Journal of the Nigerian Association of Mathematical Physics
***Volume 54* (January *2020 Issue*), pp143 – 146**

DETERMINATION OF RESONANT STATES IN A FINITE SQUARE WELL

[1]S. Kado and [2]A. Tanimu

[1]Department of Physics, Federal University Dutsinma, Katsina.
[2]Department of Physics, Umaru Musa Yar'adua University, Katsina.

Abstract

The purpose of this work is to determine the resonant states in a one-dimensional finite square well system. Resonant states are the Eigen solutions to the time independent Schrödinger's equation with outgoing wave boundary conditions. The secular transcendental equations for even and odd states were first obtained. This is done by solving the Schrödinger's wave equation with purely outgoing wave boundary conditions. The equations obtained were solved numerically in MATLAB leading to three types of states namely: bound states, antibound states and resonant states. Apart from bound states which has been covered in so many textbooks resonant states have attracted significant interest in recent time, in particular, in quantum mechanics due to rapid progress in the field of semiconductor physics were different electronic states are formed. In spite of this growing interest, many fundamental aspects of resonant states are still to be investigated. In this case the effect of changing the parameters in the system is fully observed. We observed that for a shallow well there is at least one bound state within the system. However, increasing the strength of the potential will lead to an increase in the number of bound/antibound states.

***Keywords*: Finite Square well, Bound states, Antibound states, Resonant states.**

1. Introduction

In quantum mechanics resonant states (RSs) have been studied for over a long period of time [1, 2]. They are obtained by seeking solutions to the time independent Schrödinger's equation with outgoing wave boundary conditions [3, 4, 5]. These are states with complex energy eigenvalues, causing them to decay exponentially in time [6, 7]. Because of their complex nature, resonant states have been used to model unstable particles in nuclear physics [2, 4]. Resonant state investigation is very important in a vast majority of physics areas among which are quantum physics and electrodynamics.

In this work, we demonstrate how the effect of changing the parameter affects the spectrum of a studied system [6, 8].

These spectrums include bound states, antibound states and normal resonant states. All these form a complete set of Eigen wave numbers.

We first work out the analytics obtaining secular transcendental equations for even and odd states. This is done by applying the outgoing wave boundary conditions to the one-dimensional Schrödinger's equation [9]. Solutions to these equations are obtained numerically in MATLAB and plotted in a complex k-plane.

2. Theory

2.1 Finite square well potential

The finite square well potential (also known as the finite square well) is a concept from quantum mechanics in which a particle is bounded to a box which has finite potential well [6] as shown in Fig. 1.

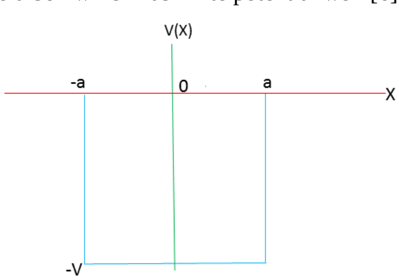

Figure 1: A schematic diagram for a finite square well potential.

Corresponding Author: Kado S., Email: skado@fudutsinma.edu.ng, Tel: +2348035304338, +2348063399084 (AT)

The time-independent Schrödinger equation for one dimensional finite square potential well is

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

Where $V(x)$ is the potential of the particle given as

$$V(x) = \begin{cases} -\alpha, & |z| < a \\ 0, & |z| > a \end{cases} \qquad (2)$$

and $E = \frac{\hbar^2 k^2}{2m}$ is the energy of the particle. For convenience, we use in the following $m = 1/2$ and $\hbar = 1$, so that $E = k^2$, where k is the eigen wave number of the particle, $\hbar$ is the Planck's constant, m is the effective mass of the particle.

Equation 1 can be written as

$$-\frac{d^2}{dx^2}\,\psi(x) = k^2\psi(x) \qquad (3)$$

where

$$k = \frac{\sqrt{-2mE}}{\hbar} \qquad (4)$$

The general solution to equation 3 is

$$\psi(x) = Ae^{-ik_n x} + Be^{ik_n x} \qquad (5)$$

Where *A* and *B* are constant

For a wave function to be normalized, the constant *A* must be zero.

Thus equation (5) becomes,

$$\psi(x) = Be^{ik_n x} \qquad (6)$$

By introducing a new constant q in region *II* i.e., $-a < x < a$, the Schrödinger's equation in equation (1) will now become

$$\frac{d^2}{dx^2}\,\psi(x) = -q^2\psi(x) \qquad (7)$$

k and q are the eigenvalues in their respective regions and are related as

$$q = \sqrt{k^2 + \alpha} \qquad (8)$$

The general solution to equation 7 is

$$\psi(x) = C\,sin(qx) + D\,cos(qx) \qquad (9)$$

In region III $x < -a,\ \alpha(x) = 0$, same case with region I

$$\psi(x) = Fe^{-ik_n x} + Ge^{ik_n x} \qquad (10)$$

In order to keep the wave function normalized we set G = 0. Thus

$$\psi(x) = Ae^{-ik_n x} \qquad (11)$$

Therefore;

$$\psi(x) = \begin{cases} Be^{ik_n x} \\ C\,sin(qx) + D\,cos(qx) \\ Fe^{-ik_n x} \end{cases} \qquad (12)$$

For a wave function to be symmetric there has to be even and odd solutions.

