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Shooting Method for Analysis of Quantum Wells with Arbitrary Potential Profiles

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Abstract — *This paper presents a simple method for accurately calculating energy eigenvalues and eigenfunctions in quantum wells by using shooting method. This method is applicable to various potential barriers and wells, including continuous variations of potential energy. Various potential structures, i.e., single finite quantum well, triple finite quantum wells and multiple irregular quantum wells, are analyzed to show the feasibility of this method. This method is useful to find the eigenfunction and energy eigenvalues, which are very important parameters to analyze and design quantum tunneling devices.*

1. INTRODUCTION

Nano devices such as single electron devices [1-3], resonance tunneling devices [4,5] etc., have attracted interest in order to solve the limitation of downscaling conventional metal-oxide-semiconductor field effect transistors (MOSFET). With the epitaxial crystal growth techniques such as MBE (molecular beam epitaxy) and MOCVD (metal organic chemical vapor deposition), it has become possible to fabricate high-quality layered semiconductor structures like quantum wells and potential barriers, which are the basic structures of the nano devices. In order to understand deeply the transport characteristics through the quantum wells and potential barriers, it is very important to calculate quantum confinement effect for those structures. However, analytical method is useful to solve Schrodinger equation only for simple potential well structures but not for the non-uniform shape of structure. So far, numerical methods based on the multistep potential approximation [6-8], piecewise-linear potential approximation [9], transmission line analogy [10] and shooting method [11] have been developed for the analysis of quantum wells.

In this work, Schrodinger equation in non-uniform shape of potential quantum well is solved by using finite difference based on shooting method [11]. Using this method, both energy eigenvalues and the eigenfunctions are easily calculated for any potential shapes. The eigenfunctions are useful to determine the electron density in the potential quantum wells.

2. CALCULATION METHOD

Time-independent Schrodinger equation in one-dimensional potential V(x) can be given by the following equation,

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

where $\psi(x)$ is the wave function representing the particle, $\hbar$ is Planck's constant, m is the effective mass of the particle and E is the energy of the particle. The equation (1) can be written as follows:

$$-\frac{\hbar^2}{2\mathrm{m}}\frac{d^2}{dx^2}\psi(x)+[\mathrm{V(x)}-\mathrm{E}]\psi(x)=0. \qquad (2)$$

The problem is to find a numerical method for the solution of both the energy eigenvalues E and the eigenfunctions $\psi(x)$ for any V(x). For this aim, it is considered the expanding second-order derivative in terms of finite difference. As shown in Fig. 1, the first derivative of any function is defined as:

$$\lim_{\Delta x\to\infty}\frac{\Delta f}{\Delta x}=\frac{df}{dx}. \qquad (3)$$

It is useful here to use the approximate form, i.e.,

$$\frac{\Delta f}{\Delta x}\approx\frac{df}{dx}=\frac{f(x+\delta x)-f(x-\delta x)}{2\delta x}. \qquad (4)$$

Hence, the second derivative follows as:

$$\frac{d^2f}{dx^2}\approx\frac{\frac{df}{dx}\Big|_{x+\delta x}-\frac{df}{dx}\Big|_{x-\delta x}}{2\delta x}. \qquad (5)$$

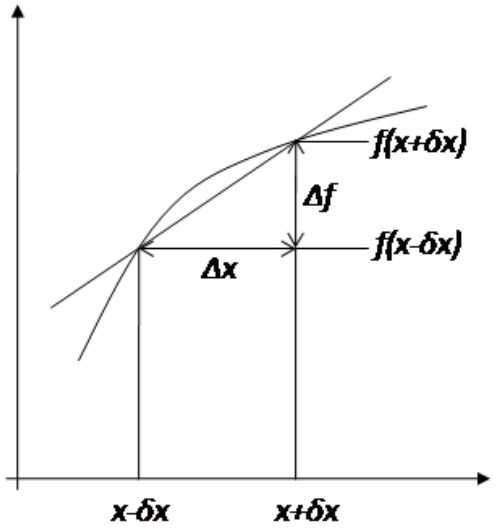


Figure 1. The first derivative of a function.

