Approximate methods to find $\mathcal{U}(\vec{r})$

Thomas-Fermi theory

1) Fermi electron gas:

Independent electrons moving in a box of size L.

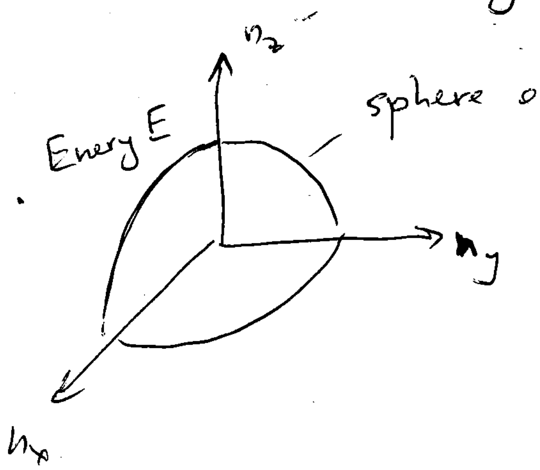
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(\vec{r}) = E\psi(\vec{r}),$$

boundary condition $\psi = 0$ at L.

the allowed energies are

$$E = \frac{\pi^2\hbar^2}{2mL^2}\left(n_x^2+n_y^2+n_z^2\right) = \frac{\pi^2\hbar^2}{2mL^2}n^2$$

What is the density of states $D(E)$?



What is the number of quantum states inside the sphere of radius n?

$$N_S = \underbrace{2}_{\substack{\text{factor which}\\ \text{accounts for } \frac{1}{2}, -\frac{1}{2} \text{ spins}}} \cdot \underbrace{\frac{1}{8}}_{\substack{\text{one octant}\\ \text{of a sphere}\\ \text{(only positive}\\ \text{values of } n_x, n_y, n_z)}} \cdot \underbrace{\frac{4}{3}\pi n^3}_{\text{volume of the sphere.}} = \frac{1}{3}\pi n^3$$

Using $V = L^3$ and

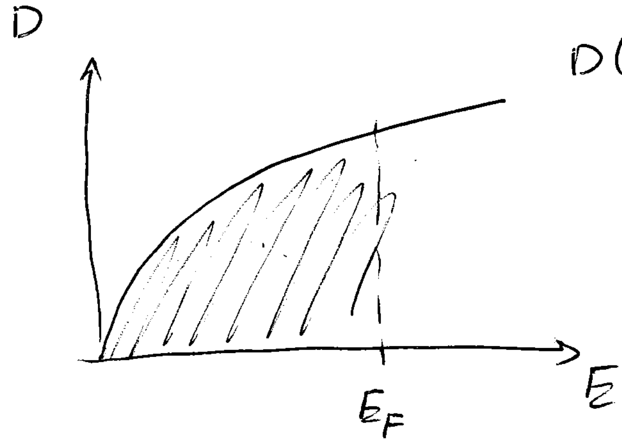
$$E = \frac{\pi^2\hbar^2}{2mL^2}n^2,$$

we can obtain

$$N_S = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E^{3/2}$$

(~~number~~ number of states within the energy range $(E, E+dE)$)

$$D(E) = \frac{dN_S}{dE} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} V E^{1/2}$$



Fermi energy.

$D(E) \sim E^{1/2}$ – the density of states as function of E

We now that system contains N electrons. So we can require that $N = \int_0^{E_F} D(E)\,dE$

We can find that $E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \rho\right)^{2/3}$, where $\underbrace{\rho = \frac{N}{V}}_{\text{uniform distribution of electrons in space.}}$

What happens if we impose some potential? What is ρ?

E_F – is the maximum energy of free moving electrons, so it is kinetic energy.

We place electrons in the potential $V(r)$

than maximum total energy is $E_{max} = E_F + V(r)$

Because E_F is the kinetic energy, we can write $E_F = \frac{k_F^2}{2m}$

Using $E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \rho\right)^{2/3}$, we can derive

$$\rho(r) = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\Big[\underbrace{E_{max} - V(\vec{r})}_{\text{electrostatic potential } -\varphi(\vec{r})}\Big]^{3/2}$$

, how to obtain $\varphi(\vec{r})$.

$\Phi(\vec{r})$ is connected to the density $\rho(\vec{r})$ by Poisson's equation $\nabla^2\Phi(\vec{r}) = -\frac{1}{\varepsilon_0}\rho(\vec{r})$

Thus we have equations

$$\rho(\vec{r}) = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[-\Phi(\vec{r})\right]^{3/2}$$

$\nabla^2\Phi(\vec{r}) = -\frac{1}{\varepsilon_0}\rho(\vec{r})$; or in spherica coordinates:

$$\boxed{\frac{1}{r}\frac{d^2}{dr^2}\left[r\Phi(r)\right] = -\frac{1}{\varepsilon_0}\rho = \frac{1}{3\pi^2\varepsilon_0}\left(\frac{2m}{\hbar^2}\right)^{3/2}\left[\Phi(r)\right]^{3/2}}$$

The boundary conditions:

$$\lim_{r\to 0}\Phi(r) = \frac{Z\bar{e}}{4\pi\varepsilon_0 r}$$ – Coulomb potential

We can assume that $r\Phi(r) = \frac{Ze}{4\pi\varepsilon_0}\chi(x)$

$x = \frac{r}{b}$ $b = \frac{(3\pi)^{2/3}}{2^{7/3}} a_0 Z^{1/3}$

We can finally obtain

$$\frac{d^2\chi(x)}{dx^2} = \frac{1}{\sqrt{x}}\chi(x)^{3/2}$$ – Thomas-Fermi equation.

so we get access to $\rho(\vec{r})$ and $V(\vec{r})$.