Lecture #18 PHYS 551

Heat Capacity of an Electron Gas

We recall from last time:

$$\text{Occupancy} \equiv \#\text{ of } e^- \text{'s with energy } \varepsilon = f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T}+1}$$

where $\mu \equiv$ chemical potential $T =$ temperature

Now the total number of electrons in our system, N, must be

$$N = \int_0^\infty f(\varepsilon)\, D(\varepsilon)\, d\varepsilon \qquad \mathcal{D}(\varepsilon) \equiv \text{ density of states}$$

$$\text{and} \qquad \overline{U} = E_{\text{Total}} = \int_0^\infty \varepsilon\, f(\varepsilon)\, \mathcal{D}(\varepsilon)\, d\varepsilon$$

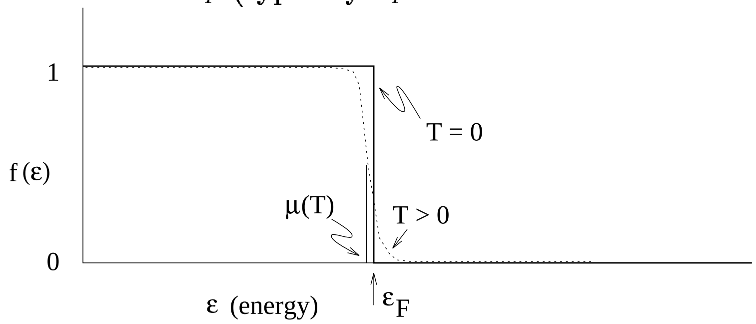
At $T = 0$

$$f(\varepsilon) = 1 \text{ for } \varepsilon < \mu \text{ where } \mu = \varepsilon_f$$

$$\text{and} \quad f(\varepsilon) = 0 \text{ for } \varepsilon > \mu$$

Clearly, these integrals are straightforward at $T = 0$. However $\mu = \mu(T) \rightarrow$ thus the above integrals are non-trivial.

Assume $T > 0$ and $T < T_F$ (typically $T_F \sim 50000$K and $T \approx 300$K or less)



Clearly, only those electrons close to μ contribute to the heat capacity. A general method was developed by Sommerfeld to handle this integral.

$$I = \int_0^\infty d\varepsilon\, f(\varepsilon)\, H(\varepsilon) \quad \text{where } H(\varepsilon) \text{ is a general function.}$$

In our case $H(\varepsilon)$ is either $\mathcal{D}(\varepsilon)$ or $\mathcal{D}(\varepsilon)\varepsilon$.

Let

$$1:\ z = (\varepsilon - \mu)/k_B T \quad 2:\ \varepsilon = k_B T z + \mu \quad 3:\ \tau = k_B T \quad 4:\ d\varepsilon = k_B T dz$$

First

$$I = \int_0^{\mu} d\varepsilon f(\varepsilon) H(\varepsilon) + \int_{\mu}^{\infty} d\varepsilon \; f(\varepsilon) \; H(\varepsilon) \qquad \text{Note: } f(\mu) = 1/2$$

and now substitute
$$I = \underbrace{\int_{-\mu/\tau}^{0} \tau \frac{1}{e^z + 1} H(\mu + \tau z) dz}_{} + \int_0^{\infty} \tau \frac{dz}{e^z + 1} H(\mu + \tau z)$$

For the first term let $\quad z' = -z$ and $dz' = -dz$

$$I = -\int_{\mu/\tau}^{0} \tau \frac{dz'}{\exp(-z') + 1} H(\mu - \tau z') + \int_0^{\infty} \tau \frac{dz}{\exp(z) + 1} H(\mu + \tau z)$$

or inverting

$$I = \int_0^{\mu/\tau} (\quad \uparrow \quad) + \int_0^{\infty} (\quad \uparrow \quad)$$

but

$$\frac{1}{e^{-z'} + 1} = 1 - \frac{1}{e^{z'} + 1} = \frac{e^{z'} + 1 - 1}{e^{z'} + 1} = \frac{e^{z'}}{e^{z'} + 1}$$

So,

$$I = \tau \int_0^{\mu/\tau} H(\mu - \tau z') dz' - \int_0^{\mu/\tau} \tau \frac{H(\mu - \tau z')}{e^{z'} + 1} dz' + \int_0^{\infty} \frac{\tau H(\mu + \tau z)}{e^z + 1} dz$$

And $\mu/\tau >>> 1 \qquad \mu/\tau \approx \infty$

$$I = \tau \int_0^{\mu/\tau} H(\mu - \tau z') dz + \int_0^{\infty} \tau \frac{H(\mu + \tau z) - H(\mu - \tau z)}{e^z + 1} dz$$

$$z' = -z = (\mu - \varepsilon)/k_B T \qquad dz' = -d\varepsilon/\tau$$

$$\mu - \tau z' = \varepsilon$$

$$I = -\int_{\mu}^{0} H(\varepsilon) d\varepsilon \; + \; \int_0^{\infty} \tau \frac{H(\mu + \tau z) - H(\mu - \tau z)}{e^z + 1} dz$$

or finally

$$I = \int_0^{\mu} H(\varepsilon) d\varepsilon \; + \; \int_0^{\infty} \tau \frac{H(\mu + \tau z) - H(\mu - \tau z)}{e^z + 1} dz$$

(one approximation made so far)

