L60-Free Electron Gas

Monday, February 15, 2016 07:31

* In a solid, the inter-atomic forces are just as important as the electron interactions.

  - some valence electrons become free, and are shared by the entire crystal

* Free electron gas model completely ignores periodicity of the force on valence electrons in the solid.

  - infinite square well where width $l_x, l_y, l_z \to \infty$ $(\sim \sqrt[3]{10^{21}}$ atoms$)$
  - alternatively one can apply periodic boundary conditions.

* examples:
  a) metals (electron Fermi gas)
  b) white dwarf (electron Fermi gas) # 5.35
  c) neutron stars (neutron Fermi gas) # 5.36
  d) nuclei (n,p gas: liquid drop model)

* 3-d solution separates into 3 copies of §2.2

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x,y,z) = \frac{-\hbar^2}{2m}\left(\partial_x^2+\partial_y^2+\partial_z^2\right)\psi = \frac{-\hbar^2}{2m}\left((ik_x)^2+(ik_y)^2+(ik_z)^2\right)\psi = E\psi$$

  - boundary conditions: $\psi = X(x)Y(y)Z(z)$ $\quad X(x) = \sin(k_{n_x}x)$, etc.

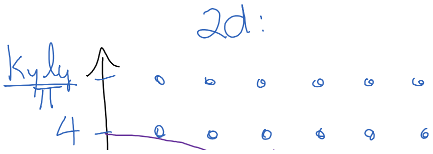
$$k_x l_x = n_x\pi \quad \text{where } n_x = 1,2,3,\ldots \quad ; \quad \text{same for } n_y, n_z$$

  - thus $\psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{8}{l_x l_y l_z}}\,\sin(k_x x)\cdot\sin(k_y y)\cdot\sin(k_z z)$

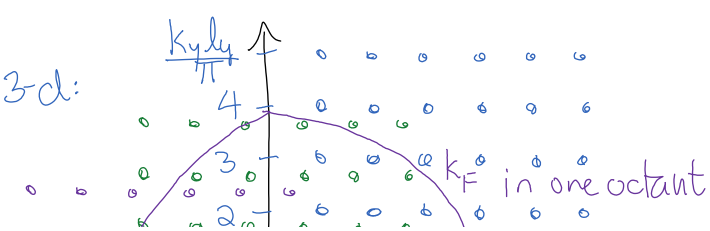
$$E_{n_x n_y n_z} = \frac{p^2}{2m} = \frac{\hbar^2 k}{2m} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{l_x^2}+\frac{n_y^2}{l_y^2}+\frac{n_z^2}{l_z^2}\right) \qquad k^2 = k_x^2+k_y^2+k_z^2$$

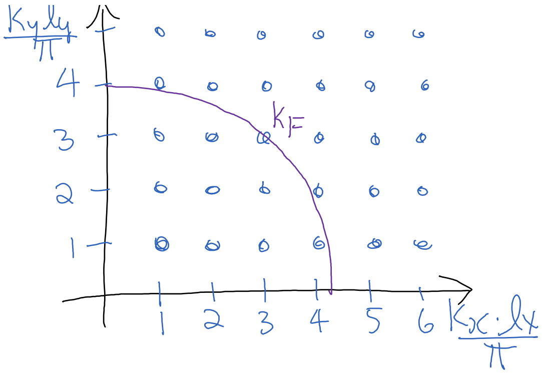
* state space: 3d lattice in $\vec{k}$

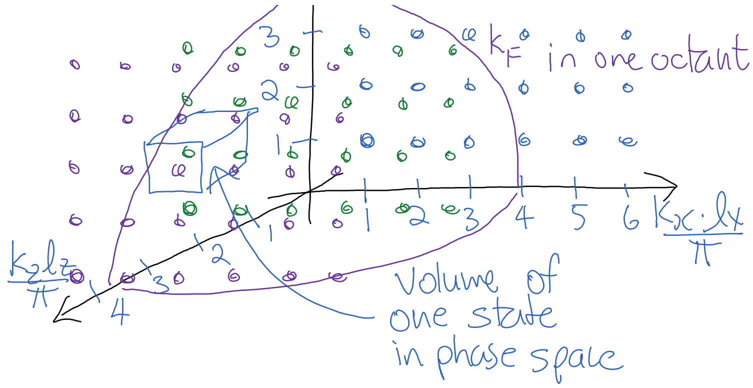
2d:



