Intro to Solid State Physics

- Free Electron Gas : Simplest model

N atoms in a box, q e^- free per atom = charge of remaining ion

— We'll choose cubic box. Shape doesn't matter if large

$$V(x,y,z) = \begin{cases} 0 & \text{for } 0 \le x,y,z \le l \\ \infty & \text{outside} \end{cases}$$

- Separation of variables gives 3 1D Schrödinger equs

$$\frac{-\hbar^2}{2m}\frac{d^2X}{dx^2} = E_x X \quad , \ \ldots \qquad E = E_x + E_y + E_z$$

- Wave functions are sine waves. Boundaries give

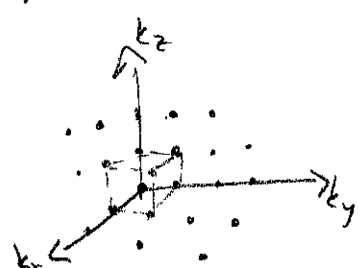
$$X(x) = \sin\left(\frac{n_x \pi}{l} x\right), \ \text{etc} \qquad k_x = \frac{\sqrt{2mE_x}}{\hbar} = \frac{n_x \pi}{l}$$

- Total 1 particle wavefunction is

$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{l^3}} \sin\left(\frac{n_x \pi}{l} x\right) \sin\left(\frac{n_y \pi}{l} y\right) \sin\left(\frac{n_z \pi}{l} z\right)$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2ml^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

- Each state is lattice point in 1st octant of (k_x, k_y, k_z) + carries unit cell of volume π^3/V



— The multiparticle state includes 2 spin choices for each (n_x, n_y, n_z). Antisymmetry allows 1 state where each e^- has different (n_x, n_y, n_z, m_s)

- This fills levels out to a total "momentum" k_F ← Fermi surface

Ground state →

$$\text{Number } e^- = Nq = \text{Number of states} = 2 \times \left(\frac{1}{8}\frac{4}{3}\pi k_F^3\right) \Big/ (\pi^3/V)$$

$$\Rightarrow \quad k_F = (3\pi^2 n)^{1/3}, \quad n = Nq/V = e^- \text{ \# density}$$

- The electron in state at Fermi surface has Fermi energy

$$E_F = \hbar^2/2m \, (3\pi^2 n)^{2/3}$$

- Statistical Mechanics / Thermodynamics
  - Total energy of all e^-

$$\sum_{\substack{\text{energy}\\\text{levels}}} \left((E)_c (\text{degeneracy}) \right) = \int_0^{k_F} \underbrace{\left(\frac{\hbar^2}{2m} k^2\right)}_{\text{energy}} \underbrace{\left(\frac{2}{8} \frac{4\pi k^2 dk}{\pi^3/V}\right)}_{\text{degeneracy}}$$

$$\Rightarrow U = E_{tot} \propto k_F^5 V \propto V^{-2/3}$$

  - Pressure follows from 1st law of thermo $dU = -PdV$

$$P = \frac{2}{3} U/V \propto k_F^5 \propto n^{5/3} \leftarrow \text{degeneracy pressure}$$

due to Pauli exclusion

Periodic Potential / Bands

- Nuclei are really uniformly placed in solid. 1D model
Leads to general periodic potential $V(x) = V(x+a)$
  - Recall $e^{+ipa/\hbar} \psi(x) = \psi(x+a)$
  For periodic potential $e^{+ipa} \cdot (V(x) \cdot \psi(x)) = V(x+a)\psi(x+a)$

$$= V(x) e^{ipa/\hbar} \psi(x) \Rightarrow [e^{+ipa/\hbar}, H] = 0$$

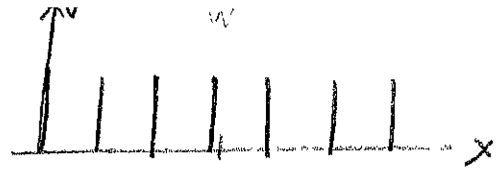
  - Therefore, choose stationary states as eigenstates of $e^{+ipa/\hbar}$.
  We saw before that eigenvalues are e^{iKa}, K real
  $\Rightarrow$ We have condition $\psi(x+a) = e^{iKa}\psi(x)$ Bloch's Theorem
  - K is determined by boundary conditions / edge effects
  To keep a truly periodic potential, make lattice truly periodic, so $\psi(x+Na) = \psi(x)$ $N =$ # of nuclei

$$\Rightarrow e^{iNKa}\psi(x) = \psi(x) \Rightarrow K = \frac{2\pi j}{Na}, \; j = 0, 1, \ldots N-1 \text{ dist.}$$

  (if $j \geq N$, e^{iKa} is same as for $j \bmod N$.)
Physics deep inside solid should be independent of b.c.

– Simplest Model : Dirac Comb

$$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - ja)$$



• In 1st unit cell $0 \le x < a$,

$$\psi(x) = A\sin(kx) + B\cos(kx), \quad k = \frac{\sqrt{2mE}}{\hbar} \text{ as free}$$

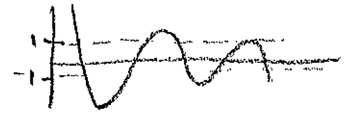
• In cell to right $-a \le x < 0$ (really $(N-1)a \le x < Na$)

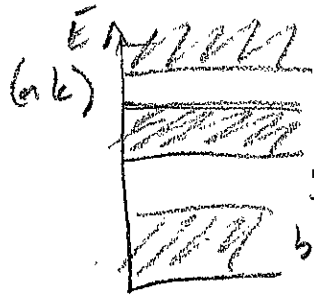
$$e^{ika}\psi(x) = A\sin(k(x+a)) + B\cos(k(x+a))$$

• The b.c. at $x=0$ $\psi(x)$ continuous, $d\psi/dx$ jumps as seen before

$$\Longrightarrow \quad \cos\left(\frac{2\pi j}{N}\right) = \cos(ka) + \frac{m\alpha}{\hbar^2 k}\sin(ka)$$

• That's a transcendental eqn.
But note $|LHS| \le 1$, RHS can go outside. This means there are bands + gaps





← eventually band goes to $E \to \infty$

gap ← $|RHS| > 1$

band ← k where $|RHS| \le 1$ ← 2N states per band (each j) $\times 2$ spins

• If $q = 1\,e^-/\text{atom}$, half 1st band full (or $n=3$ for 2nd)
= conductor = easy to excite e^- at Fermi surface

If $q = 2$, band is full = insulator = hard to excite over gap

If you "dope" material to have a few e^- in one band or a few vacancies ("holes") at top of band, semiconductor.