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ENERGY BAND STRUCTURE OF AN ELECTRON IN A ONE-DIMENSIONAL PERIODIC POTENTIAL

[1]Tanimu, A. and [*1,2]Bagudo, I. M.

[1]Department of Physics Umaru Musa Yar'adua University Katsina
[2]Ibrahim Shehu Shema Centre for Renewable Energy and Research Umaru Musa Yar'adua University Katsina

[*]Corresponding author's email: ibrahim.bagudo@umyu.edu.ng

ABSTRACT
In this work a relatively simple quantum mechanical model consisting of an electron in a one-dimensional periodic potential is presented. This model was first formulated by Kronig and Penney in 1931. Unlike more realistic model which requires rigorous numerical calculations, this model allows for a simple analytical solutions. Using this model we study the energy band structure of an electron in a one-dimensional periodic potential composed of an array of delta-like function. It has been found that, the increase or decrease in the energy band gaps depends on the choice of potential strength γ. The lager the strength of the potential the wider the energy band gaps and vice versa.

Keywords: Energy bands, Bloch's theorem, Periodic potential, Kronig-Penney model

INTRODUCTION

Energy band structure for phonons and electrons is one of the most fundamental concepts in solid state physics. The easiest to develop is the phonon structure often introduced before that for electrons (John, 1996). This is due to the accuracy of the harmonic approximation for small displacement. The concept involved is rather abstract and often have some difficulties in analyzing the implications of the model. For this reason, a simpler model such as the Kronig-Penney model (KP) is needed. The KP-model played a unique and important role in our recent understanding of the electronic states in one-dimensional systems. The model has also been playing an important role in approaching solid states physics problems. An interesting aspect of this model is not based on the analytical determination of the band structure of the crystals but also the nature of all solutions (allowed and forbidden energy gaps) can be analytically obtain and analyzed. Various calculations were performed with the KP-model to determine the electronic band structure of a one-dimensional crystal (Kronig and Penney, 1931). Unlike more sophisticated model (John, 1996, Boyd, 2001) which requires rigorous numerical calculations using a high speed computers, this model allows for a simple analytical solution. Using this model the energy band structure of an electron in a one-dimensional periodic potential superimposed of an array of delta-like function is obtained. The electronic band structure has some prominent features of many macroscopic properties of the material. Based on this, many researcher's shows overwhelming interest in investigating these materials experimentally. The KP-model is a relatively simple one-dimensional quantum mechanical model of an electron. In spite of the simplifications, the energy band structure obtained from this model resembles many important features with band structures that result from more complicated models (John, 1996).

The concept of Bloch's theorem was briefly introduced for better understanding of the model. Bloch's theorem explain that the interaction of electron with the other particles of the lattice may be replaced by approximating the potential in a periodic field (Kronig and Penney, 1931). Band theory is based on two basic approximations. The first assumes that the electronic and nuclear motions can be separated by invoking the adiabatic approximation of Born and Oppenheimer, 1927. A second simplification is made by using the one-electron approximation. In this case each of the electrons is assumed to move under the influence of a periodic potential as shown in figure 1of the current study (the Kronig-Penney model). Most literatures (Hook and Hill, 1991, Kronig and Penney, 1931, Kasap, 2005) discussed KP-model in a number of ways for different purpose but here we make use of its simplified version for clear understanding of the energy band structure of electrons in a one dimensional periodic potential. We superimposed our periodic potentials with a delta-like functions. The aim is to reduce the number of boundary conditions leading to a very big matrix (Donald, 1996). The discussion of the methods will be based on the one-dimensional electron Schrodinger's equation given of the form (Mandle, 1992, Sprung and Hua, 2000, Charles, 2004)

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

with a periodic potential

$$V(x+a) = V(x) \qquad (2)$$

where x is a vector in the lattice, *i.e.* it points from one lattice to another. The fundamental theorem regarding the motion of electrons in a periodic potential is that of Bloch (Kronig and Penney, 1931) which, in its one-dimensional form, is usually called the Bloch-Floquet theorem (Charles, 2004, Ashcroft and Mermin, 1976).

