Band Structure

Why are curves so complex?

1. Periodicity of lattice, structures + symmetries → Geometrical Effect
2. Details of \( U(x) \) and \( U(r) \) → Consequence

Tackle 1 first (Kittel tackles 2 first)

Empty Lattice Model

\[ \varepsilon = \frac{\hbar^2 k^2}{2m} \]

Two ways of plotting:
1. "Extended zone scheme": plot \( e^2, \varepsilon_r \) vs \( r \)
2. "Reduced zone scheme": plot (like plane)

\( \varepsilon_r \) are only being back by RLVs ended.

already done this for 1D

1D fairly easy to envision

3D: harder. Do simple cubic case only.
Best ideas too simple to be used.
Hass: III direction
\[ E = \frac{k^2 k^2}{2m} \Rightarrow \frac{k^2}{2m} (k + G)^2 \]

Looking for things that end up in 100 science.

More data? 
May be handout?

\[ \begin{align*}
\text{Yes! Handout for 100} \\
\text{will Mathematica} \\
\text{see next page.}
\end{align*} \]
Central Eqn (Hamiltonian)
\[ \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) = E \]

b) periodic ... expand in Fourier series

(like when we did F for lattice itself
back in Chap. 2)

\[ U(x) = \sum G e^{-ikx} \]

or 10. \[ U(x) = \sum G e^{ikx} \]

Also write \( r \) as linear combination of two solutions

\[ \Psi(x) = \sum G e^{ikx} \]

\[ \frac{d}{dx} \Psi = i \hbar \Psi \]

\[ \Psi(0) = 0 \quad \hbar \text{physical unit} \]

\[ \Psi(h) = 0 \quad \text{periodic boundary cond.} \]

\[ \Rightarrow k = 2 \pi n / a \]

Then...

\[ \frac{-\hbar^2}{2m} \sum G e^{ikx} + \sum G e^{ikG} e^{ikx} = E \sum G e^{ikx} \]

\[ k' = k+G \]

\[ \sum G e^{ikG} e^{ik'x} \]

reindex \( k' \to k \)

Extract each coeff of \( e^{ikx} \):

\[ \frac{\hbar^2 k^2}{2m} C_k + \sum G e^{ikG} C_{k+G} = E C_k \]

\[ \left( \frac{-\hbar^2}{2m} - E \right) C_k + \sum G e^{ikG} C_{k+G} = 0 \]

Again, \( k \) like a... boundary eigenvalue matrix eigenvalue prefers whole Schrödinger diff eqn.

How to use: 1) Calculate Fourier coeffs of \( U \)

2) Truncate to some appropriate number ("quasi-degenerate")

3) Solve matrix eqn to determine \( C_k \)

Then you have \( r \) (and easily \( \Psi \))