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CONSTRUCTING BOUND STATES FROM A FINITE POTENTIAL WELL OF VARYING DEPTH

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Abstract

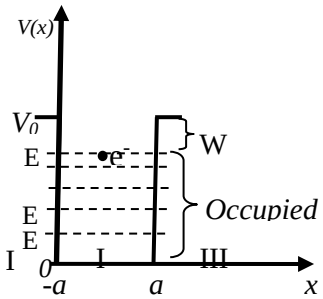
Increase in demands of smart devices, due to their current needs in every aspect of human endeavours has opened new opportunities for advances in semiconductor technology. In this study, bound states of a one-dimensional finite square well system, with a varying potential depth were determined, taking the width of the potential to be constant. The allowed energies were determined implicitly as the solutions to the transcendental equations; $\tan(z)=\sqrt{(z_o/z)^2-1}$ ***and*** $-\cot(z)=\sqrt{(z_o/z)^2-1}$. ***Energy eigenvalues are higher for odd solutions than for even solutions. The deeper a potential well is, the higher the energy eigenvalues. At varying depth of a potential well, for each corresponding level of bound states, the deepest well possesses the highest energy. Generally,*** z_0 ***controls the number of bound states, as*** z_0 ***grows, for the even solutions, the solutions tend to singularities*** $(2k+1)\pi/2$, ***where k is natural number. For the odd solutions, as*** z_0 ***grows, solutions tend to singularities that are integer multiples of*** π .

1.0 Introduction

Applications of smart devices, arising from advances in semiconductor technology are very vast in every aspect of human endeavours [1]. For instance, deterministic location of specific deep center in arsenic-on-gallium-site (AsGa or arsenic antisite), using the potential well model has found important applications in high speed light-emitting-diodes (LEDs), photodetectors, optical modulators, and nonlinear optics [2, 3]. The finite quantum well is of great practical importance because it forms the basis for understanding the structures of quantum well devices [4].

Bonfim and Griffiths [5] investigated the problem of a quantum particle in a one-dimensional finite square well. These authors used the standard approach of numerically solving transcendental equations but at a single well parameter. Palma and Raff [6] also developed a Fourier integral representation scheme for determining bound states in semiconductor materials. Applications of potential well models are vast in semiconductor technology, whereby free electrons are modeled to move freely in semiconductor materials but consistently localize electrons within a semiconductor material. Varying the well parameters and correspondingly determining the eigen energies will bring about robust characterization of semiconductor materials. To this end, this study determines bound states of a one-dimensional finite square well system of varying potential depth and constant width. The allowed energies were numerically determined by solving the transcendental equations: $\tan(z)=\sqrt{(z_o/z)^2-1}$ and $-\cot(z)=\sqrt{(z_o/z)^2-1}$. The findings from this study are expected to support the development of future models that will lead to the designs of semiconductor devices with optimum efficiency.

2.0 Formulation of the Problem



The potential can be expressed as:

$$V(x)=\begin{cases}-V_o, -a\le x\le a\\ 0, |x|>a\end{cases}$$

Figure 1: A finite square well potential model for electrons in a metal; the electrons are free inside the metal, occupying states up to a certain energy level E_n; the highest occupied energy level.

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The time-independent Schrodinger equation for a finite square potential can be expressed as:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V_o\psi(x)=E_n\psi_n(x) \quad (1)$$

From Figure 1, in region I, $x<-a$, the potential is zero, equation (1) becomes;

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}=E_n\psi_n(x) \quad (2)$$

$$\frac{d^2\psi(x)}{dx^2}-k^2\psi(x)=0 \quad (3)$$

where the wave vector $k=\sqrt{-2mE}/\hbar=\sqrt{2mE}_n/\hbar$ (E = -E_n) is real and positive. The general solution of equation (3) is of the form:

$$\psi(x)=A\exp^{-kx}+B\exp^{kx} \quad (4)$$

The term $\psi(x)=A\exp^{-kx}$ blows up as x approaches negative infinity; hence it has no physical meaning in this direction. For this reason, it is suppressed. Hence,

$$\psi(x)=B\exp^{kx} \quad (5)$$

In region II, $-a<x<a$, equation (1) becomes;

