Transactions of the Nigerian Association of Mathematical Physics
Volume 4, (July, 2017), pp27 – 30
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Electron States of a One-Dimensional Periodic Potential

Abdullahi Tanimu

Physics Department, Umaru Musa Yar'adua University, Katsina

Abstract

The quantum mechanical system consisting of an electron in a perfectly periodic potential was rigorously analysed by Bloch in 1928. Bloch's work also included a somewhat more speculative estimate of the electron motion for the case where a uniform electric field was also present. This work uses the Bloch's theorem in the absence of uniform electric field to study the electron states in a one-dimensional periodic potential superimposed with an array of delta-like function. It has been found that, the periodic potential introduces gaps in the reduced representation. The regions of non-propagating states, which give rise to energy band gaps, become smaller with increasing values of kd. The properties of wave functions for a finite-square well in terms of a mirror symmetry were also presented.

Keywords: Periodic potential, Bloch's theorem, Dispersion relation, Square-well

1.0 Introduction

The quantum mechanical system consisting of an electron in a perfectly periodic potential was rigorously analysed by Bloch [1] in 1928. Bloch's work also included a somewhat more speculative estimate [2] of the electron motion for the case where a uniform electric field was also present. Owing to its fundamental importance in the theory of solid state electronic conduction, the physical system considered by Bloch has been the subject of numerous papers since that time. The purpose of this work is to study the electron states in a one-dimensional periodic potential superimposed with an array of delta-like function. I first concentrate on bound states wave functions [3] and revisit their properties in a finite square well. My approach consists of a straight forward and well-known derivation of secular transcendental equations for a finite square-well and the energy dispersion relation for a periodic potential. My results should be useful therefore in the same general class of application of Kronig-Penney model to the motion of electron in a periodic potential.

2.0 Theory

2.1 Finite square well potential

The quantum mechanical system we use in preparation for the periodic potential is described by a one-dimensional Schrodinger equation with a finite square well potential [4]. We use it because of it is simplicity and practical importance for low dimensional structures such as quantum wells [5]. For an electron in a semiconductor structure, the time-independent Schrodinger equation in the effective mass is

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

where $E = \frac{\hbar^2 k^2}{2m}$ is the energy states of the particle. For convenience, we use in the following $2m = 1$ and $\hbar^2 = 1$, 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, $m = m_e$ for the conduction level. The potential $V(x)$ is

$$V(x) = -V_0\,, |x| < a \quad (2)$$

$$V(x) = 0\,, |x| > a \quad (3)$$

This potential has been covered in depth in many textbooks such as [6]. The solutions to Eq. (1) in terms of plane waves are

$$\psi_1 = Ae^{kx} \quad (4)$$

$$\psi_2 = Ce^{qx} + De\,-^{qx} \quad (5)$$

$$\psi_3 = Be^{-kx} \quad (6)$$

where *A, B, C* and *D* are the amplitude of the wave and k and q are the eigenvalues in their respective regions and are related as

$$q = \sqrt{k^2 + V_0} \quad (7)$$

Correspondence Author: Eze E.O., Email: obinwanneeze@gmail.com, Tel: +2348155851370, +447778111550

To find the eigenvalues, k, we require that from Eq. (1) $\psi(x)$ and $\psi'(x)$ are continuous at $x = \pm a$. Solving C and D in terms of A and B we obtain

$$C = \frac{(q+k)e^{(k-q)a}}{2q}A \quad (8)$$
$$D = \frac{(q-k)e^{(k+q)a}}{2q}A \quad (9)$$
$$C = \frac{(q-k)e^{(k+q)a}}{2q}B \quad (10)$$
$$D = \frac{(q+k)e^{(k-q)a}}{2q}B \quad (11)$$

