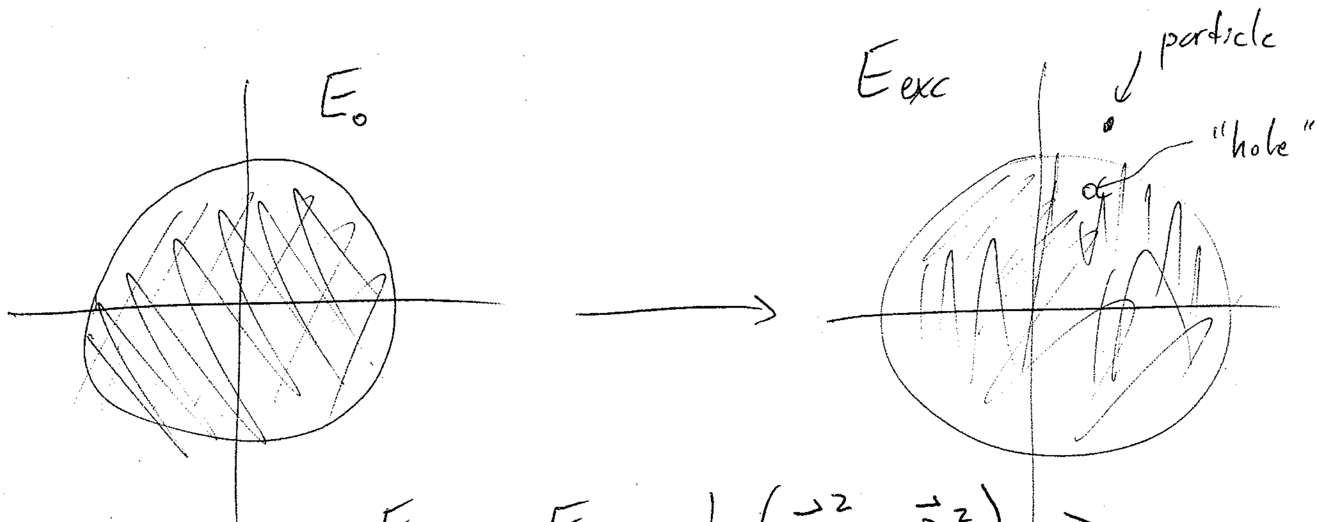
Free Fermi Gas - Nonzero Temperature

- For $T > 0$, excited states play a role. What are the low-energy excited states?

Particle-Hole Excitations



- $E_{exc} - E_0 = \frac{1}{2m}\left(\vec{p}_p^{\,2} - \vec{p}_h^{\,2}\right) > 0$
- $E_{exc} - E_0 \to 0$ as $|p_p|, |p_h| \to p_F$
- $\Rightarrow$ Low-energy excitations are <u>near</u> the Fermi surface.

- Only particles & holes with $|\varepsilon - \varepsilon_F| \lesssim k_B T$ contribute significantly.
- For $T \ll T_F$, need to think QM'ically, in terms of <u>fermi</u> gas. $T_F \sim 10^4 K$, so quantum mechanics important at room temp. & above!

Useful to work in grand canonical ensemble

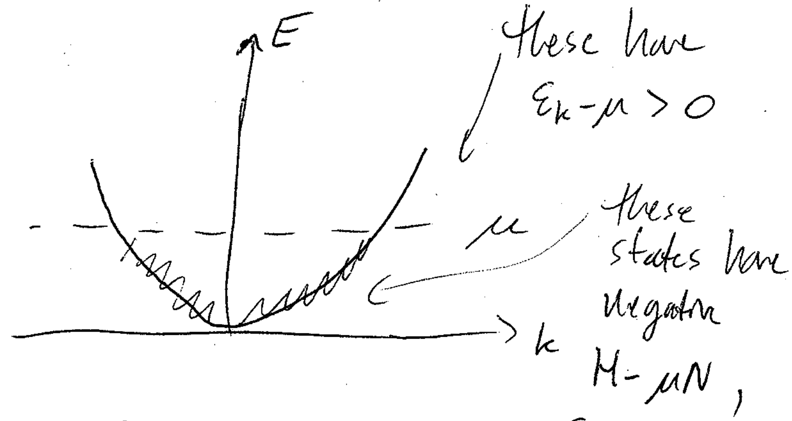
((let total # of electrons fluctuate $\leftrightarrow$ system can exchange electrons with a bath)

(call energies of this F, not E, since it's a kind of free energy)

- Then $H - \mu\hat{N}$ plays the role H played in canonical ensemble.

