PROBLEM SET 1

Physics 219A, Spring 2014

Due Monday, April 7

[1.] Consider a classical system which has three energy states $E_1 < E_2 < E_3$.
a. What is the partition function Z?
b. What is the free energy F?
c. What are the probabilities p_1, p_2, p_3 of occupying each state? Sketch $p_i(T)$ versus T and interpret.
d. Show $\langle E \rangle = \partial \ln Z / \partial \beta$ gives the same answer as $\langle E \rangle = \sum_i p_i E_i$. Sketch $\langle E \rangle(T)$ versus T.
e. Compute $C = d\langle E \rangle / dT$ and show it equals $\beta^2 (\langle E^2 \rangle - \langle E \rangle^2)$.
f. What is the entropy $S(T)$? What are its low and high temperature limits?

[2.] In this problem we'll consider the limiting behavior of the specific heat at low and high temperature and what it might tell us about the system's energy states.
a. The specific heat of the two state system we considered in class obeys $C(T \to \infty) \to 0$. On the other hand, for a classical harmonic oscillator $C(T) = k_B$ for all T, and hence does not vanish as $T \to \infty$. What can you say about the energy states of a system which would affect whether or not C vanishes at high T?
b. The specific heat of the two state system we considered in class obeys $C(T \to 0) \to 0$, while that of the harmonic oscillator remains finite. What can you say about the energy states of a system which would affect whether or not C vanishes at low T?
c. Some glasses have a specific heat which goes to zero *linearly* with T as $T \to 0$. A model for this phenomenon is that inside the glass are *many* two level systems (corresponding, perhaps, to two different positions of the atoms). Assume that these two level systems can have a distribution of energy spacings Δ and that the number of two level systems with spacing Δ is the same for all Δ. Show that this results in $C(T)$ which is linear in T.
d. The specific heat in (c) goes to zero as $T \to 0$, but does so more slowly (linearly rather than exponentially) that a single two level system of spacing Δ_0. Explain why physically. Make a general statement about what you might infer from the knowledge that $C(T)$ vanishes exponentially. (This was an important clue into the mystery of superconductivity.)

[3.] Suppose a system has an infinite number of states with discrete energies $E_n = n\Delta$ with $n > 0$. Compute the partition function Z, the free energy $F(T)$, the average energy $\langle E \rangle(T)$, and the entropy $S(T)$.

[4.] We will use the results of this exercise a fair amount in this course: Given a binomial distribution $\mathcal{P}(n) = \binom{N}{n} p^n q^{N-n}$. Evaluate $\langle n \rangle = \sum_n n \, \mathcal{P}(n)$. Hint: Consider the expression for $\sum_n \mathcal{P}(n)$ and differentiate with respect to p. Compute also $\langle n^2 \rangle$ and then $\langle n^2 \rangle - \langle n \rangle^2$. Is there any physical interpretation/importance to this result?

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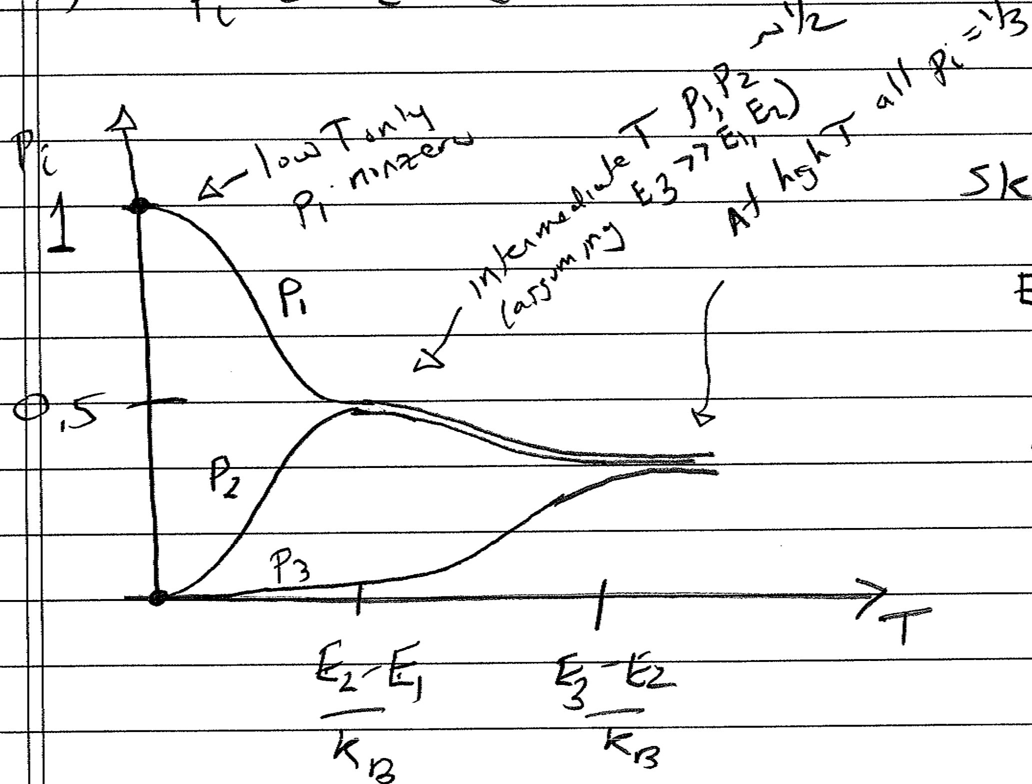
$\boxed{1}$ a) $Z = e^{-\beta E_1} + e^{-\beta E_2} + e^{-\beta E_3}$

