Chapter 6: Free Electron Fermi Gas

Read Slater Determinant: We typically use an approximation of the wavefunction for N fermions as

$$E\psi_N = \left[\frac{-\hbar}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_N$$

found using the Hartree-Fock method where we use the Slater determinant to find the energy of the system. For a system of N fermions we have a periodic potential and we can approximate this N fermions to one mean-field. Also related: Dyson Equation. When we treat the group of particles as one *mean-field* we call them *quasiparticles*. The quasiparticle must obey the charge conservation e.g. a bare electron drags a positive cloud which also drags nearby electrons as a quasi electron and the total charge of the dragged cloud is still -1. We desire small mass quasi particles for semiconductors due to a faster acceleration. For the free-electron case we assume that the electrons do not interact with each other thus, we can quanitize the single electron states.

Energy The quantized energies are related to the quantized standing waves of the particle in a box. The Hamiltonian is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n = E_n\psi_n$$

which has a sinosoidal solution of the wavefunction

$$\psi_n = A\sin\left(\frac{2\pi}{\lambda_n}x\right)$$

and the boundary condition determines the wavelength

$$n\lambda_n = 2L$$

and thus the energy of a state is

$$E_n = \frac{\hbar^2k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

Fermi (level) energy is pretty much the highest occupied state (energy). For the 1D case the wave number can only be satisfied at the states for the standing waves:

$$k_0 = 0, \quad k_2 = \pm\frac{2\pi}{L}, \quad k_4 = \pm\frac{4\pi}{L}, \quad \dots$$

the fermi level at N is

$$k = \frac{N\pi}{2L} \to \epsilon_f = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2$$

For the 3D case, we have a cube with a small box of volume $(()\frac{2\pi}{L}^3)$ and for the large number 10^{23} we get a rough estimate of a spherical shell. The fermi energy is

$$\frac{\frac{4}{3}\pi k_f^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{N}{2}$$

where the $N/2$ comes from the denegeracy of the spin states. This is equivalent to the ratio of the volume of the sphere to the volume element. The fermi momentum is

$$k_f = \left(\frac{3}{8}\sqrt{(2\pi)^3}L^3\frac{1}{\pi}\right)^{1/3}$$

or

$$K_f = \left(\frac{3\pi^2 N}{V}\right)^{1/3}$$

and the fermi energy is

$$\epsilon_f = \frac{\hbar^2}{2m}k_f^2 = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3}$$

and the electron velocity is

$$v_f = \frac{\hbar k_f}{m} = \frac{\hbar}{m}\left(\frac{3\pi^2 N}{V}\right)^{1/3}$$

much like the phonon example, we can find the density of states for the free electron gas:

$$D(\epsilon) = \frac{\mathrm{d}N}{\mathrm{d}\epsilon}$$

we can solve the fermi energy equation as a function of energy

$$N = \left(\frac{2\epsilon m}{\hbar^2}\right)^{3/2}\frac{V}{3\pi^2}$$

we also have a relation between N and k_f so we can write the volume in k space:

$$V_k = \frac{4}{3}\pi k^3$$

and since the energy is quantized as

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow k = \frac{\sqrt{2mE}}{\hbar}$$

thus

$$V_k = \frac{4}{3}\pi\frac{(2mE)^{3/2}}{\hbar^3}$$

and since the number of states is

$$N = \frac{V_k}{\left(\frac{2\pi}{L}\right)^3}\cdot 2$$
$$= \frac{V}{3\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

thus the density of states is

$$D(\epsilon) = \frac{\mathrm{d}N}{\mathrm{d}\epsilon} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$$

so the DOS is proportional to $\sqrt{E}$. Also it is proportional to the mass!

Chapter 6: Cont'd

Fermi Energy We have a 3D free electron gas with a DOS of

$$D(\epsilon) = \square\epsilon^{1/2}$$

For the 2D case we have

$$D(\epsilon) = const$$

which will look like a Heaviside step function. For the 1D case we have

$$D(\epsilon) = \frac{1}{\sqrt{\epsilon}}$$

where we have the energy dispersion relation

$$\epsilon = \frac{\hbar^2 k^2}{2m}$$

for graphene (2D material) what does the DOS look like? We would expect it to look like step function, but the electron dispersion relation is linear: $\epsilon = ck$ so the DOS is a linear function.