By using finite difference forms in equation 4 for the first derivatives, then:

$$\frac{d^2f}{dx^2} \approx \frac{\left[\frac{f(x+2\delta x)-f(x)}{2\delta x}\right]-\left[\frac{f(x)-f(x-2\delta x)}{2\delta x}\right]}{2\delta x}, \quad (6)$$

so that,

$$\frac{d^2f}{dx^2} \approx \frac{f(x+2\delta x)-2f(x)+f(x-2\delta x)}{(2\delta x)^2}. \quad (7)$$

Above equation can be simplified by substituting δx for $2\delta x$, i.e.,

$$\frac{d^2f}{dx^2} \approx \frac{f(x+\delta x)-2f(x)+f(x-\delta x)}{(\delta x)^2}. \quad (8)$$

Using this form for the second derivative in the original Schrodinger equation and taking the step length δx as sufficiently small, it can be obtained,

$$-\frac{\hbar^2}{2\mathrm{m}}\left[\frac{\psi(x+\delta x)-2\psi(x)+\psi(x-\delta x)}{(\delta x)^2}\right]+ [\mathrm{V(x)}-\mathrm{E}]\psi(x)=0. \quad (9)$$

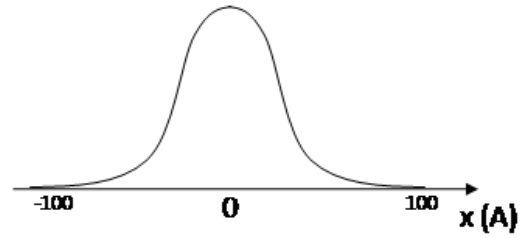
Equation (9) can be finally written as:

$$\psi(x+\delta x)=\left[\frac{2\mathrm{m}}{\hbar^2}(\delta x)^2(\mathrm{V(x)}-\mathrm{E})+2\right]\psi(x) -\psi(x-\delta x). \quad (10)$$

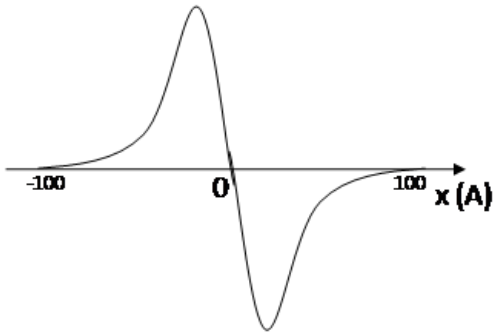
Equation above implies that if the wave function is known at the two points $(x-\delta x)$ and x, the value of the wave function at $(x+\delta x)$ can be calculated for any energy E. This iterative equation forms the basis of a standard method of solving differential equations numerically, and is known as the shooting method [11].

Using two known values of the wave function $\psi(x-\delta x)$ and $\psi(x)$, a third value, i.e., $\psi(x+\delta x)$, can be predicted. Using this new point $\psi(x+\delta x)$, together with $\psi(x)$ and by making the transformation $x+\delta x \rightarrow x$, a fourth point, $\psi(x+2\delta x)$, can be calculated, and so on. Hence the complete wave function can be deduced for any particular energy. The solutions for stationary states have wave function which satisfy the standard boundary conditions. i.e.

$$\psi(x) \rightarrow 0 \text{ and } \frac{\partial\psi(x)}{\partial x} \rightarrow 0, \text{ as } x \rightarrow \pm\infty. \quad (11)$$



(a)



(b)

Figure 2. Eigenfunctions ψ(x) for (a) the first and (b) second energy levels of square quantum well.

The solution for the wave function starts with $\psi(x_{\mathrm{left}}) = 0$ to approximate $\psi(x = \infty) = 0$, and then numerically solves the time-independent Schrodinger equation, calculating the energy eigenfunction from left to right.

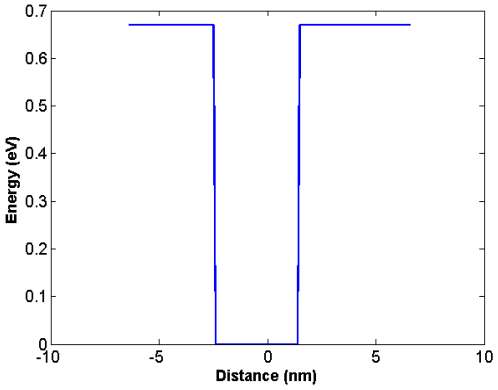
Because at the first time of calculation, two datas of wave function is needed, the following starting conditions could be chosen :

$$\psi(0) = 0; \psi(\delta x) = 1. \quad (12)$$

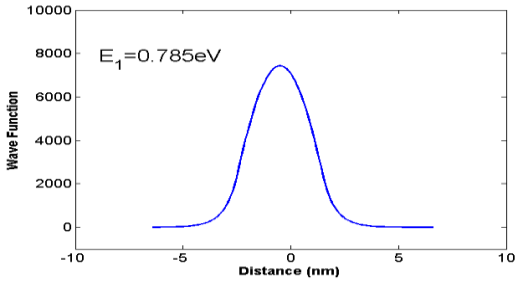
It is noted that all energy values solve the time-independent Schrodinger equation, but only some of these are referred to as energy eigenvalues which yield valid (proper) bound-state energy eigenfunctions. Figure 2 shows the example of eigenfunctions $\psi(x)$ for the first and second energy levels of square quantum well.