This yield two equations for B in terms of A

$$B = \frac{q+k}{q-k}e^{-2qa}A \quad (12)$$
$$B = \frac{q-k}{q+k}e^{2qa}A \quad (13)$$

which can only be satisfied if

$$\left(\frac{q+k}{q-k}\right)^2 = e^{4qa}. \quad (14)$$

There are two possible solutions to Eq. (14):
Solution 1 is:

$$\frac{q-k}{q+k} = -e^{2qa}, \quad (15)$$

and
solution 2 is:

$$\frac{q-k}{q+k} = e^{2qa} \quad (16)$$

which after some algebra leads to

$$k = -qcot(qa) \quad (17)$$

for odd solution.
And

$$k = qtan(qa) \quad (18)$$

for even solution.
Eq. (17) and (18) (secular transcendental equations) are solved together with equation (7) to find their eigen wave numbers. These are not presented here, but will be presented somewhere else. After I found my transcendental equations I then substitute

$$\frac{q-k}{q+k} = \pm e^{2qa}, \quad (19)$$

back into the equation giving the relations between the *A, B, C* and *D* to obtain the wave functions shown in fig. (6). I found that, if

$$\frac{q-k}{q+k} = +e^{2qa}, \quad (20)$$

then $C = D$, $A = B$, $\psi(-x) = \psi(x)$. The solutions are even and the wave functions are symmetric. If, however,

$$\frac{q-k}{q+k} = -e^{2qa} \quad (21)$$

then $C = -D$, $A = -B$, $\psi(-x) = -\psi(x)$. The solutions are odd and the wave functions are antisymmetric.

2.2 Periodic potential

Having shown the symmetric and antisymmetric wave functions in a previous subsection, the next step is to derive and analyse the energy spectrum due to an infinite array of delta-function potentials (see fig. 1).

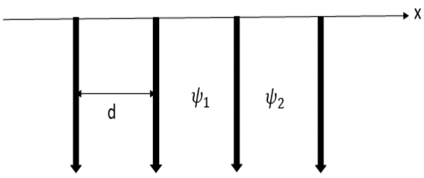

Fig. 1. Periodic delta-function potential in a one-dimensional lattice

To do this Bloch's theorem must be applied to calculate the wave functions in a periodic potential [7]. For a periodic potential, the solutions to the time-independent Schrodinger equation are of the following form

$$\psi(x) = u(x)e^{ikd} \quad (22)$$

where $u(x)$ is the Bloch's periodic parts that has the periodicity of the lattice as

$$u(x + Nd) = u(x) \quad (23)$$

Eq. (23) is Bloch's theorem and can be used to find the wave function at any point in the infinite lattice by applying the phase factor e^{ikd} to the wave function. Bloch's theorem [7] is a vital tool to derive the energy spectrum for an electron in an infinite lattice.
dispersion relation for a series of delta-well potentials (see fig. 4-5) as opposed to square well used in the Kronig-Penney Model [8]. Using the Bloch's theorem, I have

$$\psi(0) = u(0) \quad (24)$$

This work is based on one-dimensional periodic potential [2] and Bloch's theorem will be used in calculating the energy

$$\psi = u(d)e^{ikd} \tag{25}$$

$$\frac{\psi(d)}{\psi(0)} = \frac{u(d)e^{ikd}}{u(0)} = e^{ikd} \rightarrow \psi(d) = \psi(0)e^{ikd} \tag{26}$$

In fig. 1 above ψ_1 is the wave function in region 1 and ψ_2 is the wave function in region 2. For ψ_1 the electron is given a wave function like that of a free particle as

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} \tag{27}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$.

Using Bloch's theorem, we can write the wave function in region 2 in terms of the wave function in region 1 as

$$\psi_2(x) = \psi_1(x-d)e^{ikd} = [Ae^{ik(x-d)} + Be^{-ik(x-d)}]e^{ikd}. \tag{28}$$

The wave function $\psi(x)$ must be continuous at any point as

$$\psi_1(d) = \psi_2(d) \tag{29}$$

which gives:

$$A(e^{ikd} - e^{-ikd}) = B(e^{-ikd} - e^{ikd}) \tag{30}$$

but its derivative $\psi'(x)$ is discontinuous at $x = \pm d$. This is evaluated by integrating Eq. (1) across the regions of the potentials

$$\psi'(d+0_+) - \psi'(d-0_+) = V_0\psi_2(d) \tag{31}$$

Using Eq. (28) obtain the second equation relating the coefficient A and B

$$[ike^{ikd} - ike^{ikd} - V_0e^{ikd}]A = [ike^{ikd} - ike^{-ikd} + V_0e^{ikd}]B \tag{32}$$