weird li yang writing:

$$C_v \propto \alpha T^3 + \beta T$$

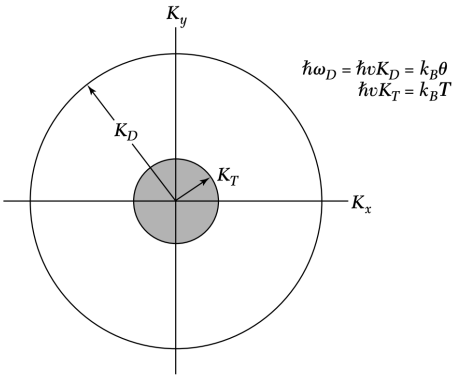

Figure 0.1: Fermi sphere

Fermi sphere at roughly 30 K the classical thermal energy is roughly $k_B T \sim 3$ meV. As the temperature goes up, there is a smearing of the shell at the edges of the fermi sphere. So there are more electrons that can be excited to hgiher energy states thus $N \propto k_B T$. The fermi energy is then roughly $N k_B T \approx T^2 \propto U$. And the heat capacity is

$$C_v \propto \frac{\partial U}{\partial T} \propto T$$

Fermi-Dirac distribution We have 3 parameters that describe the distribution

$$f(T, \epsilon, \mu) = \frac{1}{\exp\left(\frac{\epsilon - \mu}{k_B T}\right) + 1}$$

For $T \to 0$, if $\epsilon > \mu$ then $f \to 0$ and if $\epsilon < \mu$ then $f \to 1$. at very small temperatures, we have a step function. As T increases, the energy states are more smoothed out.

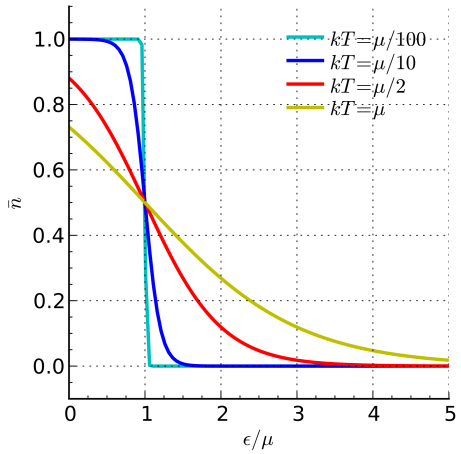

Figure 0.2: Fermi-Dirac distribution

Energy change

$$\Delta U = U(T) - U(0)$$

for $U(0)$ we have

$$U(0) = \int_0^{\epsilon_f} \mathrm{d}\epsilon\, D(\epsilon)\epsilon$$

where we are taking the density of energy and multiplying by the energy at each state and summing them up from 0 to ϵ_f. For $U(T)$ we have

$$\begin{aligned} U(T) &= \int_0^{\infty} \mathrm{d}\epsilon\, D(\epsilon)\epsilon f(\epsilon) \\ &= \left(\int_0^{\epsilon_f} + \int_{\epsilon_f}^{\infty}\right) \mathrm{d}\epsilon\, D(\epsilon)\epsilon f(\epsilon) \end{aligned}$$

where we can split this integral into two parts. So we get the change in energy

$$\Delta U = \int_{\epsilon_f}^{\infty} [\epsilon - \epsilon_f] f(\epsilon) D(\epsilon)\, \mathrm{d}\epsilon + \int_0^{\epsilon_f} [\epsilon_f - \epsilon][1 - f(\epsilon)] D(\epsilon)\, \mathrm{d}\epsilon$$

where the first term I is the part to the right of the chemical potential and the second term II is the part to the left of the chemical potential. We can then find the chemical potential in reference to the zero energy state.:

$$\begin{aligned} C_v = \frac{\mathrm{d}(\Delta U)}{\mathrm{d}T} = \int_{\epsilon_f}^{\infty} \mathrm{d}\epsilon\, (\epsilon - \epsilon_f) \frac{\partial f}{\partial T} D(\epsilon) + \int_0^{\epsilon_f} \mathrm{d}\epsilon\, (\epsilon_f - \epsilon) \left(-\frac{\partial f}{\partial T}\right) D(\epsilon) \\ = \int_0^{\infty} \mathrm{d}\epsilon\, (\epsilon - \epsilon_f) \frac{\partial f}{\partial T} D(\epsilon) \end{aligned}$$

