Homework 2

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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:

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

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

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

Furthermore, entropy may be expressed as:

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

2. (a) We need to calculate the multiplicity of the N-spin system. First and foremost, we know:

$$U = -2msB$$

We also know the N-spin system can be rewritten using:

$$2s = N_\uparrow - N_\downarrow = N_\uparrow - (N - N_\uparrow) = 2N_\uparrow - N$$

This yields:

$$U = (N - 2N_\uparrow)mB$$

We then need to form a sum to find the partition function. We can do this by knowing the boundaries of s:

$$-\frac{N}{2} \leq s \leq \frac{N}{2}$$

$$\sum_{s=-\frac{N}{2}}^{\frac{N}{2}}$$

We need to multiply the exponential term by N choose $N_\uparrow$:

$$\sum_{s=-\frac{N}{2}}^{\frac{N}{2}} \binom{N}{N_\uparrow} e^{\frac{2smB}{\tau}}$$

Since we know s can be expressed as $N_\uparrow - \frac{N}{2}$, $N_\uparrow$ can be expressed as $s + \frac{N}{2}$; furthermore, $N_\downarrow$ can be expressed as $\frac{N}{2} - s$, which gives us:

$$z = \sum_{s=-\frac{N}{2}}^{\frac{N}{2}} \frac{N!}{(\frac{N}{2}+s)!(\frac{N}{2}-s)!} e^{\frac{2smB}{\tau}}$$

To simplify, we can shift the boundaries by taking $s \to s - \frac{N}{2}$

$$z = \sum_{s=0}^{N} \frac{N!}{s!(N-s)!} e^{\frac{2mB}{\tau}\left(s-\frac{N}{2}\right)}$$

$$z = \sum_{s=0}^{N} \frac{N!}{s!(N-s)!} e^{\frac{2smB}{\tau} - \frac{NmB}{\tau}}$$

We then use $\sum_j^N \binom{N}{j} x^j = (1+x)^N$, dropping $s = 0$ because the term is extremely small:

$$e^{-\frac{NmB}{\tau}}(1+e^{\frac{2mB}{\tau}})^N = (e^{-\frac{mB}{\tau}}+e^{\frac{mB}{\tau}})^N = 2^N \cosh^N\left(\frac{mB}{\tau}\right)$$

We then differentiate z with respect to τ to get:

$$\frac{\partial z}{\partial \tau} = N2^N \cosh^{N-1}\left(\frac{mB}{\tau}\right)\left(-\frac{mB}{\tau^2}\right)\sinh\left(\frac{mB}{\tau}\right)$$

We can then express M as:

$$M = -\tau^2 \frac{\partial}{\partial \tau}\left(\ln(z)\right) \to Nm \tanh\left(\frac{mB}{\tau}\right)$$

And finally:

$$\boxed{\chi = \frac{\partial M}{\partial B} = \frac{Nm^2}{\tau}\operatorname{sech}^2\left(\frac{mB}{\tau}\right)}$$

(b) We know we can write the free energy as:

$$F = -\tau\ln(z) = -\tau\ln\left(2^N\cosh^N\left(\frac{mB}{\tau}\right)\right) = -N\tau\ln\left(2\cosh\left(\frac{mB}{\tau}\right)\right)$$

This can be rewritten as:

$$F = -N\tau\ln\left(\frac{2}{\operatorname{sech}\left(\frac{mB}{\tau}\right)}\right)$$

We know $\operatorname{sech}(t) = \sqrt{1-\tanh^2(t)}$, and, applying $x \to \frac{M}{Nm}$ we get $x = \tanh(t)$. Thus, we can write:

$$F = -N\tau\ln\left(\frac{2}{\sqrt{1-x^2}}\right)$$

Distributing the negative, we finally get:

$$\boxed{F = N\tau\ln\left(\frac{\sqrt{1-x^2}}{2}\right)}$$

(c) As $mB << \tau$, the term inside the sech^2 expression approaches zero. Thus, we can say:

$$\chi = \frac{Nm^2}{\tau}\operatorname{sech}^2(0)$$

We know, at zero $\operatorname{sech}(0) = 1$, so we can write:

$$\boxed{\chi = \frac{Nm^2}{\tau}}$$

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:

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

(b) We know the following:

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

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

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

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

$$\boxed{\sigma = \frac{\hbar\omega}{\tau\left(e^{\frac{\hbar\omega}{\tau}} + 1\right)} - \ln\left(1 - e^{-\frac{\hbar\omega}{\tau}}\right)}$$

4. First, let us define a variable related to τ to simplify calculations:

$$\alpha = \frac{1}{\tau}$$

Using the chain rule, this defines the partial with respect to τ as:

$$\frac{\partial}{\partial \tau} = \frac{\partial \alpha}{\partial \tau}\frac{\partial}{\partial \alpha} = -\frac{1}{\tau^2}\frac{\partial}{\partial \alpha}$$