b) $F = -k_B T \ln Z$

c) $p_i = Z^{-1} e^{-\beta E_i}$



Sketch is for $E_1 < E_2 < E_3$ with E_3 considerably greater than E_1, E_2

d) $Z = \sum_n e^{-\beta E_n}$ Here $n = 1, 2, 3$

$$-\frac{\partial}{\partial \beta} \ln Z = \frac{1}{Z} \sum_n E_n e^{-\beta E_n} = \sum_n E_n \frac{e^{-\beta E_n}}{Z} = \sum E_n p_n$$

(2)

general proof

e) $C = \frac{d\langle E\rangle}{dT} = \frac{d}{dT} Z^{-1} \sum E_n e^{-\beta E_n}$

$$d/dT = d\beta/dT \; d/d\beta$$

$$= -1/T^2 \, d/d\beta = -\beta^2 \, d/\partial\beta$$

$$\therefore \; C = -\beta^2 \frac{d}{d\beta} Z^{-1} \sum E_n e^{-\beta E_n}$$

$$= -\beta^2 \left[\frac{-1}{Z^2} \underbrace{\frac{dZ}{d\beta}}_{-\sum E_n e^{-\beta E_n}} \sum E_n e^{-\beta E_n} + Z^{-1} \sum_n E_n (-E_n) e^{-\beta E_n} \right]$$

$$= \beta^2 \left[Z^{-1} \sum E_n^2 e^{-\beta E_n} - \left(Z^{-1} \sum E_n e^{-\beta E_n} \right)^2 \right]$$

$$= \beta^2 \left[\langle E^2 \rangle - \langle E \rangle^2 \right]$$

f) $F = \langle E \rangle - TS$ so $S = \beta [\langle E\rangle - F]$

$$S = \frac{1}{T} \left\{ Z^{-1} \sum E_n e^{-\beta E_n} + k_B T \ln Z \right\}$$

$\boxed{2.}$ a) If the energy levels are bounded from above the specific heat must vanish at high T.

The reason physically is that C measures the ability of the system's energy to respond to changes in temperature

$$d\langle E\rangle = C\,dT$$

If E_n are bounded, the system cannot increase $\langle E\rangle$ once T is high enough. So C must vanish.

b) If there is a gap in the spectrum between E_0 and the excited states C must vanish (exponentially).

The point is that for $T \ll E_1 - E_0$ the system cannot reach E_1 (or any higher level). $\langle E\rangle$ is stuck at E_0 even as T increases (as long as $T \ll E_1 - E_0$). Note if there is no gap and $E_1 - E_0$ can be arbitrarily small this argument fails.

See part (c).

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c) $$p(\Delta) = \begin{cases} 1/\Delta_m & 0 < \Delta < \Delta_m \\ 0 & \text{otherwise} \end{cases}$$

For a two level system

$$\langle E \rangle = \Delta e^{-\beta\Delta} / (1 + e^{-\beta\Delta})$$

$$= \Delta / (e^{\beta\Delta} + 1)$$

$$C = \frac{d\langle E \rangle}{dT} = \Delta e^{\beta\Delta} / (e^{\beta\Delta} + 1)^2 \quad \Delta\beta^2 k_B$$

$$= k_B \, (\beta\Delta)^2 e^{\beta\Delta} / (e^{\beta\Delta} + 1)^2$$

$$\langle c \rangle = \int_0^{\Delta_m} \frac{d\Delta}{\Delta_m} \, k_B (\beta\Delta)^2 e^{\beta\Delta} / (e^{\beta\Delta} + 1)^2$$

Define $x = \beta\Delta$

$$\langle c \rangle = \int_0^{\beta\Delta_m} \frac{dx}{\beta\Delta_m} \, k_B \, x^2 \, e^x / (e^x + 1)^2$$

As $\beta \to \infty$ ($T \to 0$) $\beta \Delta_m \to \infty$

$$\langle c \rangle \to \frac{k_B}{\beta \Delta_m} \underbrace{\int_0^\infty x^2 \, e^x/(e^x+1)^2 \, dx}$$

This integral takes some (irrelevant) numerical value A

$$\langle c \rangle \to A k_B \left(\frac{k_B T}{\Delta_m} \right)$$ ie linear in T

(d) $\langle c \rangle$ vanishes as a power law in T because there is no gap: There is some nonzero density of levels arbitrarily close to the ground state. If $c(T)$ vanishes exponentially then there is a gap.

