Lecture 39: The Sommerfeld Expansion

Monday, April 27, 2020

At the end of the last class, we wanted to evaluate

$$I_N = \int \mathrm{d}\epsilon\, g(\epsilon)\mathcal{F}_+(\epsilon - \mu)$$

- The first assumption we will make is $\lim_{\epsilon \to -\infty} g(\epsilon) = 0$ so that there are no states below the ground state.
- The second we will make is that $g(\epsilon) \propto \epsilon^\alpha$ as $\epsilon \to \infty$.
- The third is that $g(\epsilon)$ is sufficiently smooth at $\epsilon = \epsilon_F$.
- Finally, we will define $G(\epsilon) = \int_{-\infty}^{\infty} \mathrm{d}\epsilon'\, g(\epsilon')$.

Now consider first for a fixed μ and $\tilde{f}(x) = \frac{1}{e^x + 1}$:

$$\begin{aligned}
I &= \int \mathrm{d}\epsilon\, G'(\epsilon)\tilde{\mathcal{F}}\left(\frac{\epsilon - \mu}{k_B T}\right) \\
&= -\int \mathrm{d}\epsilon\, G(\epsilon)\tilde{\mathcal{F}}'\left(\frac{\epsilon - \mu}{k_B T}\right)\frac{1}{k_B T} \\
&= -\,\mathrm{d}x \qquad \underbrace{G(\mu + k_B T x)}_{G(\mu) + x k_B T G'(\mu) + \frac{1}{2}(x k_B T)^2 G''(\mu)} \qquad \tilde{\mathcal{F}}'(x) \qquad x \equiv \frac{\epsilon - \mu}{k_B T} \\
&= -G(\mu)\int \underbrace{\mathrm{d}x\, \tilde{\mathcal{F}}'(x)}_{-1} - k_B T G'(\mu)\int \underbrace{\mathrm{d}x\, x\tilde{\mathcal{F}}'(x)}_{0} - \frac{1}{2}(k_B T)^2 G''(\mu)\underbrace{\int \mathrm{d}x\, x^2 \tilde{\mathcal{F}}'(x)}_{-\pi^2/3} + \dots \\
&= G(\mu) + \frac{\pi^2}{6}(k_B T)^2 G''(\mu) + \mathcal{O}\big(T^4\big)
\end{aligned}$$

We can think of this as a low-T expansion of the FD-distribution at fixed μ:

$$\mathcal{F}_+(\epsilon - \mu) = \Theta(\mu - \epsilon) - \frac{\pi^2}{6}(k_B T)^2 \delta'(\epsilon - \mu) + \mathcal{O}\big(T^4\big)$$

Let's apply this. Suppose $W(\epsilon) = \int_{-\infty}^{\epsilon} \mathrm{d}\epsilon'\, D(\epsilon')$:

$$N = \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, D(\epsilon)\mathcal{F}_+(\epsilon - \mu) = W(\mu) + \frac{\pi^2}{6}(k_B T)^2 W''(\mu) + \mathcal{O}\big(T^4\big)$$

Now we "just" need to solve this for $\mu(N)$. This is terribly hard, but here's a nice solution. We are going to write μ as a series expansion in $k_B T$, insert this into the right-hand side, and then expand again for small $k_B T$! Finally, we compare coefficients of $(k_B T)^n$.

$$\mu = \epsilon_F + \mu_1 k_B T + \mu_2 (k_B T)^2 + \cdots$$

$$\begin{aligned}
N &= W(\epsilon_F + \mu_1 k_B T + \mu_2 (k_B T)^2 + \dots) + \frac{\pi^2}{6}(k_B T)^2 W''(\epsilon_F + \mu_1 k_B T + \mu_2 (k_B T)^2 + \dots) + \dots \\
&= W(\epsilon_F) + W'(\epsilon_F)\left(\mu_1 k_B T + \mu_2 (k_B T)^2 + \dots\right) + \frac{1}{2}W''(\epsilon_F)\left(\mu_1 k_B T + \mu_2 (k_B T)^2 + \dots\right)^2 + \dots \\
&+ \frac{\pi^2}{6}(k_B T)^2\left[W''(\epsilon_F) + W'''(\epsilon_F)\left(\mu_1 k_B T + \mu_2 (k_B T)^2 + \dots\right) + \dots\right] \\
&= \underbrace{W(\epsilon_F)}_{N} + k_B T\underbrace{\left[W'(\epsilon_F)\mu_1\right]}_{\mu_1 = 0} + (k_B T)^2\underbrace{\left[W'(\epsilon_F)\mu_2 + \frac{1}{2}W''(\epsilon_F)\mu_1^2 + \frac{\pi^2}{6}W''(\epsilon_F)\right]}_{\mu_2 = -\frac{\pi^2}{6}\frac{W''(\epsilon_F)}{W'(\epsilon_F)} = -\frac{\pi^2}{6}\frac{D'(\epsilon_F)}{D(\epsilon_F)}} + \dots
\end{aligned}$$

$$\implies \mu(T, N) = \epsilon_F - \frac{\pi^2}{6}(k_B T^2)\frac{D'(\epsilon_F)}{D(\epsilon_F)} + \dots$$

