PHN - 006

Kronig-Penney Model

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Sub Batch – O1

Introduction

The study of condensed matter physics has played a vital role in our understanding of the behavior of electrons in materials and has led to numerous technological advancements. One important model in this field is the Kronig - Penney model, proposed by physicists Ralph Kronig and Walter Penney in the early 1930s. This model provides a theoretical framework for investigating the behavior of electrons in a one-dimensional periodic potential.

The importance of this model in explaining the energy band structure and comprehending various properties of solids, like electrical conductivity, thermal conductivity, and optical properties made me highly curious and fascinated. This was my primary motivation to dive deep into the topic.

The Kronig Penney model provides a quantum mechanical framework for understanding the behavior of electrons in a periodic potential. By solving the Schrödinger equation within this model, we can gain insights into the energy states, wave functions, and quantized properties of electrons in a crystal lattice. Hence, the model allows for the analysis of energy band structures in periodic potentials. This links the model to the study of energy bands and band theory in solids.

Also, it serves as a bridge between the microscopic behavior of individual electrons and the macroscopic properties of materials. By exploring the model's predictions, we can connect the quantum mechanical description of electrons to macroscopic phenomena, such as conductivity and thermal properties.

From above points, we can see that this model is directly related to and is an integral part of Quantum and Statistical mechanics.

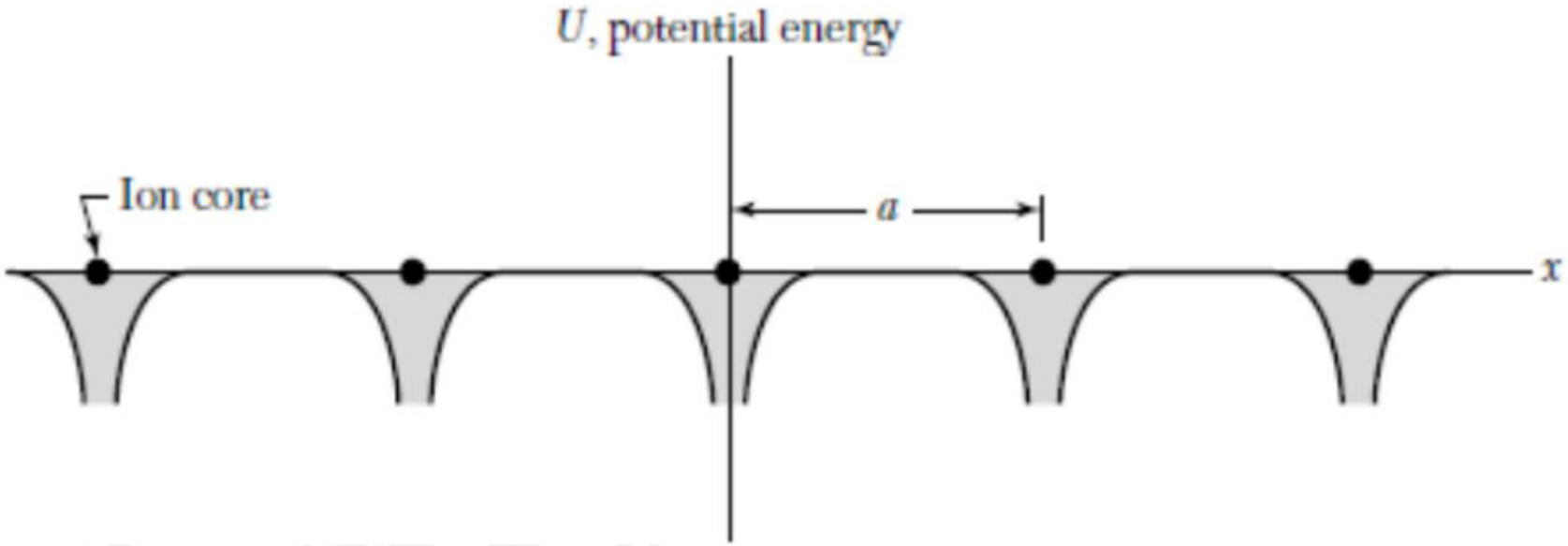
List of Topics

In this project, we aim to delve into the Kronig Penney model and investigate specific aspects of its behavior. In doing so, we will follow the following order of topics:

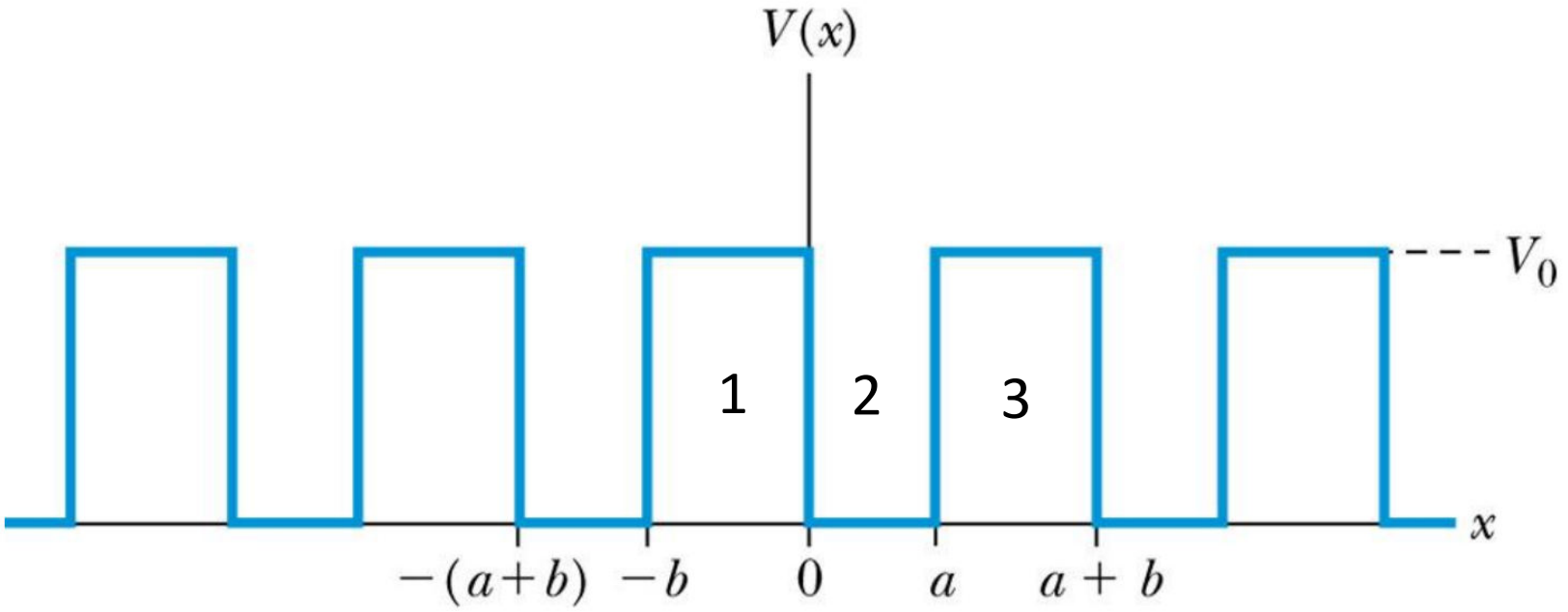
1. Electron in Periodic Potential
2. Mathematical formulation of the model
3. Bloch theorem
4. Solving the mathematical model
5. E-k diagram / Dispersion Spectrum
6. Alternate approach to solve the model
7. Applications of Kronig Penney model

Electron in Periodic Potential

- The electron in a solid can be assumed as an electron in a periodic potential which is generated due to periodic arrangement of lattice ions and also the remaining electrons in the solid.



- Hence the first step towards creating a model for an electron in solid is done by assuming the electron to be in a periodic potential as follows:



Mathematical formulation of the model

- The general 1-dimensional Schrödinger equation along x-axis is given by:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

where, E represents energy of electron and V represents potential energy of electron.

- Hence, for Region-1 and 3 it will be:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi$$

- Here, $V_0 > E$. Hence the solution of this equation will be:

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (V_0 - E)\psi \quad \Rightarrow \quad \psi_1(x) = Ae^{sx} + Be^{-sx}$$

where, s = wavevector in region 1 = $\frac{\sqrt{2m(V_0 - E)}}{\hbar}$

and, A and B are constants.

- For Region-2, it will be:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

$$\Rightarrow \quad \psi_2(x) = Ce^{iQx} + De^{-iQx}$$

where, Q= wavevector in region 2 = $\frac{\sqrt{2mE}}{\hbar}$

and, C and D are constants.

- But till now, there is no term in ψ which accounts for its periodicity. Hence, periodicity is introduced by using the Bloch function, which will be discussed now.

Bloch Theorem

- According to the Bloch theorem, the wavefunction $\psi_{\vec{k}}(\vec{r})$ of an electron in a crystal can be expressed as product of plane wave and a function $u_{\vec{k}}(\vec{r})$ which has the same periodicity as the lattice:

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r})e^{i(\vec{k}\cdot\vec{r})}$$

where, $\vec{k}$ = wavevector of De-Broglie wave of electron and $|\vec{k}| = \frac{2\pi}{\lambda}$, λ = wavelength of De-Broglie wave of electron

This is a direct consequence of the periodic nature of the potential energy function, i.e, $V(\vec{r}) = V(\vec{r} + \overrightarrow{R_n})$, where $\overrightarrow{R_n} = n_1\overrightarrow{a_1} + n_2\overrightarrow{a_2} + n_3\overrightarrow{a_3}$ is an arbitrary translation vector of crystallographic lattice and $\overrightarrow{a_1}$, $\overrightarrow{a_2}$ and $\overrightarrow{a_3}$ are unit lattice vectors. Hence,

$$u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \overrightarrow{R_n})$$

- It is important to note that Bloch function, $u_{\vec{k}}(\vec{r})$ is itself not periodic but due to the plane wave component ($e^{i(\vec{k}\cdot\vec{r})}$), $\left|\psi_{\vec{k}}\right|^2$ has the periodicity of the lattice.
- Another interesting property of the wavefunctions derived from the Bloch theorem is :

$$\psi_{\vec{k}}\left(\vec{r}+\overrightarrow{R_n}\right) = \psi_{\vec{k}}(\vec{r})$$
$$e^{i\left(\vec{k}\cdot\overrightarrow{R_n}\right)}$$

Solving the mathematical model

- Now, for wavefunction ψ to be physically acceptable, following conditions must hold true:

1. ψ and ψ' must be continuous.

$$\psi_1(0) = \psi_2(0)$$

$$\psi_1'(0) = \psi_2'(0)$$

2. Also, Bloch theorem requires ψ to satisfy periodic boundary conditions :

$$\psi_2(a) = \psi_1(-b)\, e^{ik(a+b)}$$

$$\psi_2'(a) = \psi_1'(-b)\, e^{ik(a+b)}$$

From above conditions we get the following 4 equations:

1. $A + B = C + D$
2. $s(A - B) = iQ(C - D)$
3. $Ce^{iQa} + De^{-iQa} = (Ae^{-sb} + Be^{sb})e^{ik(a+b)}$
4. $iQ(Ce^{iQa} - De^{-iQa}) = s(Ae^{-sb} + Be^{sb})\, e^{ik(a+b)}$