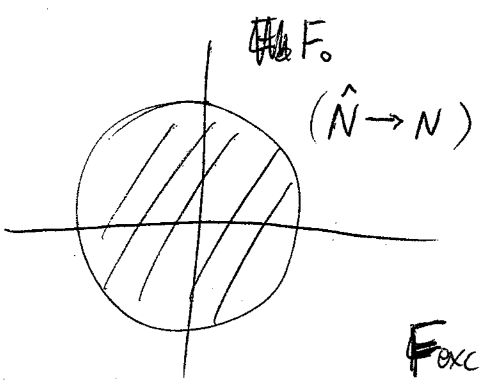
number operator

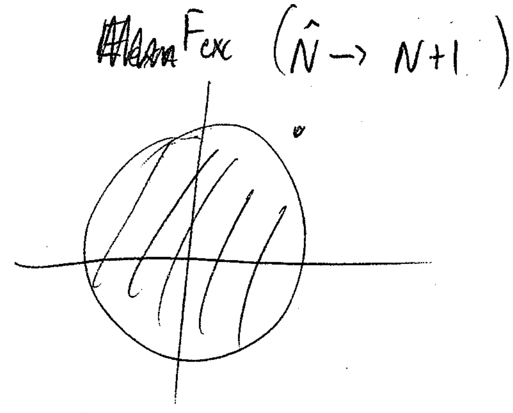
- To fill up fermi sea:



- Minimum $H-\mu N$ achieved by filling states up to ~~μ~~ $\varepsilon = \mu$ $\Rightarrow$ $\boxed{\mu(T=0) = \varepsilon_F}$

- Single particle (or hole) excitations near fermi surface are low (free) energy:





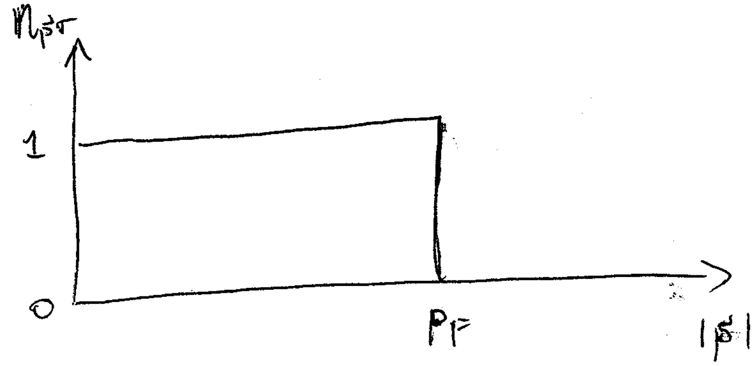
$$F_{exc} - F_0 = \frac{\vec{p}_f^{\,2}}{2m} - \mu$$

Occupation Number — will be very useful at nonzero-T

$$n_{\vec{p}\sigma} = \Theta(p_F - |\vec{p}|) \quad \text{at zero-T}$$

- Probability state $|\vec{p}\sigma\rangle$ is occupied by an electron
- Mean number of electrons in state $|\vec{p}\sigma\rangle$

→ Exercise: Show these two quantities are the same.



