

Analysis and Exploration of Kronig and Penney Potential Models in Crystal Lattice Structures



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ABSTRACT

This study delves into the intricate influence of crystal lattices on material properties, employing the Kronig and Penney potential model (KP) to understand wave functions and electronic band structures. Investigating classical and quantum mechanics, the research explores discrete atomic states through Schrödinger's equation, considering both finite and infinite potential scenarios. The results found that as (αa) increases, the energy within the +1 power scatter barrier experiences damping, reaching a constant defined by $F(\alpha a) = 6 \times [10]^{-5} (\alpha a) + 0.9888$. Electron confinement within the unit atom results in an infinite power scatter barrier, and energy (E_n) for any lattice is determined by $E_n = 13.7 n^2$. Temperature-induced variations signify increased energy, indicating free electron movement and a finite power scatter barrier. The electron's negligible velocity in the lattice plays a crucial role in determining amplitude. A decrease in ET corresponds to an increase in the velocity VT of the free electron. Extreme phonon energy in lattice structures is negligible due to its massless nature. The study notes increased energy in restricted electrons, causing a reduction in free electron energy due to an energy gap or barrier scatter. High temperatures are essential to reduce the energy band, facilitating electron transitions and resulting in an electron lifetime of $1.63 \times [10]^{-50}$ s. These insights deepen our understanding of crystal lattice dynamics, offering avenues for innovative applications in materials science and quantum physics.

Keywords:

Kronig and Penney potential,
Energy Levels,
Periodic potential,
Crystal lattice.

INTRODUCTION

The study of crystal lattice structures is fundamental to our understanding of the physical properties of materials. Crystal lattices are three-dimensional arrangements of atoms or ions, and they play a crucial role in determining the electrical, mechanical and optical properties of materials. The Kronig and Penney potential model (KP) is a mathematical framework used to describe wave function and the electronic band structure in crystalline solids. The wave is a set of rhythmic square waves that represents an idealized quantum-mechanical system (Salimen, 2020). Quantum mechanics is engaged in these phenomena to calculate them (Salimen, 2020). After taking a few steps, the restricted and permissible band gaps are finally discovered (Salimen, 2020). This proposal outlines a research project aimed at analyzing and exploring the Kronig and Penney potential model

within crystal lattice structures to deepen our understanding of their impact on material properties.

The KP model is drastically simplified one-dimensional crystallographic quantum mechanical model. Despite the model's simplifications, the electronic band structure it produces has many similarities to band structures that come from more complex well developed models (Kahl, 2005).

The primary objectives of this research project are as follows: To develop a theoretical framework to analyze the Kronig and Penney potential model within different crystal lattice structures. To utilize computational methods and software tools to perform simulations and calculations on specific crystal lattice structures. To compare the results obtained from theoretical analysis and computational simulations with experimental data were available to validate the accuracy of the Kronig and

Penney potential model in describing real-world crystal lattice structures.

Crystal lattice structures are at the heart of our understanding of the physical properties of materials, playing a pivotal role in various scientific and industrial applications. To elucidate the behavior of electrons within these structures, the Kronig and Penney potential model has been widely employed. Despite the extensive use of the Kronig and Penney model, there may still be gaps in our understanding of its intricacies and nuances. Identifying and addressing these knowledge gaps is essential for refining the model's accuracy and utility.

Resolving these issues and questions surrounding the Kronig and Penney potential model in crystal lattice structures holds significant scientific and practical importance. A comprehensive analysis of the model's accuracy, its variations, and its integration with experimental data will advance our understanding of materials and potentially open doors to designing new materials with tailored properties. This research can contribute to advancements in fields such as electronics, materials engineering, and energy storage, where crystal lattice structures play a central role.

This study will focus primarily on the theoretical aspect of Kronig and Penney potential model in crystal lattice structures. It will encompass solid state physics, quantum mechanics and mathematical modeling. While the analysis will be theoretical in nature, it may include discussions of experimental results for comparative purposes.

The Kronig-Penney model of a particle in a one-dimensional lattice has been studied using bootstrap methods from conformal field theory. These methods efficiently compute the band gaps of the energy spectrum but have trouble effectively constraining the minimum energy. To address this issue, more complex constraints involving higher powers of momenta have been proposed. Additionally, an approach for analytically constructing the dispersion relation associated with the Bloch momentum of the system has been suggested (Blacker et al., 2022). The discontinuous potentials in the Kronig-Penney model have been shown to have unusual conclusions in the solutions of the associated Schrodinger equation, with classical analogs displaying the appearance of frequency bands instead of energy bands found in the quantum domain (Oseguera, 1992). The properties of electrons moving in two dimensions in a one-dimensional periodic magnetic field, which is the magnetic analog of the Kronig-Penney problem, have also been investigated (Ibrahim et al., 1995).

MATERIALS AND METHODS

Theoretical Frame Work

Theoretical frameworks for the Kronig-Penney potential model within different crystal lattice structures have been developed and analyzed in scientific literature. One

approach is to use an accurate analytical model that considers a crystal lattice with a stepwise change in potential (Colmankhaneh et al., 2021). This model has been extensively studied and analyzed, particularly for structures with a double-cell period.

Another approach is to extend the Kronig-Penney model by introducing chiral (sub lattice) symmetry through variations in scattered separations or potential heights (Vytovtov et al., 2022). This extension allows for the existence of topological chiral symmetry protected edge states. The solution to these models can be obtained using the conventional scattering formalism used to study the Kronig-Penney model (Smith et al., 2020). Overall, these approaches provide theoretical frameworks for understanding the Kronig-Penney potential model within different crystal lattice structures.

