Lecture 5 - Band structure

Last time started to look at more realistic model for electrons in a crystal
- include interactions with ion cores

Introduced Bloch's Theorem
- If potential $U(x+a) = U(x)$
  - Single-particle
  - Energy eigenstates $2\pi \psi(x+a) = e^{iK_0 a} \psi(x)$

So in a crystal, only need to solve Sch Eqn
- For $0 \leq x < a$, get rest by translation

Example: $U(x) = \alpha \sum_\mathbb{Z} \delta(x-j\alpha)$

Not a model for a real crystal, just the simplest periodic potential we can find

Solve for states:

For $0 \leq x < a$, particle is free

$\psi(x) = A \sin kx + B \cos kx$, $E = \frac{\hbar^2 k^2}{2m}$
Need correct continuity at \( x = 0 \)

For \(-\infty < x < 0\), have

\[
\varphi(x) = e^{-i k x} \left[ A \sin(k x) + B \cos(k x) \right]
\]

where \( k \) is unknown function of \( k \)

To be determined

Need \( \varphi(0^+) = \varphi(0^-) \)

So

(1) \( B = e^{-i k x} \left( A \sin(k x) + B \cos(k x) \right) \)

And also

\[
\frac{d\varphi}{dx} \bigg|_{0^+} = \frac{d\varphi}{dx} \bigg|_{0^-} + \frac{2\pi a}{x^2} \varphi(0)
\]

Discontinuity from \( S \)-function potential

So

(2) \( k A = e^{-i k x} \left[ A \cos(k x) - B \sin(k x) \right] + \frac{2\pi a}{x^2} B \)

Solve (1) for \( A = \frac{B e^{i k x} - \cos(k x)}{\sin(k x)} \)

Substitute into (2)

(Also cancel overall \( B \) and clear \( \sin(k x) \)):

\[
k \left( e^{i k x} - \cos(k x) \right) = e^{-i k x} \left[ \left( e^{i k x} - \cos(k x) \right) \cos(k x) - \sin(k x) \right]
\]

\[
+ \frac{2\pi a}{x^2} \sin(k x)
\]

\[
= e^{-i k x} \left[ e^{i k x} \cos(k x) - 1 \right] + \frac{2\pi a}{x^2} \sin(k x)
\]

\[\begin{align*}
\cos(k x) &= \cos(k x) + \frac{2\pi a}{x^2 k \sin(k x)} \\
\cos(k x) &= \cos(k x) + \frac{ma}{\pi^2 k \sin(k x)}
\end{align*}\]
Implicitly gives \( k(K) \rightarrow E(K) \)
(recall \( K \) is our quantum number, can take any value)

Too bad we can't solve it explicitly!

Rewrite \( \cos Ka = f(\varepsilon) \)

\[
f(\varepsilon) = \cos \varepsilon + \beta \frac{\sin \varepsilon}{\varepsilon}
\]

\( \varepsilon = Ka \quad \beta = \frac{\text{max}}{r^2} \)

\( \varepsilon \) strength of potential

Plot \( f(\varepsilon) \)

No solution unless \( |f(\varepsilon)| < 1 \)

\( \Rightarrow \) only certain values of \( \varepsilon \) allowed
\( \Rightarrow \) only certain values of \( k \)
\( \Rightarrow \) certain values of \( E \)

Draw like:

```
\[
|---|---|---|---|
\]  \( \text{forbidden = "gap"} \)
```

\[
|---|---|---|---|
\]  \( \text{allowed = "band"} \)

```
This gives energies of our single particle states

For finite system length $L_x$, each band breaks up into discrete states $\Delta k \approx \frac{\pi}{L_x}$

Thens out to be $N$ states per band, $N = \#\text{ of atoms}$

(Really $2N$ states per band, including spin)

So if each atom donates $q$ electrons,
for $q$ even, fill up all bands
for $q$ odd, top band is half full, "valence band"

If valence band is full, then exciting an electron costs considerable energy
$\rightarrow$ electrical insulator (diamond, silico, mica, etc)

If valence band partial full, costs little energy to excite electrons
$\rightarrow$ electrical conductor (copper, gold, etc)

For more realistic potentials, relation between $k$ and $k$ is more complicated

But still get bands, good description of crystal behavior

--- Questions?