3. RESULTS AND DISCUSSIONS

The single quantum well is a good testing to check the numerical method discussed here. Figure 3 shows a GaAs single quantum well, surrounded by potential barrier AlGaAs of height 0.68 eV, with the same effective mass. The quantum well is shown in Fig. 3(a) and the eigenfunctions and energy eigenvalues are shown in Fig. 3(b-d). Three eigenfunctions and those energy eigenvalues are easily to be obtained from equation (10). These results are the same with the results obtained from the analytical method as discussed in any textbooks of quantum mechanics.



(a)



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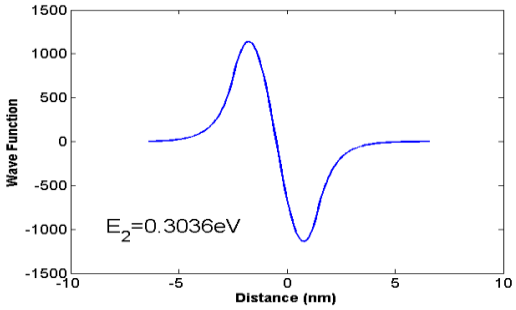

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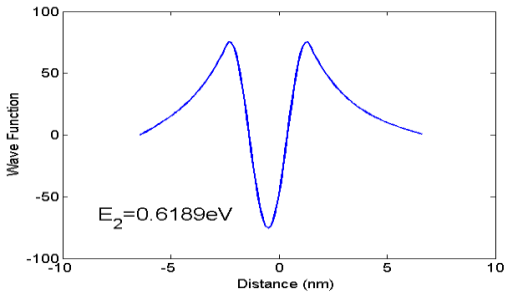
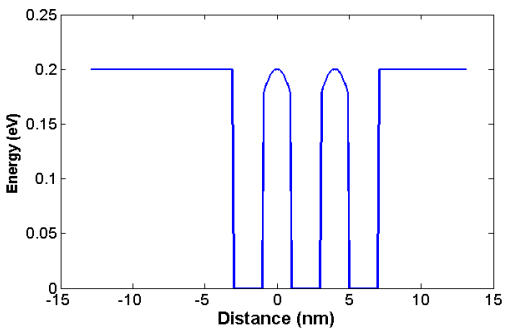


(d)

Figure 3. (a) Single quantum well formed from a GaAs coupled by a AlGaAs (AlGaAs/GaAs/ AlGaAs) and (b-d) the eigenfunctions and energy eigenvalues calculated from single quantum well in Fig. 3(a).

Figure 4 shows the calculation results of three quantum well with height of 0.2 eV. The potential barriers between the quantum well have circle shape on the top. Such quantum well structure in Fig. 4(a) is quite unique and it is not commonly obtained in the examples of Schrodinger equation solution. However, even the structure of the quantum well is unique, the eigenfunctions and energy eigenvalues can be easily calculated, as shown in Fig. 4(b-d).



(a)

