

SIMULATION OF PROBABILITY DENSITY FOR AN ELECTRON IN ONE DIMENSIONAL PERIODIC POTENTIAL

Sa'adiyya Bello Bature^{1*} and Abdulqadir Muhammad Nura²

¹Department of Physics, Umaru Musa Yar'adua University Katsina, Nigeria

²Department of Physics, Bayero University Kano, Nigeria

Abstract

The theoretical study of electronic band structures has been a challenging area in the field of study over past years. Many approximation methods have been developed to compute the eigenvalues and eigenvectors since exact analytic solutions to the Schrödinger's equation are unobtainable for some realistic potential. In this work, Intel® Visual Fortran 17.0 update 3 for windows contained in Intel® Parallel Studio XE 2017 Cluster Edition for windows was used to solve the time independent Schrödinger's equation with periodic potentials together with Visual Studio Community 2015. The Probability density functions for rectangular, saw tooth, and cosine periodic potential was calculated in the reduced zone scheme using the nearly free electron approximation. The result shows that the probability density increases with increase in the potential height and vice versa. The result shows reasonable agreement when compared with most of most of the existing results in the literature.

Keywords: Probability density, Periodic Potential, Nearly free electron approximation, Energy gap.

1.0 INTRODUCTION

Band structure is one of the most important concepts in Solid State Physics. It provides the electronic levels in (ideal) crystal structures, which are characterized by a Bloch vector k and a band index n . Here the Bloch vector is an element of the reciprocal space (in units $1/\text{length}$) and typically restricted to the first Brillouin zone. Many electronics, optical, and even some magnetic properties of crystals can be explained in terms of the band structure. Of importance is the location of the Fermi energy, until which all levels are occupied at zero temperature. If the location of Fermi energy is in a band gap, the material is insulating (or semiconducting) while it is metallic otherwise [1].

Thus, it is interesting to be able to compute the energy bands for a specific potential. Although not physically exact, the infinite periodic approximation is sufficiently good as to provide some insight into the shape of the bands in real solids. Remarkably enough, the electronic bands in one dimensional system can be numerically obtained by solving an approximate eigenvalue equation. Modeling one dimensional case is much easier than doing it for higher dimensions, since it only allows one type of periodicity, while higher dimensions allow plenty of possible periodic lattices [2].

No single method suffices for all potentials. Moreover, for most physically realistic potentials, the Schrödinger equation cannot be solved in analytic form. This is particularly true of real three-dimensional systems, such as many electron atoms, for which the potential experienced by each electron is determined by the configuration of all the other electrons in the atom [3]. For these cases and for many one-dimensional potentials it has become customary to resort to numerical approximation method, employing a computer to do the repetitive calculation involved. In contrast to analytic methods, the computer solution procedure for one-dimensional potentials can be standardized. Many attempts using different method or computer programming language have been used to obtain the energy band in one-dimensional Schrödinger equation [4].

Corresponding Author: Sa'adiyya B.B., Email: saadiyya.bello@umyu.edu.ng, Tel: +2347033943031, +2347063517772 (AMN)

Band structure of a material is very important to calculating the materials property, specifically for obtaining the electrical properties. Usually we need to have some information about the bands to simulate electron devices. Precisely there is not any analytical solution for the Schrödinger's equation in a crystal. Even it is not usually an easy and straightforward task to calculate it using existing numerical schemes because of the huge complexity involved [5].

Photonic crystal is another application of band gap engineering, which essentially changes band structure to create desired optical properties of a crystal. Both photonic crystals and thermoelectric nanostructure can be modeled by the Kronig-Penney potential and the band structure can be calculated to investigate the properties of the materials [6].

In this paper, Intel Visual Fortran 17.0 update 3 for windows which is inside the Intel® Parallel Studio XE 2017 Cluster Edition was used to solve the required Schrödinger equation with periodic potential in connection with Visual Studio Community 2015 using the computer simulation program "EnergyBands" to obtain the probability densities of an electron for $k = \frac{\pi}{a}$ in the region $-a/2 < x < a/2$.

