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Eigenvalues of Particle Bound in Single and Double Delta Function Potentials through Numerical Analysis

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Abstract**—**This study employs the use of the fourth order Numerov scheme to determine the eigenstates and eigenvalues of particles, electrons in particular, in single and double delta function potentials. For the single delta potential, it is found that the eigenstates could only be attained by using specific potential depths. The depth of the delta potential well has a value that varies depending on the delta strength. These depths are used for each well on the double delta function potential and the eigenvalues are determined. There are two bound states found in the computation, one with a symmetric eigenstate and another one which is antisymmetric.

Keywords**—**Double Delta Potential, Eigenstates, Eigenvalue, Numerov Method, Single Delta Potential

I. Introduction

THE delta function potential has an interesting property and it plays an important character in theoretical solid state physics. In the Kronig-Penney square well periodic potential, the periodic delta function is used to simplify the coefficients of the eigenstate of electrons so as to determine the accessible energy states and isolated energy bands on solids[1]. The potential has the form

$$U(x) = -\alpha\delta(x) \tag{1}$$

where α is called the delta strength. Theoretically, this has one bound state

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \tag{2}$$

and the allowed energy[2] is

$$E = -\frac{m\alpha^2}{2\hbar^2}. \tag{3}$$

This research work aims to investigate on the bound state and energy of a particle in single and double delta function potentials.

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II. Numerical Method

The Numerov Method is based on a Taylor expansion of the function and its second derivative[3]. This is the numerical

method used to solve the eigenstate of particle in delta function potential. In solving the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x), \tag{4}$$

implementing Numerov algorithm gives the eigenstate

$$\psi_{n+1} = \frac{2\left(1-\frac{5m}{6\hbar^2}h^2(E-U_n)\right)\psi_n - \left(1+\frac{1m}{6\hbar^2}h^2(E-U_{(n-1)})\right)\psi_{n-1}}{1+\frac{1m}{6\hbar^2}h^2(E-U_{(n+1)})} \tag{5}$$

This method requires two initial conditions of the eigenstate to start the iteration for the equation. It must be noted that the wave function approaches zero as the position tends to infinity. Starting conditions could be chosen as $\psi_0 = 0$ and $\psi_1 = 1$. These are reliable initial conditions and can be justified mathematically since multiplying an eigenstate with a constant does not affect the eigenvalue[4]. In all calculations, h has a value equal to 0.1 Å.

To easily get values of the wave function, a computer must be used to easily solve the iterative equation. The simulation tool used here is ROOT, an object-oriented framework aimed at solving the data analysis challenges of high-energy physics[5].

III. Single Delta Function Potential

The Dirac delta function, $\delta(x)$, is defined informally as follows[2]:

$$\delta(x) = \begin{cases} 0, \text{if } x \neq 0 \\ \infty, \text{if } x = 0 \end{cases}, \quad \text{with} \quad \int_{-\infty}^{+\infty}\delta(x)dx = 1 \tag{7}$$

It is infinitely high, infinitesimally narrow spike at the origin, whose area is 1[2]. However, in computational calculations, it is impossible to use an infinite value. So there must be a defined depth of the delta potential well. In the numerical calculations, this potential depth is the quantity that was derived using analytical eigenvalues. For an electron as the particle in consideration, delta strengths of 1.0 neV·m, 1.5 neV·m, 2.0 neV·m, 2.5 neV·m and 3.0 neV·m are used and the corresponding eigenvalues from equation 3 are utilized for the iterative equation 5. These are just arbitrary values chosen for the purpose of differentiating the behavior of the potential.

For these delta strengths, the potential energies shown in table 1 for each potential well were used in order to get the wave function that depicts the theoretical wave function.