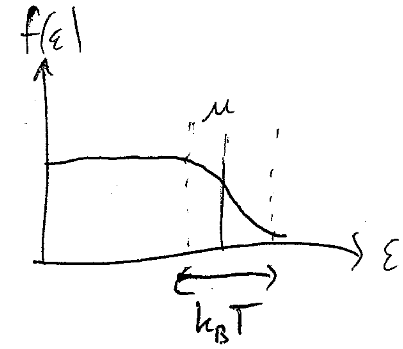
- Total # of electrons: $N = \sum_{\vec{p}\sigma} n_{\vec{p}\sigma} \Rightarrow n = \sum_{\sigma} \int \frac{d^3\vec{p}}{(2\pi)^3\hbar^3} n_{\vec{p}\sigma}$

- Ground state energy: $E = \sum_{\vec{p}\sigma} \varepsilon_{\vec{p}} n_{\vec{p}\sigma} \Rightarrow \mathcal{E} = \frac{E}{V} = \sum_{\sigma} \int \frac{d^3\vec{p}}{(2\pi)^3\hbar^3} \varepsilon_{\vec{p}} n_{\vec{p}\sigma}$

Nonzero - T

- We will skip the derivation and write down the answer. See any textbook on statistical mechanics (and also A&M ch. 2) for a derivation.

$$\boxed{n_{\vec{p}\sigma} = \underbrace{f(\varepsilon_{\vec{p}})}_{\text{"Fermi function"}} = \frac{1}{e^{(\varepsilon_p-\mu)/k_BT}+1}}$$



- Chemical potential is now a function of T:

Determined by:

$$N = \overset{\text{for spin}}{2}\sum_{\vec{k}} f(\varepsilon_{\vec{k}}) \Rightarrow n = \int_{-\infty}^{\infty} d\varepsilon\, D(\varepsilon) f(\varepsilon)$$

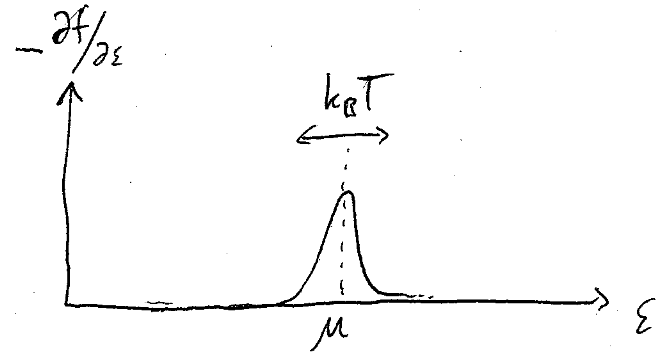
We need to know how to evaluate integrals like this
→ "Sommerfeld expansion"

- Won't go through whole derivation here. For details, see Appendix C of A&M.

General problem: calculate $I = \int_{-\infty}^{\infty} d\varepsilon \, H(\varepsilon) f(\varepsilon)$

- $H(\varepsilon) \to 0$ for $\varepsilon \to -\infty$ (sufficiently fast)
- $H(\varepsilon) \lesssim C \varepsilon^M$ for large ε (some constant C, some integer M)

Want to exploit fact that $\frac{df}{d\varepsilon}$ is very small except near $\varepsilon = \mu$:



Define: $K(\varepsilon) = \int_{-\infty}^{\varepsilon} H(\varepsilon')\, d\varepsilon' \Rightarrow H(\varepsilon) = \frac{dK(\varepsilon)}{d\varepsilon}$

Integrate by parts: $I = \int_{-\infty}^{\infty} K(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) d\varepsilon$

Expand $K(\varepsilon)$: $K(\varepsilon) = K(\mu) + \sum_{n=1}^{\infty} \left[\frac{(\varepsilon-\mu)^n}{n!} \right] \left[\frac{d^n K(\varepsilon)}{d\varepsilon^n} \right]_{\varepsilon=\mu}$

- Crucial assumption: $K(\varepsilon)$ (and $H(\varepsilon)$) is analytic near $\varepsilon = \mu$.