- These four equations form a set of homogeneous equations with A, B, C and D as variables. For determinant of coefficient matrix $\neq 0$, we will have a trivial solution which is all constants = 0, which is not of our use. Hence to get a non-trivial solution, we put determinant of coefficient matrix = 0 :

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ s & -s & -iQ & iQ \\ e^{-sb}e^{ik(a+b)} & e^{sb}e^{ik(a+b)} & -e^{iQa} & -e^{-iQa} \\ se^{-sb}e^{ik(a+b)} & se^{sb}e^{ik(a+b)} & -iQe^{iQa} & iQe^{-iQa} \end{pmatrix} = 0$$

- By solving the above determinant, we get :

$$\left[\frac{s^2 - Q^2}{2Qs}\right] \sinh(sb) \sin(Qa) + \cosh(sb) \cos(Qa) = \cos(k(a+b))$$

To further simplify the above expression and to keep in line with the realistic case, we put $b \to 0$ and $V_0 \to \infty$ such that $V_0 b$ remains constant.

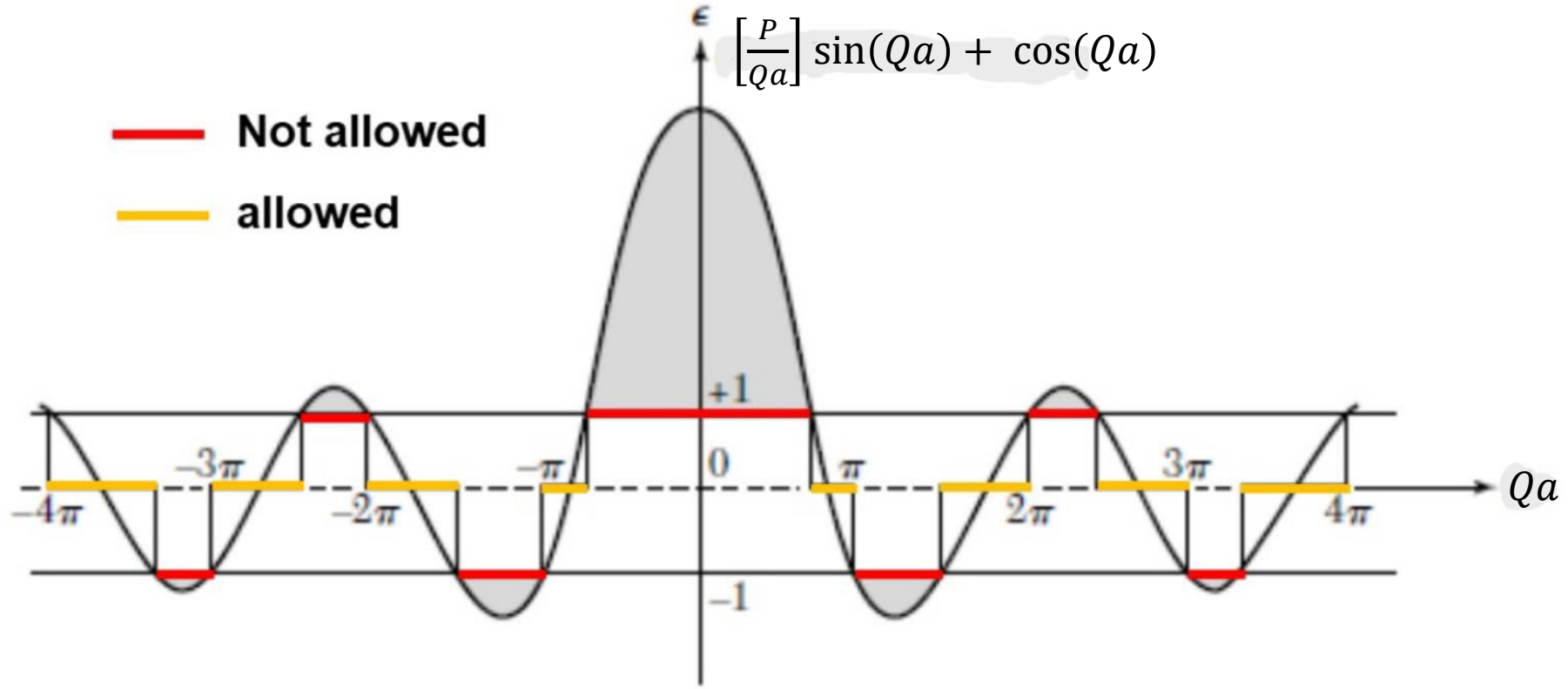
Hence, $s^2 b = \text{constant} \Rightarrow sb \to 0$; $\sinh(sb) = \frac{e^{2sb} - 1}{2e^{sb}} \to \frac{2sb}{2(1)} = sb, \cosh(sb) \to 1$

and as $s \to \infty, \frac{s^2 - Q^2}{2Qs} \to \frac{s^2}{2Qs} = \frac{s}{2Q}$.

Hence the above equation simplifies to:

$$\left[\frac{P}{Qa}\right]\sin(Qa) + \cos(Qa) = \cos(ka), \text{ where } P = \frac{s^2 ba}{2}$$

Here, the RHS of the equation is independent of the variables in LHS and it can take values only from -1 to +1 while LHS can take values even beyond -1 and +1. Hence to make the equation mathematically consistent the LHS cannot take values beyond -1 and +1 and the energy values corresponding to that region are forbidden.



Here, we can see that the red lines represent forbidden energy values while yellow lines represent the allowed energy values.

