing the numerical solutions found through the RSE against the exact solutions found in the sub-sec. (2.4). The results from sub-sec. (2.3) serves as the unperturbed basis for the RSE.

a. RSE for a symmetric triple well

Figure 1 shows that the accuracy of the perturbation is maintained by comparing the numerical solutions found through the RSE to that of the exact solutions in sub-sec. (2.4). Figure 1 (a) shows that the numerical results of the RSE match exactly with the exact values for the triple well potential for $b = 0$. This indicates a simple perturbation into the system, which is not the case for $\neq 0$, which shows some deviation due to the effect of perturbation into the system. It has been shown that for $b = 0$ only even states are perturbed while odd states do not change by this perturbation. You can deal with a 2 times smaller matrix between even states only. The graph also shows the similarity between the spectrum of the numerical solutions found through the RSE and the exact solutions to that of the unperturbed RSs. Figure 1 (b) shows the relative error between the RSE results and exact solutions for different basis size N. We can see that from the graph, there is a constant change in the relative error with an increase in the number of basis size N. As we increase N, the RSE result eventually converges to the exact solution (Doost et al., 2012).

b. RSE for anti-symmetric triple well

Figure 2 shows the convergence of the RSE to the exact values for the anti-symmetric. Here the perturbation was chosen to be away from the centre($\mathrm{i.e.}, b \neq 0$) to clearly observe the effect of the perturbation. We fixed the parameter $\gamma = \beta = 5/a$ and varied position b to notice clearly the convergence of the RSE. It was observed that the spectrum is quite different from that of the unperturbed RSs for both even and odd states. This is due to the effect of applying strong perturbations into the system.

