

# PHYS 427 - Thermal and Statistical Physics - Discussion 14 Solutions

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1. **Diffusion in three dimensions:** A drop of red dye is deposited into the center of a large tub of still water. The dye particles are jostled around randomly by collisions with thermally agitated water molecules. Over time, the dye particles *diffuse* through the water, i.e. the drop of dye spreads out.

Let  $n(\mathbf{r}, t)$  denote the number density of dye particles, where  $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$  is the position vector.

- (a) The total number of particles contained within an arbitrary subvolume  $V$  is

$$N(t) = \int_V n(\mathbf{r}, t) d^3r. \quad (1)$$

The only way for  $N(t)$  to change is if particles enter or leave  $V$ . Mathematically, this is expressed as

$$\frac{dN}{dt} = - \int_{\partial V} \mathbf{J} \cdot d\mathbf{A}, \quad (2)$$

where  $\int_{\partial V}$  denotes a surface integral over the boundary  $\partial V$  of the subvolume. We have introduced  $\mathbf{J}$ , the *particle current density*, such that  $\mathbf{J} \cdot d\mathbf{A}$  is the number of particles per second going *out* of the surface element  $d\mathbf{A}$ .

Using the divergence theorem of multivariate calculus, show that (2) is equivalent to the *continuity equation*

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = 0. \quad (3)$$

- (b) Under certain approximations, in the lecture you will derive Fick's law,

$$\mathbf{J} = -D\nabla n, \quad (4)$$

where  $D > 0$  is a constant called the *diffusion coefficient*. For now, just notice that this is the simplest, most intuitive law one could have—it says that particles flow toward less dense regions, which tends to smooth out variations in density. When Fick's law is inserted into the continuity equation, we get the *diffusion equation*

$$\frac{\partial n}{\partial t} - D\nabla^2 n = 0. \quad (5)$$

(c) Show that

$$n(\mathbf{r}, t) = \frac{N_0}{(4\pi Dt)^{3/2}} e^{-r^2/4Dt} \quad (6)$$

is a solution of the diffusion equation, where  $r = \sqrt{x^2 + y^2 + z^2}$  and  $N_0$  is a constant. *Hint: recall  $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ .*

(d) Sketch (6) as a function of  $r$  at various times. Is this what you expect a drop of dye to do?

(e) Show that

$$\int_{\text{all space}} n(\mathbf{r}, t) d^3r = N_0 \quad (7)$$

is the total number of dye particles<sup>1</sup>. *Hint:  $\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\pi/\alpha}$ .*

(f) Show that

$$\langle r^2 \rangle \equiv \frac{\int_{\text{all space}} d^3r r^2 n(\mathbf{r}, t)}{\int_{\text{all space}} d^3r n(\mathbf{r}, t)} = 6Dt. \quad (8)$$

*Hint: first observe that  $\int d^3r r^2 e^{-\alpha r^2} / \int d^3r e^{-\alpha r^2} = -\frac{d}{d\alpha} \ln \left( \int d^3r e^{-\alpha r^2} \right)$ .*

You have shown that

$$r_{rms} \equiv \sqrt{\langle r^2 \rangle} = \sqrt{6Dt}. \quad (9)$$

That is, the root-mean-square position of a dye particle, which is some measure of the “average” displacement of a dye particle from the origin, increases as  $t^{1/2}$  over time. This is the characteristic time-dependence of diffusive processes. If the diffusion constant  $D$  is bigger, then the dye particle will move more quickly on average, but still as  $t^{1/2}$ . This  $t^{1/2}$  behavior occurs for diffusion in any number of dimensions, not just three.

(g) Suppose it takes the dye about five minutes to diffuse appreciably throughout a cup of water. Estimate the value of  $D$ . *Answer:  $D \approx 10^{-4} \text{ m}^2 \text{ s}^{-1}$ .*

## SOLUTION:

(a) Inserting (1) into (2), we can bring the  $d/dt$  under the integrand to obtain

$$\int_V \frac{\partial}{\partial t} n(\mathbf{r}, t) d^3r + \int_{\partial V} \mathbf{J} \cdot d\mathbf{A} = 0. \quad (10)$$

The divergence theorem states

$$\int_{\partial V} \mathbf{F} \cdot d\mathbf{A} = \int_V \nabla \cdot \mathbf{F} d^3r, \quad (11)$$

as long as  $\mathbf{F}$  is a sufficiently “nice” vector field. Applying this to the second term in (10) yields

$$\int_V \left[ \frac{\partial}{\partial t} n(\mathbf{r}, t) + \nabla \cdot \mathbf{J} \right] d^3r = 0. \quad (12)$$

<sup>1</sup>Note that this doesn’t change over time. This is a consequence of the assumption of particle number conservation that went into the derivation of the continuity equation in part (a).