In classical mechanics it is possible to calculate, for example, the vibrational modes of a string, membrane or resonator by solving a wave equation, subject to certain boundary conditions. At the very beginning of the development of quantum mechanics, one was faced with the problem of finding a differential equation describing discrete states of an atom. It was not possible to deduce exactly such an equation from old and well-known physical principles; instead, one had to search for parallels, in classical mechanics and try to deduce the desired equation on the basis of plausible arguments. Such an equation, not derived but guessed at intuitively, would then be a postulate of the new theory, and its validity would have to be checked by experiment. This equation for the calculation of quantum-mechanical states is called the Schrodinger equation (Greiner, 2000). Insertion of this result into equation (1) yields the time-dependent wave equation:

$$\psi(x, t) = \phi(x)e^{-\frac{i\hat{E}t}{\hbar}} \quad (1)$$

If \hat{E} is real then the wave function has an amplitude $\phi(x)$ and a phase $e^{-\frac{i\hat{E}t}{\hbar}}$. The amplitude and the phase representation is convenient for many applications.

In theory, the Schrödinger's equation allows us to solve any quantum mechanical system exactly. We simply insert the potential $U(x)$ and solve for the wave function $\psi(x, t)$ and energy \hat{E} . Unfortunately, there are only very few potentials such as the finite square well or coulomb potential of the hydrogen atom, for which simple and exact solution exists. In order to make any further progress, we need to incorporate some techniques for finding approximate solutions to the Schrödinger's equation. A very important set of these techniques is called perturbation theory.

In the most simplified version of the free electron gas, the true three-dimensional potential was ignored and approximated with a constant potential (see the quantum mechanics script as well) conveniently put at 0 eV. The true potential, however, e.g. for a Na crystal, is periodic

and looks more like this (including some electronic states):

Semiconducting properties will not emerge without some consideration of the periodic potential – we therefore have to solve the Schrödinger equation for a suitable periodic potential. However, this is much easier said than done: There are several ways to do this (for real potentials always numerically), but they are all mathematically rather involved.

Luckily, as stated before, it can be shown that *all* solutions must have certain general properties. These properties can be used to make calculations easier – as well as to obtain a general understanding of the effects of a periodic potential on the behavior of electron waves.

The starting point is a potential $V(r)$ determined by the crystal lattice that has the periodicity of the lattice, i.e.

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

With a = any translation vector of the lattice under consideration. We then will obtain some wave-functions $\psi(x)$ which are solutions of the Schrödinger equation for $V(x)$. In addition, these wavefunctions have to fulfill the boundary conditions, since we are still dealing with a kind of "particle in a box" problem – the electrons are confined inside the crystal.

Bloch used straight Fourier analysis and he found that the wave differed from the plane wave of free electrons only by a periodic modulation. This was so simple to him because he did not think it could be much of a discovery, but when he showed it to Heisenberg, he said right away; "That's it!!" (F. Bloch, July, 1928) (from the book edited by Hoddeson et al., 1928).

His paper was published in 1928 [F. Bloch, Zeitschrift für Physik 52, 555 (1928)]. There are many standard textbooks which discuss the properties of the Bloch electrons in a periodic potential.

We consider the motion of an electron in a periodic potential (the lattice constant a). The system is one-dimensional and consists of N unit cells (the size $L = Na$, N : integer).

$$\varphi(x + a) = \exp(ika) \varphi(x) \quad (3)$$

This is called as the Bloch theorem. The *Bloch theorem* in essence formulates a condition that *all* solutions $\psi(r)$, for *any* periodic potential $V(r)$ whatsoever, have to meet. In one version it ascertains

$$\psi(r) = u(r)e^{ikr} \quad (4)$$

With k = any allowed wave vector for the electron that is obtained for a *constant* potential, and $u(r)$ = some functions *with the periodicity of the lattice*, i.e.

$$u(r + T) = u(r) \quad (5)$$

Any wave function meeting this requirement we will henceforth call a Bloch wave. As before, we choose periodic boundary conditions; this ensures that no restriction on the translation vectors T needs to be considered. The Bloch theorem is quite remarkable, because, as said before, it imposes very special conditions on *any* solution of the Schrödinger equation,

no matter what the form of the periodic potential might be. We notice that, in contrast to the case of the constant potential, so far, k is just a wave vector in the plane wave part of the solution. Due to the periodic potential, however, its role as an index to the wave function is *not* the same as before – as we will shortly see. Bloch's theorem is a *proven* theorem with perfectly general validity. We will first give some ideas about the proof of this theorem and then discuss what it means for real crystals. As always with hindsight, Bloch's theorem can be proved in many ways; the links give some examples. Here we only look at general outlines of how to prove the theorem:

It follows rather directly from applying *group theory* to crystals. In this case one looks at symmetry properties that are invariant under translation. It can easily be proved by working with *operator algebra* in the context of formal quantum theory Mathematics (see the quantum mechanics script again). It can be directly proved in *simple ways* – but then only for special cases or with not quite kosher "tricks". Bloch's theorem was formulated by the Swiss – born U.S physicist "FLIX BLOCH" (1905 – 1983) in 1928.

A crystal lattice is the three-dimensional structural arrangement of atoms or molecules inside a crystalline solid. It consists of repeating unit cells in different directions (Qin et al., 2023). The properties of crystalline solids are determined by the arrangement of molecules in the lattice (Quan-Qin et al., 2023). Weakening the inter-layer interaction is an effective strategy to introduce disorder between the layers of a crystalline material (Yun et al., 2023). The physio-chemical properties of a crystal lattice are highly reliant on the molecular structure of the network (Chaturvedi et al., 2020). The dissolution rates of a fused mixture and a physical mixture are expected to be the same based on solubility theory, but experimental results show non-ideal behavior. The crystal lattice energy in eutectics still limits solubility and dissolution rate.

