Electrons in solids

We have focused so far on lattice

- lattice structure
  description of
- x-ray scattering
- lattice vibrations

Turn now to electrons

An amazing thing is that a lot of properties of $e^-$
in solid can be explained by ignoring lattice!

How is it possible electrons don't scatter off ions?

Recall QM

$$\Psi(\vec{r},0) \rightarrow \Psi(\vec{r},t) \quad \text{How?}$$

Solve

$$\left[ -\frac{1}{2m} \nabla^2 + V(r) \right] \phi_n(\vec{r}) = E_n \phi_n(\vec{r})$$

Hermitean \(\quad\) complete set \(\quad\) orthogonal

Expand

$$\Psi(\vec{r},0) = \sum_n c_n \phi_n(\vec{r})$$

$$c_n = \int d^3r \Psi(\vec{r},0) \phi_n^*(\vec{r})$$
\[ \psi(\vec{r}, t) = \sum_n c_n \phi_n(\vec{r}) e^{-iE_n t/\hbar} \]

Sometimes eliminate \( c_n \) and write in fancy way

\[ \psi(\vec{r}, t) = \int d^3r' \left[ \sum_n \phi_n^*(\vec{r}') \phi_n(\vec{r}) e^{-iE_n t/\hbar} \right] \psi(\vec{r}', 0) \]

\[ G(\vec{r}, \vec{r}', t) \] "green's function" or "propagator"

But point to emphasize is that if you have \( e^- \)
in one of eigenstates initially \( \psi(\vec{r}, 0) = \phi_e(\vec{r}) \)
it never scatters out of it \( \psi(\vec{r}, t) = \phi_e(\vec{r}) e^{-iE_e t/\hbar} \)

[Analogous in a way to classical normal modes]

One has found special states (by "absorbing")
effect if ions into appropriate \( \phi_n(\vec{r}) \)

"Landau Fermi liquid theory" Perhaps

\( e^- \) in solid can be understood as free electron

(with perhaps renormalized \( m \cdot \hbar \))

CM physics
We will see other ways to understand this better in the coming weeks.

For now, let's see what comes out of a description of e⁻ in a solid as just particles in a box with no ionic potential \( V(r) = 0 \),

\[
-\frac{\hbar^2}{2m} \nabla^2 \phi_n = E_n \phi_n
\]

where

\[\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}\]

Solutions are

\[
\phi_n(x, y, z) = \sin \frac{n_x \pi x}{L} \sin \frac{n_y \pi y}{L} \sin \frac{n_z \pi z}{L}
\]

Can easily check this obeys Schrödinger Eq. with

\[
E_n = \frac{\hbar^2}{2m} \left( \frac{n_x^2}{L^2} + \frac{n_y^2}{L^2} + \frac{n_z^2}{L^2} \right)
\]

\[
k_x = \frac{n_x \pi}{L}, \quad k_y = \frac{n_y \pi}{L}, \quad k_z = \frac{n_z \pi}{L}
\]

As \( L \to \infty \), \( k_x, k_y, k_z \) continuous.
Pauli Principle: For Fermions each QM state can be occupied by at most 1 particle. (or 2 if one includes spin $\uparrow \downarrow$ as additional quantum number like $n_x n_y n_z$)

\[
E = n_x n_y n_z \quad \text{if you put 1\text{ e}^- in box at least}
\]

\[
\frac{\hbar^2 \pi^2}{2m L^2} 3 \left\{ \begin{array}{c}
1 \ 1 \ 1 \ \uparrow \downarrow \\
2 \ 1 \ 1 \ \uparrow \downarrow \\
\end{array} \right. \quad \text{Total Energy}
\]

\[
\frac{\hbar^2 \pi^2}{2m L^2} 6 \left\{ \begin{array}{c}
1 \ 2 \ 1 \ \uparrow \uparrow \\
2 \ 1 \ 1 \ \uparrow \downarrow \\
\end{array} \right. 
\]

\[
\frac{\hbar^2 \pi^2}{2m L^2} 9 \left\{ \begin{array}{c}
2 \ 2 \ 1 \ \uparrow \downarrow \\
2 \ 1 \ 2 \ \uparrow \downarrow \\
1 \ 2 \ 2 \ \uparrow \downarrow \\
\end{array} \right. \quad \text{FILLED}
\]

Fermi Energy $E_F$

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

Fermi Wave Vector $k_F$
There is a \( k \) point in every \( \left( \frac{2\pi}{L} \right)^3 \) of \( \vec{k} \) space.