We now have an equation of the form

$$\int_V f(\mathbf{r}) d^3r = 0, \quad (13)$$

and the equation must hold for all possible choices of the volume  $V$ . So we can choose the volume to be a very small box centered at  $\mathbf{r} = \mathbf{r}_0$ . If the box is small enough, then  $f(\mathbf{r}) \approx f(\mathbf{r}_0) = \text{const.}$  at all points  $\mathbf{r}$  within the box. Then

$$\int_V f(\mathbf{r}) d^3r \approx f(\mathbf{r}_0) \Delta V, \quad (14)$$

where  $\Delta V$  is the volume of the tiny box. Since this must be zero, and  $\Delta V$  is not zero, we find that  $f(\mathbf{r}_0) = 0$ . Since  $\mathbf{r}_0$  was arbitrary, we find that  $f$  is zero everywhere in space. Applying this to (12) gives the differential equation

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = 0. \quad (15)$$

The thing to remember is that this was a direct consequence of one assumption: that the number of particles is (locally) conserved. The only way for the number of particles in a particular region in space to change is if particles flowed into or out of that region. Hence the continuity equation should always be thought of as an expression of a conservation law.

(b)

(c) Applying the product rule to (6), we have

$$\frac{\partial n}{\partial t} = -\frac{3}{2} \frac{n}{t} + \frac{r^2}{4Dt^2} n. \quad (16)$$

Similarly, we have

$$\frac{\partial n}{\partial x} = -\frac{x}{2Dt} n \quad (17)$$

and

$$\frac{\partial^2 n}{\partial x^2} = -\frac{1}{2Dt} n + \frac{x^2}{4D^2t^2} n, \quad (18)$$

so

$$\nabla^2 n = -\frac{3}{2Dt} n + \frac{r^2}{4D^2t^2} n. \quad (19)$$

Multiplying this by  $D$ , we see that it is equal to (16), which is what we wanted to show.

(d) At any time, the graph of  $n$  vs.  $r$  is a Gaussian (aka bell curve, normal distribution) peaked at  $r = 0$ . As time goes on, the peak value of  $n$  decreases, and the graph broadens out. This is what we expect the dye to do as the dye particles diffuse outward away from the original location of the drop.

(e) Using the hint,

$$\int n(\mathbf{r}, t) d^3r = \frac{N_0}{(4\pi Dt)^{3/2}} \int e^{-(x^2+y^2+z^2)/4Dt} d^3r \quad (20)$$

$$= \frac{N_0}{(4\pi Dt)^{3/2}} \left( \int_{-\infty}^{\infty} e^{-x^2/4Dt} dx \right) \left( \int_{-\infty}^{\infty} e^{-y^2/4Dt} dy \right) \left( \int_{-\infty}^{\infty} e^{-z^2/4Dt} dz \right) \quad (21)$$

$$= \frac{N_0}{(4\pi Dt)^{3/2}} (\sqrt{4\pi Dt})^3 \quad (22)$$

$$= N_0. \quad (23)$$

We have found that the total number of particles in all space is equal to a constant. That had to happen, because our  $n(\mathbf{r}, t)$  is a solution to the differential equation, which itself is a *statement* of the conservation of particles.

(f) We have

$$\langle r^2 \rangle = \frac{\int d^3r \, r^2 e^{-r^2/4Dt}}{\int d^3r \, e^{-r^2/4Dt}}. \quad (24)$$

Writing  $\alpha = 1/4Dt$ , we have, following the hint,

$$\langle r^2 \rangle = \frac{\int d^3r \, r^2 e^{-\alpha r^2}}{\int d^3r \, e^{-\alpha r^2}} \quad (25)$$

$$= -\frac{d}{d\alpha} \ln \left[ \int d^3r \, e^{-\alpha r^2} \right] \quad (26)$$

$$= -3 \frac{d}{d\alpha} \ln \left[ \int_{-\infty}^{\infty} dx \, e^{-\alpha x^2} \right] \quad (27)$$

$$= -3 \frac{d}{d\alpha} \ln \sqrt{\pi/\alpha} \quad (28)$$

$$= \frac{3}{2} \frac{d}{d\alpha} \ln \alpha \quad (29)$$

$$= \frac{3}{2\alpha} \quad (30)$$

$$= 6Dt. \quad (31)$$

Note that this is just a method for evaluating the integrals involved in the expectation value of  $r^2$ . We could also use more direct methods.