2.0 THEORETICAL FOUNDATIONS

The time-independent Schrödinger's equation for an electron in one-dimension is

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

If we use the atomic units and measure energies in Rydberg's and distance in Bohr radius, then this is equivalent to setting $\hbar = 1$, $m_e = \frac{1}{2}$. Hence for an electron equation (1) takes the form:

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

where $V(x)$, the potential, is periodic with period 'a', i.e. $V(x) = V(x+ma)$ and m is an integer, and

$\psi(x)$, a complex function, can be periodic, provided it can be written as

$$\psi(x) = \exp(-i[k, x])u(x)$$

such that

$$\exp(-i[k, x]) * \exp(i[k, x]) = 1, \text{ and where } u(x+a) = u(x).$$

The probability density $\psi^*(x)\psi(x)$ then is given by:

$$\psi^*(x)\psi(x) = \exp(i[k, x])u^*(x)\exp(-i[k, x])u(x) = u^*(x)u(x) \quad (3)$$

It shows that the probability density is of period a.

For $V(x) \rightarrow 0$, $\exp(-i[k, x]) = \exp(-ikx)$, and $\psi(x) = \exp(-ikx)u_k(x)$

Wave functions of this form are known as Bloch functions. Bloch first established this result in the present connection, for the basis of periodic potential and ('periodic boundary condition').

One consequence of the form of the Bloch functions is that there are states at $k + \frac{2n\pi}{a}$ ($n = \pm 1, \pm 2, \dots$) with the same energy as a state at k. Consider the state $\psi_k(x) = \exp(ikx)u_k(x)$ and the state at $k' = k + \frac{2n\pi}{a}$;

$$\psi_{k'}(x) = \exp. (ik'x) u_{k'}(x) \quad (4)$$

$$\psi_{k'}(x) = \exp. (ikx)\exp\left(\frac{i2n\pi x}{a}\right)u_{k'}(x), \quad (5)$$

where $\exp. \left(\frac{i2n\pi x}{a}\right)$ is of period a so that $\exp. \left(\frac{i2n\pi x}{a}\right)u_{k'}(x)$ is of period a. A possible form for this function, which correspond to a solution for equation (1) is

$$\exp. \left(\frac{i2n\pi x}{a}\right)u_{k'}(x) = u_k(x), \quad (6)$$

In which case,

$$\psi_k(x) = \psi_{k'}(x) \quad (7)$$

i.e. the two states are the same.

Substituting $\psi_k(x) = \exp(ikx)u_k(x)$ into equation (2) gives

$$\left[-\frac{d^2 u_k(x)}{dx^2} - 2ik \frac{du_k(x)}{dx} + [k^2 + V(x)]u_k(x) \right] = E u_k(x). \quad (8)$$

This is another form of Schrodinger's equation, and numerical techniques can be used to obtain accurate results.

2.1 Periodic potentials

In a real crystal a periodic potential arises from the Coulomb interaction of the electron with all the atomic nuclei and all of the other electrons. In this program, the potential can be selected between number of potentials which have been selected principally with a view to their heuristic value rather than to their similarity between real crystal potentials [7]. The potentials

are of period 'a'. The origin is an inversion center, i.e. $V(x) = V(-x)$ so that it is only necessary to specify them for $0 \leq (x) \leq a/2$. The potentials are:

(i) A rectangular potential: One of the most famous potentials in theoretical mechanics, the potential is defined as

$$V(x) = \begin{cases} V_0 & 0 \leq x < \left(\frac{a}{2} - \frac{b}{2}\right) \\ 0 & \text{elsewhere} \end{cases}$$

Where a, b are the period and width of the potential respectively.

(ii) A Sawtooth potential: An asymmetric potential in the shape of a saw tooth signal, defined in each lattice unit by the formula

$$V(x) = 2V_0 \frac{x}{a}, 0 < x < \frac{a}{2}$$

This form is used so that $V(x = a/2) = V_0$.

(iii) A cosine potential: this is the simplest potential; it has only one Fourier coefficient. The frequency of the potential coincides with that of the spatial lattice, so it repeats after a distance a.

$$V(x) = V_0 \left\{ 1 - \cos\left(\frac{2\pi x}{a}\right) \right\}.$$

2.2 Probability density

The variation of E with k (or related variables) is usually the most important result of a band structure calculation. There are however situations, when the actual wave functions or related quantities are of interest [7]. The total electron probability density, which can be investigated by X-ray and neutron diffraction techniques, according to equation (3) involves the product $u_k^*(x)u_k(x)$. Now

$$u_k(x) = \sum_{l=-N}^{+N} c_l \exp\left(\frac{i2\pi lx}{a}\right) \quad (9)$$

And for systems with an inversion center, the Hamiltonian matrix is real. Subsequently the c_l 's are real, and

$$u_k^*(x) = \sum_{m=-N}^{+N} c_m \exp\left(-\frac{i2\pi mx}{a}\right). \quad (10)$$

