Lecture 6

Last time started discussion of metals.

Simplest model: free electron gas

Treat electrons as non-interacting particles in a box.

Single particle states labelled by \( \mathbf{k} \), w/ \( E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} \)

All states with \( k < k_F = \left( \frac{3\pi^2}{V} \rho \right)^{1/3} \) are filled.

empty, \( \mathbf{k} > k_F \)

Note: \( k_F \) = interparticle spacing

Electrons can't get much closer than one de Broglie wavelength

Get total energy:

Write \( E_{TOT} = \sum_{\mathbf{k}} E(\mathbf{k}) \Rightarrow \int E(\mathbf{k}) \rho(\mathbf{k}) d^3 k \)

\( \rho(\mathbf{k}) = \frac{\text{Number of states}}{\text{Volume in } k\text{-space}} = \text{"density of states"} \)

\( = \frac{2}{(\Delta k)^3} = \frac{2V}{\pi^3} \quad \text{(inc. spin)} \)

So \( E_{TOT} = \int_0^{k_F} \frac{E(\mathbf{k})}{2m} \frac{2V}{\pi^3} \frac{4\pi k^2 dk}{8\rho \chi} \)

\( = \frac{V}{2\pi^2} \frac{\pi^2}{3} \frac{k_F^5}{5} \)

\( = \frac{V}{10\pi^2} \frac{\pi^2}{3} \left( \frac{3\pi^2}{V} \rho \right)^{5/3} \)
average energy / particle = \( \frac{E_{Tot}}{\rho V} \)

\[ = \frac{3}{10} \frac{\frac{\hbar^2}{m}}{(3\pi^2 \rho)^{\frac{1}{3}}} = \frac{3}{5} \rho \frac{E_F}{m} \]

For \( E_F = \) Fermi energy \( \equiv \frac{\hbar^2 k_F^2}{2m} \)

Put in some numbers: if \( \rho = \frac{1 \text{ electron}}{(10^{-6} \text{ m})^3} \), then \( k_F = 3 \times 10^{10} \text{ m}^{-1} \)

Then \( E_F = 5.5 \times 10^{-15} \text{ J} = 3.4 \text{ eV} \)

That's a lot of energy... corresponds to \( \sim 400,000 \text{ °C} \)

See how important exchange effects are.

Turns out that electron-electron interactions really are negligible in most cases, in electrons never get very close to each other.

But ionic cores are important... electrons do get close to them.

Can introduce idea of how this affects things.

In crystal, ions make periodic lattice

\[ x \]

\[ \text{Spacing} = a \]
(Note most solids are crystals or microscopic level; glasses are not, and are more complicated.)

We want to see what effect this has on single particle states.

Key tool: Bloch's theorem

Says: If $V(x+a)=V(x)$ then energy eigenstates have form $\hat{2}q(x)$ for real quantum number $q$ and with $\hat{2}q(x+a)=e^{iqa}\hat{2}q(x)$

Proof in book, not here. I'll try to give intuitive motivation.

- Certainly want $|2\hat{q}(x+a)|^2=|2\hat{q}(x)|^2$, observables should be periodic.

But that allows $2\hat{q}(x+a)=e^{iqa}\hat{2}(x)$

Bloch says $\phi$ independent $x$.

- Free space $V=0$ satisfies $V(x+a)=V(x)$, for any $a$ we know eigenstates $\hat{2}k(x)=e^{ikx}$ so $\hat{2}k(x+a)=e^{ika}\hat{2}k(x)$

Here $\phi$ independent $x$.

- Bloch's theorem ties these together. Says for $a$, lattice period, $\hat{2}$ translates like free states.
Makes some sense to me. See that $q$ in crystal $n$ $k$ of free particle

Call $q_n$ = quasi-momentum.

See example: 1D system with $V(x) = \frac{a}{2} \sum_j \delta(x - ja)$

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

Solve for states at energy $E$:

For $0 < x < a$, free particle:

$2\psi(x) = A \sin kx + B \cos kx$ for $k = \sqrt{\frac{2mE}{h}}$

For $-a < x < 0$, have $2\psi(x+a) = e^{-iqa} 2\psi(x)$ from Bloch

Here $q$ is unknown function of $k$, need to determine.

Use continuity:

$\psi(x+a) = \psi(x) = A \sin kx + B \cos kx$
Also need \( \frac{d^2 y}{dx^2} |_{0+} = \frac{d^2 y}{dx^2} |_{0-} + \frac{2\pi a}{\lambda} \quad \text{for} \quad \lambda = 2\pi \)

Discontinuity from S-fcn, see Eq. 2.125 to look

Gives

\[ kA = e^{-iqa} \quad k \left( A \cos(ka) - B \sin(ka) \right) + \frac{2\pi a}{\lambda} B \]

Two equations, three unknowns \((A, B, q)\)

But one of \(A/B\) is overall normalization, drops out any way,

Do a little algebra, get

\[ \cos qa = \cos ka + \frac{ma}{k^2} \sin ka \]

Look at graphically

Write as \( \cos qa = \cos z + \beta \frac{\sin z}{z} = f(z) \)

\( z = ka \), \( \beta = \frac{ma}{k^2} \)

Plot \( f(z) \)

Sinusoidal, amplitude decreasing from \( 1 + \beta \) to 1

No solution for \( q \) unless \( |f(z)| \leq 1 \)
So only certain values of z allowed
  => certain values of k
  => certain values of E

Draw like:

\[ \begin{array}{c}
\text{forbidden} = "\text{gap}" \\
\text{allowed} = "\text{band}"
\end{array} \]

Now, I haven't otherwise restricted k at all.

For finite system of length Lx, each band breaks into discrete states, \( \Delta \xi \sim \frac{\pi}{\xi} \)

Works out to \( N \) states per band, \( N = \# \text{ of atoms} \)

\( 2N \) states including spin.

Each atom donates \( Q \) electrons.

For \( Q \) even, fill \( Q/2 \) bands

For \( Q \) odd, top band is half full

If top band is full, exciting an electron costs a lot of energy
  \( \Rightarrow \) crystal is insulator.

Partially filled band easy to excite: \( \Rightarrow \) conductor