Density of States for Fermi Gas

In our development we'll call the density of orbitals the density of states. That's because we're using the approximation that the energy eigenstates of the multifermion system are obtained by popping fermions into single particle orbitals ...

So. A "density of states" is what? –

A tool for converting sums / integrals over $\vec{n}$ (the quantum #s vector) into integral over energy ε

We wish to write

$$\sum_{\vec{n}} (\cdots) \longrightarrow \int d\varepsilon \, \mathcal{D}(\varepsilon) \, (\cdots)$$

$\mathcal{D}(\varepsilon)\, d\varepsilon$ is the # of orbitals in between energy ε and energy $\varepsilon + d\varepsilon$

Let's call that infinitesimal # dN

i.e. $dN = \mathcal{D}(\varepsilon)\, d\varepsilon$ or $\boxed{\mathcal{D}(\varepsilon) \equiv \frac{dN}{d\varepsilon}}$

we had

$$\varepsilon_F = \frac{\hbar^2}{2M}\left(3\pi^2 n\right)^{2/3} = \frac{\hbar^2}{2M}\left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

so let's find $N(\varepsilon_F)$:

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

$$N = \frac{V}{3\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2} \varepsilon_F^{3/2} \quad \leftarrow$$

\# of orbitals filled up to energy ε_F (×2 for spin)

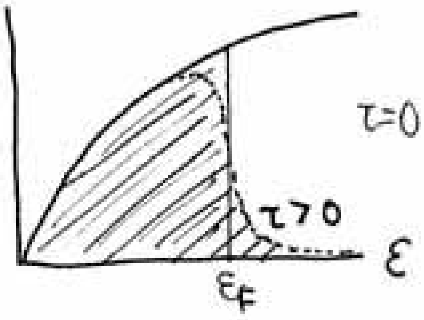
so $$\mathcal{D}(\varepsilon) = \frac{dN}{d\varepsilon} = \boxed{\frac{V}{2\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} = \mathcal{D}(\varepsilon)}$$

This is the density of states which are in principle available.

There is also a quantity which tells us the average occupation of levels: $f(\varepsilon)$

So the density of occupied orbitals is

$$f(\varepsilon)\,\mathcal{D}(\varepsilon)$$



Then

$$N = \int_0^\infty d\varepsilon \, \mathcal{D}(\varepsilon) f(\varepsilon)$$

$$\langle \varepsilon \rangle = \int_0^\infty d\varepsilon \, \mathcal{D}(\varepsilon) f(\varepsilon) \, \varepsilon$$

For the ground state ONLY, f is a step function:

$$N_0 = \int_0^{\varepsilon_F} d\varepsilon \, \mathcal{D}(\varepsilon)$$

$$U_0 = \int_0^{\varepsilon_F} d\varepsilon \, \mathcal{D}(\varepsilon) \, \varepsilon$$

Heat Capacity

We know that our Fermi gas has energy U_0 even at absolute zero. We'd like to know what happens when we heat it up to temperature τ, and compute the heat capacity.

We don't want to include $\frac{\partial U_0}{\partial \tau}$ in our computation, because we're interested in only what it takes to bump up fermions above $\tau = 0$

Therefore, we want

$$C = \frac{\partial}{\partial \tau} \left\{ \int_0^\infty d\varepsilon \, \mathcal{D}(\varepsilon) f(\varepsilon) \cdot \varepsilon \; - \; \int_0^{\varepsilon_F} d\varepsilon \, \mathcal{D}(\varepsilon) \, \varepsilon \right\}$$

Now who in $\{\ldots\}$ depends on τ ?

Well, $\mathcal{D}(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}$ doesn't

But $f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/\tau} + 1}$ does.

It's annoying to have $\int_0^{\varepsilon_F}$ in the second term and not $\int_0^\infty \ldots$ so we need a trick.

