Quantum Theory of Solids

In a classical theory of electrons as a gas of free particles, any electron can have any energy, move at any directions, etc.

But electrons are fermions — no two electrons can occupy the same state! That means two electrons at the same place cannot move within the same wave vector.

Uncertainty principle, $\Delta x \cdot \Delta p_x \sim \frac{\hbar}{2}$, $\Delta p_x = \hbar k_x$

$\Delta x \cdot \Delta k_x \sim \frac{1}{2} \implies$ more precisely $\Delta x \cdot \Delta k_x \sim 2\pi$

One electron "requires" some "space" in real coordinates and wave-vector space.

$$1e \rightarrow \frac{dx \cdot dk_x}{2\pi} \cdot \frac{dy \cdot dk_y}{2\pi} \cdot \frac{dz \cdot dk_z}{2\pi} = \frac{dV \cdot d^3 k}{(2\pi)^2}$$

Simple example — fermions in a 1-D square well

Fermi energy for 6 electrons

$\begin{array}{c}
n=4 \\
\downarrow \\
n=3 \\
\downarrow \\
n=2 \\
\downarrow \\
n=1 \\
\end{array}$

Only 2 electrons per level are allowed (Pauli exclusion principle).

Depending on the number of electrons, we can always calculate the highest energy they can have — Fermi energy.
Fermi energy \( E_F \) is defined as the highest energy for the electrons at their lowest energy state \((T=0)\)

We can also define \( k_F \) by using

\[
E_F = \frac{\hbar^2 k_F^2}{2m} \Rightarrow k_F = \sqrt{\frac{2m E_F}{\hbar^2}}
\]

highest wave number electrons can have

For a quantum gas of \( N \) free electrons

\[
N = 2 \cdot \int \int \frac{dV \, d^3k}{(2\pi)^2}
\]

volume of the conductor all possible \( k \)-vectors "volume" per one electron

two possible spin orientations

\[
N = 2 \cdot \sqrt{V} \int_0^{k_F} \frac{d^3k}{(2\pi)^2} = 2\sqrt{V} \int_0^{k_F} \frac{4\pi k^2 dk}{(2\pi)^3}
\]

move to spherical coordinates

\[
\frac{N}{\sqrt{V}} = \frac{1}{\pi^2} \int_0^{k_F} k^2 dk = \frac{k_F^3}{3\pi^2}
\]

electron density

\[
n = \frac{k_F^3}{3\pi^2} = \left(\frac{2m E_F}{\hbar^2}\right)^{3/2} \frac{1}{3\pi^2}
\]

Solving for the Fermi energy

\[
E_F = \left(3\pi^2 n\right)^{2/3} \cdot \frac{\hbar^2}{2m}
\]

Fermi energy very weakly depends on temperature
Fermi-Dirac distribution

\[ f(E) = \frac{1}{e^{\frac{E-E_F}{k_BT}} + 1} \]

The probability of finding an electron in a state with a particular energy.

\( T=0 \)

All states with \( E<E_F \) are filled, all states with \( E>E_F \) are empty.

\( T>0 \)

Fermi velocity \( V_F = \frac{\hbar k}{m} = \sqrt{\frac{2E_F}{m_e}} \)

\( E_F \approx \) a few eV \( \) (Copper \(-7\) eV)

\( V_F \approx 1.6 \times 10^6 \) m/s

Faster than classical prediction, and does not depend on temperature.
We can estimate mean free path

\( l_{\text{mfp}} \approx 390 \text{Å} \) for copper

(from experimentally measured conductivity)

\( \approx 150 \times \text{distance } \) b/w Cu atoms!

How come electrons don't bump into crystal lattice?!

We have to treat electrons as waves

\[ \text{electron} \rightarrow \]

Lattice ions