- From the above graph, we can see that the forbidden energy gap decreases and the width of allowed energy bands increases with increase in the magnitude of Qa .

Case – 1: $P = 0$

$$\left[\frac{P}{Qa}\right]\sin(Qa) + \cos(Qa) = \cos(ka) \Rightarrow \cos(Qa) = \cos(ka) \Rightarrow Q = k$$

$$\Rightarrow \qquad E = \frac{\hbar^2 k^2}{2m} \text{ (free electron energy)}$$

This is the case of a completely free electron which can have all possible values of energy. This is the case of conductor.

Case – 2: $P \to \infty$

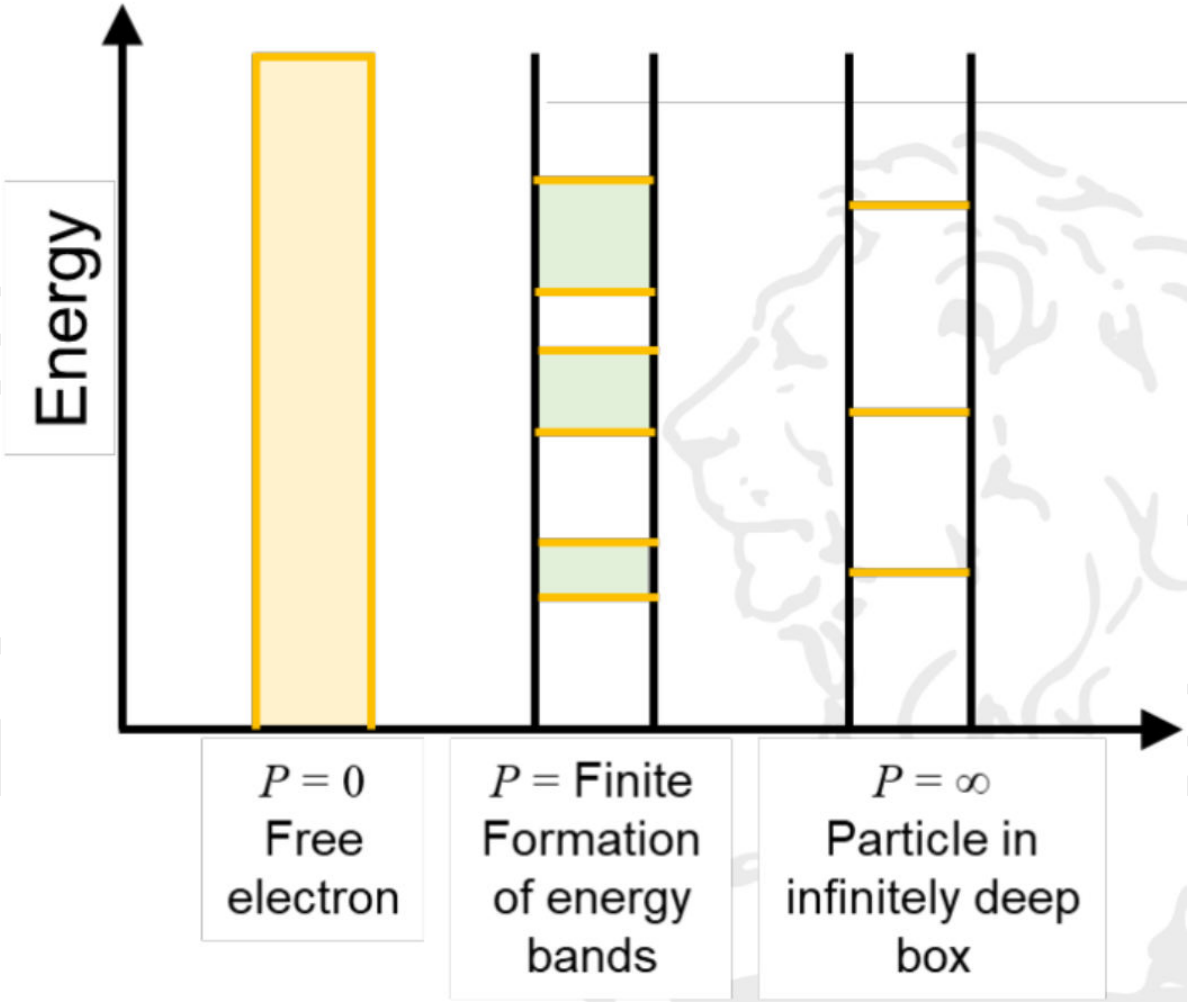
$$\left[\frac{P}{Qa}\right] \sin(Qa) + \cos(Qa) = \cos(ka) \Rightarrow \sin(Qa) = 0 \text{ (To keep LHS finite)}$$

$$\Rightarrow \quad Qa = n\pi$$

$$\Rightarrow \quad E = \frac{n^2\pi^2\hbar^2}{2ma^2} \text{ (Bound electron case)}$$

This is the result which is obtained for a particle in a box of atomic dimensions with infinite potential, i.e, electron is tightly bound and tunneling through the barrier becomes improbable. This shows the case of an insulator.

- In crystals, P has a non-zero finite value and hence energy bands exist.