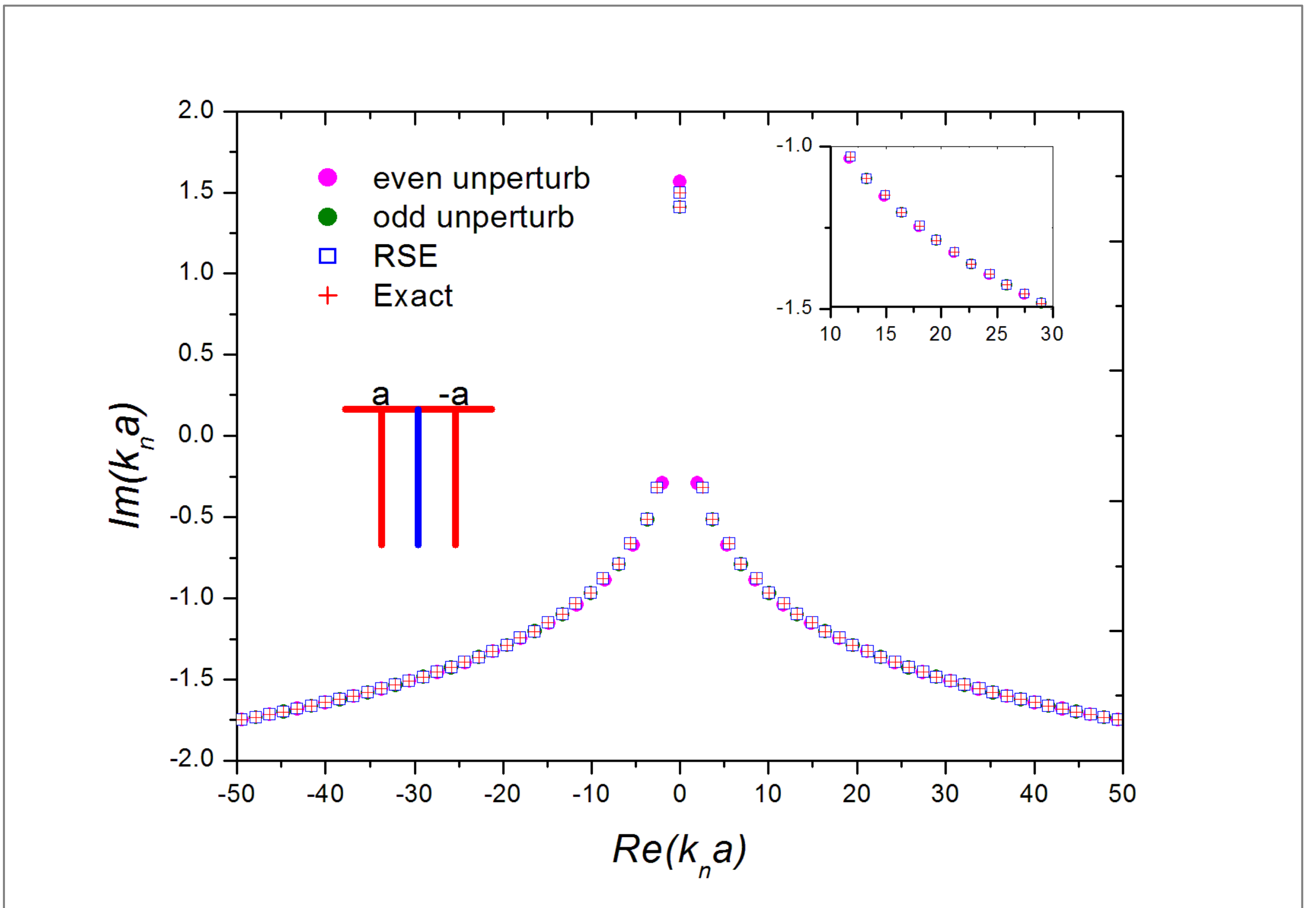

Figure 1 (a): Perturbed wave numbers plotted in the complex k-plane for a triple well potential for b = 0, γ =β = 2 with unperturbed RSs wave numbers for a double well potential calculated via Equation (13). The RSE results are calculated via Equation (6), while the exact solutions for a symmetric potential are calculated using Equation (15)

