HW 5 Solutions. [augmented after grading]

1. [Easy review question of canonical ensemble]
A set of N noninteracting (classical) spins are in a magnetic field B (in the z-direction) as the example we discussed in Chapter 1: The spin-magnetic field interaction energy is

$$H = -\mu B \sum_{i=1}^{N} \sigma_i,$$

Obtain the specific heat under constant magnetic field of this spin system.

Solution
[Strictly speaking, the internal energy $E = 0$ for this example; the generalized enthalpy $J = E - MB$ is called the 'internal energy' in the conventional textbooks and courses. We know $dJ = TdS - MdB$, so

$$C_B = T \left.\frac{\partial S}{\partial T}\right|_B = \left.\frac{\partial J}{\partial T}\right|_B.$$

You can of course use S to compute C_B, but this formula says C_B via J is easier. Do not stick to a single method; before jumping into a full computational activity, think a bit. Do not jump into a bathtub without checking its T.

Notice that $(\partial E/\partial T)_B = C_B + B(\partial M/\partial T)_B$ and is not equal to C_B (0 in our case!), generally speaking.]

Let us use the 'canonical' formalism:

$$\hat{Z} = \sum_{\sigma} e^{\beta B \sum \sigma_i} = (2\cosh \beta B)^N.$$

J may be obtained by the Gibbs-Helmholtz relation or

$$J = \left.\frac{\partial \log Z}{\partial \beta}\right|_B = -NB\frac{\sinh \beta B}{\cosh \beta B} = -NB \tanh \beta B.$$

cf (1.5.31). Therefore,

$$C_B = -\left.\frac{\partial NB \tanh \beta B}{\partial T}\right|_B = -BN\frac{1}{\cosh^2 \beta B}\left(-\frac{B}{k_B T^2}\right) = Nk_B\left(\frac{\beta B}{\cosh \beta B}\right)^2.$$

The abuse, $\hat{Z} \to Z$, $J \to E$, etc., is OK as long as you clearly recognize the abuse.

2. Calculate the fluctuation of the internal energy, i.e., $\langle \delta E^2 \rangle$. You may assume that the Gibbs relation of the system is $dE = TdS - PdV$ (i.e., you need not worry about δN). There are many ways, but perhaps the most 'unsophisticated' is to use $\delta E = T\delta S - P\delta V$. However, you may use any correct method, needless to say.

Solution
There are a few people who calculated $\langle \delta E^2 \rangle$ using the canonical ensemble. Although I did not penalize this solution (far easier than the true answer of this question), I wish you to know clearly that the fluctuation you get from this calculation is under constant volume. In the usual fluctuation problem, any quantity can fluctuate without constraints. In the present case we could imagine a very flexible 'bag' containing N particles and then ask what

the internal energy in the bag is. Its volume is not constant, and the pressure inside is not constant, either.

The 'unsophisticated' approach is indeed unsophisticated, and does not use what we already know: $\langle \delta X \delta y \rangle = 0$. To exploit this to reduce the amount of computation, let us use T and V as independent variables:

$$\delta E = T \left(\left.\frac{\partial S}{\partial T}\right|_V \delta T + \left.\frac{\partial S}{\partial V}\right|_T \delta V \right) - P\delta V.$$

We know

$$\left.\frac{\partial S}{\partial T}\right|_V = \frac{C_V}{T}, \quad \left.\frac{\partial S}{\partial V}\right|_T = \frac{\partial(S,T)}{\partial(V,T)} = \frac{\partial(S,T)}{\partial(-P,V)} \frac{\partial(-P,V)}{\partial(V,T)} = \left.\frac{\partial P}{\partial T}\right|_V.$$

Therefore,

$$\delta E = C_V \delta T + \left(T \left.\frac{\partial P}{\partial T}\right|_V - P \right) \delta V.$$

We need

$$\langle \delta T^2 \rangle = k_B T^2 / C_V$$

(this we already computed) and the fluctuation-response relation gives us[1]

$$\langle \delta V^2 \rangle = -k_B T \left.\frac{\partial V}{\partial P}\right|_T.$$

(Do not forget that the conjugate of V is $-P$.) Therefore,

$$\langle \delta E^2 \rangle = C_V^2 \langle \delta T^2 \rangle + \left(T \left.\frac{\partial P}{\partial T}\right|_V - P \right)^2 \langle \delta V^2 \rangle = k_B T^2 C_V - k_B T \left(T \left.\frac{\partial P}{\partial T}\right|_V - P \right)^2 \left.\frac{\partial V}{\partial P}\right|_T.$$

If we use $\delta E = T\delta S - P\delta V$, we need

$$\langle \delta S^2 \rangle = k_B T \left.\frac{\partial S}{\partial T}\right|_P = k_B C_P, \ \langle \delta S \delta V \rangle = k_B T \left.\frac{\partial S}{\partial P}\right|_T.$$

Therefore,

$$\langle \delta E^2 \rangle = k_B T^2 C_P - 2 k_B T^2 P \left.\frac{\partial S}{\partial P}\right|_T - k_B T P^2 \left.\frac{\partial V}{\partial P}\right|_T$$

or

$$\langle \delta E^2 \rangle = k_B T^2 C_P + 2 k_B T^2 P \left.\frac{\partial V}{\partial T}\right|_P - k_B T P^2 \left.\frac{\partial V}{\partial P}\right|_T.$$

[The original version had sign errors.]