- If we try to find an explicit expression for E in terms of k from the equation $\left[\frac{P}{Qa}\right] \sin(Qa) + \cos(Qa) = \cos(ka)$, we would find that it has discontinuity at :

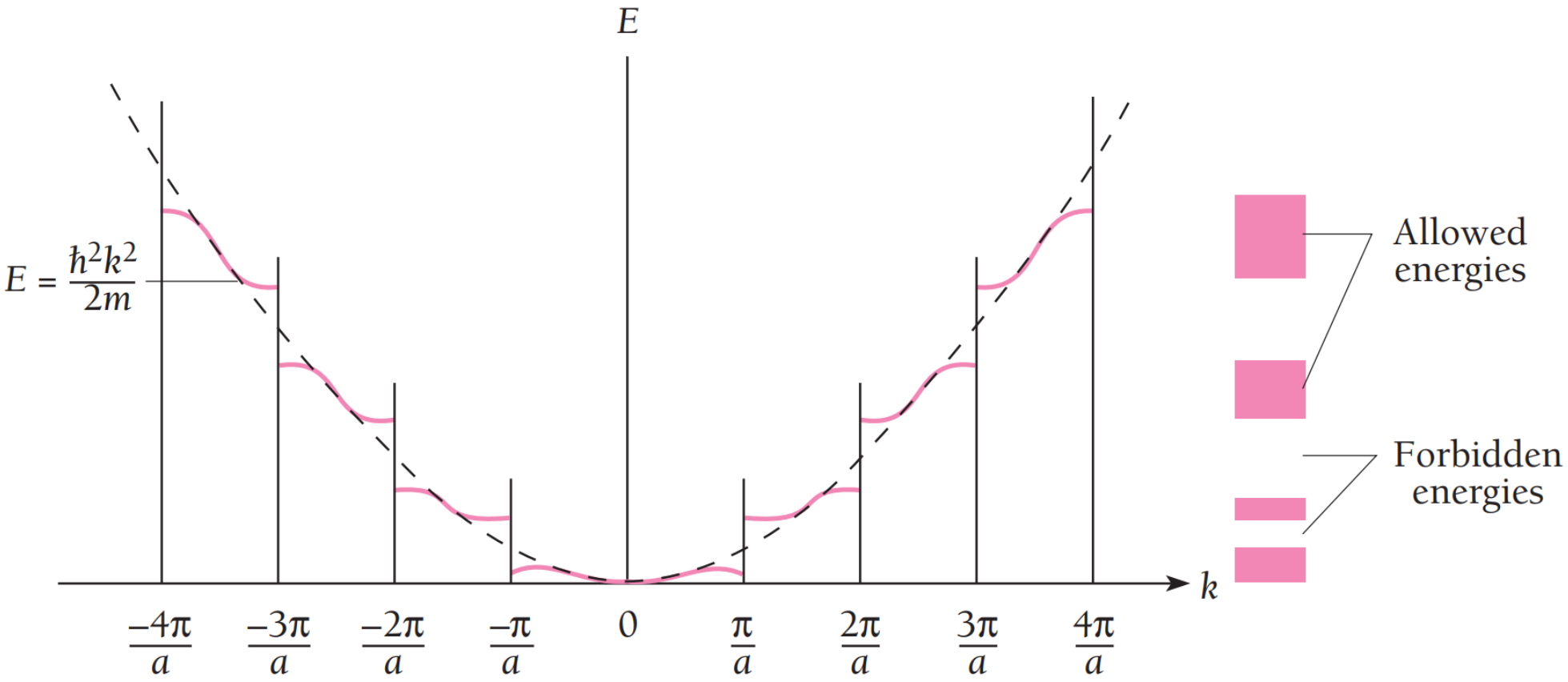
$$k = \pm \frac{n\pi}{a} \text{ , n = 1,2,3,....}$$

Hence for same value of k, E has two possible values. There is a definite gap between those two values and this gives rise to the forbidden energy band.

The discontinuity in expression of E at $k = \pm \frac{n\pi}{a}$ becomes even more evident when we consider the alternate approach to solve the model, which is using Bragg's reflection of the De-Broglie waves associated with electron.

E- k Diagram / Dispersion Spectrum

- From the previous conclusion, we can obtain the graph of E vs k, which is as follows:



Alternate approach to solve the model

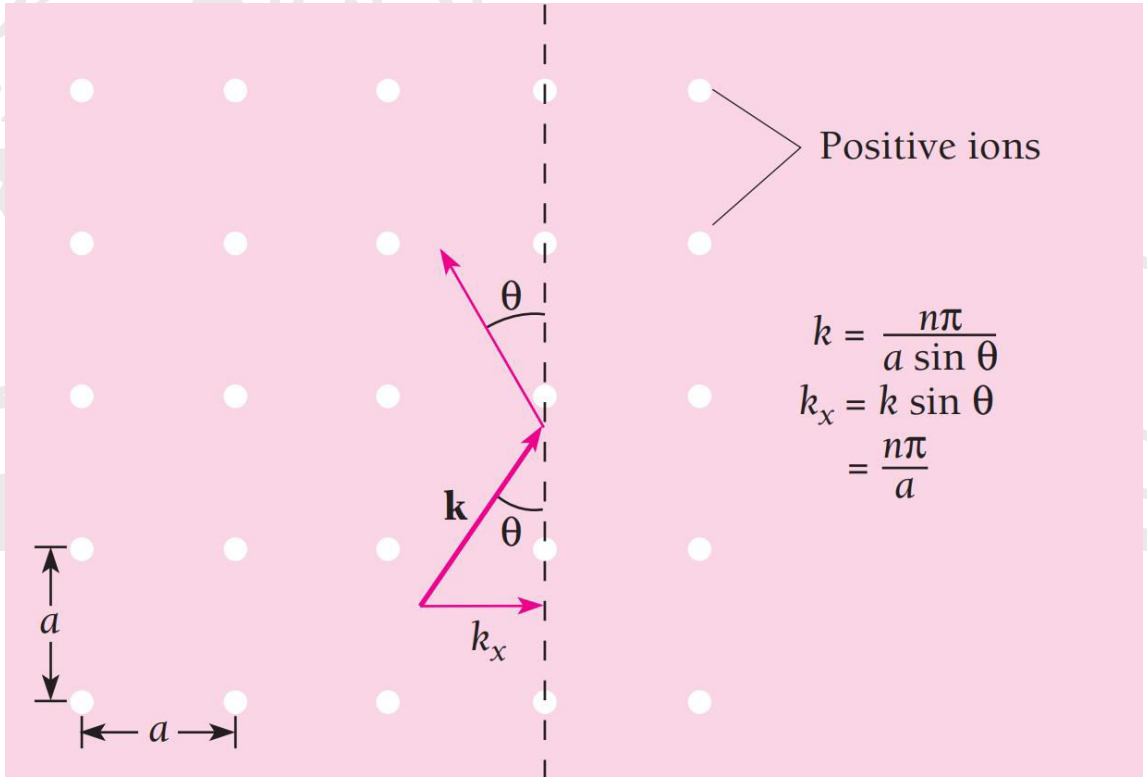
- In this approach, we consider electron as its De-Broglie wave. When electron moves inside the lattice, it can undergo Bragg's reflection from the lattice layers, which can limit the momentum of electron and in turn restricts the value of its energy to certain allowed values. But this will happen only when De-Broglie wavelength of electron λ is comparable to the lattice spacing a .