Theory

Bloch's Theorem

The concept of Bloch theorem was briefly introduced here. It was first developed by Felix Bloch in 1928 (Kronig and Penney, 1931, Mike, 2011) to describe the conduction of electrons in crystalline solids. Independent mathematical proves was provided by (John, 1996, Boyd, 2001). As a result, a variety of nomenclatures are common: applied to ordinary deferential equations, it's called Floquet theory. The general form of a one-dimensional periodic potential equation is Hill's equation (Charles, 2004)

$$\frac{d^2y}{dt^2} + f(t)y = 0 \qquad (3)$$

where $f(t)$ is a periodic potential. Such periodic one-dimensional equations include the KP-model (Kronig and Penney, 1931) and Mathieu's equation (Charles, 2004).

Mathematically Bloch's theorem states that for any periodic potential $u(x)$ all solutions $\psi_{nk}(x)$, must fulfill the following condition

$$\psi_{nk}(x) = e^{ikx}u_{kj}(x) \qquad (4)$$

with the periodic part

$$u_{kj}(x + a) = u_{kj}(x) \qquad (5)$$

for all a in the lattice. The indexes k, j are the electron wave vector and electron bands respectively. Eq.(4) and Eq.(5) imply that

$$\psi_{kj}(x + a) = e^{ika}\psi_{kj}(x). \qquad (6)$$

Dropping the indexes Bloch's theorem can be written as a product of a plane wave and a periodic function which has the same periodicity as a potential

$$\psi(x + a) = e^{ika}\psi(x) \qquad (7)$$

such that for every a in the lattice the Eigen states of the Hamiltonian H can be chosen so that each ψ is associated with a wave vector k.

Kronig-Penney model

The Kronig-Penney model (KP) was first formulated in 1931 by R. de L. Kronig and W. G. Penney (Kronig and Penney, 1931). Although the KP-model was discussed in a number of solid-state physics text books (Hook and Hill, 1991, Ascroft and Mermin, 1976, Charles, 2004) using different techniques, it is usually developed in such way that it will give a clear understanding about the periodic potential. The representation of this model is giving by the one-dimensional periodic potential shown in fig.1. Unlike most literatures (John, 1996, Donald, 1996), here we make use of a delta-function potential for its simplicity and explicit analytical solvability to show how the energy band structures are formed in a one-dimensional periodic potential. Another advantage of using delta-function is in order to reduce the number of boundary conditions which may require a very big matrix (Donald, 1996).

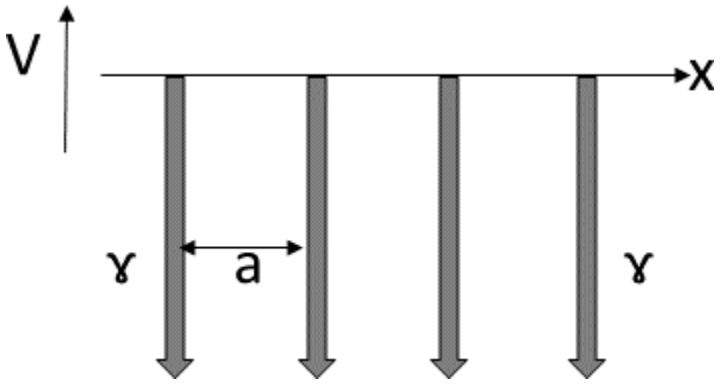

Figure 1. Sketch of a Kronig-Penney model with δ-function potentials

Despite being it a one-dimensional model, it is periodicity of the potential will open gaps in the energy dispersion relation. The electrons interaction with a given lattice will also lead to energy band gaps (Kasap, 2005, Tanimu and Babaji, 2012).