Computational methods and calculations can be utilized on specific crystal lattice structures in several ways. One approach is to use machine learning-based methods to automatically classify structures by crystal symmetry (Ziletti et al., 2017). This involves representing crystals by calculating a diffraction image and constructing a deep-learning neural-network model for classification. Another method is to use various techniques such as plane-wave methods, orthogonalized plane waves, linear combination of atomic orbitals, and Kronig Penney perturbation theory to calculate the band structure of solids (Fischetti et al., 2016). Additionally, intermolecular potentials can be used to calculate lattice frequencies and crystal structures, taking into account the effects of different potential terms (Righini, 1985). Furthermore, a phase-field crystal model can be employed to create complex three- and two-dimensional

crystal structures by energetically favoring specific inter planar angles (Alster et al, 2017). Finally, a solvent-independent approach based on crystal lattice properties can be used to calibrate ion parameters for accurate simulations of aqueous systems (Hmao et al., 2012). Software tools are available to perform simulations and calculations on specific crystal lattice structures. These tools enable researchers to investigate the quality of force fields, correlate simulated ensembles to experimental structure factors, and extrapolate behavior in lattices to behavior in solution (Cerutti et al., 2019). Modern high-level programming languages allow for the development of internal domain-specific languages (DSL) for lattice-based operations in simulation models (Hawick, 2012). Crystallographers can use professional software for structure refinement, but non crystallographers may not have access to it. However, a simple method has been proposed to study the sensitivity of crystal lattice energy to changes in structural parameters, providing a diagnostic tool to test the quality of crystal structure files (Jinjin li et al., 2014). Additionally, a new method has been developed to calculate the free energy difference between two crystalline structures, particularly advantageous for highly harmonic systems (Ackland et al., 1997). These software tools and methods enhance the study of crystal structures and their properties in various scientific fields (Righini et al., 1985).

The Schrödinger's Equation, Bloch theorem, matrix and Hyperbolic functions. The researcher used rectangular square wells and berries with periodicity (a-b) to explain the behavior of an electron in 1-D periodic potential. The possible states that the electron can occupy are determined by the Schrödinger equation. In this case, the potential V is in the form of array of rectangular square wells and berries with periodicity (a-b).

$$\frac{d^2\varphi}{dx^2} + \frac{8\pi^2m}{h^2}E\varphi = 0 \quad (6)$$

and

$$\frac{d^2\varphi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V)\varphi = 0 \quad (7)$$

Making use of Bloch's theorem, the solution can be written in the form of

$$\varphi_x = u_k(x)e^{-ikx} \quad (8)$$

Assuming that the total energy E of the electron is less than the potential energy $V_{(x)}$, we define two real quantities α and β such that

$$\alpha^2 = \frac{8\pi^2m}{h^2}E \quad (9)$$

And

$$\beta^2 = \frac{8\pi^2m}{h^2}(V_0 - E) \quad (10)$$

Thus,

$$\frac{d^2\varphi}{dx^2} + \alpha^2\varphi = 0 \quad (11)$$

and

$$\frac{d^2\varphi}{dx^2} - \beta^2\varphi = 0 \quad (12)$$

The solution that will be appropriate for both the regions suggested by Bloch is the form

$$\varphi_x = u_k(x)e^{-ikx} \quad (13)$$

On differentiating the equation (13), one get

$$\frac{d\varphi}{dx} = \frac{du_k}{dx}e^{-ikx} + u_k ike^{-ikx} \quad (14)$$

$$\frac{d^2\varphi}{dx^2} = \left(\frac{d^2u_k}{dx^2} + \frac{du_k}{dx}2ik - k^2u_k\right)e^{-ikx} \quad (15)$$

Substituting equation (15) into equation (11) and (12), we get

$$\frac{d^2u_1}{dx^2} + \frac{du_1}{dx}2ik + (\alpha^2 - k^2)u_1 = 0 \quad (16)$$

and

$$\frac{d^2u_2}{dx^2} + \frac{du_2}{dx}2ik - (\beta^2 + k^2)u_2 = 0 \quad (17)$$

Where u_1 represents the value of $u_k(x)$ in the interval $0 < x < a$ and u_2 the value of $u_k(x)$ in the interval $-b < x < 0$. The solution of the differential equation (16) is of the form:

$$u_1 = e^{mx} \quad (18)$$

$$\frac{du_1}{dx} = me^{mx} \quad (19)$$

$$\frac{d^2u_1}{dx^2} = m^2e^{mx} \quad (20)$$

Substituting equations (18), (19) and (20) into equation (16), we get

$$m^2e^{mx} + 2ikme^{mx} + (\alpha^2 - k^2)e^{mx} = 0 \quad (21)$$

This implies that,

$$m^2 + 2ikm + (\alpha^2 - k^2) = 0 \quad (22)$$

Therefore,

$$m = \frac{-2ik \pm \sqrt{4k^2 - 4(\alpha^2 - k^2)}}{2} = -ik \pm i\alpha$$

$$m_1 = i(\alpha - k) \quad (23a)$$

$$m_2 = -i(k + \alpha) \quad (23b)$$

Thus, the general solution is

$$u_1 = Ae^{m_1x} + Be^{m_2x} \quad (24)$$

By substituting equations 23a and 23b into equation 24, we get

$$u_1 = Ae^{i(\alpha-k)x} + Be^{-i(\alpha+k)x} \quad (25)$$

Where A and B are constants. Similarly equation (16) can be written as:

$$m^2e^{mx} + 2ikme^{mx} - (\beta^2 + k^2)e^{mx} = 0 \quad (26)$$

This implies that,

$$m^2 + 2ikm - (\beta^2 + k^2) = 0 \quad (27)$$

Therefore,

$$m = \frac{-2ik \pm \sqrt{4k^2 + 4(\beta^2 + k^2)}}{2} = -ik \pm \beta$$

$$m_1 = (\beta - ik) \quad (28a)$$

and

$$m_2 = -(\beta + ik) \quad (28b)$$

Thus, the general solution is

$$u_2 = Ce^{m_1x} + De^{m_2x} \quad (29)$$

By substituting equations (28a) and (28b) into equation (29), we get

$$u_2 = Ce^{(\beta-ik)x} + Be^{-(\beta+ik)x} \quad (30)$$

where C and D are constants. The values of the constants A, B, C and D can be obtained by applying the boundary conditions:

$$[u_1(x)]_{x=0} = [u_2(x)]_{x=0} \quad (31a)$$

$$[u_1'(x)]_{x=0} = [u_2'(x)]_{x=0} \quad (31b)$$

and

$$[u_1(x)]_{x=a} = [u_2(x)]_{x=-b} \quad (32a)$$

$$[u_1'(x)]_{x=a} = [u_2'(x)]_{x=-b} \quad (32b)$$

By applying these conditions, we get

$$[Ai(\alpha - k)e^{i(\alpha-k)x} - Bi(\alpha + k)e^{-i(\alpha+k)x}]_{x=0} \\ = [C(\beta - ik)e^{(\beta-ik)x} - D(\beta + ik)e^{-(\beta+ik)x}]_{x=0}$$

