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Analytical and Numerical Study of the Kronig–Penney Model in One Dimension

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ABSTRACT
The Kronig–Penney model is a foundational exactly solvable problem in solid state physics that illustrates the emergence of energy band structure in periodic potentials. This paper presents both an analytical solution of the model for a one-dimensional periodic delta-function potential and a numerical validation of the resulting band gaps. The analytical approach solves the time-independent Schrödinger equation by applying Bloch's theorem and continuity conditions, leading to a transcendental equation relating the energy and the Bloch wavenumber. Numerically, the band structure is computed using a transfer matrix method, and the results are compared with the analytical dispersion relation. The study confirms the existence of alternating allowed and forbidden energy bands and demonstrates how the model potential strength affects the band gap widths.

INTRODUCTION

Understanding electronic energy levels in crystalline solids is central to modern condensed matter physics. In an ideal periodic lattice, electrons experience a spatially varying potential that forms energy bands separated by band gaps (Ashcroft & Mermin, 1976). While realistic potentials are highly complex, the Kronig–Penney model (Kronig & Penney, 1931) simplifies this by providing an exactly solvable, one-dimensional (1D) representation of periodic potential barriers or wells (see Figure 1).

In its most common configuration, the model replaces finite-width barriers with Dirac delta functions to make the Schrödinger equation analytically tractable. A compelling feature of this framework is that it goes beyond merely determining crystal band structures; it also enables researchers to analytically derive and evaluate the nature of all solutions, explicitly revealing both allowed and forbidden energy gaps. Consequently, the model elegantly reproduces core elements of band theory, such as the dependence of band gaps on the strength of the periodic potential.

In this work we derive analytically the dispersion relation for the 1D Kronig–Penney model. This is done by applying the relevant boundary conditions. Unlike in (Tanimu & Muljarov, 2018), which uses different approach, here, a numerical solution was implemented using a transfer matrix method, and lastly, we compare analytical predictions with numerical results across varying potential parameters.

MATERIALS AND METHODS

Analytical Formulation of the Kronig–Penney model

The Kronig–Penney model was first introduced in 1931 (Kronig & Penney, 1931). While widely treated in literature for diverse purposes (Hook & Hill, 1991; Kasap, 2005; Griffiths & Schroeter, 2018), we adopt a simplified version here to clarify how electron energy bands form in a 1D periodic potential. By superimposing the periodic potential with delta-like functions, we minimize the number of boundary conditions that typically yield a complex matrix system (Donald, 1996). This analysis relies on the 1D Schrödinger equation (Charles, 2004; Mandle, 1992; Tanimu & Muljarov, 2018) given in Equation 1. Structurally, the model features an array of Dirac delta functions separated by a lattice constant a (see Figure 1) (Tanimu & Bagudo, 2020).

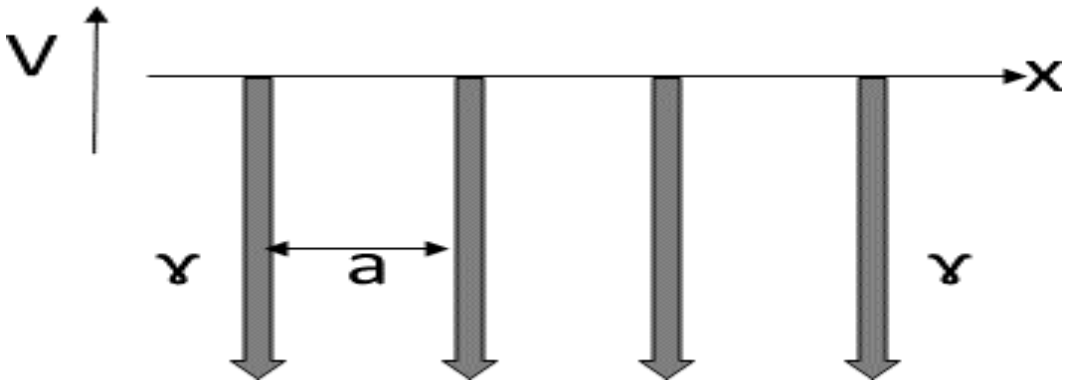

Figure 1: Sketch of a Kronig–Penney model with δ function potentials

Even though the model is one-dimensional, the periodicity of the potential opens gaps in the energy dispersion relation (John, 1996). We start from the one-dimensional time-independent Schrödinger equation:

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

$$V(x) = \gamma \sum_{n=-\infty}^{\infty} \delta(x - na) \quad (2)$$

where $\gamma > 0$ represents the strength of the repulsive potential. Between the delta functions (i.e., for$0 < x < a$), the potential vanishes, so the solution is a plane wave:

$\psi(x) = Ae^{iqx} + Be^{-iqx}$, where $q = \frac{\sqrt{2mE}}{\hbar}$

According to Bloch's theorem which was first developed by Felix Bloch in 1928 (Felix Bloch, 1928), the wave function satisfies $\psi(x + a) = e^{ika}\psi(x)$ with Bloch wavenumber k in the first Brillouin zone $\frac{-\pi}{a} < k \leq \frac{\pi}{a}$. Imposing continuity of ψ at $x = 0$ and a jump condition for ψ' due to the delta function (obtained by integrating the Schrödinger equation across the singularity) yields:

$$\psi'(0^+) - \psi'(0^-) = \frac{2m\gamma}{\hbar^2}\psi(0) \quad (3)$$

Applying these conditions leads to a system of equations for the coefficients *A, B*. After algebraic manipulation, the dispersion relation is obtained (Griffiths & Schroeter, 2018):

$$cos(ka) = cos(qa) + \frac{m\gamma}{\hbar^2 q} sin(qa) \quad (4)$$

Define the dimensionless parameter $P = \frac{m\gamma a}{\hbar^2}$. Then the equation becomes:

$$cos(ka) = cos(qa) + P\frac{sin(qa)}{qa} \quad (5)$$

This secular transcendental equation determines the allowed values of $E = \frac{\hbar^2 q^2}{2m}$ for a given real k.

The importance of this equation is that it provides a restriction on the allowed values of k. Solutions exist only when the right-hand side lies in the interval [−1, 1]; otherwise, k becomes complex, corresponding to forbidden energy gaps.

Numerical Method

To solve the dispersion relation numerically, we scan over $q$or E and compute the left-hand side as

$$f(qa) = cos(qa) + P\frac{sin(qa)}{qa} \quad (6)$$

For a given P, values of qa for which $|f(qa)| \leq 1$ correspond to allowed bands. The corresponding ka is obtained as $ka = arcos[f(qa)]$.

Alternatively, a transfer matrix approach can simulate wave propagation through multiple periods and extract the band structure via the eigenvalues of the unit cell transfer matrix (Markos & Soukoulis, 2008). The transfer matrix across one period from $x = 0^-$ to $x = a^-$ is:

$$M = \begin{pmatrix} \left(1 - \frac{iP}{qa}\right)e^{-iqa} & \frac{iP}{qa}e^{iqa} \\ \frac{-iP}{qa}e^{-iqa} & \left(1 - \frac{iP}{qa}\right)e^{iqa} \end{pmatrix} \quad (7)$$

We implement a simple numerical script in MATLAB that iterates over qa from 0 to 10π and plots the function $f(qa)$ alongside the ± 1 boundaries.

RESULTS AND DISCUSSION

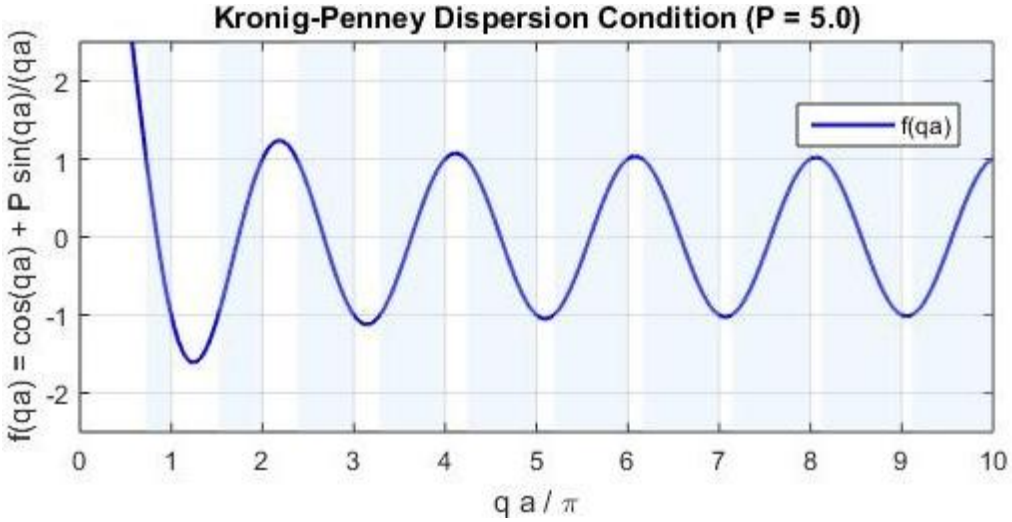

Figure 2: Plot of the function $f(qa) = cos(qa) + P\frac{sin(qa)}{qa}$ for the parameter $P = 5.0$

