

## Physics 112 - Intro to Statistical and Thermal Physics - Spring 2023

### Problem Set 05

Due Thursday, March 2 at 11:59 PM (PST)

Last Update: February 26, 2023

---

---

- **Highlighted/Most Relevant Reading for the material on this week's problem set:**

- Schroeder, Sections 2.1, 2.4, 2.5. Appendices B.1 and B.2 for background on Gaussian integrals and Gamma functions.

- **Reading for next week:**

- Schroeder, Sections 2.2-2.6; 3.1-3.3.
- 
- 

## Problem 5.1 - Paramagnets and the 1D Ising Model

Just as we used the van der Waals gas to explore many aspects of classical thermodynamics in Part I of the course, we will use one common system to explore many different aspects of classical statistical mechanics for Part II of the class - the *paramagnet*.

Our model of a paramagnet is a binary model system consisting of  $N$  spins placed in an external magnetic field of strength  $B$ . Each individual spin can be in one of two states, either aligned with the magnetic field - what we will call *spin-up*  $\uparrow$ , or anti-aligned with the magnetic field - what we will call *spin-down*  $\downarrow$ .

We will use the index  $i \in \{1, \dots, N\}$  to label the spins and let  $\sigma_i = \pm 1$  denote the  $i$ -th spin, with  $\sigma_i = +1$  for spin-up and  $\sigma_i = -1$  for spin-down. The *microstates* of this system are given by specifying each of the  $N$  spin values  $\sigma_i$ . Each spin acts like a tiny dipole magnet with magnitude of magnetic dipole moment  $\mu$ .<sup>1</sup> The energy of the  $i$ -th spin is therefore

$$U_i = -\mu B \sigma_i = \begin{cases} -\mu B, & \text{Spin aligned with field} \\ +\mu B, & \text{Spin anti-aligned with field} \end{cases}.$$

If we let  $N_\uparrow$  be the number of up-spins in a microstate and  $N_\downarrow = N - N_\uparrow$  be the number of down-spins then we can define the *magnetization* as

$$M \equiv \sum_i \mu \sigma_i = \mu(N_\uparrow - N_\downarrow) = \mu(2N_\uparrow - N).$$

The energy of the paramagnet is

$$U = \sum_i U_i = -\mu B \sum_i \sigma_i = -\mu B(N_\uparrow - N_\downarrow) = -BM.$$

We can equivalently define the *macrostate* in terms of the number of up-spins  $N_\uparrow$ , the magnetization  $M$ , or the energy  $U$ .

---

<sup>1</sup>Note: I'm sorry that we have a finite symbol set. For this problem we will *not* be working with the chemical potential. Rather,  $\mu$  will stand for the magnetic dipole moment, an entirely different physical quantity.

In the previous problem set we explored the multiplicity of this macrostate,

$$\Omega(U) = \binom{N}{N_{\uparrow}} = \frac{N!}{(N_{\uparrow})!(N - N_{\uparrow})!}, \quad N_{\uparrow} = \frac{1}{2} \left( N - \frac{U}{\mu B} \right).$$

Finally, we will define the **entropy** of a macrostate via the Boltzmann formula,

$$S(U) = k_B \ln \Omega(U).$$

(a) For an  $N$ -spin paramagnet, use Stirling's approximation to find an expression for  $S(N_{\uparrow})$ , the entropy as a function of energy.

(b) **Extra Part** (*Not for Credit*) Non-dimensionalize your expression from (a) by using  $\tilde{S} \equiv S/k_B$  and  $u \equiv U/\mu B$ . Then graph your function. Based on your graph, is the function  $S(U)$  convex as we expect from Problem 3.3?

Oooh! Now we're dealing with our old familiar thermodynamic concepts "internal energy" and "entropy" that we spent so much time with in the first part of the course! Hmm... I seem to recall that there was some relationship between energy, entropy, and *temperature*...

(c) How do we find the temperature if we know the entropy as a function of energy,  $S(U)$ ? Use this to find the temperature for our paramagnetic system,  $T(U)$ .

*Answer (highlight to reveal):*  $[T = \frac{2\mu B}{k_B} \left[ \ln \left( \frac{N - U/\mu B}{N + U/\mu B} \right) \right]^{-1}]$

Before going on, I think we should take the *best trigonometric detour ever!!* That is, we will look at the hyperbolic trigonometric functions.<sup>2</sup> As we journey through statistical mechanics we will see a lot of the hyperbolic trigonometric functions. **Hyperbolic cosine** and **hyperbolic sine** are defined analogously to the Euler formula for sine and cosine, only with real arguments for the exponentials,

$$\cosh x \equiv \frac{e^{+x} + e^{-x}}{2}, \quad \sinh x \equiv \frac{e^{+x} - e^{-x}}{2}.$$

We define the other hyperbolic versions of trig functions using these. For example, the **hyperbolic tangent**  $\tanh x \equiv \sinh x / \cosh x$  and **hyperbolic secant**  $\operatorname{sech} x \equiv 1 / \cosh x$ .

(d) Show the following useful hyperbolic trigonometric identities

- $\frac{d}{dx} \cosh x = \sinh x$ .
- $\frac{d}{dx} \sinh x = \cosh x$ .
- $\cosh^2 x - \sinh^2 x = 1$ .
- $\frac{d}{dx} \tanh x = \operatorname{sech}^2 x$ .

(e) Invert your formula for  $T(U)$  from part (c) to find  $U(T)$ . From this, determine the magnetization  $M(T)$  and the heat capacity at constant magnetic field  $C_B(T) \equiv \left( \frac{\partial U}{\partial T} \right)_B$ .

