SIGNATURE ____________________ NAME ______________________

Student ID # ____________________

Physics 404
Spring 2011
Prof. Anlage
First Mid-Term Exam
10 March, 2011
CLOSED BOOK, NO Calculator Permitted, CLOSED NOTES

Point totals are given for each part of the question.

If you run out of room, continue writing on the back of the same page. If you do so, make a note on the front part of the page!
Note: You must solve the problem following the instructions given in the problem. Correct answers alone will not receive full credit.

Partial Credit:

→ Show Your Work! Answers written with no explanation will not receive full credit.

→ You can receive credit for describing the method you would use to solve a problem, even if you missed an earlier part.

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Problem	Credit	Max. Credit
1		25
2		25
3		25
4		25
TOTAL		100

$$\int_{-\infty}^{+\infty} \exp(-x^2)dx = \pi^{1/2} \qquad \int_{-\infty}^{+\infty} x^2 \exp(-x^2)dx = \frac{\pi^{1/2}}{2} \qquad n! \cong (2\pi n)^{1/2} n^n \exp\left[-n + \frac{1}{12n}\right] \qquad \frac{1}{1-x} = \sum_{n=0}^{\infty} x^n$$

$$F = -\tau \log(Z) = U - \tau\sigma \qquad dU(\sigma, V) = \tau d\sigma - PdV \qquad dF(\tau, V) = -\sigma d\tau - PdV$$

$$Z = \sum_s Exp[-\varepsilon_s/\tau] \qquad \frac{1}{\tau} = \partial\sigma/\partial U|_{V,N} \qquad C_V = \frac{\partial U}{\partial \tau}|_V \qquad \langle N \rangle = \sum_s f(\varepsilon_s)$$

$$d(XY) = X\,dY + Y\,dX \quad \log(AB) = \log(A) + \log(B) \quad \log(A+B) \neq \log(A) + \log(B)$$

$$g(N, s) = \frac{N!}{\left(\frac{N}{2}+s\right)!\left(\frac{N}{2}-s\right)!} \cong \sqrt{\frac{2}{\pi N}}\, 2^N\, e^{-2s^2/N} \qquad g(s) = \sum_s g_1(s_1) g_2(s - s_1)$$

$$P(\varepsilon_s) = \text{Exp}\left(-\frac{\varepsilon_s}{\tau}\right)/Z \qquad \langle X \rangle = \sum_s X(s)P(s) \qquad p = -\left(\frac{\partial U}{\partial V}\right)|_\sigma = \tau\left(\frac{\partial \sigma}{\partial V}\right)|_U = -\left(\frac{\partial F}{\partial V}\right)|_\tau$$

1. **a.)** Explain clearly the differences between the microcanonical and canonical ensembles of statistical mechanics. Give your answer as a legible, grammatically-correct paragraph or two, carefully defining any terms that you use in the paragraph or in any equations that you write. *(5 points)*

b.) For the microcanonical and canonical ensembles, what is the probability that the system will be in a particular quantum state s? *(5 points)*

c.) A closed system has an internal insulating wall that divides the system in half. If the wall is removed, what are the possible consequences, in terms of the total entropy of the system? *(5 points)*

d.) Consider two systems, one initially at a higher temperature than the other. Show that energy cannot spontaneously flow from a low-temperature system to a high-temperature system. Hint: write $\Delta\sigma$ in terms of $(\partial\sigma/\partial U)|_{N,V}\,\Delta U$, etc. *(10 points)*

a.) The microcanonical ensemble applies to a closed system. Such a system has a fixed energy U. The fundamental assumption of statistical mechanics is that all accessible states of such a system are equally likely to be occupied. Multiplicty is the number of states with distinct lists of quantum numbers that have the same energy. The entropy is the logarithm of the multiplicity. In practice one state, and a small number of similar states, is far more likely (has the highest multiplicity) than all the rest. The macroscopic properties of the system are dominated by those states. Whenever a constraint internal to the system is relaxed, the entropy of the system will either stay the same or increase. The temperature of the system is given by the energy derivative of the entropy of the system: $\frac{1}{\tau} = \partial\sigma/\partial U|_{V,N}$.

The canonical ensemble applies to a system that is in thermal equilibrium with a far larger reservoir at temperature τ. The system is able to exchange energy with the reservoir and explore many possible states with different energy ε_s. Hence the energy of the system is not fixed. The probability of occupation of that state is not a constant, but given by its Boltzmann factor divided by the partition function: $P(\varepsilon_s) = \mathrm{Exp}\left(-\frac{\varepsilon_s}{\tau}\right)/Z$, where the partition function is $Z = \sum_s Exp[-\varepsilon_s/\tau]$.

b.) In the microcanonical ensemble the probability of occupation of any accessible state is equal to a constant, which is the reciprocal of the total number of accessible states. For the canonical ensemble the probability of occupation of that state is not a constant, but given by its Boltzmann factor divided by the partition function: $P(\varepsilon_s) = \mathrm{Exp}\left(-\frac{\varepsilon_s}{\tau}\right)/Z$, where the partition function is $Z = \sum_s Exp[-\varepsilon_s/\tau]$.