We can insist this is our expression for $\mathcal{F}_+(\epsilon-\mu)$:

$$
\begin{aligned}
\mathcal{F}_+(\epsilon-\mu) &= \Theta\left(\epsilon_F - \frac{\pi^2}{6}(k_BT)^2\frac{D'}{D} + \cdots - \epsilon\right) - \frac{\pi^2}{6}(k_BT)^2\delta'\left(\epsilon - \epsilon_F + \frac{\pi^2}{6}(k_BT)^2\frac{D'}{D} + \cdots\right) + \mathcal{O}(T^4) \\
&= \Theta(\epsilon_F) + \Theta'(\epsilon_F)\left(-\frac{\pi^2}{6}(k_BT)^2\frac{D'}{D} + \dots\right) + \dots - \frac{\pi^2}{6}(k_BT)^2(\epsilon-\epsilon_F) + \dots \\
&= \Theta(\epsilon_F - \mu) - \frac{\pi^2}{6}(k_BT)^2\left[\frac{D'(\epsilon_F)}{D(\epsilon_F)}\delta(\epsilon-\epsilon_F) + \delta'(\epsilon-\epsilon_F)\right] + \dots
\end{aligned}
$$

We can use this expansion in our potential expression:

$$
\begin{aligned}
\Omega(T,\mu) &= -\int \mathrm{d}\epsilon\, W(\epsilon\mathcal{F}_+(\epsilon-\mu)) \\
&= -\int_{-\infty}^{\mu}\mathrm{d}\epsilon'\, W(\epsilon') - \frac{\pi^2}{6}(k_BT)^2 D(\mu) + \mathcal{O}(T^4)
\end{aligned}
$$

$$
\begin{aligned}
F(T,N) &= \max_\mu\{\Omega(T,\mu) - \mu N\} = \Omega(T,\mu(T,N)) \\
&= -\int_{-\infty}^{\mu}\mathrm{d}\epsilon'\, W(\epsilon') - \frac{\pi^2}{6}(k_BT)^2 D(\mu) + N\mu \\
&= -\int_{-\infty}^{\epsilon_F - \frac{\pi^2}{6}(k_BT)^2\frac{D'}{D}\cdots}\mathrm{d}\epsilon\, W(\epsilon) - \frac{\pi^2}{6}(k_BT)^2 D(\epsilon_F) + N\left(\epsilon_F - \frac{\pi^2}{6}(k_BT)^2\frac{D'}{D}\dots\right)\dots \\
&= -\int_{-\infty}^{\epsilon_F}\mathrm{d}\epsilon\, W(\epsilon) - \left(-\frac{\pi^2}{6}(k_BT)^2\frac{D'}{D}\right)W(\epsilon_F) - \frac{\pi^2}{6}(k_BT)^2 D(\epsilon_F) - N\epsilon_F - \frac{\pi^2}{6}(k_BT)^2\frac{D'}{D}N + \dots \\
&= -\int_{-\infty}^{\epsilon_F}\mathrm{d}\epsilon\int_{-\infty}^{\epsilon}\mathrm{d}\epsilon'\, D(\epsilon') - \frac{\pi^2}{6}(k_BT)^2 D(\epsilon_F) + N\epsilon_F + \dots \\
&= -\int_{-\infty}^{\epsilon_F}\mathrm{d}\epsilon'\int_{\epsilon'}^{\epsilon_F} D(\epsilon') + (\text{the other terms}) \\
&= -\int_{-\infty}^{\epsilon_F}\mathrm{d}\epsilon'\, D(\epsilon')(\epsilon_F - \epsilon') + (\text{the other terms}) \\
&= -\epsilon_F N + U_0 + (\text{the other terms})
\end{aligned}
$$

so

$$
\begin{gathered}
F(T,N) = U_0 - \frac{\pi^2}{6}(k_BT)^2 D(\epsilon_F) + \mathcal{O}(T^4) \\
S(T,N) = -\frac{\partial F(T,N)}{\partial T} = \frac{\pi^2}{3}k_B^2 T D(\epsilon_F) + \mathcal{O}(T^3) \\
U(T,N) = F(T,N) + TS(T,N) = U_0 + \frac{\pi^2}{6}(k_BT)^2 D(\epsilon_F) + \mathcal{O}(T^4) \\
c_V(T,N) = \frac{\partial U}{\partial T} = \frac{\pi^2}{3}k_B^2 T D(\epsilon_F) + \mathcal{O}(T^3)
\end{gathered}
$$

This is linear in T!