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}-V_o\psi(x)=E_n\psi_n(x) \quad (6)$$

$$\frac{d^2\psi(x)}{dx^2}+k'^2\psi(x)=0 \quad (7)$$

where the wave vector $k'=\frac{\sqrt{2m(E+V_o)}}{\hbar}=\frac{\sqrt{2m(V_o-E_n)}}{\hbar}$. The solution is of the form

$$\psi(x)=C\sin(k'x)+D\cos(k'x)$$

By Symmetry, the solution of equation (1) in region III, where $x>a$ is of the form:

$$\psi(x)=F\exp^{-kx}+G\exp^{kx} \quad (8)$$

where, again, $k=\sqrt{2mE}/\hbar$. The term $\psi(x)=Ge^{kx}$ blows up as x approaches positive infinity; hence, the term is suppressed, therefore;

$$\psi(x)=Fe^{-kx} \quad (9)$$

Using the boundary conditions, and matching the wave functions and their derivatives at the boundaries of the potential well ($\pm a$), we have the even and odd solutions, B=F for even solutions and B=-G for odd solutions, where B, C, D, F, and G are constants.

$$\psi_{even}(x)=\begin{cases}Fe^{-kx}, x>a\\ D\cos(k'x), -a<x<a\\ Fe^{kx}, x>-a\end{cases} \quad (10a)$$

$$\psi_{odd}(x)=\begin{cases}Ge^{-kx}, x>a\\ C\sin(k'x), -a<x<a\\ -Ge^{kx}, x>-a\end{cases} \quad (10b)$$

The solution with cosine term is even, while the solution with sine term is odd. The above constants can be found by normalizing the odd and even wave functions for the bound states. To solve for the allowed energies, the boundaries conditions will be imposed. At x = a, the wave function and its derivative are continuous.

$$\psi(x)=Fe^{-ka}=D\cos(k'a) \quad (11)$$

Also, $\frac{d\psi(x)}{dx}=-kFe^{-ka}=-k'D\cos(k'a)$ (12)

Dividing equation (12) by equation (11), we have $k = k' \tan(k'a)$

This is the equation for the allowed energies. Since k and k' are both functions of *E*, we can solve for *E* by introducing the following variables; $z = k'a$, $z_o = \frac{a}{\hbar}\sqrt{2mV_o}$. From the definitions of k and k', the even solution is in tangent form, while the odd solution is in a negative cotangent form,

$$\tan(z) = \sqrt{\left(\frac{z_o}{z}\right)^2 - 1} \qquad (13a)$$

$$-\cot(z) = \sqrt{\left(\frac{z_o}{z}\right)^2 - 1} \qquad (13b)$$

3.0 Computational Method

The transcendental equations (13a & b) cannot be solved analytically but graphically [5]: $f(z) = \tan(z)$, $g(z) = -\cot(z)$, $q(z) = \sqrt{\left(\frac{z_o}{z}\right)^2 - 1}$ are plotted against *z*, for varying value of z_0 (2, 4, 8, 16, 32). Values of *z* on the horizontal axis are carefully taken to be a little above z_0 at a major axis tick size of $\pi/2$ and an equal step-size of $\pi/10$. z_0 is the potential well parameter, defined as; $z_o = \frac{a}{\hbar}\sqrt{2mV_o}$, while $z = k'a$. We assume that the well's width is 2 *nm*, and constant all through the simulation scheme, with varying well depth V_0, all other parameters are constant. Each point of intersection of the plots on the *z* axis implies a bound state, and each of the bound state can be used to infer an allowed energy value. The energy eigenvalues were numerically determined by using $z_n = \frac{a}{\hbar}\sqrt{2mE_n}$

4.0 Results and Discussion

In this finite square potential problem formulation, we determined the bound states for varying potential depth for a quantum particle in a one-dimensional finite square well [7]. In the standard approach the allowed energies are determined implicitly as the solutions to the transcendental equations (13a & b) [8]. The parameter z_0 defines the depth, V_0 and width, *2a* of the well, with a particle of mass m inside the potential well. By implication, a very deep and/or wide potential has very large z_0, while a very shallow and/or narrow potential has small z_0. However, in this study, the author has assumed a situation whereby the width of the potential well is 2 *nm*, and constant all through the numerical experiment. Consequently, the only varying term is the depth of the well. In Figures 2–6, as the well gets deeper, z_0 grows to create more bound states. The bound states are represented by the intersections in the plot with red heavy dots for both the even and odd solutions.