Therefore

$$Ai(\alpha - k) - Bi(\alpha + k) = C(\beta - ik) - D(\beta + ik) \quad (33)$$

$$Ae^{i(\alpha-k)a} + Be^{-i(\alpha+k)a} = Ce^{-(\beta-ik)b} + De^{(\beta+ik)b} \quad (34)$$

$$[Ai(\alpha - k)e^{i(\alpha-k)x} - Bi(\alpha + k)e^{-i(\alpha+k)x}]_{x=a} = [C(\beta - ik)e^{(\beta-ik)x} - D(\beta + ik)e^{-(\beta+ik)x}]_{x=-b}$$

Therefore,

$$Ai(\alpha - k)e^{i(\alpha-k)a} - Bi(\alpha + k)e^{-i(\alpha+k)a} = C(\beta - ik)e^{-(\beta-ik)b} + D(\beta + ik)e^{(\beta+ik)b} \quad (35)$$

Equations (33), (34) and (35) will have non – vanishing solution if and only if the determinant of the coefficient A, B, C and D vanishes.

This requires that:

$$\begin{vmatrix} 1 & 1 & -1 & -1 \\ i(\alpha - k) & -i(\alpha + k) & (\beta - ik) & -(\beta + ik) \\ e^{i(\alpha-k)a} & e^{-i(\alpha+k)a} & e^{-(\beta-ik)b} & e^{(\beta+ik)b} \\ i(\alpha - k)e^{i(\alpha-k)a} & -i(\alpha + k)e^{-i(\alpha+k)a} & (\beta - ik)e^{-(\beta-ik)b} & -(\beta + ik)e^{(\beta+ik)b} \end{vmatrix} = 0 \quad (36)$$

This implies that,

$$(2i\alpha\beta - 2k^2)[e^{i(\alpha-k)a} - e^{-(\beta-ik)b}][e^{-i(\alpha+k)a} - e^{(\beta+ik)b}] + (-2i\alpha\beta - 2k^2)[e^{i(\alpha-k)a} - e^{(\beta+ik)b}][e^{-(\beta-ik)b} - e^{-i(\alpha+k)a}] = (\alpha^2 - 2k^2 - \beta^2)[e^{-i(\alpha+k)a} - e^{i(\alpha-k)a}][e^{(\beta+ik)b} - e^{-(\beta-ik)b}] \quad (37)$$

The R.H.S of equation (36) can be expands as

$$= (\alpha^2 - 2k^2 - \beta^2)[e^{-i(\alpha+k)a}e^{\beta b}e^{ikb} + e^{-i(k-a)a}e^{-\beta b}e^{-ikb} - e^{-i(\alpha+k)a}e^{-\beta b}e^{ikb} - e^{ik(b-a)}e^{\beta b}e^{i\alpha a}]$$

The L.H.S of equation (36) can be expands as

$$= (2i\alpha\beta - 2k^2)[e^{i(\alpha-k)a-i(\alpha+k)a} - e^{-(\beta+k)a-i(\alpha+k)a} + e^{-(\beta-ik)b+(\beta+ik)b} - e^{i(\alpha+k)a+(\beta+ik)b}] + (-2i\alpha\beta - 2k^2)[e^{-(\beta-ik)b+i(\alpha-k)a} + e^{-i(\alpha+k)a+(\beta+ik)b} - e^{-i(\alpha+k)a+i(\alpha-k)a} - e^{(\beta+ik)b-(\beta+ik)b}]$$

R.H.S is further simplified as:

$$= (\alpha^2 - \beta^2 - 2k^2)[e^{ik(b-a)}e^{\beta b}e^{-i\alpha a} + e^{ik(b-a)}e^{-\beta b}e^{i\alpha a} - e^{ik(b-a)}e^{-\beta b}e^{-i\alpha a} - e^{ik(b-a)}e^{\beta b}e^{i\alpha a}] \\ = (\alpha^2 - \beta^2 - 2k^2)(e^{ik(b-a)}[e^{\beta b}(e^{-i\alpha a} - e^{i\alpha a}) + e^{-\beta b}(e^{i\alpha a} - e^{-i\alpha a})])$$

L.H.S is further simplified as:

$$= (2i\alpha\beta - 2k^2)[e^{-2i\alpha k} + e^{2ikb} - e^{ik(b-a)}e^{-b\beta}e^{-i\alpha a} - e^{ik(b-a)}e^{b\beta}e^{i\alpha a}] \\ + (2i\alpha\beta - 2k^2)[e^{ik(b-a)}e^{-b\beta}e^{i\alpha a} + e^{ik(b-a)}e^{-b\beta}e^{-i\alpha a} - e^{-2i\alpha k} - e^{2ikb}] \\ = (2i\alpha\beta - 2k^2)[e^{ik(b-a)}[e^{-2i\alpha k-ik(b-a)} + e^{2ikb-ik(b-a)} - e^{-b\beta-i\alpha a} - e^{i\alpha a+b\beta}]] \\ + (2i\alpha\beta - 2k^2)[e^{ik(b-a)}[e^{-\beta b+i\alpha a} + e^{b\beta-i\alpha a} - e^{-2i\alpha k-ik(b-a)} - e^{2ikb-ik(b-a)}]]$$

Since $e^{ik(b-a)}$ is a common factor both for the L.H.S and R.H.S, the equation is simplified and written as under:

$$R.H.S. \\ = (\alpha^2 - \beta^2)[e^{\beta b}(e^{-i\alpha a} - e^{i\alpha a}) + e^{-\beta b}(e^{i\alpha a} + e^{-i\alpha a})] - 2k^2[e^{\beta b}(e^{-i\alpha a} - e^{i\alpha a}) + e^{-\beta b}(e^{i\alpha a} - e^{-i\alpha a})]$$