(g) We want to know how long it takes for the root mean square displacement of a dye particle to be approximately equal to the radius of a cup of water, which is about  $r_{rms} \approx 5 \times 10^{-2}$  m. We also set  $t = 300$  s to obtain

$$5 \times 10^{-2} \text{ m} \approx \sqrt{1800 \text{ s} \times D} \implies D \approx 10^{-6} \text{ m}^2 \text{ s}^{-1}. \quad (32)$$

**2. Paramagnet (review):** A simple model for a paramagnet consists of a lattice with  $N$  sites, each of which can be in either a “spin up” or “spin down” state. The spins do not interact with each other, but each spin interacts with the external magnetic field. If a spin is “up”, it contributes an energy  $\mu B$ . If it is “down”, it contributes an energy  $-\mu B$ .

- (a) Consider the paramagnet as a closed system with fixed energy  $U$ , compute the entropy.
- (b) Plot the entropy as a function of  $U$ . For what values of  $U$  is the temperature negative?
- (c) Suppose the paramagnet is prepared with a negative temperature. If it is put into thermal contact with a “normal” system, i.e. one which can only have a positive temperature, which way will energy spontaneously flow?

**SOLUTION:**

(a) We have

$$N = N_{\uparrow} + N_{\downarrow} \implies N_{\downarrow} = N_{\uparrow} - N. \quad (33)$$

Then

$$U = \mu B N_{\uparrow} - \mu B N_{\downarrow} = \mu B (2N_{\uparrow} - N) \implies N_{\uparrow} = \frac{N}{2} \left( 1 + \frac{U}{\mu B N} \right) \quad (34)$$

The multiplicity  $\Omega(U)$  is the number of microstates accessible to the system when its energy is  $U$ . Equivalently, this is the number of possible ways to assign  $N_{\uparrow}$  of the spins to be up (and the rest to be down). This is

$$\Omega = \binom{N}{N_{\uparrow}} \quad (35)$$

$$= \frac{N!}{N_{\uparrow}!(N - N_{\uparrow})!}. \quad (36)$$

The entropy is, using Sterling's approximation,

$$S/k_B = \ln \Omega \quad (37)$$

$$= \ln N! - \ln N_{\uparrow}! - \ln(N - N_{\uparrow})! \quad (38)$$

$$\approx N \ln N - N - N_{\uparrow} \ln N_{\uparrow} + N_{\uparrow} - (N - N_{\uparrow}) \ln(N - N_{\uparrow}) + (N - N_{\uparrow}) \quad (39)$$

$$= N \ln N - \frac{N}{2} \left( 1 + \frac{U}{\mu B N} \right) \ln \left[ \frac{N}{2} \left( 1 + \frac{U}{\mu B N} \right) \right] - \frac{N}{2} \left( 1 - \frac{U}{\mu B N} \right) \ln \left[ \frac{N}{2} \left( 1 - \frac{U}{\mu B N} \right) \right]. \quad (40)$$

From this expression, we can see that  $S(U) = S(-U)$ , i.e.  $S(U)$  is an even function. This is to be expected, because changing  $U$  to  $-U$  is like flipping all the spins simultaneously, which can't change  $\Omega$ . Furthermore, one can show by Taylor expanding this expression when  $U/\mu B N \ll 1$  that  $S(U) \approx -CU^2$ , where  $C$  is a constant. This is also to be expected, because  $\Omega$ , and therefore  $S$ , should reach its maximum when half the spins are up and half the spins are down, corresponding to  $U = 0$ .

(b) The graph of  $S(U)$  vs.  $U$  looks roughly like a semicircle peaked at  $U = 0$ . Therefore, when  $U > 0$ , the slope of  $S(U)$  is negative. By the definition of temperature,  $1/T = (\partial S / \partial U)$ , we find that  $T < 0$  when  $U > 0$ .

(c) Energy will spontaneously flow toward the positive-temperature object, no matter what, because this will cause the total entropy of the combined system (paramagnet + normal system) to increase, in accordance with the second law of thermodynamics.

One can see this by drawing  $S(U)$  for both systems. For the normal system,  $S(U)$  has positive slope, so its entropy will increase if it gains energy. Meanwhile, the paramagnet's entropy will increase if it loses energy (because  $S(U)$  has negative slope for the negative-temperature paramagnet). Therefore both systems will gain entropy if energy is transferred from the paramagnet to the normal system.