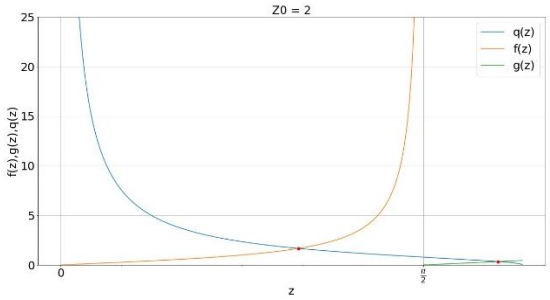

Figure 2: Plots of *g(z)*, *f(z)*, and *q(z)* against *z* for $z_0 = 2$

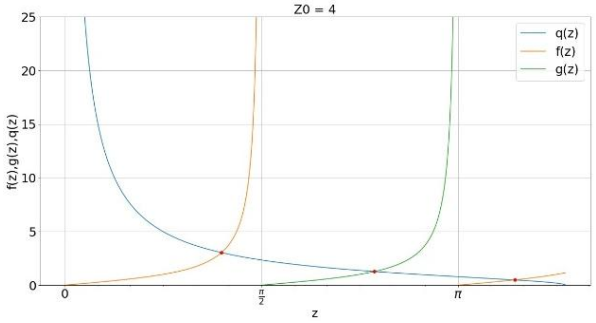

Figure 3: Plots of *g(z)*, *f(z)*, and *q(z)* against *z* for $z_0 = 4$

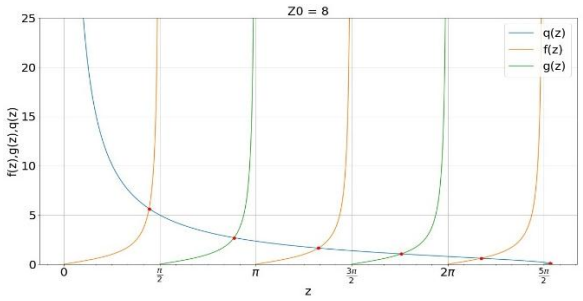

Figure 4: Plots of *g(z)*, *f(z)*, and *q(z)* against *z* for $z_0 = 8$

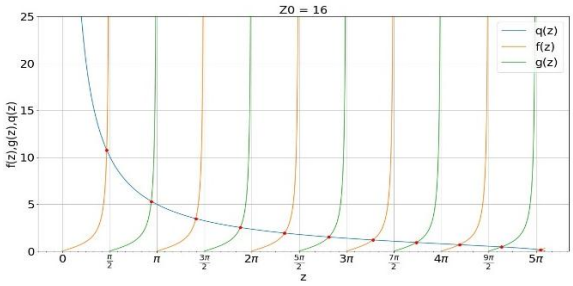

Figure 5: Plots of *g(z)*, *f(z)*, and *q(z)* against *z* for $z_0 = 16$

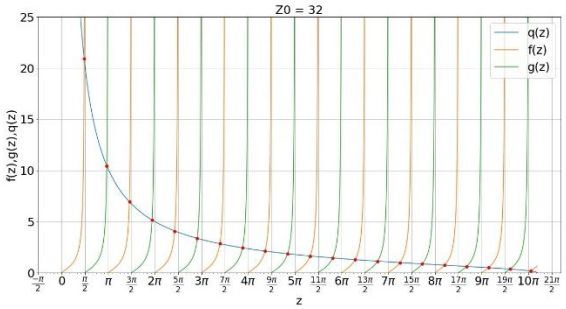

Figure 6: Plots of *g(z)*, *f(z)*, and *q(z)* against *z* for $z_0 = 32$

In Figure 2, for $z_0 = 2$, there is one point of intersection each for both even and odd solutions, which means single bound state each for the even and odd solutions, at $z_1 = 1.03$ and 1.90, respectively, with energy eigenvalues of 0.010 *eV* and 0.034 *eV* . The summary of the bound state values and their energy eigenvalues is presented in Tables 1 and 2. Thus, at least one bound state exists; irrespective of how shallow a finite well is, because an intersection of the functions always exists. As z_0 increases, the number of points of intersection also increases. From Figure 6, when $z_0 = 32$, for the even solutions, the first intersection was recorded at $z_1 = 1.52$ and energy eigenvalue of 0.022 *eV* (Table 1). The second intersection is z_2 is 4.57 with a corresponding energy eigenvalue of 0.200 *eV*. On the other hand, for the odd solutions at large z_0 ($z_0 = 32$), the first intersection takes place at $z_1 = 3.05$ and energy eigenvalue of 0.089 *eV* (Figure 6, Table 2). The second intersection is z_2 is 6.09 with a corresponding energy eigenvalue of 0.354 *eV*.