$\boxed{3.}$ $$Z = \sum_n e^{-\beta E_n} = \sum_{n=1}^{\infty} (e^{-\beta\Delta})^n$$

$$= e^{-\beta\Delta}/1 - e^{-\beta\Delta} = 1/e^{\beta\Delta} - 1$$

$$F = -k_B T \ln Z = k_B T \ln(e^{\beta\Delta} - 1)$$

$$\langle E \rangle = -\frac{\partial}{\partial\beta} \ln Z = +\frac{\partial}{\partial\beta} \ln(e^{\beta\Delta} - 1)$$

$$= (e^{\beta\Delta} - 1)^{-1} e^{\beta\Delta} \Delta$$

$$S = \frac{1}{T} (\langle E \rangle - F)$$

$$= k_B \left\{ \beta\Delta e^{\beta\Delta} (e^{\beta\Delta} - 1)^{-1} - \ln(e^{\beta\Delta} - 1) \right\}$$

You can ask about limits, eg what happens to $\langle E \rangle$ at high T, $(\beta \to 0)$

$$\langle E \rangle \to (1 + \beta\Delta - 1)^{-1} \, 1 \, \Delta$$

$$= 1/\beta = k_B T.$$

$\boxed{4}$ $$p(n) = \binom{N}{n} p^n q^{N-n}$$

$$\sum_{n=0}^{N} p(n) = (p+q)^N = \sum_{n=0}^{N} \binom{N}{n} p^n q^{N-n}$$

Taking $\partial/\partial p$ $$N(p+q)^{N-1} = \sum_{n=1}^{N} \binom{N}{n} n p^{n-1} q^{N-n}$$

$$= \frac{1}{p} \sum_{1}^{N} \binom{N}{n} p^n q^{N-n} n$$

$$= \frac{1}{p} \sum_{1}^{N} p(n) n$$

Now setting $p+q=1$ we get

$$Np = \sum_{1}^{\infty} n\, p(n) = \langle n \rangle$$

Note this differentiation trick is also useful in doing geometric sums

$$\sum_{0}^{\infty} x^n = 1/(1-x)$$

differentiate wrt x $$\sum_{1}^{\infty} n x^{n-1} = 1/(1-x)^2$$

$$\sum_{1}^{\infty} n x^n = x/(1-x)^2.$$

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$$\langle n^2 \rangle = \sum_n n^2 \mathcal{P}(n)$$

We have $$pN(p+q)^{N-1} = \sum_1^N n \binom{N}{n} p^{n-1} q^{N-n}$$

Differentiate wrt p again

$$N(N-1)(p+q)^{N-2} = \sum_2^N n(n-1)\binom{N}{n} p^{n-2} q^{N-n}$$

$$= \frac{1}{p^2} \sum_2^N n(n-1) \underbrace{\binom{N}{n} p^n q^{N-n}}_{\mathcal{P}(n)}$$

Have to be a little careful with limits of summation

$$\sum_2^\infty n(n-1)\mathcal{P}(n) = \sum_2^\infty n^2 \mathcal{P}(n) - \sum_2^\infty n \mathcal{P}(n)$$

$$= \sum_1^\infty n^2 \mathcal{P}(n) - \mathcal{P}(1) - \left(\sum_1^\infty n \mathcal{P}(n) - \mathcal{P}(1) \right)$$

$$= \langle n^2 \rangle - \underbrace{\langle n \rangle}_{Np}$$

Setting $p+q=1$

$$N(N-1) = \frac{1}{p^2}\left(\langle n^2 \rangle - Np\right) = \frac{\langle n^2 \rangle}{p^2} - \frac{N}{p}$$

$$\langle n^2 \rangle = N^2 p^2 - N p^2 + Np$$

$$\underbrace{\langle n^2 \rangle - \langle n \rangle^2}_{Np} = N^2 p^2 - N p^2 + Np - N^2 p^2$$

$$= Np(1-p) = Npq$$

$\langle n^2 \rangle - \langle n \rangle^2$ measures square of fluctuations in $\langle n \rangle$

The fluctuations in $\langle n \rangle$ go as $\sqrt{N}\sqrt{pq}$

Even though $\langle n \rangle$ grows linearly in $\langle N \rangle$

fluctuations are $\sqrt{N}$. Thus $\langle n \rangle$/fluctuations

falls as $1/\sqrt{N}$, the standard result,