L.H.S is:

$$= (2i\alpha\beta)[e^{-2i\alpha k-ik(b-a)} + e^{2ikb-ik(b-a)} - e^{-b\beta-i\alpha a} - e^{i\alpha a+b\beta}] - 2k^2[e^{-2i\alpha k-ik(b-a)} + e^{2ikb-ik(b-a)} - e^{-b\beta-i\alpha a} - e^{i\alpha a+b\beta}] \\ + (2i\alpha\beta)[e^{-\beta b+i\alpha a} + e^{b\beta-i\alpha a} - e^{-2i\alpha k-ik(b-a)} - e^{2ikb-ik(b-a)}] - 2k^2[e^{-\beta b+i\alpha a} + e^{b\beta-i\alpha a} - e^{-2i\alpha k-ik(b-a)} - e^{2ikb-ik(b-a)}]$$

On expanding k^2 terms of both L.H.S and R.H.S and equating them, we find the result yields zero value. Now by equating L.H.S and R.H.S and simplifying

$$(-\alpha^2 + \beta^2)(e^{i\alpha a} - e^{-i\alpha a})(e^{\beta b} - e^{-\beta b}) = (2i\alpha\beta)[2e^{-ik(b+a)} + 2e^{ik(b+a)}] - 2i\alpha\beta[(e^{i\alpha a} + e^{-i\alpha a})(e^{\beta b} + e^{-\beta b})] \\ \frac{(-\alpha^2 + \beta^2)}{(2i\alpha\beta)}(e^{i\alpha a} - e^{-i\alpha a})(e^{\beta b} - e^{-\beta b}) = [2e^{-ik(b+a)} + 2e^{ik(b+a)}] - [(e^{i\alpha a} + e^{-i\alpha a})(e^{\beta b} + e^{-\beta b})] \quad (38)$$

Dividing equation 38 throughout by 2

$$\frac{(-\alpha^2 + \beta^2)}{(2\alpha\beta)}\left[\frac{(e^{i\alpha a} - e^{-i\alpha a})}{2i}(e^{\beta b} - e^{-\beta b})\right] = [e^{-ik(b+a)} + e^{ik(b+a)}] - [(e^{i\alpha a} + e^{-i\alpha a})\frac{(e^{\beta b} + e^{-\beta b})}{2}] \quad (39)$$

But from hyperbolic function:

$$\frac{(e^{i\alpha a} - e^{-i\alpha a})}{2i} = \sin \alpha a \quad (40a)$$

$$(e^{i\alpha a} + e^{-i\alpha a}) = 2 \cos \alpha a \quad (40b)$$

$$\frac{(e^{\beta b} + e^{-\beta b})}{2} = \cosh \beta b \quad (40c)$$

$$(e^{\beta b} - e^{-\beta b}) = 2 \sinh \beta b \quad (40d)$$

$$[e^{-ik(b+a)} + e^{ik(b+a)}] = 2 \cos k(a+b) \quad (40e)$$

Now by substituting equations (40a), (40b), (40c), (40d), and (40e) into equation (39), we get

$$\frac{(-\alpha^2 + \beta^2)}{(2\alpha\beta)} 2 \sin \alpha a \sinh \beta b = 2 \cos k(a+b) - 2 \cos \alpha a \cosh \beta b \quad (41)$$

Thus, the solution of the determinant (equation 36) can be written as:

$$\frac{(-\alpha^2 + \beta^2)}{(2\alpha\beta)} \sin \alpha a \sinh \beta b + \cos \alpha a \cosh \beta b = \cos k(a+b)$$

Equation (41) is complicated but a simplification is possible. Kronig and Penney considered the possibility that V_{0b} remains finite. Such function is called delta function. Under these circumstances

$$\sinh \beta b \rightarrow \beta b$$

And

$$\cosh \beta b \rightarrow 1 \text{ as } b \rightarrow 0.$$

Hence equation 42 becomes

$$\frac{(-\alpha^2 + \beta^2)}{(2\alpha\beta)} \beta b \sin \alpha a + \cos \alpha a = \cos ka \quad (42)$$

Now

$$\beta^2 - \alpha^2 = \frac{8\pi^2 m}{h^2} (V_0 - E) - \frac{8\pi^2 m}{h^2} E = \frac{8\pi^2 m}{h^2} (V_0 - 2E)$$

since $V_0 \gg E$

$$\beta^2 - \alpha^2 = \frac{8\pi^2 m}{h^2} (V_0) \quad (43)$$

By substituting equation (43) into the equation (42), we get

$$\frac{8\pi^2 m (V_0)}{(2\alpha\beta h^2)} \beta b \sin \alpha a + \cos \alpha a = \cos ka \quad (44)$$

where $p = \frac{mV_0 ab}{h^2}$

$$\left(\frac{mV_0 ab}{h^2}\right) \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

$$p \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad (45)$$

The term V_{0b} is called the barrier strength. The term p in equation (45) is sometime referred as the scattering power of the potential barrier. It is a measure of the strength with which electron in crystal attracted to the ions on the crystal lattice sites. Also,

$$\alpha^2 = \frac{8\pi^2 m}{h^2} E$$

$$E = \frac{\alpha^2 h^2}{8\pi^2 m}$$

and

$$k = \frac{2\pi}{\lambda} \quad (46)$$

Equation 48 is a condition of the existences of a solution for the electron wave function.

There are only two variables in equation (45), namely α and k . The R.H.S of equation (45) is bounded since it can only assume values within 0 and 1. If we plot the L.H.S of this equation against αa , it will be possible to determine those values of α (and hence energy) which are

permissible; that is, permit $p \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ to take value between 0 and 1. When each of these values is set equal to $\cos(ka)$, K is determined. Then α can be found from equation (13). Periodic potential is obtained by solve above equation. L.H.S of the equation is bounded by R.H.S (\pm).