From Tables 1 and 2, for instance, at $z_0 = 2$, 8, and 32 for the even solutions; $E_1 = 0.010$, 0.019, and 0.020, respectively, and the corresponding E_3 = nil, 0.445, and 0.552. For the odd solutions; $E_1 = 0.034$, 0.074, and 0.089, respectively, and the corresponding E_3 = nil, 0.604, and 0.796. Comparatively, energy eigenvalues are higher for odd solutions than for even solutions. Furthermore, the deeper a potential well is, the higher the associated energy eigenvalues. We can also see from Tables 1 and 2, that for $z_0 = 2$, 4, 8, 16, and 32; the least energy eigenvalue, say at bound state z_1 was recorded for $z_0 = 2$ and the highest for $z_0 = 32$. This trend repeated all though our numerical experiment for all z_n. Consequently, at varying depth of a potential well, for each corresponding level of bound state, the deepest well possesses the highest energy.

Generally, z_0 controls the number of bound states, as z_0 grows, for the even solutions, the points of intersection of $f(z)$ curve with the $q(z)$-curves tends to singularities $(2k+1)\pi/2$, where k is natural number. The odd solutions showed a feature of a shift in the even solutions by $\pi/2$. For the odd solutions, as z_0 grows, the points of intersection of $g(z)$curve with the $q(z)$-curves tends to singularities that are integer multiples of π.

In semiconductor technology, the numerical scheme from this study can be used to model free electrons as they move freely in semiconductor materials at predetermined potential wells and barriers [9]. The electrons occupy states up to a certain energy level E_n [10], the highest occupied energy level (Fermi energy). As shown in the problem formulation (Figure 1), for an electron to be released from a semiconductor material/metal, energy W, representing the work function of the metal must be overcome.

Table 1: Energy eigenvalues derived from the points of intersection of the even bound states solutions for a 2 *nm* width potential well of varying depth.

n	$Z_0 = 2$		$Z_0 = 4$		$Z_0 = 8$		$Z_0 = 16$		$Z_0 = 32$	
	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$
1	1.90	0.034	2.47	0.058	2.79	0.074	2.96	0.084	3.05	0.089
2					5.52	0.291	5.91	0.333	6.09	0.354
3					7.96	0.604	8.84	0.745	9.14	0.796
4							11.74	1.314	12.18	1.414
5							14.56	2.021	15.21	2.205
6									18.24	3.172
7									21.26	4.309
8									24.27	5.615
9									27.26	7.084
10									30.18	8.683

Table 2: Energy eigenvalues derived from the points of intersection of the odd bound states solutions for a 2 *nm* width potential well of varying depth

n	$Z_0 = 2$		$Z_0 = 4$		$Z_0 = 8$		$Z_0 = 16$		$Z_0 = 32$	
	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$	Z_n	$E_n(eV)$
1	1.03	0.010	1.25	0.015	1.40	0.019	1.48	0.021	1.52	0.022
2			3.60	0.124	4.16	0.165	4.43	0.187	4.57	0.200
3					6.83	0.445	7.37	0.518	7.61	0.552
4							10.30	1.011	10.66	1.080
5							13.17	1.654	13.69	1.787
6							15.85	2.395	16.73	2.668
7									19.75	3.719
8									22.77	4.943
9									25.77	6.331
10									28.73	7.869
11									31.58	9.507

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5.0 Conclusion

This study determined the bound states of a one-dimensional finite square well system, with a varying potential depth [11, 12]. We assumed a situation whereby the width of the potential well is 2 *nm*, and constant all through the numerical experiment, so that the only varying term is the depth of the well. As the well gets deeper, more bound states were generated [13]. Irrespective of how shallow a finite well may be, there is always at least one bound state. Comparatively, energy eigenvalues are higher for odd solutions than for even solutions. Furthermore, the deeper a potential well is, the higher the energy eigenvalues. At varying depth of a potential well, for each corresponding level of bound state, the deepest well possesses the highest energy. Generally, z_0 controls the number of bound states, as z_0 grows, for the even solutions, the solutions tend to singularities $(2k+1)\pi/2$, where k is natural number. For the odd solutions, as z_0 grows, solutions tend to singularities that are integer multiples of π. This numerical scheme is expected to enhance future modeling of the behaviours of free electrons in semiconductor technology.

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