Algebraically, we can write the previous paragraph as follows. Let  $P$  denote the paramagnet and  $N$  the normal system. We have  $dS_P = T_P dU_P$  and  $dS_N = T_N dU_N$  by the definition of temperature. We also have  $dU_N = -dU_P$  by conservation of energy. Therefore  $dS_{\text{tot}} = dS_P + dS_N = dU_N(T_N^{-1} - T_P^{-1})$ . The factor in parenthesis is positive, so we must have  $dU_N > 0$  in order for  $dS_{\text{tot}} > 0$ .

We can summarize this by saying “negative temperature is hotter than any positive temperature”. That's because of what is meant by the word “hot”. We say that a stove is hot because it transfers energy spontaneously to your hand if you touch it.

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3. **Rotational partition function (review):** Consider a diatomic molecule whose moment of inertia is  $I$ . The center of mass of the molecule is at rest, but it is allowed to rotate. In quantum mechanics, one finds that the energy eigenstates are labelled by two integers  $\ell = 0, 1, 2, \dots$  and  $m = -\ell, -\ell+1, \dots, \ell$  with corresponding energies

$$E_{\ell m} = \frac{\hbar^2}{2I} \ell(\ell+1). \quad (41)$$

Note that the energy does not depend on  $m$ .

- (a) Suppose the molecule is in contact with a thermal reservoir. Express its canonical partition function as a sum over  $\ell$  only.
- (b) Keeping the two smallest terms, write down an approximate form for  $Z$  which is valid at very low temperature. What does “very low temperature” mean quantitatively? (use the symbol  $\gg$  in your answer)
- (c) Show that the average rotational energy at low temperatures is

$$U_{\text{rot}} \approx \frac{3\hbar^2}{I} e^{-\beta\hbar^2/I} \quad (42)$$

- (d) At very high temperature, the sum in  $Z$  can be approximated by an integral. Justify this statement and evaluate the integral to obtain an approximate expression for  $Z$ . *Answer:*  $Z \approx k_B T / (\hbar^2/2I)$ .
- (e) Compute the average rotational energy at high temperatures.
- (f) Use your answers to (c) and (e) to make a rough sketch of the graph of  $U_{\text{rot}}(T)$  over all temperatures. Roughly indicate where  $T = E_{00}/k_B$  is located on this sketch.
- (g) Calculate the heat capacity of the molecule at high temperatures. Does your result agree with the equipartition theorem?

### SOLUTION:

(a)

$$Z = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} e^{-\beta E_{\ell m}} \quad (43)$$

$$= \sum_{\ell=0}^{\infty} (2\ell+1) e^{-\beta \frac{\hbar^2}{2I} \ell(\ell+1)}. \quad (44)$$

(b) If  $\hbar^2/(2Ik_B T) \gg 1$ , i.e.  $k_B T \ll \hbar^2/2I$ , then  $e^{-\beta\hbar^2/2I}$  is very small and terms in the sum with higher  $\ell$  are smaller than previous terms. Hence we can approximate  $Z$  by keeping only the  $\ell = 0$  and  $\ell = 1$  terms:

$$Z \approx 1 + 3e^{-\beta\hbar^2/I}. \quad (45)$$

(c) We compute

$$U_{\text{rot}} \approx -\frac{1}{1 + 3e^{-\beta\hbar^2/I}} \frac{\partial}{\partial \beta} (1 + 3e^{-\beta\hbar^2/I}) \quad (46)$$

$$= \frac{\hbar^2}{I} \frac{1}{\frac{1}{3}e^{\beta\hbar^2/I} + 1}. \quad (47)$$

Again we note that if  $T$  is small, so that  $\beta$  is large, then we can drop the 1 in the denominator in comparison to the exponential.

$$U_{\text{rot}} \approx \frac{3\hbar^2}{I} e^{-\beta\hbar^2/I}. \quad (48)$$

Note that this is always the type of behavior one should expect at low temperatures for any system where there is a “gap” in energy between the ground state and the first excited state. In any such system, the energy behaves exponentially with inverse temperature at low temperature, and correspondingly the specific heat  $C = dU/dT$  has an exponentially decaying factor as well. Hence there is a directly measurable characteristic of the existence of a gap (an exponentially decaying specific heat at low  $T$ ).