where we first redefine $\tau = k_B T$, and

$$f(\epsilon, \tau, \mu) = \frac{1}{\exp\left(\frac{\epsilon - \mu}{\tau}\right) + 1}$$

so

$$\frac{\partial f}{\partial T} = k_B \frac{\partial f}{\partial \tau} = \frac{\epsilon - \epsilon_f}{\tau^2} \frac{\exp\left(\frac{\epsilon - \mu}{\tau}\right)}{\left(\exp\left(\frac{\epsilon - \mu}{\tau}\right) + 1\right)^2}$$

as $\mu to \epsilon_f$. We can define another variable

$$x = \frac{\epsilon - \mu}{\tau}$$

So

$$C_v = k_B^2 T D(\epsilon_f) \int_{-\epsilon_f/\tau}^{\infty} \mathrm{d}x\, x^2 \frac{\exp(x)}{(\exp(x)+1)^2}$$

and at $T \to 0$ we get reduce this to

$$C_v = k_B^2 T D(\epsilon_f) \int_{-\infty}^{\infty} \mathrm{d}x\, x^2 \frac{\exp(x)}{(\exp(x)+1)^2}$$

and the analytical solution gives us

$$\frac{\pi^2}{3}$$

e.g. for the free electron gas with a DOS

$$D(\epsilon_f) = \frac{3N}{2k_B T_f}$$

the heat capacity is

$$C_v = \frac{1}{2}\pi^2 N k_B \frac{T}{T_f}$$

Electrical Conductivity for an electron the force is

$$\mathbf{F} = -e\mathbf{E} = m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}$$

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -eE \qquad \Delta U = -\frac{eE}{m}\Delta t$$

From the Drude model, we have a mean free path that explains the motion of the electrons. This Δt is related to teh scattering (where high τ means less scattering). And from the Drude model we can define the current density:

$$\mathbf{j} = ne\mathbf{v} = n\frac{e^2\tau\mathbf{E}}{m}$$

with conductance

$$\sigma = \frac{ne^2\tau}{m}$$

the overall collision time is

$$\frac{1}{\tau} = \frac{1}{\tau_1} + \frac{1}{\tau_2} + \dots$$

So applying an electric field will shift the center of the fermi sphere since the electric field will apply a force on the electrons.

Chapter 6: Cont'd

From the conductance eq, we usually see that well conductive materials have a lighter effective mass.

Hall Effect: Consider a 2D material with a longitudinal electric field E_x and a orthogonal magnetic field $\mathbf{H} = B_z$. There will be a resulting voltage drop(electric field) in the transverse direction E_y: We first define the longitudinal conductance

$$\rho(H) = \frac{E_x}{J_x}$$

and the Hall coefficient is

$$R_H = \frac{E_y}{J_x H}$$

from the Lorentz force we have

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = q(\mathbf{E} + \frac{\mathbf{p}}{m} \times \mathbf{H}) - \frac{\mathbf{p}}{\tau}$$

where $\mathbf{p}$ is the momentum. We can assume that this is a steady state:

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = 0$$

and we can a set of equations for the steady state:

$$\begin{cases} 0 = qE_x - \omega_c p_y - \frac{p_x}{\tau} \\ 0 = qE_y + \omega_c p_x - \frac{p_y}{\tau} \end{cases}$$

where $\omega_c = \frac{qH}{mc}$ is the cyclotron frequency. Or in terms of the conductance and resistivity:

$$\begin{cases} -\sigma_0 E_x = \omega_c \tau j_y + j_x \\ -\sigma_0 E_y = -\omega_c \tau j_x + j_y \end{cases}$$

and since $j_y = 0$ we get

$$\begin{aligned} -\sigma_0 E_x = j_x; \qquad \sigma_0 &= -\frac{j_x}{E_x}, \\ -\sigma_0 E_y = -\omega_c \tau j_x; \quad E_y &= \frac{\omega_c \tau}{\sigma_0} j_x \end{aligned}$$

substituing back into the Hall coefficient we get

$$\begin{aligned} R_H = \frac{E_y}{j_x H} = \frac{\omega_c \tau}{\sigma_0 H} &= \frac{q\tau}{mc\sigma_0} \\ \text{using} \quad \sigma_0 &= n\frac{q^2\tau}{m} \\ R_H &= \frac{1}{ncq} \end{aligned}$$