Hence

$$u_k^*(x)u_k(x) = \sum_{m=-N}^{+N} c_m \exp\left(-\frac{i2\pi mx}{a}\right) \sum_{l=-N}^{+N} c_l \exp\left(\frac{i2\pi lx}{a}\right),$$

$$= \sum_{m=-N}^{+N} \sum_{l=-N}^{+N} c_m c_l \exp\left(i2\pi[l - m] \frac{x}{a}\right),$$

$$= \sum_{m=-N}^{+N} \sum_{l=-N}^{+N} c_m c_l \cos\left(2\pi[l - m] \frac{x}{a}\right),$$

$$= 1 + 2 \sum_{m=-N}^{+N} \sum_{l=m+1}^{+N} c_m c_l \cos\left(2\pi[l - m] \frac{x}{a}\right), \quad (11)$$

as, $\sum_{m=-N}^{+N} c_m^2 = 1$ and $u_k^*(x)u_k(x)$ is real.

3.0 METHODOLOGY

The subroutine F02ABF inside the program "Energy Band" written by Clarke and Martin, in Physics Program edited by A. D. Boardman, (1980) for calculating the eigenvectors of the Hamiltonian (H), was replaced with DSYEV (double precision symmetric eigenvalues and eigenvectors) from LAPACK 3.6 (linear algebra package), that is inside the Mathematical Kernel Library (MKL) which is inside the Intel Parallel Studio XE 2017 Cluster edition for windows together with Visual Studio Community 2015. The potential was varied from 0, 5 and 10Ry for rectangular, saw tooth and cosine potentials. The spacing of $a = 1.5a_0$, range of distance $x - a/2 < x < a/2$, and $k = \pi/a$ where chosen. All inputs and outputs are in atomic units, that is the unit of distance is Bohr radius symbolized a_0 (1 Bohr radius = 0.529A⁰).

4.0 RESULTS AND DISCUSSION

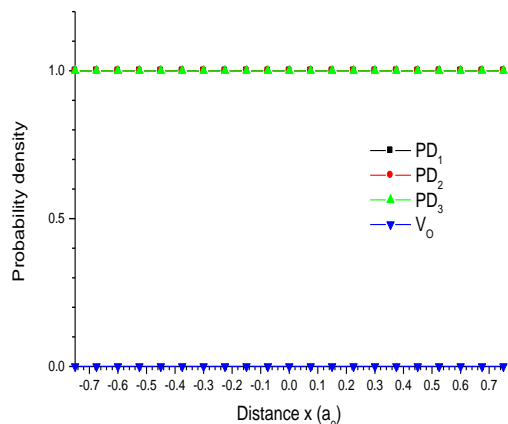


Figure 1: Probability density versus distance x for rectangular, sawtooth, and cosine periodic potentials with $V_0 = 0\text{Ry}$ for the first three energy levels.

As stated earlier, our program considers a rectangular, sawtooth and cosine periodic potential in a one dimensional lattice. Figure 1 shows the probability density function versus distance x for rectangular, sawtooth and cosine periodic potentials with $V_0 = 0$ at $k = \pi/a = 2.0944$ for the first three energy levels for spacing $a = 1.5$ and $x = -a/2$ to $a/2$. It shows that when the potential $V_0 = 0$, the probability density is zero for the second and third energy levels, but 1.0 for first energy level, hence the electron resides in the ground state and there is no band gap. This implies that in the absence of potential the energy gap cannot be found. This applies to the three potentials.

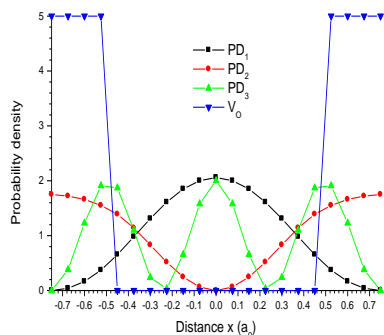


Figure 2: Probability density versus distance x for rectangular potential with $V_0 = 5\text{Ry}$ for the first three energy levels.