- Bragg's reflection condition: $n\lambda = 2a\sin\theta$, n = 1,2,3,…

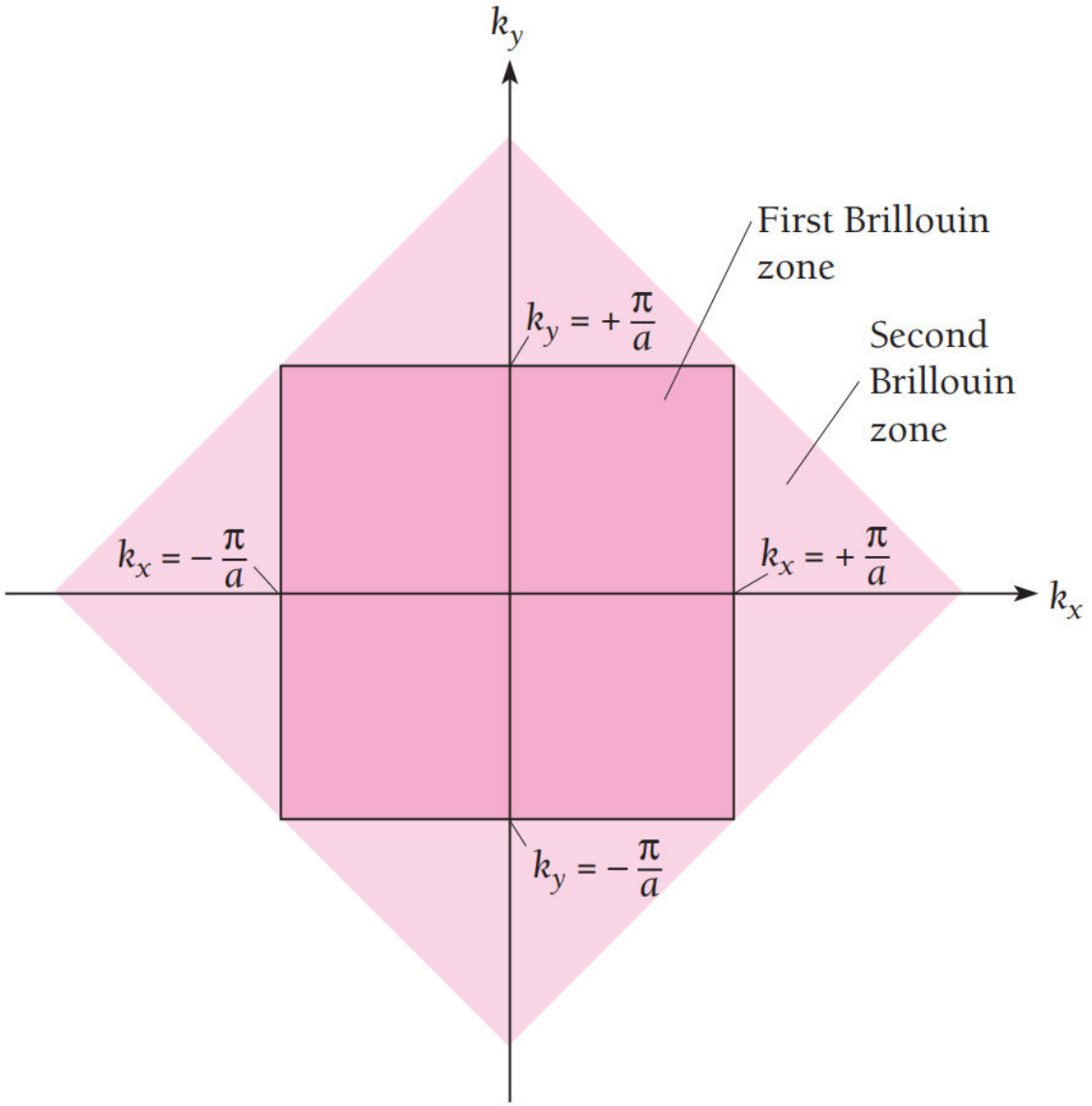
  In terms of wavevector k, it is:

$$k = \frac{n\pi}{a\sin\theta}$$

- From the below diagram, we can see that the electrons are Bragg-reflected from the vertical row of ions, when $k_x = \frac{n\pi}{a}$ and similarly they are Bragg-reflected from horizontal row of ions when $k_y = \frac{n\pi}{a}$.