For even solutions

$$\psi^+_{(x)} = \begin{cases} Be^{ik_n x} \\ D\,cos(qx) \\ Be^{-ik_n x} \end{cases} \qquad (13)$$

For odd solutions

$$\psi^-_{(x)} = \begin{cases} -Be^{ik_n x} \\ Csin(qx) \\ Be^{-ik_n x} \end{cases} \quad . \qquad (14)$$

Applying boundary conditions (for even solutions)

At $x = a$

$\psi^+_{(x)} = \psi^-_{(x)}$. And $\psi'^+_{(x)} = \psi'^-_{(x)}$.

$$Be^{ik_n a} = Dcos(qa) \qquad (15)$$

$$ikBe^{ik_n a} = -qDsin(qa) \qquad (16)$$

Dividing equation 15 and 16 and after some algebra we have solution for even state as

$$k = iq_n\,tan(qa) \qquad (17)$$

Following the same procedure as above we have solution for odd state as

-$k = iq_n\, cot(qa)$ (18)

Equations 17 and 18 are the two secular equations corresponding to the even and odd states. These equations are to be solved numerically with the help of Newton-Raphson procedure in MATLAB. Solutions to these are plotted in complex k-plane as shown in section 3 of this work.

3.0 Result and Discussion

3.1 Resonant states wave numbers

Fig. 2 shows the plots of the complex wave numbers in equations (17) and (18). For α = 3 the graph has only bound states and resonant states within the spectrum while for α = 10 the graph shows all types of states (Bound states, antibound states and RSs) within the spectrum.

Bound states are located at the position where $Im\ k > 0$ with positive imaginary axis [5, 6]. Antibound states are located at the region where $Im\ k < 0$ with negative real axis. The remaining states in the spectrum are resonant states. The resonant states are symmetric about the imaginary axis and contain symmetric pair of states.

It has observed that irrespective of the quantum well depth there is at least one bound state in a square well potential. It can be seen from these figures that, for α = 3 we have only two bound states in the spectrum. However, increasing the depth of the potential will lead to an increase in the number of bound states and antibound states in the system (see Figure for α = 10).

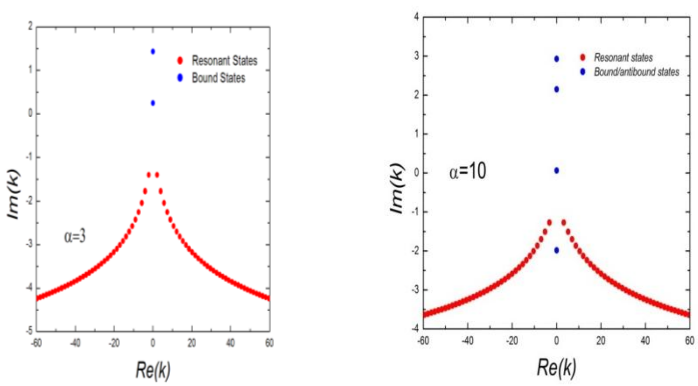

Figure 2: Eigen wavenumbers k plotted in the complex plane with α = 3 and α = 10.

4.0 Summary and Conclusion

In this work, we consider a well-known problem in quantum mechanics, the finite square well to study the spectrum of resonant sates (RSs) in a finite square well potential. RSs were studied by seeking solutions to one-dimensional time independent Schrödinger equation. After application of boundary conditions to the Schrödinger's wave equation, a system of equations was generated and written in form of secular transcendental equations. These equations were solved numerically with the help of Newton-Raphson procedure in MATLAB.

We have demonstrated that for a finite square well the full set of RSs are obtained by applying the outgoing wave boundary conditions. We have also demonstrated that the decrease or increase in the number of bound/antibound states depends on the choice of parameter α.

References

[1] G. Gamow, (1928). Zur quantentheorie des atomkernes. *Zeitschrift fur Physik,* **51**, 204–212, 1928.

[2] A. J. F. Siegert, (1939). On the Derivation of the Dispersion Formula for Nuclear Reaction. phys. Rev. **56**,750

[3] R. M. More, (1971). Theory of Decying States. Phys. Rev A, **4**, 1782.

[4] N. Hatano, (2008). Some properties of the resonant state in quantum mechanics and its computation. Prog. Theor. Phys. **119,** 187.

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

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

[7] M. B. Doost, W. Langbein, and E. A. Muljarov, (2012). Resonant state expansion applied to planar open optical systems. Phys. Rev. A, **85**, 023835.
[8] Sprung D. W. L. and Hua Wu, (2000). Bound states of a finite periodic potential, Am. J. of Phys. **68**, 715
[9] Mandle F. (1992). Quantum Mechanics (1st Edition), Wiley, 50010.