If H(ε) is *slowly varying* around $\varepsilon = \mu$ (or $\tau z = 0$)
We can expand H($\mu \pm \tau z$) in a *TAYLOR SERIES*

$$H(\mu + \tau z) = H(\mu) + \frac{dH}{d(\tau z)}\Big|_{\tau z = 0} \tau z + H'' \frac{(z\tau)^2}{2} + ...$$

$$H(\mu - \tau z) = H(\mu) - \quad H' \qquad \tau z \; + H'' \frac{(z\tau)^2}{2} + ...$$

$\rightarrow$ <u>EVEN H terms cancel</u>

So

$$I = \int_0^{\mu} H(\varepsilon) d\varepsilon + 2H'(\mu)\tau^2 \int_0^{\infty} \frac{z dz}{e^z + 1} + \frac{2}{6} H'''(\mu) \tau^4 \int_0^{\infty} \frac{z^3 dz}{e^z + 1} + ...$$

$$\text{But} \quad \int_0^\infty \frac{z^{2n-1}dz}{e^z+1} = \frac{2^{2n-2}-1}{2^n}\pi^{2n}B_n$$

where B_n are the Bernoulli numbers

$$B_1 = \frac{1}{6} \quad B_2 = \frac{1}{30} \quad 1 - \frac{x}{2}\cot\frac{x}{2} = \frac{B_1 x^2}{2!} + \frac{B_2 x^4}{4!} + \frac{B_3 x^6}{6!} + ...$$

Thus

$$I = \int_0^\mu H(\varepsilon)d\varepsilon + \frac{\pi^2}{6}\tau^2 H'(\mu) + \frac{7\pi^4}{360}\tau^4 H'''(\mu) + ...$$

Now

$$H'(\mu) = \frac{dH(\mu \pm \tau z)}{d\tau \ z}|_{z\tau=0} = \frac{dH(\varepsilon)}{d\varepsilon}|_{\mu=\varepsilon} \quad \text{and so on.}$$

For the 3-D CASE:

$$\begin{aligned} H(\varepsilon) &= \mathcal{D}(\varepsilon) = \frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\varepsilon^{1/2} \qquad I \text{ now becomes } N \\ H'(\mu) &= \frac{V}{2\pi^2}(\frac{2m}{\hbar})^{3/2}\frac{1}{2}\mu^{-1/2} \end{aligned}$$

$$N = \int_0^\mu \mathcal{D}(\varepsilon)d\varepsilon + \frac{\pi^2}{6}\tau^2\frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\frac{1}{2}\mu^{-1/2}$$

We need to solve for $\mu(\tau)$, which is *NOT TRIVIAL*

$$\begin{aligned} \text{Let} \quad F(\mu) &\equiv \int_0^\mu \mathcal{D}(\varepsilon)d\varepsilon \quad \text{and} \quad \mu = \mu_F + \delta\mu \\ F(\mu_F + \delta\mu) &= F(\mu_F) + F'(\mu_F)\delta\mu \qquad F'(\mu_F) = \mathcal{D}(\mu_F) \\ &\text{Now} \quad F(\mu_F) = \int_0^{\mu_F} \mathcal{D}(\varepsilon)d\varepsilon = N \\ F(\mu_F + \delta\mu) &= N + F'(\mu_F)\delta\mu \qquad F'(\mu_F) \Rightarrow \mathcal{D}'(\mu) \approx \mathcal{D}'(\mu_F) \end{aligned}$$

$$\begin{aligned} N &= N + \delta\mu\ \mathcal{D}(\mu_F) + \frac{\pi^2}{6}\ \tau^2\ \mathcal{D}'(\mu_F) \\ 0 &= \delta\mu\ \mathcal{D}(\mu_F) + \frac{\pi^2}{6}\ \tau^2\ \mathcal{D}'(\mu_F) \\ \delta\mu &\approx -\frac{\pi^2}{6}\tau^2\mathcal{D}'(\mu_F)/\mathcal{D}(\mu_F) \\ \delta\mu &\approx -\frac{\pi^2}{6}\tau^2(\frac{1}{2}\frac{1}{\mu_F}) = -\frac{\pi^2}{12}\frac{\tau^2}{\mu_F} \end{aligned}$$

$$\boxed{\mu = \mu_F - \frac{\pi^2}{12}\frac{\tau^2}{\mu_F}}$$

Now we can solve for U, $H(\varepsilon) = \varepsilon\mathcal{D}(\varepsilon)$

$$\begin{aligned} U &= \int_0^\mu \varepsilon\mathcal{D}(\varepsilon)d\varepsilon + \frac{\pi^2}{6}\tau^2 H'(\mu) + \mathcal{O}(\tau^4) \\ U &= \frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\ \frac{2}{5}\ \mu(T)^{5/2} + \frac{3}{2}\tau^2\frac{\pi^2}{6}\frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2}\mu(T)^{1/2} + ... \end{aligned}$$

Substitute for $\mu(\tau)$ and turn the crank

$$
\begin{aligned}
U &= \frac{3}{5}N\varepsilon_F + \frac{2\pi^2}{12}\tau^2\mu_F^{1/2}\frac{V}{2\pi^2}(\frac{2m}{\hbar^2})^{3/2} \\
U &= \frac{3}{5}N\varepsilon_F + \frac{\pi^2}{4}N\tau^2/\varepsilon_F \\
C_V &= \frac{\pi^2}{2}k_B N\tau/\varepsilon_F + \mathcal{O}(\tau^3)
\end{aligned}
$$

If τ is small $C_{V_{\mathrm{electron}}} \propto \tau$!!! $(\tau = k_B T)$