From Eq. (30) and (32) we obtain

$$\cos(Kd) = \cos(kd) + V_0\frac{\sin(kd)}{kd}, \tag{33}$$

where K is the quasi momentum, derived from Bloch's theorem and k is the wave number associated with the energy of the particle. However, for the energy above the potential, Eq. (33) is not valid since $k = \sqrt{\frac{2mE}{\hbar^2}}$. But for the energies below the potential, the trigonometric functions turn hyperbolic giving

$$\cos(Kd) = \cos(kd) + V_0\frac{\sinh(kd)}{kd}, \tag{34}$$

where $k = \sqrt{\frac{-2mE}{\hbar^2}}$.

Eq. (33) and (34) were solved with the help of Newton-Raphson procedure in MATLAB to show how the dispersion relation changes with the energy of the particle.

3.0 Result and Discussion

3.1 Regions of allowed wave numbers

Fig. 2 and 3 shows the regions of allowed wave numbers for different strength of the potential. The allowed regions are those that lie between $-1 \leq \cos(Kd) \leq 1$ as found by plotting the right-hand side of Eq. (33). The regions of non-propagating states, which give rise to energy band gaps, become smaller with increasing values of kd [2]. As can be seen, the widths of the forbidden bands decreases and the width of the allowed bands increases with increasing kd is due to the decrease in the amplitude of the sine term.

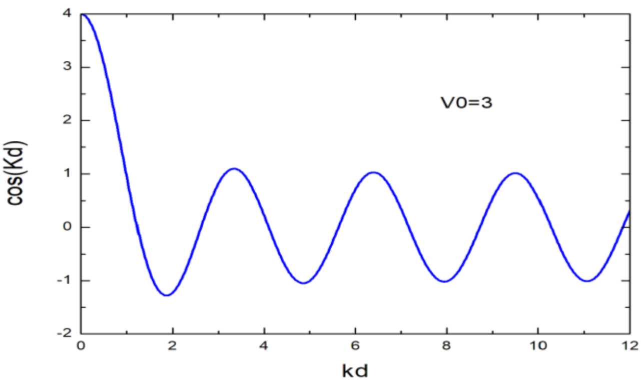

Fig. 2. Plot of the real solutions of equation (33) for $V_0 = 3$

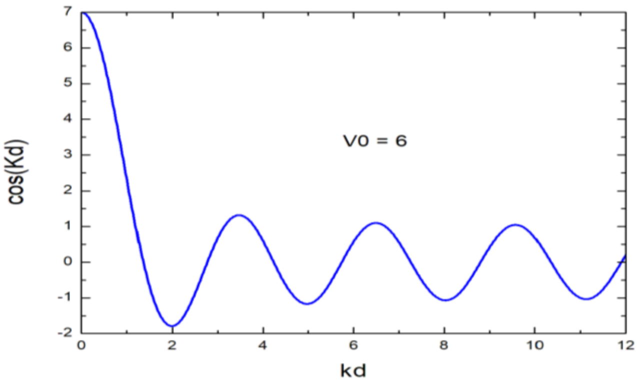

Fig. 3. Plot of the real solutions of equation (33) for $V_0 = 6$

3.2 Dispersion Relation

The graphs of dispersion relation for a particle in a periodic potential are presented in fig. (4) and (5). This curves shows the extended and reduced representations respectively [9]. It can be seen that, the periodic potential introduces a gaps in the reduced representation. This graphs are consistent with fig. (2) and (3) as they show the lowest band gap having the greatest magnitude in separation and then decreasing in size as the energy increases [2]. From these figures, it was clear to see the effect between different potential strength (V_0).

The very clear effect was that for any value of V_0 used, the spectrum tends towards that of the free electron dispersion relation as the energy increases [8]. It was also found that, the larger the strength of the potential the wider the energy band gaps and vice versa.