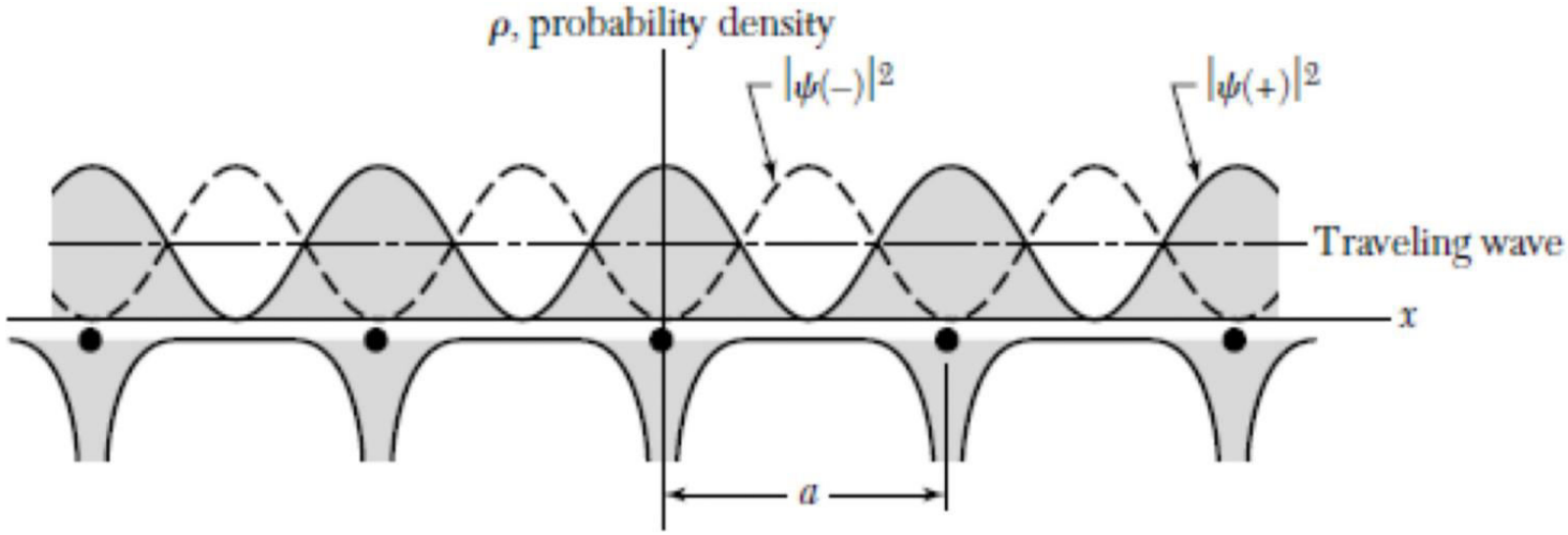
- So, electrons whose wave numbers are sufficiently small, they do not undergo Bragg's reflection and they form first Brillouin zone. When $k = \frac{\pi}{a}$, they are prevented from moving in x and y – directions by reflection. The more k exceeds $\frac{\pi}{a}$, the more limited the possible directions of motion, until when $k = \frac{\pi}{asin45°}$ the electrons are reflected, even when they move diagonally through the lattice.
- Electrons having $\frac{2\pi}{a} > k > \frac{\pi}{a}$ do not fit into the first zone yet they have sufficiently small wave numbers to avoid diffraction by the diagonal sets of atomic plane. Further zones can be constructed similarly.
- At $k = \frac{\pi}{a}$, E has two values, the lower belonging to the first Brillouin zone and the higher to the second zone. There is a definite gap between the possible energies in the first and second Brillouin zones which corresponds to a forbidden band. The same pattern continues as successively higher Brillouin zones are reached.


k_y
First Brillouin zone
$k_y = +\frac{\pi}{a}$
Second Brillouin zone
$k_x = -\frac{\pi}{a}$
$k_x = +\frac{\pi}{a}$
k_x
$k_y = -\frac{\pi}{a}$

- Also, the values of k at which discontinuity occurs in E corresponds to standing wave instead of travelling wave.
- For simplicity, we consider electron moving along x – direction. When $k = \pm\frac{\pi}{a}$, as we have seen, the waves are Bragg-reflected back and forth, and so the only solutions of Schrödinger's equation consist of standing waves whose wavelength is equal to the periodicity of the lattice. There are two possibilities for these standing waves for n = 1 :