Case I: when $p \rightarrow \infty$, $\sin \alpha a = 0$

and

$$\alpha a = n\pi \Rightarrow \alpha = \frac{n\pi}{a}$$

By squaring both side

$$\alpha^2 = \left(\frac{n\pi}{a}\right)^2$$

But

$$\alpha^2 = \frac{2m}{h^2} E \quad (47)$$

Equating equation (3.11) and (3.46) we get

$$\frac{2m}{h^2} E = \left(\frac{n\pi}{a}\right)^2$$

Therefore

$$E = \frac{h^2}{2m} \left(\frac{n\pi}{a}\right)^2 \quad (48)$$

$$a = \frac{n\lambda}{2} \quad (49a)$$

$$\lambda = \frac{c}{f} \Rightarrow t = \frac{1}{f}$$

Therefore

$$\lambda = ct \quad (49b)$$

By putting equations (49a) and (49b) into (44) we get

$$E = \frac{2h^2 \pi^2}{mc^2 \tau^2} \quad (50)$$

Where τ in the equation (48) is the time

Case II: When $p \rightarrow 0$,

$$\cos \alpha a = \cos ka \quad (51)$$

$$\alpha = k, \Rightarrow \alpha^2 = k^2,$$

$$k^2 = \frac{2\pi^2}{\lambda^2}$$

$$E = \frac{\pi^2 h^2}{\lambda^2 m} \quad (52)$$

From de-Broglie hypothesis

$$\lambda^2 = \frac{h^2}{p^2} \Rightarrow \lambda^2 p^2 = h^2$$

$$h^2 = \frac{h^2}{8\pi^2}$$

$$\frac{1}{\lambda^2} = \frac{4\pi^2 p^2}{h^2}$$

$$E = \frac{\pi^2 h^2}{m 8\pi^2} \frac{4\pi^2 p^2}{h^2}$$

$$E_{\text{extreme}} = \frac{p^2}{2m} = \frac{1}{2} m v^2 \quad (53)$$

$$E_T = \frac{3}{2} k_B T \quad (54)$$

By equating E_{extreme} and E_T we get

$$\frac{3}{2} k_B T = \frac{1}{2} m v^2$$

$$v = \sqrt{\frac{3k_B T}{m}} \quad (55)$$

Equation (55) is the velocity of free electron in lattice, it is extreme velocity. By equating equation (50) and equation (54) we get

$$\frac{3}{2} k_B T = \frac{2h^2 \pi^2}{mc^2 \tau^2}$$

$$\tau = \sqrt{\frac{4h^2 \pi^2}{3mk_B T c^2}} \quad (56)$$

Equation (54) is the average time (τ) per temperature (k)

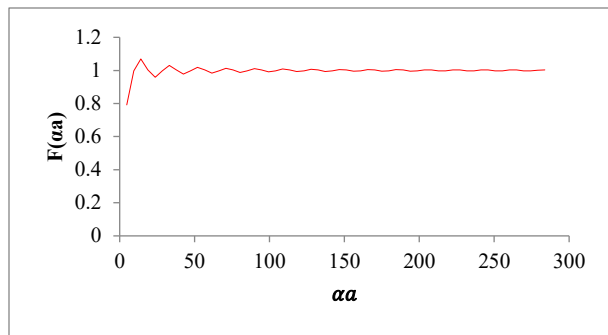
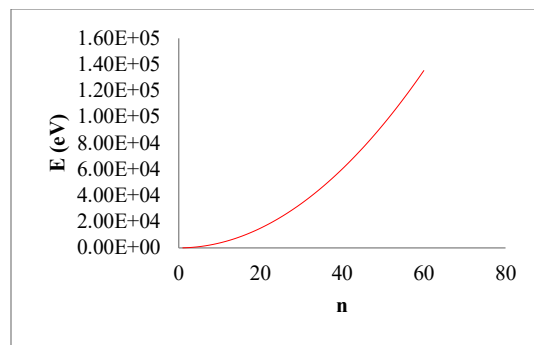
RESULTS AND DISCUSSION

Table 1: Variation of Power Scatter Barrier Depending on Different αa

n	$E_n(J)$	$\lambda(m)$	k	ka	α	αa	$F(\alpha a)$
1	3.76E+01	3E-10	6.073E-21	9.11E-31	3.E+10	4.7296615	0.7918
2	1.50E+02	1.5E-10	1.215E-20	1.822E-30	6.E+10	9.459323	0.9964
3	3.38E+02	1E-10	1.822E-20	2.733E-30	9.E+10	14.188985	1.06932
4	6.02E+02	7.5E-11	2.429E-20	3.644E-30	1.E+11	18.918646	1.00359
5	9.40E+02	6E-11	3.037E-20	4.555E-30	2.E+11	23.648308	0.95851
6	1.35E+03	5E-11	3.644E-20	5.466E-30	2.E+11	28.377969	0.99641
7	1.84E+03	4.3E-11	4.251E-20	6.377E-30	2.E+11	33.107631	1.02953
8	2.41E+03	3.8E-11	4.859E-20	7.288E-30	3.E+11	37.837292	1.00359
9	3.05E+03	3.3E-11	5.466E-20	8.199E-30	3.E+11	42.566954	0.97714
10	3.76E+03	3E-11	6.073E-20	9.11E-30	3.E+11	47.296615	0.99642
11	4.55E+03	2.7E-11	6.681E-20	1.002E-29	3.E+11	52.026277	1.01859
12	5.41E+03	2.5E-11	7.288E-20	1.093E-29	4.E+11	56.755938	1.00357
13	6.35E+03	2.3E-11	7.895E-20	1.184E-29	4.E+11	61.4856	0.98438
14	7.37E+03	2.1E-11	8.503E-20	1.275E-29	4.E+11	66.215261	0.99644
15	8.46E+03	2E-11	9.11E-20	1.367E-29	5.E+11	70.944923	1.01342
16	9.63E+03	1.9E-11	9.717E-20	1.458E-29	5.E+11	75.674584	1.00355
17	1.09E+04	1.8E-11	1.032E-19	1.549E-29	5.E+11	80.404246	0.98828
18	1.22E+04	1.7E-11	1.093E-19	1.64E-29	6.E+11	85.133907	0.99646
19	1.36E+04	1.6E-11	1.154E-19	1.731E-29	6.E+11	89.863569	1.01037
20	1.50E+04	1.5E-11	1.215E-19	1.822E-29	6.E+11	94.59323	1.00353