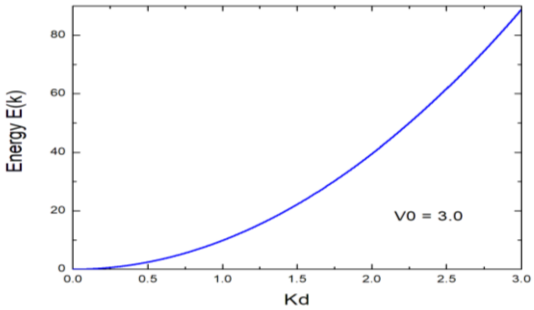

Fig. 4. Plot of dispersion relation in the extended zone representation

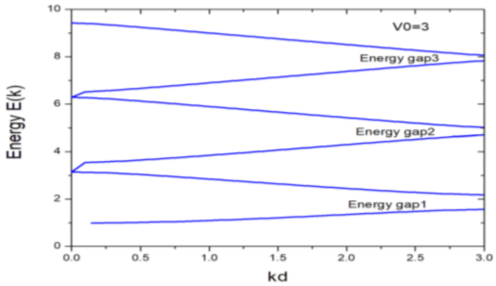

Fig. 5(a). Plot of dispersion relation in the reduced zone representation for $V_0 = 3$

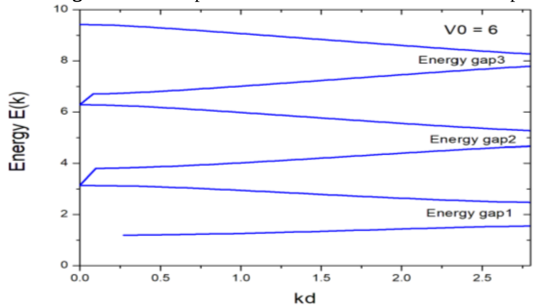

Fig. 5(b). Plot of dispersion relation in the reduced zone representation for $V_0 = 6$

3.3 Wave functions for a finite square well

Fig. 6. shows the plots of the absolute values of the ground state, 1st excited state, and 2nd excited state wave functions for a square well potential. These are obtained by applying the boundary conditions to the set of eigenfunctions from two discrete sets, one remain unchanged under mirror transformation (i.e. if we change *x* to *-x*), and the other changes sign. As we can see from this figure the wave functions exhibit even and odd symmetries about *x=0*. Functions of this kind of behaviour are said to have a definite parity [10].
If $\psi(x) = \psi(-x)$ the parity is said to be even, and if $\psi(-x) = -\psi(x)$ the parity is said to be odd.

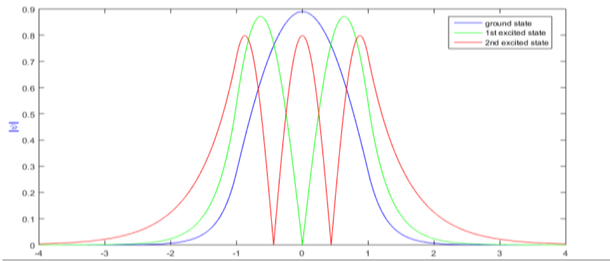

Fig. 6. Normalized wave function for a finite square well

4.0 Summary and Conclusion

In this work, we study the electron states in a one-dimensional periodic potential superimposed with an array of a delta-like function. On implementing the boundary conditions of the continuity of the wave function, problems were solved using Schrodinger's wave equation and a derivation for a secular transcendental equation has been shown. Bloch's theorem was derived in order to calculate the wave function of an electron at any periodic point in the potential. These wave functions were substituted into the boundary conditions that defines the delta-like potential to derive the dispersion relation equation. Once the formulae had been calculated, the energy spectrums of different scenarios could be analysed, these were made for $V_0 = 3$ and $V_0 = 6$.
From the figures generated for dispersion relation in the reduced representation it was found that for any value of V_0 used, the spectrum tends towards that of the free electron dispersion relation as the energy increases. It was also found that, the larger the strength of the potential V_0 the wider the energy band gaps and vice versa. However, the dispersion relation in the extended representation agree with the exact result in the literature.
The wave functions for a finite square well have been shown for ground, 1st and 2nd excited states. These wave functions exhibit even and odd symmetries about $x = 0$

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