3-d:







- density of states in phase space: a new interpretation of h!
- applies to Pauli Exclusion Principle, not just Heisenberg Uncertainty Principle

$$\underbrace{\Delta k_x \Delta k_y \Delta k_z}_{V_{\vec{k}}} \cdot \underbrace{l_x l_y l_z}_{V_{\vec{r}}} = \pi^3 \quad \rightarrow \quad \Delta\phi = (\Delta p \cdot \Delta x = 2h)^3 = \boxed{8h^3}$$

volume of one state in phase space.

* Pauli Exclusion principle: 2 electrons $(\uparrow, \downarrow)$ per (n_x, n_y, n_z) state.

- ground state will fill lowest k^2 states up to $|\vec{k}| < k_F$ (the Fermi momentum or energy: $E_F \equiv \hbar^2 k_F^2 / 2m$

- \# states in one octant $(k_x, k_y, k_z > 0)$: \#atoms (N) x \# free electrons (q)
  = volume of phase space $V_{\vec{k}} \cdot V_{\vec{r}}$ x density of states $(\frac{1}{\pi^3})$ x spin degeneracy (2)

$$Nq = \frac{2}{8} \cdot \frac{4}{3}\pi k_F^3 \cdot \frac{V_r}{\pi^3} \qquad k_F^3 = 3\pi^2 \rho \quad \text{where } \rho = \frac{Nq}{V_r} = \text{free electron density}$$

- then $$E_F = \frac{\hbar^2 k_F^2}{2m} = \boxed{\frac{\hbar^2}{2m}(3\pi^2\rho)^{2/3}}$$ (Fermi energy)

  - (exclusion) degeneneracy has forced electron to have energies up to E_F!

* thermodynamics of electron gas: internal energy U:

$$U = \int_0^{k_F} E\, d^3(Nq) = \int_0^{k_F} \frac{\hbar^2 k^2}{2m} \cdot \frac{2}{8} \cdot \underbrace{4\pi k^2 dk}_{\text{volume of shell}} \cdot \frac{V_r}{\pi^3} = \frac{\hbar^2}{2m}\frac{V_r}{\pi^2}\int_0^{k_F} k^4 dk = \boxed{\frac{\hbar^2 k_F^5 V_r}{10\pi^2 m}}$$

but $k_F = \left(3\pi^2 \frac{Nq}{V}\right)^{1/3}$ so $$U = \frac{\hbar^2 (3\pi^2 Nq)^{5/3}}{10\pi^2 m} V^{-2/3} = a V^{-2/3}$$

- isentropic expansion $(\Delta S = 0)$ $\rightarrow$ pressure: $dU = PdV + T\cancel{dS}^{\,0}$

note: this model assumes $T \approx 0 \rightarrow$ ground state.
$T > 0 \rightarrow$ excitations above $k_F \rightarrow$ conduction.

$$dU = d(aV^{-2/3}) = -\frac{2}{3}\frac{U\,dV}{V} = P\,dV$$

degeneracy pressure

$$\Rightarrow P = \frac{2}{3}\frac{U}{V} = \frac{2}{3}\frac{\hbar^2 k_F^5}{10\pi^2 m} = \frac{\hbar^2}{5m}(3\pi^2)^{2/3}\rho^{5/3}$$

ideal gas: $P = kT \cdot \rho \xrightarrow{T\to 0} 0$