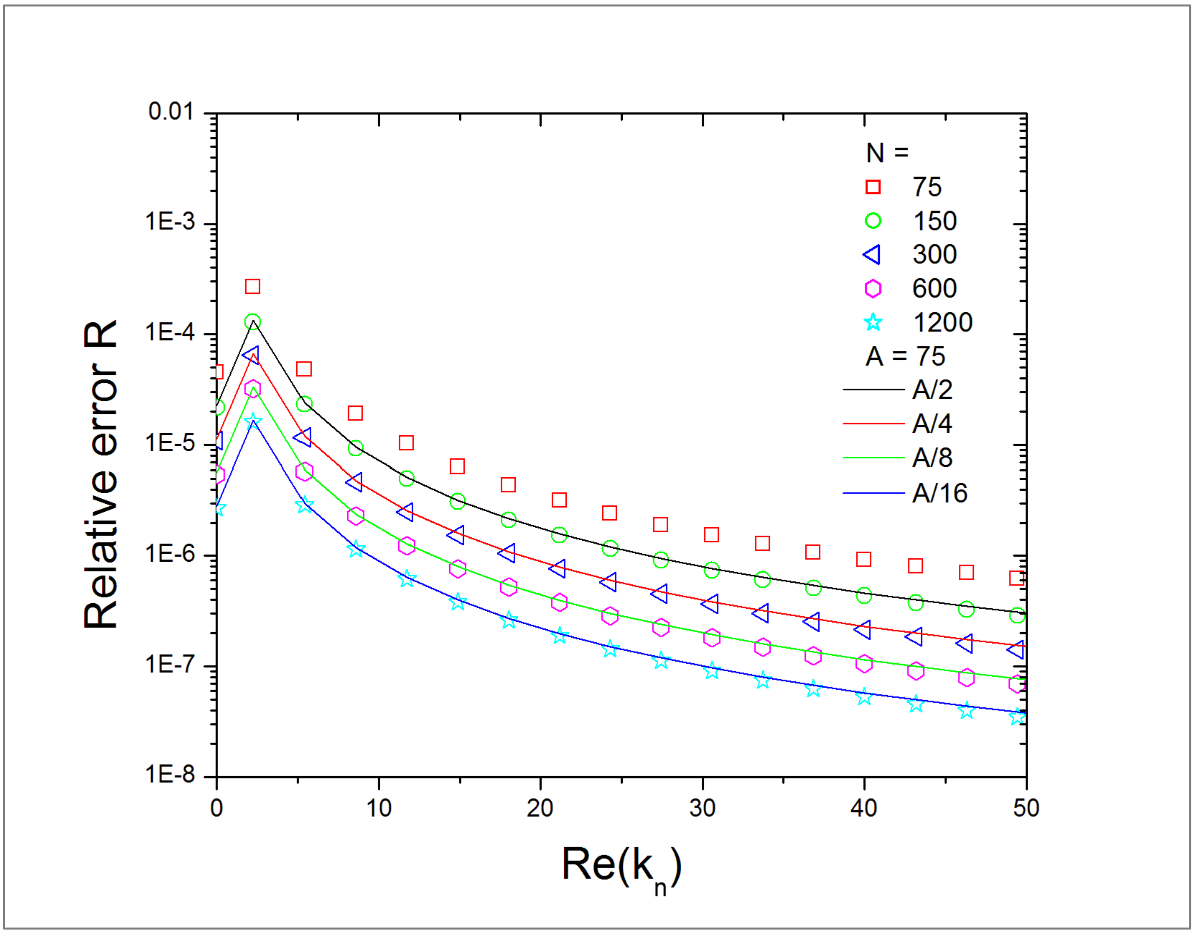

Figure 1(b): Relative error between the RSE results and exact solutions for different basis size *N*.