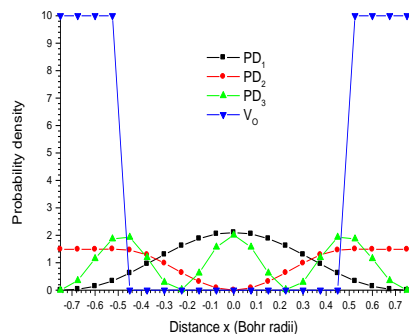


Figure 3: Probability density versus distance x for rectangular potential with $V_0 = 10\text{Ry}$ for the first three energy levels. Figures 2 and 3 show the probability density function versus distance x for the rectangular potential $V_0 = 5$ and 10Ry .

It was observed that for $V_0 = 5\text{Ry}$, the probability density is at its peak for $x=0, a, 2a, \dots$, for the first energy band, but zero for the second energy band, while the first energy band has probability density zero at $a/2, 3a/2, \dots$, with the second energy band having its peaks there. This gives the origin of energy gap. Also as the potential V_0 increases from 5 to 10, the probability density increases as well as the energy gap, and vice versa. The blue line represents the potential height V_0 .

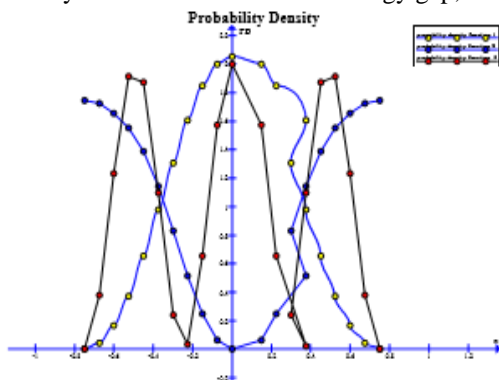


Figure 4: Graph for probability density function for the first three energy levels employing the rectangular potential based on nearly free approximation [7].

Figure 4 shows the comparison between our results and that in the literature. The simulated results of the rectangular potential was compared and produces reasonable agreement with previous results.

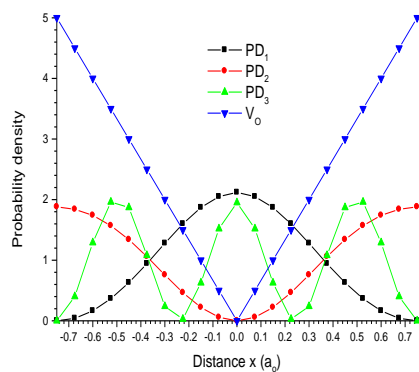


Figure 5: Probability density versus distance x for sawtooth potential with $V_0 = 5\text{Ry}$ for the first three energy levels.

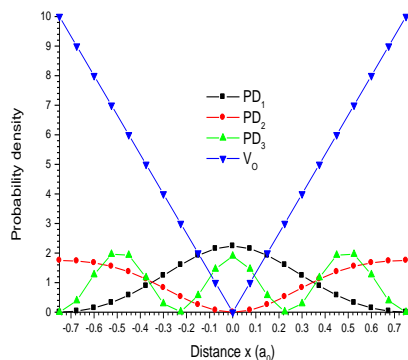


Figure 6: Probability density versus distance x for sawtooth potential with $V_0 = 10\text{Ry}$ and for the first three energy levels. Figures 5 and 6 show the results for the probability density, for the sawtooth potential varying from 5Ry to 10Ry while keeping the spacing fixed. It was observed that the probability density is at its peak for $x=0, a, 2a, \dots$, for the first energy band, but zero for the the second energy band, while the first energy band has probability density zero at $a/2, 3a/2, \dots$, with

the second energy band having it's peaks there. This give the origin of energy gap. Also as the potential V_0 increases from 5 to 10Ry, the probability density also increases as well as the energy gap and vice versa. The blue line represents the potential height V_0 . Hence the band gaps increases with increase in the potential.

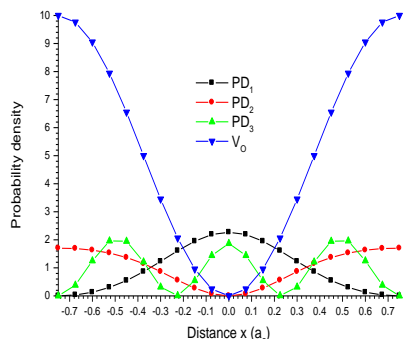


Figure 7: Probability density versus distance x for cosine potential with $V_0 = 5Ry$ for the first three energy levels.