We can then express the partition function and its differentials as:

$$z = \sum_{s}\left(e^{-\alpha\varepsilon_s}\right)$$

$$\frac{\partial}{\partial \alpha} z = \sum_{s}\left(-\varepsilon_s e^{-\alpha\varepsilon_s}\right)$$

$$\frac{\partial^2}{\partial \alpha^2} z = \sum_s \left(\varepsilon_s^2 e^{-\alpha \varepsilon_s} \right)$$

We then express the energy as:

$$U = -\frac{\partial}{\partial \alpha} \ln(z)$$

Which then becomes:

$$\frac{\partial U}{\partial \tau} = \frac{\partial \alpha}{\partial \tau} \frac{\partial U}{\partial \alpha} = -\frac{1}{\tau^2} \frac{\partial U}{\partial \alpha}$$

We then insert the expression for U:

$$\frac{1}{\tau^2} \left(\frac{\partial}{\partial \alpha} \left(\frac{\frac{\partial}{\partial \alpha} z}{z} \right) \right) = \frac{1}{\tau^2} \left(\frac{\frac{\partial^2 z}{\partial \alpha^2} z - \left(\frac{\partial z}{\partial \alpha} \right)^2}{z^2} \right) = \frac{1}{\tau^2} \left(\frac{\frac{\partial^2 z}{\partial \alpha^2}}{z} - \frac{\left(\frac{\partial z}{\partial \alpha} \right)^2}{z^2} \right)$$

Thus, we see that:

$$\langle \varepsilon^2 \rangle = \frac{\frac{\partial^2 z}{\partial \alpha^2}}{z} \quad \text{and} \quad \langle \varepsilon \rangle^2 = \frac{\left(\frac{\partial z}{\partial \alpha} \right)^2}{z}$$

Which gives us:

$$\frac{\partial U}{\partial \tau} = \frac{1}{\tau^2} \left(\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2 \right)$$

And finally:

$$\boxed{\tau^2 \frac{\partial U}{\partial \tau} = \left(\langle \varepsilon^2 \rangle - \langle \varepsilon \rangle^2 \right)}$$

8. First and foremost, for the ground orbital, we know $n_x, n_y, n_z = 1$. We must then check ψ for normalization:

$$\int_0^L \sin^2 \left(\frac{n_x \pi x}{L} \right) dn_x = \left(n_x - \frac{n_x}{2} - \frac{L}{4\pi x} \sin \left(\frac{2 n_x \pi x}{L} \right) \right) \Big|_0^L$$

Evaluating the integral, we are left with:

$$\left(L - \frac{L}{2} - 0 - (0 - 0 - 0) \right) = \frac{L}{2}$$

Which gives us:

$$\langle\psi|\psi\rangle = A^2 = \frac{8}{L^3}$$

Then solving, we can apply the formula for kinetic energy in terms of momentum:

$$\frac{p^2}{2m} = \frac{3\pi^2}{2mL^2}$$

Since we know $n = \frac{1}{L^3}$, we can rewrite this as:

$$\frac{3\pi^2}{2m}n^{\frac{2}{3}} = T \rightarrow n^{\frac{2}{3}} = \frac{2mT}{3\pi^2}$$

Then we are left with:

$$n = \left(\frac{2mT}{3\pi^2}\right)^{\frac{3}{2}}$$

We then substitute $T = \frac{\tau}{\hbar^2}$ to get:

$$n = \left(\frac{2m\tau}{3\pi^2\hbar^2}\right)^{\frac{3}{2}}$$

We know that the quantum concentration may be written as $n_Q = \left(\frac{m\tau}{2\pi\hbar^2}\right)^{\frac{3}{2}}$, thus n is a factor multiple of n_Q, so we can use:

$$\frac{n}{n_Q} = \left(\frac{4}{3\pi}\right)^{\frac{3}{2}}$$

And finally, we can confirm n_0, by expressing this as:

$$\boxed{n = \left(\frac{4}{3\pi}\right)^{\frac{3}{2}} n_Q}$$

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

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

Thus, we know:

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

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

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

Using the formula for free energy, we can find:

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

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 $y = \dfrac{2\hbar^2\pi}{L^2m}$ to simplify:

$$\sigma = -\frac{\partial}{\partial\tau}\left(\frac{1}{2}N\tau \ln\left(\frac{y}{\tau}\right)\right)$$

$$-\frac{N}{2}\ln\left(\frac{y}{\tau}\right) - \frac{N\tau}{2}\frac{\partial}{\partial\tau}\left[\ln\left(\frac{y}{\tau}\right)\right] = -\frac{N}{2}\ln\left(\frac{y}{\tau}\right) - \frac{N\tau^2}{2y}\frac{\partial}{\partial\tau}\left[\frac{y}{\tau}\right]$$

$$-\frac{N}{2}\ln\left(\frac{y}{\tau}\right) - \frac{N\tau^2}{2y}\left(-\frac{y}{\tau^2}\right) = \frac{N}{2}\left(1 - \ln\left(\frac{y}{\tau}\right)\right)$$

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