We can use the fact that the # of particles is the same no matter τ:

$$N = \int_0^{\varepsilon_F} d\varepsilon \, \mathcal{D}(\varepsilon) = \int_0^\infty d\varepsilon \, f(\varepsilon) \mathcal{D}(\varepsilon)$$

so $\int_0^{\varepsilon_F} d\varepsilon \, \mathcal{D}(\varepsilon) \, \varepsilon_F = \int_0^\infty d\varepsilon \, f(\varepsilon) \mathcal{D}(\varepsilon) \, \varepsilon_F$

i.e.

$C = \frac{\partial}{\partial \tau} \left\{ u(\tau) - u(0) \right\}$ where

$U(\tau) - U(0)$

$$= \int_0^\infty d\epsilon\, \mathcal{D}(\epsilon) f(\epsilon)\, \epsilon - \int_0^{\epsilon_F} d\epsilon\, \mathcal{D}(\epsilon)\, \epsilon$$

$$+ N\epsilon_F - N\epsilon_F$$

$$= \int_0^\infty d\epsilon\, \mathcal{D}(\epsilon) f(\epsilon) (\epsilon - \epsilon_F) - \int_0^{\epsilon_F} d\epsilon\, \mathcal{D}(\epsilon) (\epsilon - \epsilon_F)$$

$$= \int_{\epsilon_F}^\infty d\epsilon\, (\epsilon - \epsilon_F)\, f(\epsilon)\, \mathcal{D}(\epsilon) + \int_0^{\epsilon_F} d\epsilon\, (\epsilon_F - \epsilon)(1 - f(\epsilon))\mathcal{D}(\epsilon)$$

energy needed to take election from
ϵ_F to $\epsilon > \epsilon_F$;
$f(\epsilon)\, \mathcal{D}(\epsilon)\, d\epsilon$ = infinitesimal #
elevated from ϵ_F to ϵ

$1 - f(\epsilon)$ is probability e^-
removed from orbital @ ϵ

So !

$$C_{el} = \frac{\partial}{\partial \tau}\left(U(\tau) - U(0)\right) = \int_{\epsilon_F}^\infty d\epsilon\, (\epsilon - \epsilon_F)\, \frac{\partial f}{\partial \tau}\, \mathcal{D}(\epsilon)$$

$$+ \int_0^{\epsilon_F} d\epsilon\, (\epsilon_F - \epsilon) \cdot \frac{-\partial f}{\partial \tau}\, \mathcal{D}(\epsilon)$$

In other words,

$$C_{el} = \int_0^\infty d\varepsilon \, (\varepsilon - \varepsilon_F) \frac{\partial f}{\partial \tau} \mathcal{D}(\varepsilon)$$

Now: $\frac{\partial}{\partial \tau} \frac{1}{e^{(\varepsilon-\mu)/\tau} + 1} = ?$

(For $\tau \ll \varepsilon_F$ ignore temperature dependence on μ says book.) & Replace μ by ε_F

$$\frac{\partial f}{\partial \tau} = -\frac{(\varepsilon-\varepsilon_F)}{\tau^2} \cdot \frac{-1}{(e^{(\varepsilon-\varepsilon_F)/\tau} + 1)^2} \cdot e^{(\varepsilon-\varepsilon_F)/\tau} .$$

Now let $x \equiv \frac{(\varepsilon - \varepsilon_F)}{\tau}$.

$$\Rightarrow \quad C_{el} = \tau \int_{-\varepsilon_F/\tau}^{\infty} dx \, \frac{x^2 e^x}{(e^x+1)^2} \mathcal{D}(\varepsilon)$$

what will we do with this?

For $\varepsilon_F \gg \tau$, f only has a noticeable derivative near $\varepsilon = \varepsilon_F$. $\Rightarrow$ approximate as $\mathcal{D}(\underline{\underline{\varepsilon_F}})$.