This graph shows the Kronig–Penney dispersion function plotted using the potential strength, $P = 5.0$. In this model, electron energies are allowed only when $|f(qa)| \leq 1$as shown by plotting the right hand side of equation (6). The shaded vertical regions indicate these allowed solutions. This is the region corresponding to real k that is whenever the function lies outside this region [−1, 1]; no real wave vector k exists, resulting in energy band gaps or forbidden energy regions. For$P = 5.0$, as shown in the current study the oscillatory function exceeds the limits ∓ 1several times, creating multiple separated allowed regions. This demonstrates that a stronger periodic potential significantly modifies the free-electron energy spectrum and leads to the formation of distinct energy bands. It can be shown that the first few allowed regions are relatively narrow, indicating stronger electron confinement within the lattice.

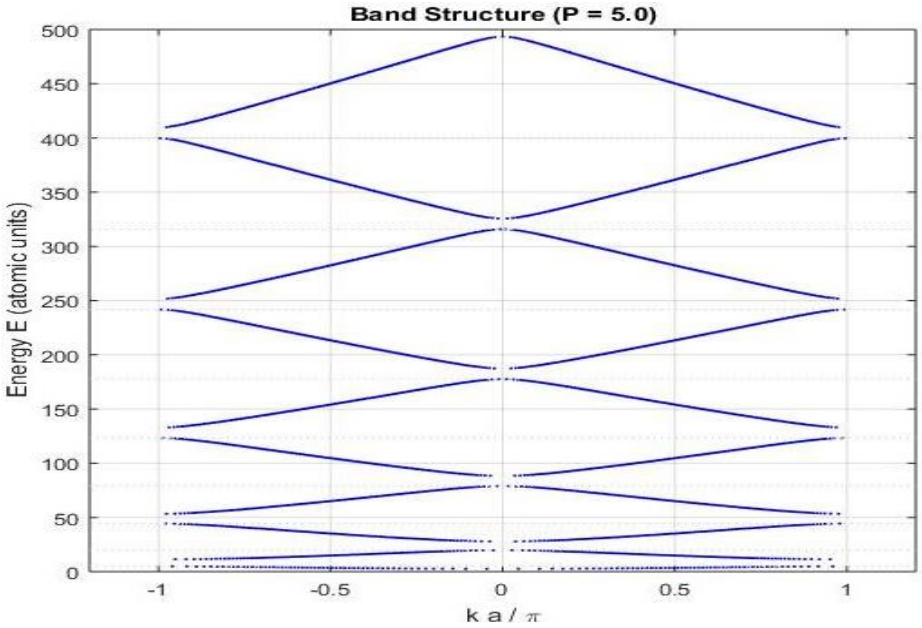

Figure 3: Plot of E versus k showing allowed bands (continuous curves) and band gaps (white regions) for $P = 5.0$

This graph presents the resulting energy bands as a function of crystal wave number$k$. As shown in this figure, the energy bands are symmetric about $k = 0$, reflecting the periodicity and inversion symmetry of the lattice. The allowed energies form continuous bands separated by forbidden gaps. It is observed that, band edges occurs at the Brillouin-zone boundaries ($k = \pm\frac{\pi}{a}$) and at the zone center ($k = 0$). The energy gaps become more pronounced due to the relatively large value of P. Similar features were observed in Figure 2 of (Tanimu & Bagudo, 2020) and in figure 5 of (Mike, 2011) using different parameters. It can be seen that the lowest band is narrow compared to higher bands, implying larger effective

electron mass and reduced electron mobility. As energy increases, the bands become wider, indicating that higher-energy electrons behave more like free particles and are less affected by the periodic potential. The existence of forbidden gaps is a fundamental consequence of Bragg reflection of electron waves at the crystal lattice. These gaps determine whether a material behaves as a conductor, semiconductor, or insulator.