TABLE I
POTENTIAL DEPTH OF THE WELL

Delta Strength α (10^{-20} eV·m)	Potential energy of the well (10^{-20} eV)
1.0	–10.36381494819571
1.5	–15.83707646222841
2.0	–21.52314586178961
2.5	–27.43775238467572
3.0	–33.59757028209128

The corresponding potential energy of the potential well for certain values of the delta strengths

This showed a more realistic model since it is impossible in actual physical systems to have wells or barriers with infinite depth or height.

The eigenstate for the first delta potential, with delta strength equals $1\ x\ 10^{-20}$ eV·m is graphed and shown on figure 1. Different delta strengths would still show a similar behavior of the curve.

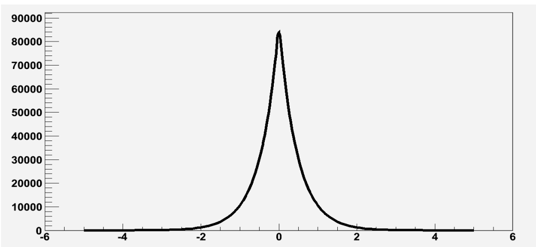

Fig. 1 Graph of the eigenstate of an electron influenced by an attractive delta potential with delta strength $1\ x\ 10^{-20}$ eV·m. Horizontal axis shows the position of the electron while the vertical axis represents the values of eigenstate

IV. DOUBLE DELTA FUNCTION POTENTIAL

Using the potentials depths derived in part III, the double delta function potential could be analyzed easier now. The double delta function is much more interesting because it gives a quick way to study the properties of a narrow deep double well[6]. Let the potential be of the form

$$U(x) = -\alpha[\delta(x-a) + \delta(x-a)] \tag{8}$$

The delta strength used will still be the same with that of the single delta potential with corresponding potential depths. For a =1.0 Å, the eigenvalues determined is shown in table II.

TABLE II
EIGENVALUE OF BONDING STATES FOR a = 1.0 Å

Depth of the delta potentials (10^{-20} eV)	Eigenvalue (10^{-20} eV)
–10.36381494819571	– 1.081062871017
–15.83707646222841	– 2.373951456076
–21.52314586178961	– 4.207072725867
–27.43775238467572	– 6.570993061844
–33.59757028209128	– 9.461779956832

Eigenvalue of an electron bound in a double delta function potential for different potential depths derived in part III with a = 1.0 Å for bonding states.

Figure 2 shows the eigenstate of the particle influenced by this delta function potential. However, for this double delta potential, another bound state also exists. This eigenstate, unlike the symmetric graph shown in figure 2, is antisymmetric. Bonding and antibonding states exist for double delta function potential, respectively with even and odd parity[7]. Table III shows the eigenvalues of for the antibonding states.

TABLE III
EIGENVALUE OF ANTIBONDING STATES FOR a = 1.0 Å

Depth of the delta potentials (10^{-20} eV)	Eigenvalue (10^{-20} eV)
–10.36381494819571	– 1.018041401387
–15.83707646222841	– 2.356725108829
–21.52314586178961	– 4.203336265901
–27.43775238467572	– 6.570281057373
–33.59757028209128	– 9.461655042166

Eigenvalue of an electron bound in a double delta function potential for different potential depths derived in part III with a = 1.0 Å for antibonding states.

For other values of a, at 1.5 Å and 2.0 Å, the eigenvalues for symmetric eigenstates are shown in tables 4 and 6. Eigenvalues for antisymmetric eigenstates are also calculated and shown in tables V and VII.

TABLE IV
EIGENVALUE OF BONDING STATES FOR a = 1.5 Å

Depth of the delta potentials (10^{-20} eV)	Eigenvalue (10^{-20} eV)
–10.36381494819571	– 1.05509022589
–15.83707646222841	– 2.36579662427
–21.52314586178961	– 4.20523563474
–27.43775238467572	– 6.57063901021
–33.59757028209128	– 9.46171761553

Eigenvalue of an electron bound in a double delta function potential for different potential depths derived in part III with a = 1.5 Å for bonding states.