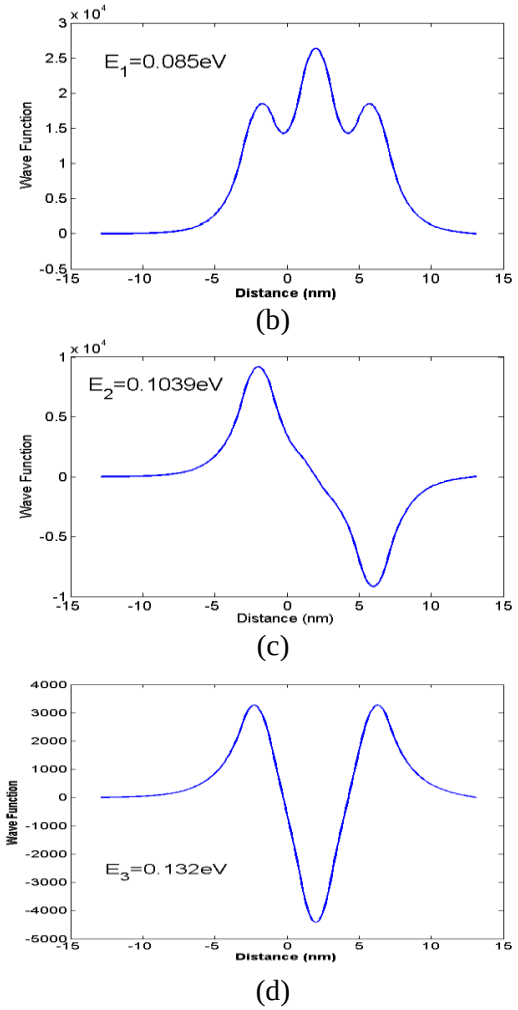
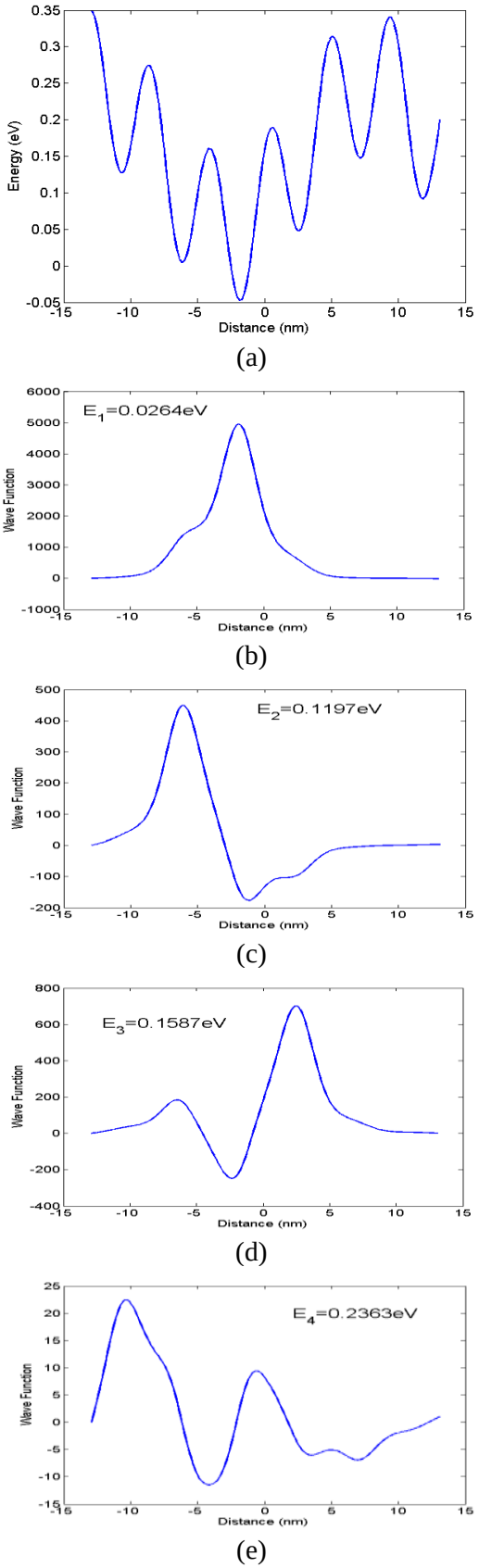
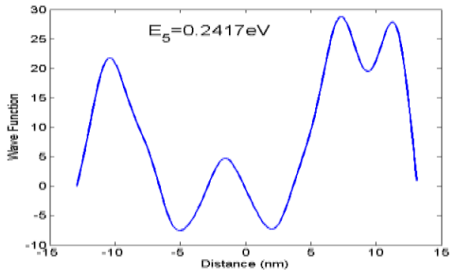


Figure 4. (a) Three quantum wells with potential height of 0.2 eV and (b-d) their eigenfunctions and energy eigenvalues.

Figure 5 shows the application of method to the irregular multi quantum wells and numerically obtained wave functions and their energy eigenvalues. Such irregular quantum wells are formed in multiple quantum dots structure having different size of dots. It can be seen that, even the quantum wells are irregular with total numbers of 6 wells, the wave functions and their energy eigenvalues are easily to be calculated.





(f)

Figure 5. (a) Irregular multi quantum wells and (b-f) numerically obtained wave functions and their energy eigenvalues.

From these 3 types examples of the quantum wells, it is concluded that the simple numerical method discussed here can be used for the calculations of the eigenfunctions and energy eigenvalues of arbitrary quantum well structure. It is noted that the wave functions obtained from this numerical method are not normalized, i.e., they do not satisfy:

$$\int_{all\ space} \psi^*(x)\psi(x)dx = 1\ . \qquad (13)$$

Therefore, the following transformation is needed for normalization,

$$\psi(x) \rightarrow \frac{\psi(x)}{\sqrt{\int_{all\ space} \psi^*(x)\psi(x)dx}}\ . \qquad (14)$$

4. CONCLUSIONS

Shooting method has been applied to calculate eigenfunctions and energy eigenvalues in quantum well with arbitrary potential profiles. The calculation is based on the solution of one-dimensional Schrodinger equation in the quantum well system. The validity of the method is confirmed by calculating the eigenstates of simple square quantum well, triple quantum well and multiple irregular quantum wells. Therefore, the present method is shown to be useful for analyzing and designing the quantum size effect devices.

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