Also for $\tau \ll \varepsilon_F$, lower limit $\sim -\infty$

$$\Rightarrow \quad C_{el} \simeq \tau \mathcal{D}(\varepsilon_F) \underbrace{\int_{\infty}^{+\infty} dx \frac{x^2 e^x}{(e^x+1)^2}}_{} \Rrightarrow \boxed{C_{el} \cong \frac{\pi^2}{3} \tau \mathcal{D}(\varepsilon_F)}$$

We had

$$\mathcal{D}(\epsilon) = \frac{V}{2\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2}\epsilon^{1/2} \qquad \text{and}$$

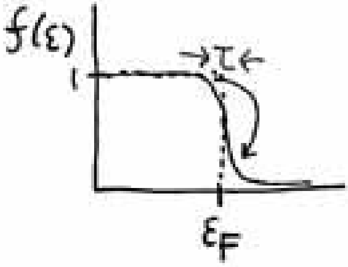
$$N = \frac{V}{3\pi^2}\left(\frac{2M}{\hbar^2}\right)^{3/2}\epsilon_F^{3/2}.$$

so $\mathcal{D}(\epsilon_F)\cdot\epsilon_F = \frac{3}{2}N$

so

$$\boxed{C_{el} \underset{\tau \ll \epsilon_F}{\cong} N\frac{\pi^2}{2}\frac{\tau}{\epsilon_F}}$$

Linear in τ



Why did this happen?

excited e^-'s for low-τ

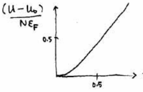
is $\sim N\dfrac{\tau}{\epsilon_F}$

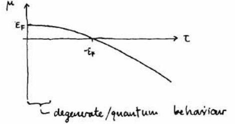
and energy increase $\Big\} \sim \tau$

so $U(\tau) - U(0) \sim \dfrac{N\tau^2}{\epsilon_F}$

so $C_{el} \sim N\left(\dfrac{\tau}{\epsilon_F}\right)$.

Energy & Chemical Potential for Fermi Gas





Application : 'Gas' of conduction electrons in metals

Contribution to heat capacity from Fermi gas behaviour is linear in τ.

Recall also Debye theory –

Debye story said that at low enough temperature, upper bound of 3N on # of phonon modes was not "felt"

so phonon gas acted like photon gas & had $U \propto \tau^4 \Rightarrow C_V \propto \tau^3$

So for a metal, C_V has 2 contributions

(a) atomic lattice vibrations

$$C_V^{(at)} \equiv A\tau^3$$

(b) electron gas

$$C_V^{(el)} \equiv \gamma\tau$$

and $\gamma = \frac{\pi^2}{2} N Z \frac{1}{\varepsilon_F}$

while $A = \frac{12\pi^4}{5} N \frac{1}{(k_B \underset{\uparrow \text{Debye temperature}}{\Theta_D})^3}$

Notice that by our usual definition $C_V \equiv \left(\frac{\partial U}{\partial \tau}\right)_V$ C_V is <u>dimensionless</u>.

Let's look harder at these $\uparrow$ formulae :

$$C_V = \gamma\tau + A\tau^3$$

$$= \frac{\pi^2}{2} N \left(\frac{\tau}{\varepsilon_F}\right) + \frac{12\pi^4}{5} N \left(\frac{\tau}{k_B\theta_D}\right)^3$$

We can write $\varepsilon_F \equiv k_B T_F$

then

$$\left(\frac{C_V}{N}\right) = \left(\frac{\pi^2}{2}\right)\left(\frac{T}{T_F}\right) + \left(\frac{12\pi^4}{5}\right)\left(\frac{T}{\theta_D}\right)^3$$

$$\nwarrow \quad \nearrow$$

Both terms here are of the form

$(\text{math \#'s}) \left(\frac{T}{T_{\text{characteristic}}}\right)^{\#}$ $\nwarrow$ integer power

This is another example of dimensional analysis at work in physics, and it's deep.

The N is there because C_V is extensive.

Characteristic temperatures?

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

"Fermion Elbows"

cf. $\theta_D = \frac{\hbar c}{k_B}\left(6\pi^2\frac{N}{V}\right)^{1/3}$

Experiments on metals?

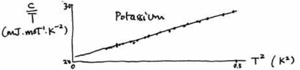
(1) ε_F is order 1 eV for

Alkali metals (Li, Na, K, Rb, Cs)

and Copper, Silver, Gold

(2) Curves of $\frac{C_V}{\tau} \equiv \gamma + A\tau^2$ from theory

are, experimentally,



$\frac{C}{T} = 2.08 + 2.57T^2$ in these units