Kronig-Penney Model

$b \to 0 \quad U_0 \to \infty \quad , \quad \frac{Q^2 ab}{2} = P = \text{constant}$

$$\frac{P}{Ra} \sin(Ra) + \cos(Ra) = \cos(ka)$$

$$\frac{\hbar^2 Q^2}{2m} = U_0 - E \qquad \frac{\hbar^2 R^2}{2m} = E$$

Goal: Use the periodicity of the lattice (Bloch's condition) to rewrite the Schrödinger Equation as an algebraic equation.

Expand the potential energy/in a Fourier space transform

$$U(\vec{r}) = \sum_{\substack{k_x, k_y, k_z \\ \vec{G}}} \tilde{U}_{\vec{G}} \, e^{i\vec{G}\cdot\vec{r}}$$

$U(x)$ is real : $\tilde{U}_{-G}^{*} = \tilde{U}_{G}$

$$\vec{G} = \nu_1 \vec{b}_1 + \nu_2 \vec{b}_2 + \nu_3 \vec{b}_3$$

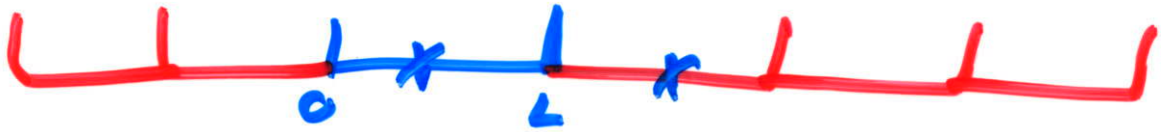
$$\vec{T} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$$

$$U(\vec{r}+\vec{T}) = \sum_{\vec{G}} \tilde{u}_{\vec{G}} \, e^{i\vec{G}\cdot\vec{r}} \cdot \underbrace{e^{i\vec{G}\cdot\vec{T}}} = U(\vec{r})$$

$$e^{i\vec{G}\cdot\vec{T}} = e^{i[\nu_1 n_1 \underbrace{\vec{a}_1\cdot\vec{b}_1}_{2\pi} + \cdots + \cdots]} = 1$$

$$\psi_{(x)} = \sum_{\vec{J}} \tilde{C}_{\vec{J}} e^{iJx}$$

must periodic boundary conditions



$$\psi_{(x+L)} = \psi_{(x)} \Rightarrow \vec{J} = \frac{\pm 2\pi i n}{L}$$

Schrödinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_{(x)} + U_{(x)}\psi_{(x)} = E\psi_{(x)}$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \sum_{G} \tilde{U}_G e^{iGx}\right]\left(\sum_J \tilde{C}_J e^{iJx}\right)$$

$$= E\left(\sum_J \tilde{C}_J e^{iJx}\right)$$

$$\sum_J \frac{\hbar^2 J^2}{2m} \tilde{C}_J e^{iJx} + \sum_G \sum_J \tilde{U}_G \tilde{C}_J e^{i(G+J)x}$$

$$= E \sum_J \tilde{C}_J e^{iJx}$$

$k = G + J$

$J = k - G$

e^{ikx} are linearly independent basis functions that span the space (Hilbert space) closure.

Multiply the previous equation by e^{-ikx} and integrate over x.

Pick out the e^{ikx} coefficients

$$\underbrace{\frac{\hbar^2 k^2}{2m}}_{\lambda_k} \tilde{C}_k + \sum_G \tilde{U}_G \tilde{C}_{k-G} = E \tilde{C}_k$$

$$(\lambda_k - E)\tilde{C}_k + \sum_G \tilde{U}_G \tilde{C}_{k-G} = 0$$

$\tilde{C}_k \ll 1$ for large $k > G_{min} = \frac{2\pi}{a} \equiv g$

Only need k's near zero.

$$G \in \{-2g, -g, 0, g, 2g\}$$

$$U(x) \text{ real} \rightarrow \tilde{U}_g = +\tilde{U}_{-g} = \tilde{U}$$

$$(\lambda_{k-2g} - E)\tilde{C}_{k-2g} + \hat{U}_g \tilde{C}_{k-3g} + \hat{U}_{-g} \tilde{C}_{k-g} = 0$$

$$(\lambda_{k-g} - E)\tilde{C}_{k-g} + \hat{U}_g \tilde{C}_{k-2g} + \hat{U}_{-g} \tilde{C}_{k} = 0$$

$$(\lambda_{k} - E)\tilde{C}_{k} + \hat{U}_g \tilde{C}_{k-g} + \hat{U}_{-g} \tilde{C}_{k+g} = 0$$

$$(\lambda_{k+g} - E)\tilde{C}_{k+g} + \hat{U}_g \tilde{C}_{k} + \hat{U}_{-g} \tilde{C}_{k+2g} = 0$$

$$(\lambda_{k+2g} - E)\tilde{C}_{k+2g} + \hat{U}_g \tilde{C}_{k+g} + \hat{U}_{-g} \tilde{C}_{k+3g} = 0$$

$$\underline{\underline{M}} \cdot \begin{pmatrix} C_{k+2g} \\ C_{k+g} \\ C_k \\ C_{k-g} \\ C_{k-2g} \end{pmatrix} \quad \vdots$$

$$\underline{\underline{M}} = \cdots \begin{pmatrix} \lambda_{k-2g}-E & U & 0 & 0 & 0 \\ U & \lambda_{k-g}-E & U & 0 & 0 \\ 0 & U & \lambda_k-E & U & 0 \\ 0 & 0 & U & \lambda_{k+g}-E & U \\ 0 & 0 & 0 & U & \lambda_{k+2g}-E \end{pmatrix} \cdots$$

$$\vdots$$