c.) Whenever a constraint internal to the system is released, the entropy of the system will either stay the same or go up. When a constraint is lifted, the system is able to explore new states, increasing the multiplicity and therefore the entropy (which is the logarithm of the multiplicity).

d.) Suppose energy ΔU is transferred from the hot system to the cold system. The change of entropy of the entire system is $\Delta\sigma = \left(\frac{\partial\sigma_1}{\partial U_1}\right)_{N_1}(-\Delta U) + \left(\frac{\partial\sigma_2}{\partial U_2}\right)_{N_2}(\Delta U)$, where the first term is the entropy given up from the system 1 (the hot system), and the second term is the increase in entropy of system 2 (the cold system). The pre-factors are in fact the temperatures of each system: $\Delta\sigma = \left(-\frac{1}{\tau_1} + \frac{1}{\tau_2}\right)\Delta U$. Since $\tau_1 > \tau_2$ the term in parentheses is positive and the change in entropy is positive. If the energy flowed from the cold object to the warm object, the change in entropy would be negative, violating the second law of thermodynamics.

2. Consider a system consisting of N constituent particles, each of which can occupy four spin-3/2 quantum states, with energies: $E_1 = -\frac{3}{2}\varepsilon$, $E_2 = -\frac{1}{2}\varepsilon$, $E_3 = +\frac{1}{2}\varepsilon$, $E_4 = +\frac{3}{2}\varepsilon$, and multiplicities 1, 3, 3, and 1, respectively. The system is in thermal equilibrium with a reservoir at temperature τ.

a.) Calculate the partition function Z_N of the N-particle system assuming that the particles are distinguishable. *Hint: the one-particle partition function Z_1 can be written as the cube of a simple function. (10 points)*

b.) Calculate the Helmholtz free energy F of the system *(5 points)*

c.) Calculate the entropy σ of the system *(5 points)*

d.) Calculate the energy U of the system *(5 points)*

a) Start with the 1-particle partition function $Z_1 = \sum_s e^{-\varepsilon_s/\tau} = \sum_i g(E_i)\, e^{-E_i/\tau}$

$$Z_1 = 1e^{-3\varepsilon/2\tau} + 3e^{-\varepsilon/2\tau} + 3e^{\varepsilon/2\tau} + 1e^{3\varepsilon/2\tau}$$

$$= \left(e^{-\varepsilon/2\tau} + e^{\varepsilon/2\tau}\right)^3 \quad \text{following the hint}$$

$g(E_i)$	E_i
1	$3\varepsilon/2$
3	$\varepsilon/2$
3	$-\varepsilon/2$
1	$-3\varepsilon/2$

$$Z_1 = \left(2\cosh\left(\tfrac{\varepsilon}{2\tau}\right)\right)^3$$

Now use the fact that the particles are distinguishable, so $Z_N = Z_1^N$

$$Z_N = \left(2\cosh\left(\tfrac{\varepsilon}{2\tau}\right)\right)^{3N}$$

b) The Helmholtz free energy $F = -\tau \log Z_N = -\tau \log Z_1^N = -N\tau \log Z_1$

$$F = -3N\tau \log\left(2\cosh\left(\tfrac{\varepsilon}{2\tau}\right)\right)$$

c) The entropy can be derived from the temperature derivative of the Helmholtz free energy $\sigma = -\partial F/\partial\tau|_V$

$$\sigma = -\frac{\partial F}{\partial \tau}\Big|_V = 3N\log\left(2\cosh\left(\tfrac{\varepsilon}{2\tau}\right)\right) + 3N\tau\,\frac{2\left(\frac{-\varepsilon}{2\tau^2}\right)\sinh\left(\frac{\varepsilon}{2\tau}\right)}{2\cosh\left(\frac{\varepsilon}{2\tau}\right)}$$

$$= 3N\log\left(2\cosh\left(\tfrac{\varepsilon}{2\tau}\right)\right) - \frac{3N\varepsilon}{2\tau}\tanh\left(\tfrac{\varepsilon}{2\tau}\right)$$

d) The energy can be found from the Helmholtz free energy and the entropy:

$$U = F + \tau\sigma$$

$$= \cancel{-3N\tau\log\left(2\cosh\left(\tfrac{\varepsilon}{2\tau}\right)\right)} + \cancel{3N\tau\log\left(2\cosh\left(\tfrac{\varepsilon}{2\tau}\right)\right)} - \frac{3N\varepsilon}{2}\tanh\left(\tfrac{\varepsilon}{2\tau}\right)$$

$$= -\frac{3N\varepsilon}{2}\tanh\left(\tfrac{\varepsilon}{2\tau}\right)$$

3. Consider the following descriptions of a thermodynamic system.

a.) The multiplicity of a system with energy U occupying volume V is given by $g(U,V) = \alpha\, Exp[\beta\sqrt{UV}]$, where α and β are constants. Determine the entropy as a function of temperature τ, volume V, and the constants α and β. *Hint: make sure you write the entropy in terms of the quantities requested! (5 points)*

b.) The entropy of a system, consisting of N particles within a volume V having internal energy U, is given by $\sigma(N,U,V) = \gamma - \delta\frac{N^2V^2}{U^3}$, where γ and δ are constants. Derive the expression for energy U as a function of temperature τ, volume V, number of particles N, and the constants γ and δ. *(10 points)*

c.) The partition function of a system is given by $Z = (Exp[\beta\tau^3 V])^N$, where β is a constant. Calculate the pressure p, the entropy σ, and the internal energy U of the system. *(10 points)*

a) Multiplicity $g(u,v) = \alpha e^{\beta\sqrt{uv}}$. The entropy is $\sigma(u,v) = \log(g(u,v))$