![Fermi Sphere Diagram]

\[ \# \text{ points inside} = \frac{4}{3} \pi k_F^3 \]

\[ \left( \frac{2\pi}{L} \right)^3 \]

\[ \Rightarrow \# \text{ electrons} N \text{ is related to } k_F, E_F \text{ by} \]

\[ N = \frac{2}{3} \pi k_F^3 \left( \frac{2\pi}{L} \right)^3 = \frac{k_F^3}{\frac{3\pi^2}{2}} \]

For spin \( \frac{N}{V} = \frac{n}{3\pi^2} \)

\[ E_F = \frac{k^2}{2m} k_F^2 = \frac{k_F^2}{2m} \left( 3\pi^2 n \right)^{2/3} \]
$E_F$ is a typical kinetic energy of an electron in a metal. In fact, you can show

$$<KE> = \frac{3}{5} E_F \quad \text{A good exercise}$$

Spin

$$<KE> = \frac{1}{N} \int \frac{k_F}{2\pi} \frac{k^2}{2m} dk \left( \frac{1}{2\pi} \right)^3 \frac{k^2}{2m}$$

$$= \frac{1}{N} \left( \frac{L}{2\pi} \right)^3 \frac{8\pi}{5} \frac{L^2}{Zm} \frac{k_F^5}{5}$$

$$\approx \frac{L^3}{N \pi^2} \frac{1}{5} E_F \frac{k_F^3}{5}$$

$$\approx \frac{1}{5} E_F \frac{3\pi^2 N}{L^3}$$

$$= \frac{3}{5} E_F$$

How big is $E_F$? Any guesses?

What is $KE$ of air molecule?

$$\frac{3}{2} k_B T = \frac{3}{2} \left( 1.38 \times 10^{-23} \frac{J}{K} \right) \left( 300 \text{ K} \right)$$

$$= 6.21 \cdot 10^{-21} \text{ J}$$
velocity \quad \frac{1}{2} mv^2 = 6.21 \cdot 10^{-21} J

32 \left(1.67 \cdot 10^{-27}\right) kg

v = 4.82 \cdot 10^2 m/s

Fermi Energy

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

= \frac{(1.055 \cdot 10^{-34})^2 \left(3\pi^2 \cdot 10^2 \cdot 10^{29}\right)^{2/3}}{2 \left(9.11 \cdot 10^{-31}\right)}

= \frac{(1.055)^2 \left(3\pi^2 \cdot 100\right)^{2/3}}{2(9.11)}

= 5.1 \cdot 10^{-19} J

= 3 eV

Another important application is astrophysical...

prevent collapse of neutron star: gravity favors smaller radius but if n increases so does KE cost
Neutron star \( N \) neutrons

\[
PE \sim -\frac{9m^2}{r} N^2 \sim -\frac{9m^2}{r} \cdot \# \text{ pairs}
\]

typical separation \( \sim V^{1/3} \)

\[
KE \sim t N E_F = N \frac{\hbar^2}{2m} \left( \frac{3\pi^2 N}{V} \right)^{2/3}
\]

\[
\sim \frac{\hbar^2}{2m} \left( \frac{3\pi^2}{V} \right)^{2/3} N^{5/3} V^{-2/3}
\]

If \( V \to V/8 \) PE increases by \( \times 2 \)

KE increases by \( \times 4 \)

Balance between 2 \( \to \) neutron star radius

Need to know \( N \), typical \# of neutrons

\[
\Delta = +B \sqrt{V^{2/3}}
\]

seen before where?
Neutron Star number

\[ E = PE + KE \]
\[ = -\frac{GM^2 N^2}{r} + \frac{\hbar^2}{2M} \left(\frac{3\pi^2}{2}\right)^{2/3} N^{5/3} \frac{1}{r^2} \]

\[ g = 6.67 \times 10^{-11} \]
\[ M = 1.67 \times 10^{-27} \]
\[ \hbar = 1.055 \times 10^{-34} \]
\[ r_0 = \frac{\hbar^2 (3\pi^2)^{2/3}}{GM^3} N^{-5/3} \]

\[ N = \frac{2.16 \times 10^{-30}}{1.67 \times 10^{-27}} \]

\[ r_0 = \frac{(1.055 \times 10^{-34})^2 \left(\frac{3\pi^2}{2}\right)^{2/3} \left(\frac{2}{1.67}\right)^{1/3} \left(10^{-57}\right)^{-1/3}}{1.67 \times 10^{-11} \left(1.67 \times 10^{-27}\right)^3} \]

\[ \approx 10^{-68} 10^{-19} 10^{11} 10^{81} \]

\[ \approx \frac{(1.055)^2 (3\pi^2)^{2/3} \left(\frac{2}{1.67}\right)^{1/3}}{(6.67)(1.67)^3} \]

\[ 10^5 \text{ m} \]

\[ 10^5 \text{ m} \approx 10^5 \text{ km} \]
Specific heat of solid

\[ c(T) = \gamma T + AT^3 \]

Crude argument

Fermi Energy \( \sim 5 \times 10^{-19} \) J

\[ k_B T \sim 4 \times 10^{-21} \) J

cannot give energy \( \sim \) electron
(deep) inside Fermi sphere because all
neighboring states filled (Pauli Blocked)

Only states within \( k_B T \) of \( E_F \) can
absorb energy (respond to increase in \( T \))

\[ c \sim Nk_B \frac{k_B T}{E_F} \]

\[ c \sim \gamma T \]

classical Pauli
ideal gas Blocking reduction
answer
This is all at $T=0$; assume $\text{e}^-$ have minimum possible energy by occupying lowest states possible.

From our review of stat mech, as $T$ increases, we begin to occupy higher states.

$E_n$ can be occupied or empty but not multiply occupied.