We start with a one-dimensional time independent Schrodinger equation Eq.(1). Since the electron moves in a spatially periodic potential (John, 1996, Tanimu and Muljarov, 2018)

$$V(x) = \gamma \sum_{n=-\infty}^{\infty} \delta(x - na) \qquad (8)$$

it's wave function must satisfy Bloch's theorem for any choice of potential

$$\psi(x + a) = e^{ika}\psi(x) \qquad (9)$$

where γ is the depth of each potential well, $\delta(x)$ is the Dirac delta function, a is the distance between the potentials while k is the Eigen wave number associated with the direction of electronic motion. To solve this problem we need to recall the solutions to Eq.(1)

$$\psi_1(x) = Ae^{ik_n x} + Be^{-ik_n x}. \qquad (10)$$

The second solution can be written in terms of Bloch theorem Eq.(7)

$$\psi_2(x) = \psi_1(x-a)e^{i\kappa_n a} = \left[Ae^{ik_n(X-a)} + Be^{-ik_n(X-a)}\right]e^{i\kappa_n a} \quad (11)$$

Where $k = \sqrt{E}$ and $\kappa = \sqrt{(\gamma - E)}$ for $2m = \hbar = 1$. Applying the continuity condition to the wave function *i.e.*

$$\psi_1(a) = \psi_2(a) \quad (12)$$

which gives

$$(A-B)e^{i\kappa_n a} = Ae^{i\kappa_n a} + Be^{-i\kappa_n a}. \quad (13)$$

Therefore,

$$A\left(e^{i\kappa_n a} - e^{i\kappa_n a}\right) = B\left(e^{-i\kappa_n a} - e^{i\kappa_n a}\right). \quad (14)$$

The continuity of the first derivative is not satisfied when $V(x)$ is a δ-function. Using the expression for $\psi_2(a)$, we can derive the equation relating the coefficients *A* and *B*

$$\left[ik_n e^{i\kappa_n a} - ik_n e^{ik_n a} - \gamma e^{i\kappa_n a}\right]A = \left[ik_n e^{i\kappa_n a} - ik_n e^{-ik_n a} + \gamma e^{i\kappa_n a}\right]B. \quad (15)$$

Expressing Eq.(14) and Eq.(15) leads to the following final expression (Mike, 2011)

$$\cos(\kappa_n a) = \gamma a \frac{\sin(k_n a)}{k_n a} + \cos(k_n a). \quad (16)$$

Eq.(16) gives the relationship between the energy and wave-vector k_n. The importance of this equation is that it provides a restriction on the allowed values of k_n (Kasap, 2005) in the periodic potential. The left hand side of this equation is bounded in the region of (−1, 1) which leads to that restrictions. For detailed calculation of Eq.(16) see (Mike, 2011). There are many numerical methods for solving equation (16) but here we make use of Newton-Raphson procedure in MATLAB because of its arbitrarily high precision and a good convergence factor.

RESULT AND DISCUSSION

Figure 2 shows the energy band structures calculated for different strengths of the potential well and barrier. These structures are the allowed and forbidden band gaps. The allowed bands are those that lie between $-1 \leq \cos(\kappa_n a) \leq 1$ as shown by plotting the right hand side of Eq.(16). This is shown for $\gamma = -1$ and $\gamma = 1$ in the current study and also in figure 5 of (Mike, 2011) using different parameters. This is the region in which k_n is real and thus the particle can propagate. The sinusoidal curve out of this range corresponds to an energy band gap (forbidden band). This can be seen by plotting the graphs for $\gamma = -5, -10,$ and $\gamma = 5, 10$ for barrier and well respectively. For the electron in a metal the energy gap is missing because bands overlap the energy gaps (Bayoumi and Rafat, 2014). However, overlapping of the energy gaps doesn't affect the energy gap in a semiconductor. It has been found that the greater the strength of the potential well or barrier γ the wider the energy gap and vice versa. It can be seen that there is a wider gap for lower wave number k_n and becomes smaller for increasing k_n. The boundary between the wave numbers for barrier and well starts in the middle of a band gap, therefore half of the band gap will be in the positive and negative regions of the dispersion curve (see for e.g. Mike, 2011).

