Using our 2nd quantized approach we saw

\[ \epsilon_A, \epsilon_B = \epsilon + \Delta (-1)^l = \epsilon + \Delta e^{il\pi} \]

Laue levels

\[ \epsilon - \Delta \quad \epsilon + \Delta \]

\[ A \quad B \quad A + B \]

coupled \( k \) to \( k + \pi \) only, leading to a

simple 2x2 matrix

\[
\begin{pmatrix}
\epsilon_k & \Delta \\
\Delta & \epsilon_{k+\pi}
\end{pmatrix}
\]

whose eigenvalues are

\[
\frac{1}{2} \left[ \epsilon_k \pm \sqrt{\epsilon_k^2 + \Delta^2} \right]
\]

We will now see how this "restricted coupling" of \( k \) only to a "small" of other \( k \) values

"first quantized only"
Expand sol'n \( \psi(\vec{r}) \) to sch eqn in plane waves

\[
\psi(\vec{r}) = \sum_k \xi_k e^{i\vec{k} \cdot \vec{r}}
\]

chosen to obey periodic bc

\( \psi(\vec{r}) \) will be \underline{periodic} over whole crystal

\[ N = L^3 \text{ atoms} \]
\[ L \text{ atoms in each direction} \]
\[ \La = \text{size of crystal side} \]

\[
\psi(\vec{r} + \La \hat{x}) = \psi(\vec{r})
\]

This means \( k = \frac{2\pi}{\La} \{1, 2, \ldots, L \} \)

Meanwhile the potential \( U(\vec{r}) \) is periodic when we move from cell to cell inside the big crystal

\[
U(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}} e^{i\vec{G} \cdot \vec{r}} \quad \vec{G} = \frac{2\pi}{\La} \{0, \La, 2\La, \ldots, \La \}
\]

There are \underline{many, many more} \( k \) values than \( \vec{G} \)

\[
k = \frac{2\pi}{\La} \{1, 2, \ldots, L \}
\]

\[
\vec{G} = \frac{2\pi}{\La} \{0, \frac{\La}{2}, \La, \ldots \}
\]
\( U(\hat{r}) \) is real \( U_0 = u^k \)

Choose \( U_0 = 0 \) as origin of energy

\[
\begin{align*}
\frac{\hat{p}^2}{2m} \psi &= -\frac{\hbar^2}{2m} \nabla^2 \psi = \sum_k \frac{\hbar^2 k^2}{2m} c_k e^{i k \cdot \vec{r}} \\
U \psi &= \sum_q U_q c_q e^{i q \cdot \vec{r}} \sum_k c_k e^{i k \cdot \vec{r}} \\
&= \sum_q U_q c_k e^{i (q + k) \cdot \vec{r}} = \sum_q U_q c_{k-q} e^{i k' \cdot \vec{r}} \quad (\text{rename } k' \rightarrow k)
\end{align*}
\]

\( k^\perp = q + k \) \\
\( k = k^\perp - q \)

\[
\text{The "Central Eqn"} \Rightarrow (\frac{\hbar^2 k^2}{2m} - \varepsilon) c_k + \sum_q U_q c(k - q) = 0
\]

\( \text{NOTE: Just as in second quantized approach, each } k \text{ value (very dense) coupled only to } k + q \)
degree set \( D \) 2x2 problem of 16 values

\[
\begin{align*}
X_1 + X_2 &= 7 \\
X_1 - 3X_2 &= 9 \\
X_3 - X_4 &= 2 \\
2X_3 + X_4 &= 1
\end{align*}
\]

100 equations in 100 unknowns

Real space looks like all 100 coupled

\[ k \text{ space: realize only coupled in pairs} \leftarrow \text{our easy problem} \]

\[ k \text{ space: only coupled } k, k + \frac{\pi}{2} \leftarrow \text{our Schrödinger picture} \]

New form is numerical

so if you look inside electronic structure (DFT) code.

(kittel gives an example)
So we need to look at $k_{\ell m} \left( \frac{-\pi}{a}, \frac{\pi}{a} \right)

and then these $k$ get coupled by $G$ to all other $k$ values.

First step in process is then to "fold" all free energy bands back to $(-\pi a, \pi a)$ and then consider what $U_g$ does to them.

Let's describe that process for simple cubic lattice

(your HW is here)
\[ \varepsilon(k_x, k_y, k_z) = \frac{\hbar^2}{2m} \left( \vec{k} + \vec{q} \right)^2 \]

\[ = \frac{\hbar^2}{2m} \left[ (k_x + q_x)^2 + (k_y + q_y)^2 + (k_z + q_z)^2 \right] \]

Consider \( \vec{q} = 0 \) and examine \( \varepsilon \) along \((k_x, 0, 0)\)

\( \vec{q} = 0: \quad \varepsilon(k_x, 0, 0) = \frac{\hbar^2}{2m} k_x^2 \) \quad " band 1"

\( \vec{q} = \pm \frac{2\pi}{a}: \quad \varepsilon(k_x, 0, 0) = \frac{\hbar^2}{2m} \left( k_x + \frac{2\pi}{a} \right)^2 \) \quad " band 2, 3"

\( \vec{q} = \pm \frac{2\pi}{a} \frac{\hat{y}}{2}: \quad \varepsilon(k_x, 0, 0) = \frac{\hbar^2}{2m} \left[ k_x^2 + \left( \frac{2\pi}{a} \right)^2 \right] \) \quad " bands 4, 5, 6, 7"