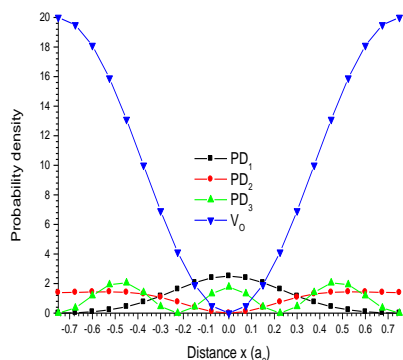


Figure 8: Probability density versus distance x for cosine potential with $V_0 = 10Ry$ and for the first three energy levels.

Figures 7 and 8 shows the results of probability density for cosine potential varying from $V_0 = 5$, to 10Ry the probability density is at its peak for $x=0, a, 2a, \dots$, for the first energy band, but zero for the second energy band, while the first energy band has probability density zero at $a/2, 3a/2, \dots$, with the second energy band having it's peaks there which give the origin of energy gap, also as the potential V_0 increases from 5 to 10, the probability density also increases and vice versa. The blue line represents the potential height V_0 . It shows that as the potential increases from 5 to 10Ry, the band gap also increases. The simulated results reproduced well when compared with the results of Figure 9.

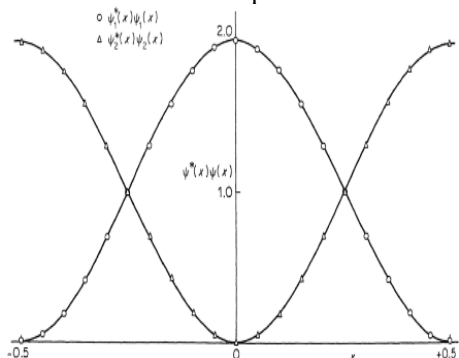


Figure 9: The results of the computer program for the probability density function at $k = \pi/a$ for the first (O) and the second band (Δ) for sawtooth potential of period 1.0 with $V_0 = 1.0$. The solid curves show the predictions of nearly-free electron approximation. Note that for the lower energy band the probability density is high where $V(x)$ is low; but for higher energy band the probability density is high where $V(x)$ is high [4].

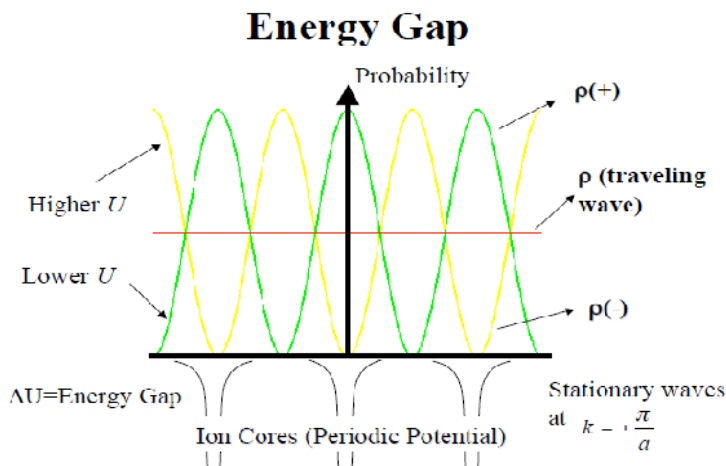


Figure 10 Shows the relation between the probability density of two energy bands and energy gap, where AU stands for average potential [8].

5.0 CONCLUSION

The probability density function for rectangular, saw tooth and cosine potential for electron in a one dimensional periodic potential have been investigated based on nearly free electron approximation in the reduced zone scheme using the program “Energy Bands” from Physics program edited by A. D. Boardman which was modified by replacing the Numerical Algorithm Groups (NAG) subroutine F02ABF with DSYEV obtained from LAPACK 3.6 which is part of the MKL in Intel Visual Fortran 17.0 update 3 for windows which is inside the Intel Parallel Studio XE 2017 Cluster edition for windows. The probability density function which is the origin of the energy gaps in solids, indicates that as the potential V_0 increases the band gap also increases as a result of the increase in the difference between the probability density for the two energy bands. The solutions are standing waves (as a result of forward and backward Bragg scattering). The higher energy solution has larger probability density in the region of higher potential.

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