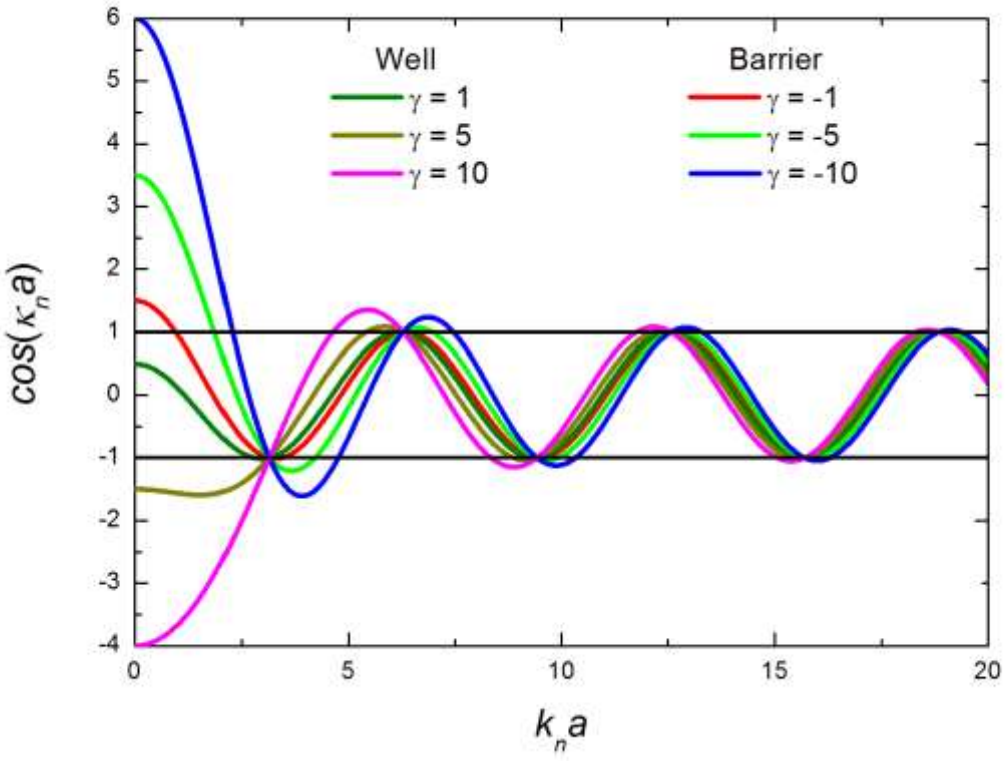

Figure 2. Plot of the function $\cos(\kappa_n a) = \gamma a \frac{\sin(k_n a)}{k_n a} + \cos(k_n a)$ for barrier and well. Forbarrier we use the parameter $\gamma = -1, -5,$, and -10 while for the well we use the parameter $\gamma = 1, 5,$ and 10

SUMMARY AND CONCLUSION

In this work we study the energy band structure of an electron in a one-dimensional periodic potential. We revisit the application of KP-model in an electron superimposed with an array of delta-like function. This is done by introducing the concept of Bloch's theorem to calculate the wave functions of an electron in a periodic potential. These wave functions were substituted in to the boundary conditions that define the delta-like function potential to derive the overall equation. This equation were solved numerically in MATLAB. Once this is achieved, the energy band structures for different potential strengths could be analyzed, these were calculated for $\gamma = -1, -5,$ and-10 for barrier and $\gamma = 1, 5,$ and 10 for the well. It has been shown using the KP-model that a one-dimensional periodic potential composed of a delta-like potential yields energy bands and energy gaps. Similar results (Kasap, 2005, Bayoumi and Rafat, 2014) were shown that the interaction of the electrons with the lattice lead to the energy gaps. It was found that the increase or decrease of energy bands gaps depends on the choice of the potential strength γ. The lager the strength of the potential the wider the energy band gaps and vice versa.

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