Are this result and the above result identical? Let us check this.

$$\begin{aligned} 2k_B T^2 P \left.\frac{\partial P}{\partial T}\right|_V \left.\frac{\partial V}{\partial P}\right|_T &= 2k_B T^2 P \frac{\partial(P,V)}{\partial(T,V)} \frac{\partial(V,T)}{\partial(P,T)} = -2k_B T^2 P \frac{\partial(P,V)}{\partial(S,T)} \frac{\partial(S,T)}{\partial(P,T)} \\ &= -2k_B T^2 P \left.\frac{\partial S}{\partial P}\right|_T = -2k_B T^2 P \left.\frac{\partial S}{\partial P}\right|_T. \end{aligned}$$

[1] Notice that in this case extensive quantities can fluctuate without any constraint, so we may consider the fluctuation in the ensemble with constant intensive variables.

This implies that the second term shows up from the cross terms obtained by the expansion of the square. We further know

$$dS = \frac{C_V}{T}dT + \left.\frac{\partial S}{\partial V}\right|_T dV,$$

so

$$\frac{C_P}{T} = \frac{C_V}{T} + \left.\frac{\partial S}{\partial V}\right|_T \left.\frac{\partial V}{\partial T}\right|_P .$$

Notice that

$$-k_BT^3\left.\frac{\partial P}{\partial T}\right|_V \left.\frac{\partial P}{\partial T}\right|_V \left.\frac{\partial V}{\partial P}\right|_T = -k_BT^3\left.\frac{\partial P}{\partial T}\right|_V \frac{\partial(P,V)}{\partial(T,V)}\frac{\partial V,T)}{\partial(P,T)} = k_BT^3\left.\frac{\partial P}{\partial T}\right|_V \left.\frac{\partial V}{\partial T}\right|_P = k_BT^3\left.\frac{\partial S}{\partial V}\right|_T \left.\frac{\partial V}{\partial T}\right|_P$$

Thus, these two results are identical.

3. There is a pendulum of length ℓ (on the earth's surface) with mass m. What is the mean square amplitude of this pendulum at temperature T? [Hint: reversible work required determines fluctuations.]

Solution
Let θ be the angular displacement of the pendulum from the vertical. Then, the increase of the potential energy is

$$\Phi = mg\ell\cos\theta - 1 = +\frac{1}{2}mgl\theta^2.$$

Therefore,

$$P(\theta) \propto \exp\left[-\beta\frac{1}{2}mgl\theta^2\right]$$

Thus, we can read the result off:

$$\langle\theta^2\rangle = k_BT/mg\ell$$

Therefore, the displacement δx in the horizontal direction reads

$$\langle\delta x^2\rangle = k_BT\ell/mg$$

Notice that m matters.

If you think the pendulum in 3D has 2 degrees of freedom in x and y directions, then the amplitude squared is $\langle\delta x^2 + \delta y^2\rangle = 2\langle\delta x^2\rangle$ gives the amplitude.

You may use the equipartition of energy, but I believe the fluctuation theory is more direct and easier to use.

4. Let the transversal displacement be $y(x)$ at x along a string of length L with tensile force F. Then, the extra elastic energy due to this displacement can be calculated as

$$\Phi[y] = \frac{F}{2}\int_0^L \left(\frac{dy}{dx}\right)^2 dx.$$

Assuming that the system is in equilibrium at temperature T. What is the transversal fluctuation of the string at $x \in (0, L)$, that is, $\langle y(x)^2\rangle$?

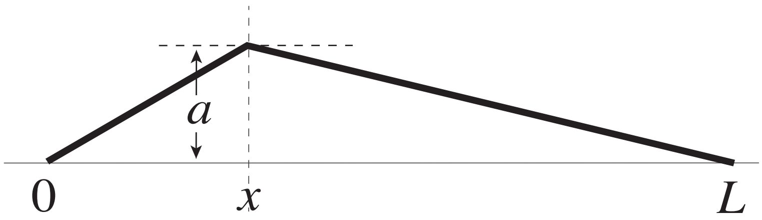

Figure 1: The configuration of the string $y(x)$ that gives a displacement of a at x with the minimum extra energy.

[Hint. The fluctuation probability is $\propto e^{-W_R/k_BT}$, where W_R is the reversible minimum work required to create the desired fluctuation.]

Solution
As you can easily guess, the way to produce the displacement we wish with the minimum work must be as illustrated in the figure (as someone actually did, using the variational calculus, you can demonstrate this shape is indeed the minimum displacement energy required to produce the deviation a).

We need the slopes: up to x it is a/x; beyond x it is $a/(L-x)$. Therefore, the minimum work needed is

$$\Phi[y] = \frac{F}{2}\int_0^x \left(\frac{a}{x}\right)^2 dx' + \frac{F}{2}\int_x^L \left(\frac{a}{L-x}\right)^2 dx' = \frac{1}{2}Fa^2\left(\frac{1}{x}+\frac{1}{L-x}\right)$$

Hence,

$$\langle a^2\rangle = \frac{k_BT}{F\left(\frac{1}{x}+\frac{1}{L-x}\right)} = \frac{k_BT}{FL}x(L-x).$$