Lecture #33 Solids

In a solid, a few loosely bound outermost valence electrons in each atom become detached and roam throughout the material.

Simple model \(\Rightarrow\) Free electron gas

\[ V = 0 \quad \text{inside} \]
\[ \infty \quad \text{outside metal} \]

Consider a box of length \(l_x, l_y, l_z\)

Solve Schrödinger Eq.

\[ -\frac{\hbar^2}{2m} \nabla^2 \Psi = E\Psi \]

in Cartesian coordinates

\[ \Psi = \frac{1}{\sqrt{l_x l_y l_z}} \sin \left( \frac{n_x \pi x}{l_x} \right) \sin \left( \frac{n_y \pi y}{l_y} \right) \sin \left( \frac{n_z \pi z}{l_z} \right) \]

with \(n_x, n_y, n_z = 1, 2, 3, \ldots\)

\[ E = \frac{\hbar^2}{2m} \left( \frac{n_x^2}{l_x^2} + \frac{n_y^2}{l_y^2} + \frac{n_z^2}{l_z^2} \right) = \frac{\hbar^2 k^2}{2m} \]
Wave vector \( \mathbf{r} = (k_x, k_y, k_z) \)

\[ k^2 = \pi^2 \left( \frac{n_x^2}{\ell_x^2} + \frac{n_y^2}{\ell_y^2} + \frac{n_z^2}{\ell_z^2} \right) \]

Fill energy levels \( \lambda \) at a time (with \( \lambda = 2 \) spin degeneracy)

until some maximum \( E_{\text{max}} = E_F \)

\[ E \leq E_F \]

Fermi energy

\[ E_F = \frac{k^2_F}{2m} \]

defines Fermi momentum \( k_F \)

Counting states: Total of \( N_{\text{tot}} \)

electrons in system of volume \( V \)

\[ V = \ell_x \ell_y \ell_z \]

Number density of electrons

\[ \rho = \frac{N_{\text{tot}}}{V} \quad \text{(units \, \text{poles} \, \text{per} \, \text{cm}^3)} \]

Interested in \( N_{\text{tot}} \) very large \( \sim 10^{24} \)
Consider cubic cell \( l_x = l_y = l_z = \lambda \).

Fill all states \( n_x, n_y, n_z \) such that

\[
    n_x^2 + n_y^2 + n_z^2 \leq n_{last}^2
\]

\[
    n_{last} = k_F \left( \frac{\lambda^2}{\pi^2} \right)
\]

Count

\[
    n_x^2 + n_y^2 + n_z^2 \leq n_{last}^2 \quad 1 \leq n \leq n_{last}
\]

\[
    N_{\text{total}} = \sum_{n_x, n_y, n_z} n_x n_y n_z = 1 \rightarrow \frac{\lambda^3}{8} \text{ only positive } n
\]

\[
    k_x = \frac{2\pi}{\lambda} n_x \Rightarrow d^3k = \frac{\pi^3}{\lambda^3} d^3n
\]

\[
    N_{\text{total}} = \frac{\lambda}{8} \frac{\lambda^3}{\pi^3} \int d^3k
\]

\[
    \rho = \frac{N_{\text{total}}}{V} - k_F \int d^3k
\]

\[
    \rho = \frac{\lambda}{8\pi^3} \int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta d\theta \int_0^\pi k^2 dk
\]

\[
    \rho = \frac{\lambda}{8\pi^3} \left( \frac{k_F^3}{2} \right) = \frac{\lambda}{6\pi^2} k_F^3 = \frac{k_F^3}{3\pi^2}
\]
Fermi momentum \( p_F = \frac{\hbar}{k_F} \)

\[ k_F = (3\pi^2)^{1/3} \]

grows with density.

Total energy

\[ E_{\text{tot}} = -\frac{\hbar^2}{2m} \frac{\pi^2}{k^2} \left( n_x n_y n_z \right) \]

\[ = -\frac{\hbar^2}{2m} \frac{4\pi V}{k_F} \int_0^{k_F} k^2 dk \]

\[ = -\frac{\hbar^2}{2m} \frac{4\pi V}{k_F} \frac{k_F^5}{5} \frac{k^2}{2m} \]

\[ = -\left( \frac{\hbar^2}{2m} \right) V \left( \frac{k_F}{2\pi^2 m} \right)^5 \left( \frac{N_{\text{tot}}}{V} \right)^{5/3} \]

\[ \lambda = 2 \]

\[ E_{\text{tot}} = \frac{k^2}{16\pi^2 m} \left( \frac{3\pi^2}{2\pi^2 m} \right)^{5/3} \frac{N_{\text{tot}}^{5/3}}{V} \]

\[ \frac{dE_{\text{tot}}}{dV} = -2 \frac{E_{\text{tot}}}{V} = -P \]

4
If you compress the gas the energy rises and the electrons press harder against the walls of the box.

\[ P = \frac{2}{3} \frac{E_{\text{el}}}{{\nu}} = \frac{k^2 k_F^5}{10 \pi^2 m} \]

\[ P \propto \nu^{-5/3}, \quad \text{so} \quad k_F \propto \nu^{1/3} \]

**Metallic Hydrogen**

At normal density and pressure solid hydrogen is a molecular compound with electrons confined into \( \frac{1}{2} \) molecules.

However, as you increase the pressure you can induce a transition to a metallic state with the electrons forming a more or less free Fermi sea inside the material, like last elections in a sodium crystal.

This takes \( 5 \) million atmospheres.

Comp between Coulomb energy \( \sim \frac{1}{\nu^{1/3}} \)

attracting electron into molecule \( F \) and

Fermi energy \( \sim \frac{k^2 k_F^2}{2m} \sim \nu^{-2/3} \)
at high density Fermi energy wins and you have nearly free Fermi gas of electrons. This is called pressure ionization.

Core of Jupiter is metallic H.

Our Sun will event run out of H fuel in ~ 5 billion years and puff up to become a red giant that burn He to C + O and run out of He. Finally without nuclear burning to keep core hot it will collapse all the way to a white dwarf.

White dwarf is a planet sized object of ~ solar mass which is supported against gravity by Fermi pressure of electrons.

Example: Sirius B (companion to Sirius A) has \( M = 1.053 \pm 0.028 \, M_\odot \) and \( r = 0.0074 \pm 0.0006 \, R_\odot \).