Table 2: Variation of Energy with Temperature and Principle Quantum Number

n	$E_n(J)$	$\lambda(m)$	$v_n(m/s)$	$T(k)$	$v_T(k/kg)$	$E_{per\ temp}(J)$	$\log E_{per\ temp}$	$\tau(s^2m^{-2}k^{-1})$
1	3.76E+01	3E-10	4.50945E-74	273	1.114E+05	5.6511E-21	-20.2479	6.71E-51
2	1.50E+02	1.5E-10	9.0189E-74	337	1.238E+05	6.9759E-21	-20.1564	7.46E-51
3	3.38E+02	1E-10	1.35284E-73	473	1.466E+05	9.7911E-21	-20.0092	8.84E-51
4	6.02E+02	7.5E-11	1.80378E-73	276	1.120E+05	5.7132E-21	-20.2431	6.75E-51
5	9.40E+02	6E-11	2.25473E-73	609	1.664E+05	1.26063E-20	-19.8994	1.00E-50
6	1.35E+03	5E-11	2.70567E-73	745	1.840E+05	1.54215E-20	-19.8119	1.11E-50
7	1.84E+03	4.3E-11	3.15662E-73	279	1.126E+05	5.7753E-21	-20.2384	6.79E-51
8	2.41E+03	3.8E-11	3.60756E-73	881	2.001E+05	1.82367E-20	-19.7391	1.21E-50
9	3.05E+03	3.3E-11	4.05851E-73	1017	2.150E+05	2.10519E-20	-19.6767	1.30E-50
10	3.76E+03	3E-11	4.50945E-73	282	1.132E+05	5.8374E-21	-20.2338	6.82E-51
11	4.55E+03	2.7E-11	4.9604E-73	1153	2.289E+05	2.38671E-20	-19.6222	1.38E-50
12	5.41E+03	2.5E-11	5.41134E-73	1289	2.420E+05	2.66823E-20	-19.5738	1.46E-50
13	6.35E+03	2.3E-11	5.86229E-73	285	1.138E+05	5.8995E-21	-20.2292	6.86E-51
14	7.37E+03	2.1E-11	6.31323E-73	1425	2.545E+05	2.94975E-20	-19.5302	1.53E-50
15	8.46E+03	2E-11	6.76418E-73	1561	2.663E+05	3.23127E-20	-19.4906	1.61E-50
16	9.63E+03	1.9E-11	7.21512E-73	288	1.144E+05	5.9616E-21	-20.2246	6.90E-51
17	1.09E+04	1.8E-11	7.66607E-73	1697	2.777E+05	3.51279E-20	-19.4543	1.67E-50
18	1.22E+04	1.7E-11	8.11701E-73	1833	2.886E+05	3.79431E-20	-19.4209	1.74E-50
19	1.36E+04	1.6E-11	8.56796E-73	291	1.150E+05	6.0237E-21	-20.2201	6.93E-51
20	1.50E+04	1.5E-11	9.0189E-73	1969	2.991E+05	4.07583E-20	-19.3898	6.71E-51

Figure 1(a): Graph of $F(\alpha a) = p \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ against αa Figure 1(b): Graph of $E(\text{eV})$ against n

In Figure 1(a), the graph depicts $F(\alpha a)$ against (αa) , revealing that energy is damped within the +1 power scatter barrier. As (αa) increases, the energy of the phonon in the crystal lattice decreases until it reaches a point of constant $F(\alpha a)$. The power scatter barrier for any crystal lattice can be determined using the model

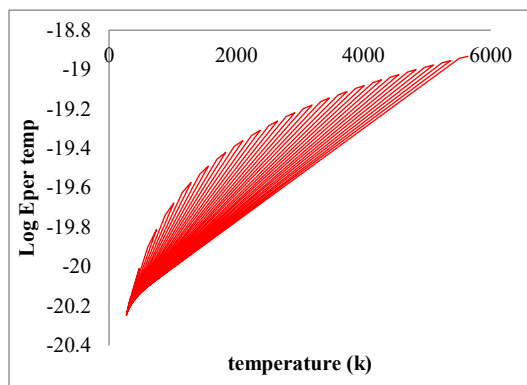
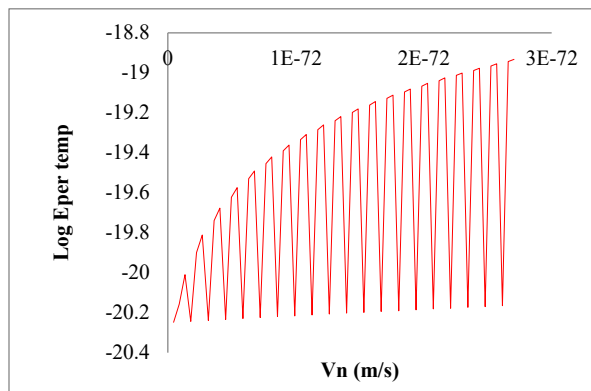
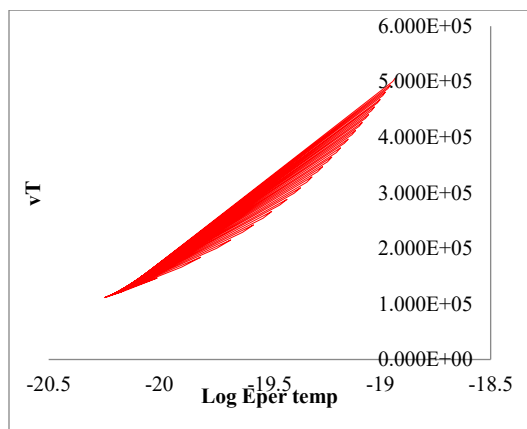
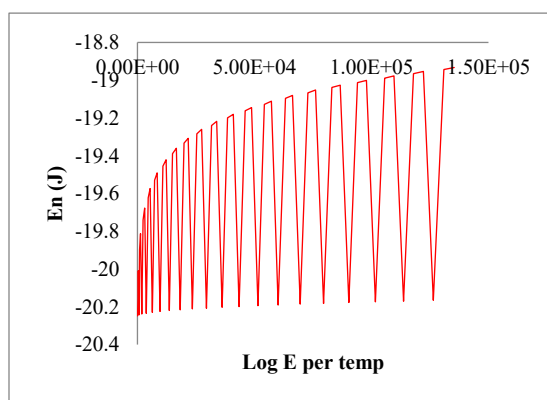
$$F(\alpha a) = 6 \times 10^{-5}(\alpha a) + 0.9888.$$