Result:

$$\int_{-\infty}^{\infty} d\varepsilon \, H(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\mu} H(\varepsilon)\, d\varepsilon + \frac{\pi^2}{6}(k_B T)^2 \left[\frac{dH}{d\varepsilon}\right]_{\varepsilon=\mu} + \mathcal{O}(T^4)$$

T- dependence of μ

$$n = \int_{-\infty}^{\mu} d\varepsilon \, D(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 \left[\frac{dD}{d\varepsilon}\right]_{\varepsilon=\mu} + \mathcal{O}(T^4)$$

Guess: $\mu(T) = \varepsilon_F + c(k_B T)^2 + (\text{higher order})$

↑ want to know this.

$$n = \underbrace{\int_{-\infty}^{\varepsilon_F} d\varepsilon \, D(\varepsilon)}_{=n} + \int_{\varepsilon_F}^{\varepsilon_F + c(k_B T)^2} d\varepsilon \, D(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 \left[\frac{dD}{d\varepsilon}\right]_{\varepsilon=\varepsilon_F}$$

$$\Rightarrow 0 = c(k_B T)^2 D(\varepsilon_F) + \frac{\pi^2}{6}(k_B T)^2 \left[\frac{dD}{d\varepsilon}\right]_{\varepsilon=\varepsilon_F}$$

$$\Rightarrow c = -\frac{\pi^2}{6 D(\varepsilon_F)} \left[\frac{dD}{d\varepsilon}\right]_{\varepsilon=\varepsilon_F} = -\frac{\pi^2}{12 \varepsilon_F}$$

$$\Rightarrow \boxed{\mu(T) = \varepsilon_F - \frac{\pi^2}{12}\frac{(k_B T)^2}{\varepsilon_F} + \ldots}$$

small change $\sim \left(\frac{k_B T}{\varepsilon_F}\right) k_B T \ll k_B T$.

Specific Heat (a.k.a. Heat Capacity)

Defined by: $$C_V = \frac{1}{V}\left(\frac{\partial E}{\partial T}\right)_{N,V} = \left(\frac{\partial u}{\partial T}\right)_{N,V}$$

~~constant~~ energy density

- Significance: Measures how effective ΔT is in generating excitations of the system.
- Measurable: Put in heat $Q = \Delta E$, measure ΔT, $C_V = \frac{\Delta E}{\Delta T}$.

Let's calculate $u(T)$:

$$u(T) = \int_{-\infty}^{\infty} d\varepsilon\, \varepsilon D(\varepsilon) f(\varepsilon) \qquad \left(H(\varepsilon) = \varepsilon D(\varepsilon)\right)$$

$$= \int_{-\infty}^{\mu} d\varepsilon\, \varepsilon D(\varepsilon) f(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2\left[\mu D'(\mu) + D(\mu)\right]$$

$$\approx \underbrace{\int_{-\infty}^{\varepsilon_F} d\varepsilon\, \varepsilon D(\varepsilon) f(\varepsilon)}_{u_0} + \int_{\varepsilon_F}^{\varepsilon_F + c(k_B T)^2} d\varepsilon\, \varepsilon D(\varepsilon) f(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2\left[\varepsilon_F D'(\varepsilon_F) + D(\varepsilon_F)\right]$$

$$= u_0 + \left[\varepsilon_F D(\varepsilon_F)\right]\left[-\frac{\pi^2}{6}(k_B T)^2 \frac{D'(\varepsilon_F)}{D(\varepsilon_F)}\right] + \frac{\pi^2}{6}(k_B T)^2\left[\cancel{\varepsilon_F D'(\varepsilon_F)} + D(\varepsilon_F)\right]$$

$$= u_0 + \frac{\pi^2}{6}(k_B T)^2 D(\varepsilon_F)$$

$$\Rightarrow \boxed{C_V(T) = \frac{\pi^2}{3} k_B^2 T D(\varepsilon_F)}$$

again, D.O.S. at Fermi energy determines low-T physics!

- Comment: $C_v(T)$ much smaller than in classical gas, $C_v^{class}(T) = \frac{3}{2} k_B n \to$ const. at low T.

Here, $C_v(T) = \frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) n k_B \cancel{\approx \frac{\pi^2}{3}\left(\frac{k_B T}{\varepsilon_F}\right) C_v^{class}(T)}$

$$\frac{C_v(T)}{C_v^{class}(T)} \sim 10^{-1} - 10^{-2} \text{ at room temp!}$$

$\to$ Thermal excitations of electrons far from Fermi surface are frozen out.