$\sigma = \log(\alpha e^{\beta\sqrt{uv}}) = \log(\alpha) + \beta\sqrt{uv}$. But we want $\sigma(\tau, v)$, so find τ

$\frac{1}{\tau} = \frac{\partial\sigma}{\partial u}\Big|_v = \frac{\beta}{2}\sqrt{\frac{v}{u}}$. Solving for u yields $u = V\left(\frac{\tau\beta}{2}\right)^2$. The entropy now becomes $\sigma(\tau, V) = \log(\alpha) + \beta^2\tau V/2$

b) Entropy $\sigma(N,U,V) = \gamma - \delta\frac{N^2V^2}{U^3}$. The temperature is given by $\frac{1}{\tau} = \frac{\partial\sigma}{\partial u}\Big|_v$

or $\frac{1}{\tau} = 3\delta\frac{N^2v^2}{u^4}$. Solving for energy u yields $U = (3\delta N^2 v^2 \tau)^{1/4}$

c) The partition function is $Z = (e^{\beta\tau^3 v})^N$. The Helmholtz free energy is $F = -\tau\log Z = -N\tau\log(e^{\beta\tau^3 v}) = -N\beta\tau^4 V$

The entropy is $\sigma = -\partial F/\partial\tau\big|_{v,N} = 4N\beta\tau^3 V$

The pressure is $p = -\partial F/\partial V\big|_\tau = N\beta\tau^4$

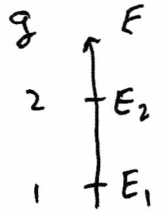
The energy U is given by $U = F + \tau\sigma$

$$U = -N\beta\tau^4 V + 4N\beta\tau^4 V$$
$$= 3N\beta\tau^4 V$$

4. Consider a system with only two accessible energy levels E_1 and E_2 in thermal equilibrium with a reservoir at temperature τ. The lower level (E_1) is nondegenerate, while the upper level (E_2) is twofold degenerate.

a.) Determine the probability that the lower level is occupied. *(5 points)*

b.) Find the thermal average energy $U = \langle \varepsilon \rangle$ of this system. *(5 points)*



c.) Consider the very high temperature limit $\tau \gg E_1, E_2$. Find the probability that the lower level is occupied and the thermal average energy in this limit. *(5 points)*

d.) Starting with the definition of the partition function, derive the general result for the thermal average energy $U = \langle \varepsilon \rangle$,

$$<\varepsilon>= \tau^2 \frac{\partial}{\partial \tau} \log(Z) \qquad \textit{(10 points)}$$

a) First calculate the partition function $Z = \sum_s e^{-\varepsilon_s/\tau} = e^{-E_1/\tau} + 2e^{-E_2/\tau}$

The probability of being in the lower state is given by the normalized Boltzmann factor $\quad P(1) = \dfrac{e^{-E_1/\tau}}{Z} = \dfrac{e^{-E_1/\tau}}{e^{-E_1/\tau} + 2e^{-E_2/\tau}}$

b) The thermal average energy is given by $\langle \varepsilon \rangle = \sum_s \varepsilon_s \dfrac{e^{-\varepsilon_s/\tau}}{Z}$

$$\langle \varepsilon \rangle = \frac{1}{Z}\left(E_1 e^{-E_1/\tau} + 2E_2 e^{-E_2/\tau} \right)$$

$$= \frac{E_1 e^{-E_1/\tau} + 2E_2 e^{-E_2/\tau}}{e^{-E_1/\tau} + 2e^{-E_2/\tau}}$$

c) In the high temperature limit $\tau \gg E_1, E_2$, so $e^{-E_1/\tau}, e^{-E_2/\tau} \to 1$ and we get

$$P(1) \simeq \frac{1}{1+2} = \frac{1}{3}$$

$$\langle \varepsilon \rangle \simeq \frac{E_1 + 2E_2}{1+2} = \frac{E_1 + 2E_2}{3}$$

d) The termal average energy is given by $\langle \varepsilon \rangle = \frac{1}{Z} \sum_s \varepsilon_s e^{-\varepsilon_s/\tau}$

The sum can be derived from the partition function.

Note that $\quad \dfrac{dZ}{d\tau} = \dfrac{1}{\tau^2} \sum_s \varepsilon_s e^{-\varepsilon_s/\tau} \quad$ so that

$$\langle \varepsilon \rangle = \frac{1}{Z} \tau^2 \frac{dZ}{d\tau}, \text{ or } \quad \langle \varepsilon \rangle = \tau^2 \frac{d(\log Z)}{d\tau}$$