Moving to Figure 1(b), the graph of E_n against n illustrates that as the principal quantum number (n) increases, the energy (E_n) also increases. This indicates that the electron within the crystal lattice is confined to

its orbital in the unit atom, and at that point, the power scatter barrier is infinite. The energy E_n for any crystal lattice can be determined using the model

$$E_n = 13.7 n^2.$$

In Figure 1(c), the graph of ET against Temperature demonstrates that as the temperature increases, the energy also increases. This suggests that the electron inside the lattice is freely moving throughout, and at that point, the power scatter barrier is finite.

Figure 1(c): Graph of $\text{Log } E_{\text{per temp}}$ against $T(\text{K})$ Figure 1(d): Graph of $\text{Log } E_{\text{per temp}}$ against $v(\text{m/s})$ Figure 1(e): Graph of $\text{Log } E_{\text{per temp}}$ against v_T Figure 1(f): Graph of $\text{Log } E_{\text{per temp}}$ against $E_n(\text{J})$

Finally, in Figure 1(d), the graph of ET against $v(m/s)$ indicates that the velocity of the phonon is negligible inside the lattice. However, this relationship is applicable for determining the amplitude of the electron.

Discussion

In Figure 1(a), the graph depicts $F(\alpha\alpha)$ against $(\alpha\alpha)$, revealing that energy is damped within the +1 power scatter barrier. As $(\alpha\alpha)$ increases, the energy of the phonon in the crystal lattice decreases until it reaches a point of constant $F(\alpha\alpha)$. The power scatter barrier for any crystal lattice can be determined using the model

$$F(\alpha\alpha) = 6 \times 10^{-5}(\alpha\alpha) + 0.9888.$$

Moving to Figure 1(b), the graph of E_n against n illustrates that as the principal quantum number (n) increases, the energy (E_n) also increases. This indicates that the electron within the crystal lattice is confined to its orbital in the unit atom, and at that point, the power scatter barrier is infinite. The energy E_n for any crystal lattice can be determined using the model

$$E_n = 13.7n^2.$$

In Figure 1(c), the graph of ET against Temperature demonstrates that as the temperature increases, the energy also increases. This suggests that the electron inside the lattice is freely moving throughout, and at that point, the power scatter barrier is finite.

Finally, in Figure 1(d), the graph of ET against $v(m/s)$ indicates that the velocity of the phonon is negligible inside the lattice. However, this relationship is applicable for determining the amplitude of the electron.

Fig 1(e): The graph of E_T against v_T shows that the E_T is decreasing the velocity v_T of the free electron is also increasing. While for the fact that in a lattice the extreme energy of the phonon is negligible, because it is massless. Figure 1(f): Graph of $\log E_{\text{per temp}}$ against $E_n (J)$ shows that as the energy of the restricted electron increase the energy of free electron is reduced due to the energy gap or barrier scatter. The researcher noticed that to reduce the energy band one must have a high temperature in the crystalline.

CONCLUSION

The findings derived from this research offer valuable conclusions: The energy within the +1 power scatter barrier experiences damping as $(\alpha\alpha)$ increases, reaching a constant point of $F(\alpha\alpha)$. The power scatter barrier for any crystal lattice can be determined using the model $F(\alpha\alpha) = 6 \times 10^{-5}(\alpha\alpha) + 0.9888$. The electron within the crystal lattice is confined to its orbital in the unit atom, resulting in an infinite power scatter barrier. The energy E_n for any crystal lattice can be determined from the model $E_n = 13.7n^2$. Increasing temperature leads to a corresponding increase in energy, indicating that the electron inside the lattice is freely moving, and the power scatter barrier is finite. The velocity of the electron inside the lattice is negligible, yet

it is instrumental in determining the electron's amplitude. The decrease in E_T corresponds to an increase in the velocity v_T of the free electron. In a lattice, the extreme energy of the phonon is negligible due to its massless nature. The energy of the restricted electron increases, causing a reduction in the energy of the free electron due to the presence of an energy gap or barrier scatter. Moreover, the study highlights that to reduce the energy band, a high temperature in the crystalline structure is necessary. Electron transition from the valance band to the conducting band requires elevated temperatures facilitating movement, leading to an electron lifetime of $1.63 \times 10^{-50} s$ during this transition. Conduct additional research to delve deeper into the mechanisms of energy damping within the +1 power scatter barrier as $(\alpha\alpha)$ increases. Extend studies to comprehensively understand the consequences and applications of an infinite power scatter barrier when the electron is restricted to its orbital in the unit atom. Explore the temperature-dependent energy characteristics in crystal lattices in more detail. Investigate how variations in temperature impact electron mobility, energy states, and the finite nature of the power scatter barrier. Further refine the understanding of the negligible velocity of electrons inside the lattice and its role in determining electron amplitude. Conduct a comprehensive analysis of energy transitions within the crystal lattice, especially those associated with reductions in energy bands. Validate the conclusions drawn from this study through experimental validations and practical applications. Encourage collaboration with researchers in related fields to share insights and data. By addressing these recommendations, future research endeavors can build upon the foundation laid by this study, expanding our knowledge of crystal lattice dynamics and opening avenues for innovative applications in materials science and quantum physics.

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