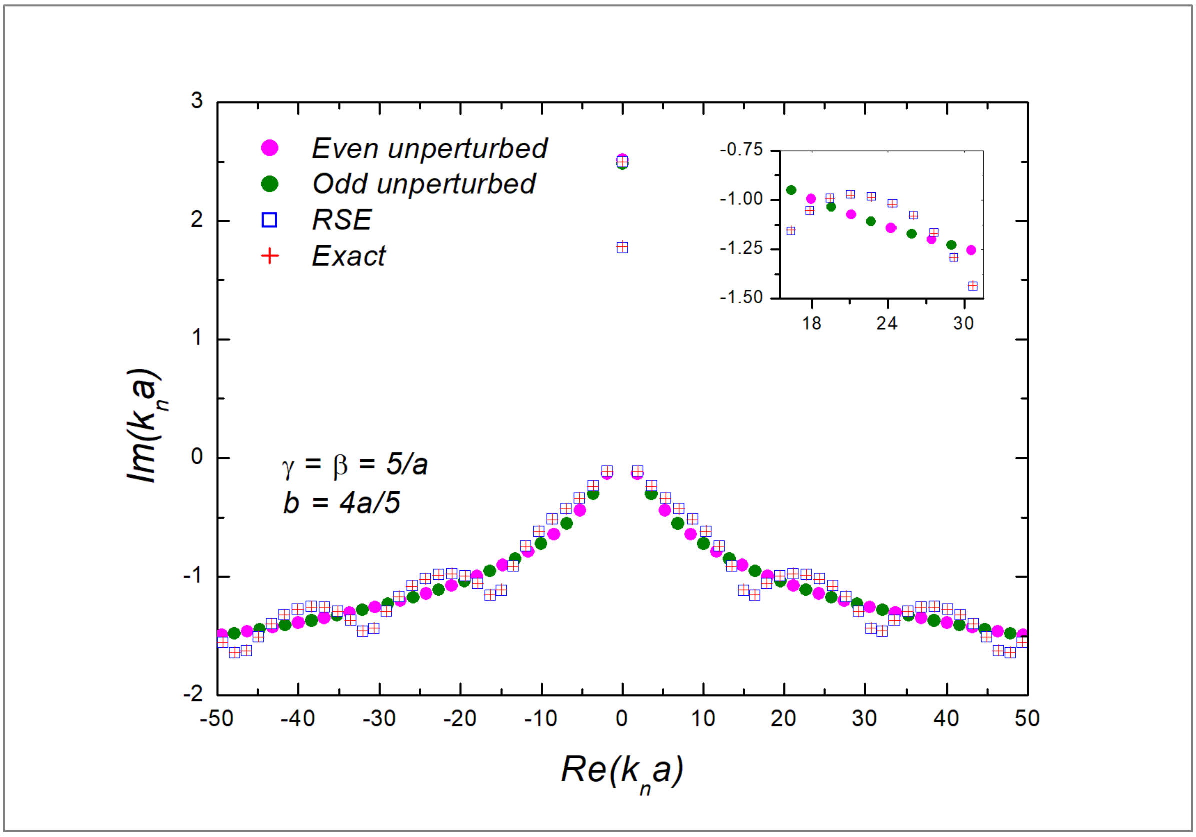

Figure 2: As in Fig. 1 (a), but for $b = 4a/5$, $\gamma = \beta = 5/a$

CONCLUSION

The RSE has been re-introduced into a non-relativistic wave equation in one dimension. In this work, we test the method on exactly solvable one-dimensional systems of triple well potential. Our work appears to be careful and thorough, looking at the convergence testing the accuracy of the perturbation as the number of basis sizes increases for both symmetric and anti-symmetric cases. A standard form of normalization used in the RSE is given. The graphs show that the accuracy is maintained for almost all the states considered within the spectrum, with inaccuracies only occurring at the extreme end of the real axis. Unlike other available commercial solvers, this method has shown to be quite an efficient and well-suited computational tool for calculating high-quality RSs.

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REFERENCES

Armitage, L. J.,Doost, M. B., Langbein, W., and Muljarov, E. A. (2014). Resonant state expansion applied to planer waveguides. Phys. Rev. A 89, 053832. [Crossref]

Doost, M. B., Langbein, W., and Muljarov, E. A. (2012). Resonant state expansion applied to planer open optical systems.Phys. Rev. A 85, 023835. [Crossref]

Gamow, G. (1928). Zurquantentheorie des atomkernes. Zeitschriftfur physic. 51, pg. 204-212. [Crossref]

Hatano, N. (2008). Some properties of the Resonant states in quantum mechanics and its computations. Prog. Theor.Phys. 119, pg. 187. [Crossref]

Lind, P. (1992). Completeness relations and resonant state expansion. Physical Review C 47, pg. 1903. [Crossref]

Mostert, M. (2014). Resonant states and Resonant states expansion in Quantum Mechanics, Year 4 Physics report

Muljarov, E. A., Langbein, W., and Zimmermann, R. (2010). Brillouin-Wigner Perturbation theory in open electromagnetic systems.EPL 92, pg. 5. [Crossref]

Siegert,A. J. F. (1939). On the Derivation of the Dispersion Formula for Nuclear Reactions. Physical Review 56, pg. 750. [Crossref]

Tanimu, A., and Muljarov, E. A. (2018). Resonant state expansion applied to one-dimensional quantum systems. Phys. Rev. A 98, 022127. [Crossref]

Tanimu, A., and Muljarov, E. A. (2018). Resonant states in double and triple quantum wells. J. Phys. Commun. 2, 115008. [Crossref]

Tanimu, A., and Bagudo, I. M. (2020). Resonant states in a one-dimensional quantum system.FJS.4, pg. 300. [Crossref]

Tanimu, A., and Bagudo, I. M. (2022). Resonant states expansion of the one-dimensional Schrödinger equation. BAJOPAS. 13, pg. 320.