$$\psi(+) = A\sin(\frac{\pi x}{a})$$

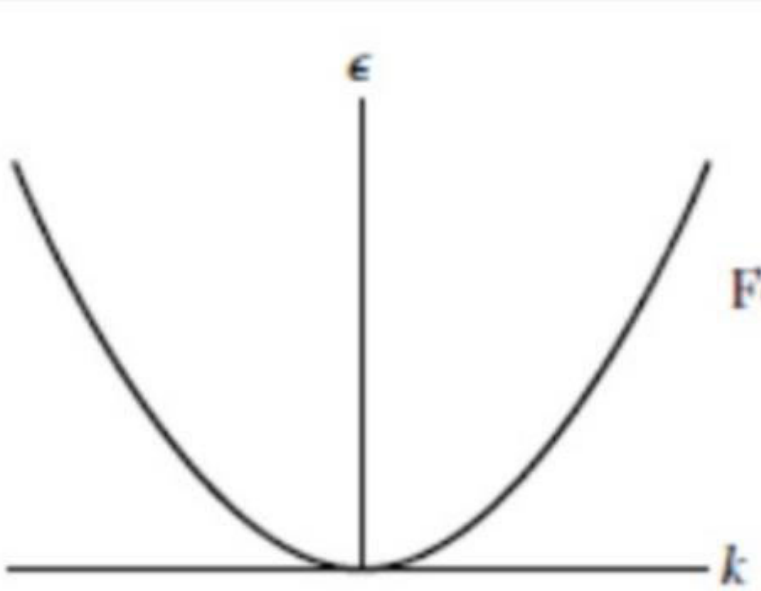
$$\psi(-) = A\cos(\frac{\pi x}{a})$$



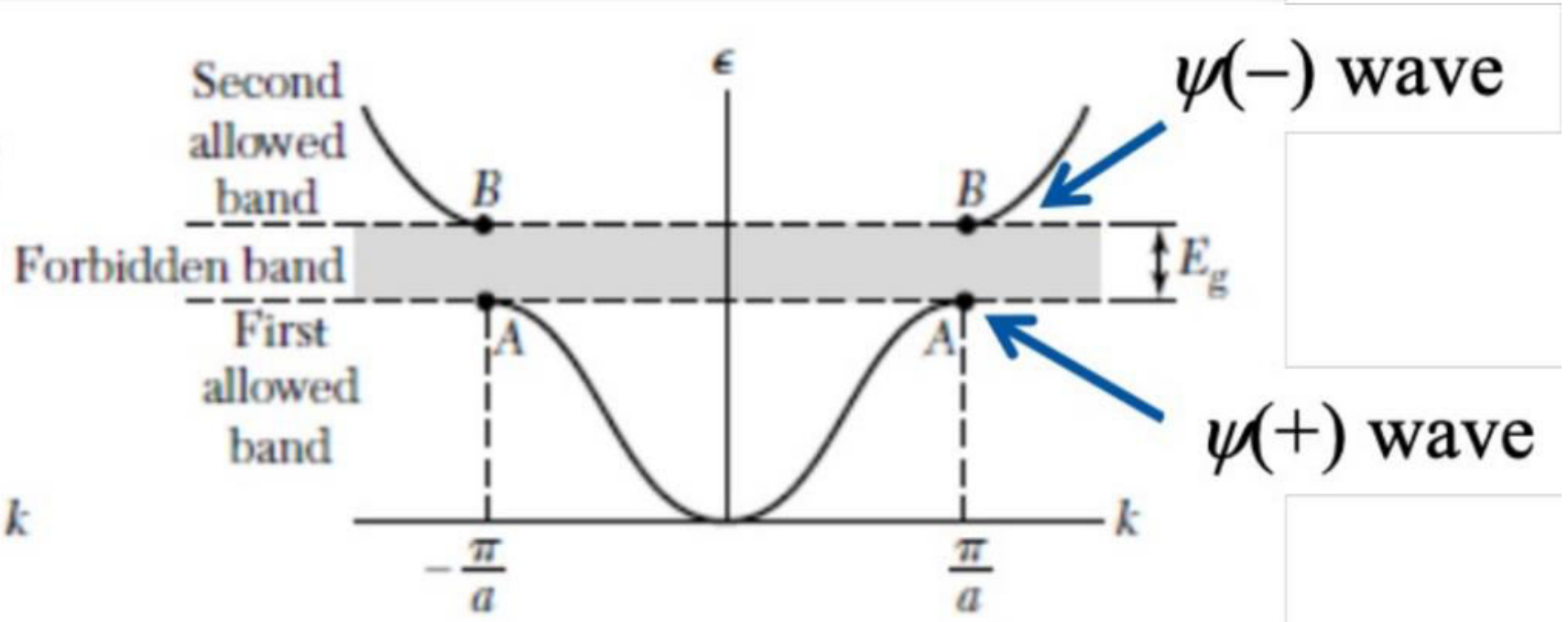
- Hence, here $\psi(+)$ piles up electrons on ions and $\psi(-)$ piles up electrons between the ions.

$$\rho(+) = |\psi(+)|^2 \propto \cos^2 \pi x/a$$

$$\rho(-) = |\psi(-)|^2 \propto \sin^2 \pi x/a$$



Free electron model



Nearly Free electron model

Applications of Kronig – Penney Model

- Kronig – Penney model is a crucial model which provides insights into the electronic properties of materials, particularly in one-dimensional periodic structures :

1. Band structure analysis: The Kronig-Penney model helps in understanding the band structure of crystalline materials. By solving the model, one can determine the allowed energy levels (bands) and forbidden energy regions (band gaps) for electrons in a periodic potential. This information is crucial for studying the electrical and optical properties of materials.
2. Semiconductor Physics: The model aids in analyzing the electronic behavior of semiconductors. By applying appropriate potentials to represent the crystal lattice, one can investigate the formation of energy bands, band gaps, and the conductivity properties of semiconductors. This understanding is essential in designing and optimizing semiconductor devices like transistors and diodes.

3. Topological Insulators: The Kronig-Penney model has been used to understand the behavior of electrons in topological insulators. These are materials that possess unique conducting surface states while being insulating in the bulk. By applying the model to such systems, one can investigate the formation of topological edge states and their potential applications in spintronics and quantum computing.

4. Bloch Oscillations: In certain conditions, electrons subjected to a periodic potential can exhibit Bloch oscillations, which are oscillations of the electron's center of mass motion. The Kronig-Penney model allows the study of Bloch oscillations and their manifestation in transport phenomena, such as electron motion in superlattices under an applied electric field.

Overall, the Kronig-Penney model provides a valuable framework for studying the electronic properties of periodic structures and has applications in various areas of solid-state physics, semiconductor devices, photonics, and emerging fields like topological materials.

Reference

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