(d) If on the other hand  $k_B T \gg \hbar^2/2I$ , then the exponential factor varies slowly as a function of  $\ell$ . Therefore the summand is a slowly varying function of  $\ell$ , and the sum can be viewed as a Riemann sum which well approximates the integral

$$Z \approx \int_0^\infty d\ell (2\ell + 1) e^{-\beta\frac{\hbar^2}{2I}\ell(\ell+1)}. \quad (49)$$

If this isn't clear, try sketching the value of the summand as a function of  $\ell$ . The integral can be evaluated by changing variables to  $u = (\beta\hbar^2/2I)\ell(\ell+1)$ , so that  $d\ell (2\ell + 1) = du (2I/\beta\hbar^2)$  and

$$Z = \frac{2I}{\beta\hbar^2} \int_0^\infty du e^{-u} = \frac{2I}{\beta\hbar^2}. \quad (50)$$

(e) Now we compute

$$U_{\text{rot}} = -\beta\hbar^2/2I \frac{\partial}{\partial\beta} (2I/\beta\hbar^2) \quad (51)$$

$$= \frac{1}{\beta} = k_B T. \quad (52)$$

(f) The sketch should be linear at high temperatures and exponentially decaying at low temperatures, with a smooth curve connecting these two limits.

(g) The heat capacity at high temperature is simply

$$\frac{dU_{\text{tot}}}{dT} \approx k_B. \quad (53)$$

This agrees with the equipartition theorem, because the system (a *single* molecule) has exactly two axes about which it can rotate. At high temperatures, these two rotations are classical quadratic degrees of freedom. The equipartition theorem says that each classical quadratic degree of freedom contributes  $\frac{1}{2}k_B$  to the heat capacity, and, famously,  $2 \times \frac{1}{2} = 1$ .

4. **2d magnon gas (review):** Magnons are quantized spin-waves; they are bosonic collective excitations that emerge in the low-temperature description of certain models of magnetism. Magnons are analogous to phonons, which are quantized sound waves that emerge when analyzing the vibrations of a crystal lattice using quantum mechanics.

Consider a system of  $N$  spins on a 2d square lattice, and assume the low-energy description of the system is a non-interacting gas of magnons with energies  $\varepsilon_{\vec{k}} = \hbar\omega_{\vec{k}}$ , where

$$\omega_{\vec{k}} = \frac{Ja^2}{2}|\vec{k}|^2. \quad (54)$$

In this dispersion relation, “ $J$ ” represents the coupling between neighbouring spins and “ $a$ ” is the lattice spacing. Because of the discrete structure of the lattice, the wavevectors are quantized according to  $\vec{k} = \pi\vec{n}/L$  where  $n_x = 1, 2, \dots, N_x$  and  $n_y = 1, 2, \dots, N_y$  with  $L = N_x a = N_y a$  and  $N = N_x N_y$ .

Furthermore, although the original degrees of freedoms are spins, there is only one “type” of magnon (i.e. there is no spin degeneracy as one might guess).

- (a) Compute the magnon density of states  $\mathcal{D}(\omega)$  and the Debye frequency  $\omega_D$ .

That is, show for  $N \gg 1$  (the thermodynamic limit) that we can replace certain sums over wavevectors by an integral over frequency, namely

$$\sum_{\vec{k}} F(\omega_{\vec{k}}) \approx \int_0^{\omega_D} d\omega \mathcal{D}(\omega) F(\omega), \quad (55)$$

where  $F(\omega)$  is an arbitrary function.

- (b) Compute the energy of the system as a function of temperature. *Note: your final answer can be left in terms of a dimensionless integral.*
- (c) Show that the heat capacity goes like  $T$  at low temperatures and approaches a constant at high temperatures. Compute the value of the constant.

### SOLUTION:

(a) Let us take the direct approach, which we haven’t done in a while in the discussion solutions. We start by observing that, when  $N \gg 1$ , the spacing between allowed  $k_x$  and  $k_y$  becomes very small, so we can approximate the sum by a wavevector integral.

$$\sum_{k_x=0}^{\pi N_x/L} \sum_{k_y=0}^{\pi N_y/L} F(\omega_{\vec{k}}) = \frac{1}{\Delta k_x} \frac{1}{\Delta k_y} \sum_{k_x=0}^{\pi N_x/L} \sum_{k_y=0}^{\pi N_y/L} \Delta k_x \Delta k_y F(\omega_{\vec{k}}) \quad (56)$$

$$= \left(\frac{L}{\pi}\right)^2 \sum_{k_x=0}^{\pi N_x/L} \sum_{k_y=0}^{\pi N_y/L} \Delta k_x \Delta k_y F(\omega_{\vec{k}}) \quad (57)$$

$$\approx \left(\frac{L}{\pi}\right)^2 \int_0^{\pi N_x/L} dk_x \int_0^{\pi N_y/L} dk_y F(\omega_{\vec{k}}). \quad (58)$$