TABLE V
EIGENVALUE OF ANTIBONDING STATES FOR a = 1.5 Å

Depth of the delta potentials (10^{-20} eV)	Eigenvalue (10^{-20} eV)
–10.36381494819571	– 1.04743093704
–15.83707646222841	– 2.36506161400
–21.52314586178961	– 4.20517992302
–27.43775238467572	– 6.57063530228
–33.59757028209128	– 9.46171738847

Eigenvalue of an electron bound in a double delta function potential for different potential depths derived in part III with a = 1.5 Å for antibonding states.

TABLE VI
EIGENVALUE OF BONDING STATES FOR a = 2.0 Å

Depth of the delta potentials (10^{-20} eV)	Eigenvalue (10^{-20} eV)
–10.36381494819571	– 1.0517617849625
–15.83707646222841	– 2.3654450304468
–21.52314586178961	– 4.2052081952484
–27.43775238467572	– 6.5706371659047
–33.59757028209128	– 9.4617175022064

Eigenvalue of an electron bound in a double delta function potential for different potential depths derived in part III with a = 2.0 Å for bonding states.

TABLE VII
EIGENVALUE OF ANTIBONDING STATES FOR a = 2.0 Å

Depth of the delta potentials (10^{-20} eV)	Eigenvalue (10^{-20} eV)
–10.36381494819571	– 1.05082651718
–15.83707646222841	– 2.36541366367
–21.52314586178961	– 4.20520736457
–27.43775238467572	– 6.57063714659
–33.59757028209128	– 9.46171750179

Eigenvalue of an electron bound in a double delta function potential for different potential depths derived in part III with a = 2.0 Å for antibonding states.

The bonding states refer to the symmetric state shown in figure 2. This is the graph of the eigenstate for a = 2.0 Å. All other potential depths and other values of a would also show a similar graph of eigenstates.

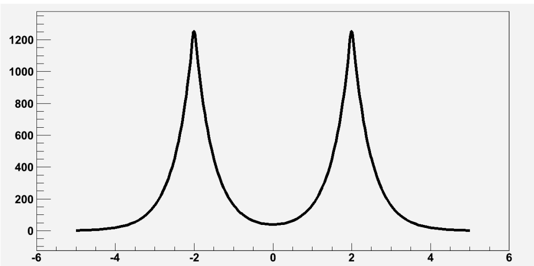

Fig. 2 Symmetric eigenstate of an electron in a double delta function potential well with kinks at a = 2.0 Å. Horizontal axis acts for the position of the electron while the vertical axis represents the values of eigenstate

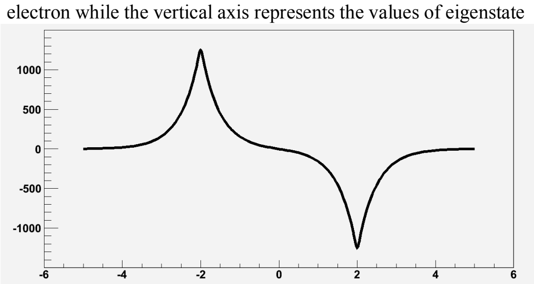

Fig. 3 Antiymmetric eigenstate of an electron in a double delta function potential well with kinks at a = 2.0 Å. Horizontal axis acts for the position of the electron while the vertical axis represents the values of eigenstate.

Figure 3 shows the antisymmetric eigenstate for a = 2.0 Å. The rest of the antibonding states for different values of a and potential depths also exhibit a similar graph of eigenstate.

V. CONCLUSION

The Numerov algorithm followed in this paper showed success in determining eigenvalues and eigenstates of an electron bound in single and double delta potential wells. For the single delta potential well, it was found that there should be a specified potential depth to get the required eigenstate of the particle considered. The potential depths were found to be dependent on the delta strength of the delta function. For the double delta function potential well, whose potential depths are those that were derived from the single well, two allowed eigenvalues were computed showing the symmetric eigenstate corresponding to the bonding state and the antisymmetric eigenstate for the antibonding state.

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