

Homework 2

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September 30, 2023

1. (a) First, we know that:

$$z(\varepsilon) = e^{-\frac{\varepsilon}{\tau}}$$

Plugging in the respective values of $\varepsilon = 0$ and $\varepsilon = \varepsilon_o$:

$$z = z(0) + z(\varepsilon_o) = 1 + e^{-\frac{\varepsilon_o}{\tau}}$$

Free energy can also be expressed in terms of z :

$$F = -\tau \ln(z) \rightarrow -\tau \ln\left(1 + e^{-\frac{\varepsilon_o}{\tau}}\right)$$

- (b) We know the energy may be expressed as:

$$\begin{aligned} U &= -\tau^2 \frac{\partial}{\partial \tau} \left(\frac{F}{\tau} \right) \\ &= \tau^2 \frac{\partial}{\partial \tau} \left(\ln \left(1 + e^{-\frac{\varepsilon_o}{\tau}} \right) \right) \\ &= \tau^2 \left(\frac{ae^{-\frac{\varepsilon_o}{\tau}}}{\tau^2 \left(1 + e^{-\frac{\varepsilon_o}{\tau}} \right)} \right) \\ &= \frac{\varepsilon_o e^{-\frac{\varepsilon_o}{\tau}}}{\left(1 + e^{-\frac{\varepsilon_o}{\tau}} \right)} \end{aligned}$$

Furthermore, entropy may be expressed as:

$$\begin{aligned} \sigma &= -\frac{\partial F}{\partial \tau} \\ &= \frac{\partial}{\partial \tau} \left(\tau \ln \left(1 + e^{-\frac{\varepsilon_o}{\tau}} \right) \right) \\ &= \ln \left(1 + e^{-\frac{\varepsilon_o}{\tau}} \right) + \frac{\varepsilon_o e^{-\frac{\varepsilon_o}{\tau}}}{\tau \left(1 + e^{-\frac{\varepsilon_o}{\tau}} \right)} \end{aligned}$$

2. (a)
- (b)
- (c)
3. (a) We want to find the free energy over all values of s . Thus, we set up a sum:

$$z = \sum_0^{\infty} e^{-\frac{s\hbar\omega}{\tau}}$$

We can find by reversing the expansion:

$$\sum_0^{\infty} e^{-\frac{s\hbar\omega}{\tau}} = \frac{1}{1 - e^{-\frac{\hbar\omega}{\tau}}}$$

Using the formula for free energy, we obtain:

$$F = -\tau \ln(z) = \tau \ln\left(1 - e^{-\frac{\hbar\omega}{\tau}}\right)$$

- (b) We know the following:

$$\sigma = -\frac{\partial F}{\partial \tau}$$

Taking the partial derivative with respect to τ , we find:

$$\begin{aligned} -\frac{\partial F}{\partial \tau} &= -\frac{\partial}{\partial \tau} \left(\tau \ln\left(1 - e^{-\frac{\hbar\omega}{\tau}}\right) \right) \Rightarrow \\ &= -\left(\ln\left(1 - e^{-\frac{\hbar\omega}{\tau}}\right) + \tau \frac{\partial}{\partial \tau} \left[\ln\left(1 - e^{-\frac{\hbar\omega}{\tau}}\right) \right] \right) = -\ln\left(1 - e^{-\frac{\hbar\omega}{\tau}}\right) - \tau \left[-\frac{\hbar\omega e^{-\frac{\hbar\omega}{\tau}}}{\tau^2 \left(1 - e^{-\frac{\hbar\omega}{\tau}}\right)} \right] \Rightarrow \\ &\sigma = \frac{\hbar\omega}{\tau \left(e^{\frac{\hbar\omega}{\tau}} + 1\right)} - \ln\left(1 - e^{-\frac{\hbar\omega}{\tau}}\right) \end{aligned}$$

- 4.
- 5.
6. From quantum mechanics, we know the energy of such a particle, with a single n (because it is unidimensional), may be expressed as:

$$\varepsilon = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

Thus, we know:

$$z = \sum_{n=1}^{\infty} e^{-\frac{\varepsilon}{\tau}}$$

If we define some value $x = \frac{\hbar\pi}{L\sqrt{2m\tau}}$, we can write this as a Gaussian integral:

$$z = \int_0^{\infty} e^{-x^2 n^2} dn = \frac{\sqrt{\pi}}{2x}$$

Using the formula for free energy, we can find:

$$-\tau \ln(z) \rightarrow N\tau \ln\left(\frac{2x}{\sqrt{\pi}}\right) = N\tau \ln\left(\frac{2\hbar\pi}{L\sqrt{2m\tau\pi}}\right)$$

To simplify our calculations, we can take out the square root:

$$N\tau \ln\left(\frac{2\hbar\pi}{L\sqrt{2m\tau\pi}}\right) = \frac{1}{2}N\tau \ln\left(\frac{2\hbar^2\pi}{L^2m\tau}\right)$$

Now we take the partial derivative with respect to τ to find the entropy, using $y = \frac{2\hbar^2\pi}{L^2m}$ to simplify:

$$\begin{aligned} \sigma &= -\frac{\partial}{\partial\tau} \left(\frac{1}{2}N\tau \ln\left(\frac{y}{\tau}\right) \right) \\ -\frac{N}{2} \ln\left(\frac{y}{\tau}\right) - \frac{N\tau}{2} \frac{\partial}{\partial\tau} \left[\ln\left(\frac{y}{\tau}\right) \right] &= -\frac{N}{2} \ln\left(\frac{y}{\tau}\right) - \frac{N\tau^2}{2y} \frac{\partial}{\partial\tau} \left[\frac{y}{\tau} \right] \\ -\frac{N}{2} \ln\left(\frac{y}{\tau}\right) - \frac{N\tau^2}{2y} \left(-\frac{y}{\tau^2} \right) &= \frac{N}{2} \left(1 - \ln\left(\frac{y}{\tau}\right) \right) \\ \sigma &= \frac{N}{2} \left(1 - \ln\left(\frac{2\hbar^2\pi}{L^2m\tau}\right) \right) \end{aligned}$$