In the second-to-last step, I used the fact that the spacing between allowed  $k_x$  values is  $\Delta k_x = L/\pi$ . Now we have an integral over a square region in  $\vec{k}$ -space, which is difficult to deal with. Debye’s approximation is to replace this square region by a quarter circle region with the same  $\vec{k}$ -space area as the square.



The square has area  $(\pi N_x/L)(\pi N_y/L) = \pi^2 N/L^2$ , and we want to set this equal to the area of the quarter circle with radius  $k_D$ , i.e. to  $\frac{1}{4}\pi k_D^2$ . This yields  $k_D = \sqrt{4\pi N/L^2}$ . Then the new integral is, in momentum-space polar coordinates  $k$  and  $\phi$ ,

$$\sum_{\vec{k}} F(\omega_{\vec{k}}) \approx \left(\frac{L}{\pi}\right)^2 \int_0^{\pi/2} d\phi \int_0^{k_D} k dk F(\omega_k). \quad (59)$$

Note that we have used the fact that  $\omega_{\vec{k}}$  actually only depends on  $k = |\vec{k}|$  (i.e. the dispersion relation is isotropic). Now we can perform the  $\phi$  integral to get an overall factor of  $\pi/2$ , and change variables in the remaining integral to  $\omega = Ja^2 k^2/2$ , so that  $k dk = d\omega/Ja^2$ . We get

$$\sum_{\vec{k}} F(\omega_{\vec{k}}) = \frac{L^2 \pi}{\pi^2} \frac{1}{2} \frac{1}{Ja^2} \int_0^{\omega_D} d\omega F(\omega) = \int_0^{\omega_D} d\omega \mathcal{D}(\omega) F(\omega), \quad (60)$$

where  $\mathcal{D}(\omega) = L^2/(2\pi Ja^2) = N/(2\pi J)$  is the density of states and the Debye frequency is given by

$$\omega_D = Ja^2 k_D^2/2 = 2\pi Ja^2 N/L^2 = 2\pi J. \quad (61)$$

Here we used the fact that  $L^2 = (N_x a)(N_y a) = Na^2$ .

(b) The magnon states are specified by  $\vec{k}$ . The state with wavevector  $\vec{k}$  has energy  $\hbar\omega_{\vec{k}}$  and the average number of magnons present with that  $\vec{k}$  is given by the Bose distribution  $f(\hbar\omega_{\vec{k}}) = (e^{\beta\hbar\omega_{\vec{k}}} - 1)^{-1}$ . So the average total energy of the system is

$$U = \sum_{\vec{k}} \hbar\omega_{\vec{k}} \frac{1}{e^{\beta\hbar\omega_{\vec{k}}} - 1} \approx \int_0^{\omega_D} d\omega \mathcal{D}(\omega) \hbar\omega \frac{1}{e^{\beta\hbar\omega} - 1}. \quad (62)$$

We insert the value of  $\mathcal{D}(\omega)$  and make the variable substitution  $x = \beta\hbar\omega$  to find

$$U = \frac{N}{2\pi J} \frac{k_B^2 T^2}{\hbar} \int_0^{\Theta_D/T} dx \frac{x}{e^x - 1}, \quad (63)$$

where we have introduced the Debye temperature  $k_B \Theta_D \equiv \hbar\omega_D = 2\pi\hbar J$ .

(c) At low  $T$ , we can replace the upper limit of the integral with  $\infty$  and we find  $U \sim T^2$ . Therefore  $C = dU/dT \sim T$ . At high  $T$ , the domain of integration is a very short interval, and over that interval the integrand has a constant value (equal to  $\lim_{x \rightarrow 0} \frac{x}{e^x - 1} = 1$ ). Therefore the integral can be replaced by  $\Theta_D/T$  and we find  $U \sim T$ , so  $C \rightarrow \text{const.}$ . More precisely,

$$U \rightarrow \frac{N}{2\pi J} \frac{k_B^2 T^2}{\hbar} \frac{\Theta_D}{T} = N k_B T \implies C = N k_B. \quad (64)$$

This is precisely what we would expect from the equipartition theorem for a system with two quadratic degrees of freedom.