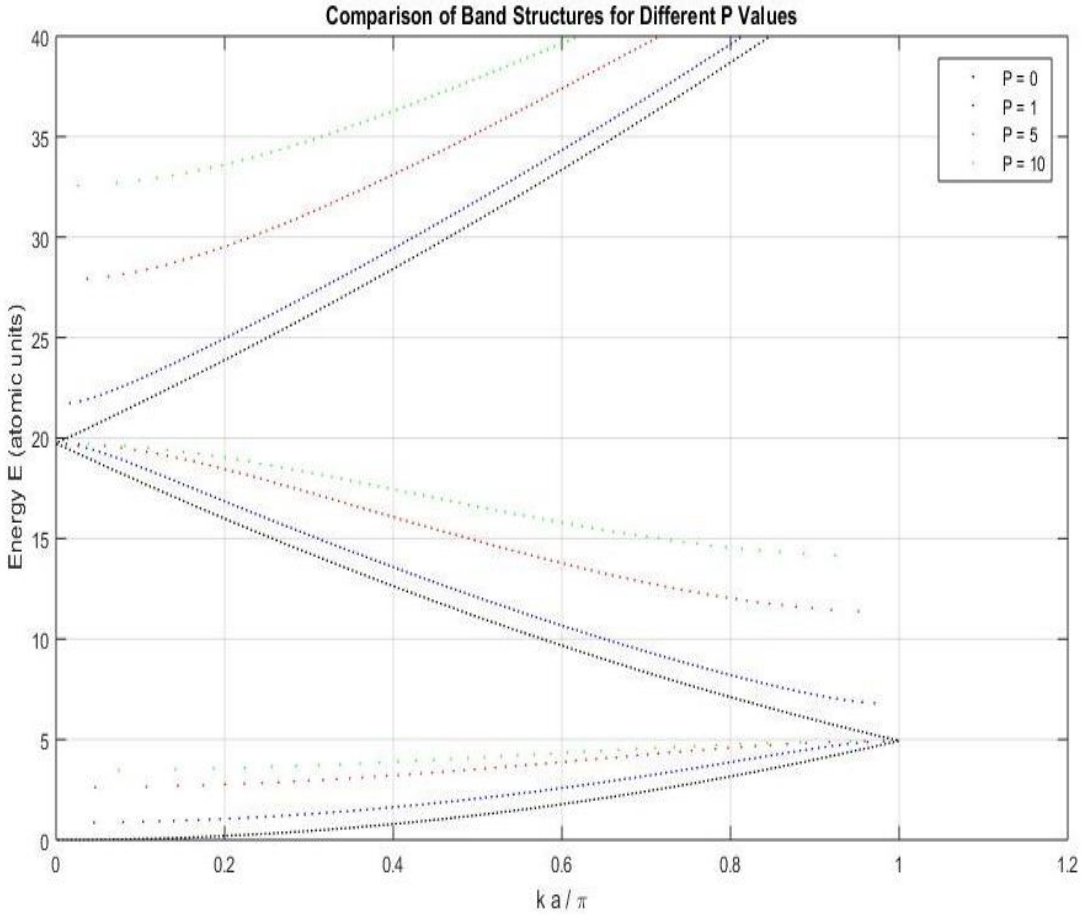

Figure 4: Plot of E versus k showing comparison of Band Structures for Different Values of P

This graph compares the electronic band structures across varying potential strengths (P = 0, 1, 5) and (10). In the free electron limit (P = 0), the periodic potential vanishes, allowing the electron to behave as a free particle whose energy varies smoothly with (k), creating a continuous free-electron parabola folded into the Brillouin zone without any band gaps. Introducing a weak potential (P = 1) initiates weak interactions between the electrons and the lattice, causing small gaps to emerge at the Brillouin-zone boundaries while largely preserving the overall free-electron profile. As the potential reaches an intermediate strength (P = 5), stronger scattering of electron waves by the periodic lattice yields clearly visible band gaps, distinct separation of allowed bands, and a noticeable decrease in bandwidth. At the extreme of a very strong potential (P = 10), it is observed that the allowed bands narrow significantly and the band gaps widen considerably; this severely restricts electron mobility, increases localization around lattice sites, and drives the system toward the limit of isolated atomic states with discrete energy levels rather than broad conduction bands.

CONCLUSION

A detailed analytical and numerical investigation of the one-dimensional Kronig–Penney model has been presented. The dispersion relation was derived from first principles using the Schrödinger equation and Bloch's theorem. The analytical solution yields a compact transcendental equation that is straightforward to solve numerically. Numerical solutions obtained through MATLAB demonstrated the formation of electronic energy bands and band gaps. The present study confirms that potential strength (P) strongly influence the electronic spectrum. Physically, the parameter (P) serves as a direct metric for the strength of the periodic potential experienced by the electrons. Elevating the value of (P) systematically enlarges the forbidden energy gaps, narrows the allowed bands, enhances electron localization, and curtails electron mobility, effectively shifting the behavior of the crystal toward that of a semiconductor or an insulator. Conversely, diminishing (P) reduces lattice interactions and minimizes the energy gaps, resulting in wider bands and a transition toward the metallic behavior characteristic of a free-electron system. The Kronig–Penney model therefore remains

a powerful framework for understanding electron dynamics in periodic structures and modern semiconductor devices.

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