*Hint (highlight to reveal):* [Gee, I think we went on our *hyperbolic tangent* for a reason...<sup>3</sup>]

<sup>2</sup>Geometry wordplay!

<sup>3</sup>Sorry for all the puns and wordplay.<sup>4</sup>

<sup>4</sup>Not really. I love puns. Complaints can be sent to aphycist28@berkeley.edu but they really just spur me on further.

We can refine our non-interacting paramagnet model by introducing a simplified interaction between neighboring spins - the **one-dimensional Ising model** which consists of a set of  $N + 1$  spins arranged in a 1D array. Two neighboring spins can interact with each other because each spin not only interacts with magnetic fields but is itself the *source* of a tiny magnetic field. Assuming no external magnetic field, the energy of an  $(N + 1)$ -spin 1D Ising model is given by the following “nearest-neighbor” Hamiltonian,

$$U = \frac{\epsilon}{2} \sum_{i=1}^N (1 - \sigma_i \sigma_{i+1}),$$

where again  $\sigma_i$  is the spin of the  $i$ -th site and can be either  $+1$  for spin-up or  $-1$  for spin-down.

**(f) Extra Part (Not for Credit)** What is the contribution to the energy from a pair of spins that are *aligned*? Anti-aligned? Which configuration is energetically preferable?

Because of the results from part (f), rather than talking about the individual  $N + 1$  different spins, we can talk about the  $N$  different *pairs* of neighboring spins. Each pair (1-2, 2-3, 3-4, etc.) is defined by whether they are aligned or anti-aligned. We call an anti-aligned pair a **domain wall** since it separates regions (**domains**) of aligned spins. For example, in the configuration  $\uparrow\uparrow\uparrow\downarrow\downarrow$ , there are two domains (the first three up-spins and last two down-spins) and one domain wall at the pair of 3rd and 4th spins. While the individual spins are *coupled* by the energy function, each *pair* can be treated independently, giving a new  $N$ -element binary model system with  $U = N_a \epsilon$ , where  $N_a$  is the number of domain walls/anti-aligned pairs.

**(g)** Argue or show that the multiplicity of the macrostate defined by having  $N_a$  domain walls (or, equivalently, the macrostate defined by energy  $U = N_a \epsilon$ ) is

$$\Omega(N_a) = 2 \cdot \frac{N!}{N_a!(N - N_a)!}.$$

Why is that factor of 2 there? How does multiplying the multiplicity by a factor of 2 change the entropy? Is this significant when  $N \gg 1$ ?

*Hint (highlight to reveal):* [Think about a 3-spin system and try explicitly writing down all the microstates. For each microstate write down the equivalent “neighboring pairs” microstate. For example, the microstate  $\uparrow\uparrow\downarrow$  becomes the neighboring pairs microstate PA, where P represents spins 1 and 2 being aligned and A represents spins 2 and 3 being anti-aligned. Note that to fully specify our microstate we need one more bit (literally) of information on top of whether each pair is parallel or anti-parallel.]

**(h) Extra Part (Not for Credit)** Find  $S(N_a)$  in the limit where the Stirling approximation is valid. Repeat the steps from earlier in the problem to find the specific heat as a function of temperature  $C(T)$ .

*Hint (highlight to reveal):* [You already did most of the work for this.]

## Problem 5.2 - Entropy of the Ideal Gas

The goal of this problem is to lay the groundwork for studying the microstates and macrostates of an ideal gas system. Unlike our paramagnet model where we had a finite and discrete number of possible microstates, for an  $N$ -particle ideal gas the state space is given by a continuous **phase space** of  $6N$ -dimensions (three position coordinates and three momentum coordinates for each of the  $N$  particles). Rather than do combinatorial counting like in the previous problem, the number of microstates corresponding to a macrostate will involve taking an integral in this gigantic-dimensional phase space. Luckily, we have ways to do this! We will start in 1-dimension and work our way up...

---

The **gamma function** is defined via

$$\Gamma(n) \equiv \int_0^\infty x^{n-1} e^{-x} dx. \quad (1)$$

(a) **Extra Part (Not for Credit)** Evaluate the integral  $\int_0^\infty e^{-\alpha x} dx$ . Then take the  $n$ -th derivative with respect to alpha on both the original integral expression and on the result you found. Evaluate this at  $\alpha = 1$  to derive the relation

$$\Gamma(n+1) = \int_0^\infty x^n e^{-x} dx = n!.$$

---

**Commentary:** As we see, when  $n$  is a positive integer,  $\Gamma(n) = (n-1)!$  and therefore the gamma function is a natural extension of the factorial to the real numbers. In particular, the gamma function and factorial share a similar recursion relation,

$$\Gamma(n+1) = n\Gamma(n), \quad n! = n(n-1)!$$

---

One of the most important definite integrals to remember across all physics is the result of the **Gaussian integral**,

$$\int_{-\infty}^\infty e^{-x^2} dx = \sqrt{\pi}. \quad (2)$$

There is a nice derivation of this result in Schroeder Appendix B.1 (along with a million other online sources and textbooks). Let's see how this is related to the gamma function.

(b) First exploit the symmetry of the integrand to rewrite Eq. 2 as an integral with limits 0 to  $\infty$ . Then perform a  $u$ -substitution with  $u = x^2$  to convert your result into the form of Eq. 1 and thus show  $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$ .

[Note: We can also express this relation as  $(-\frac{1}{2})! = \sqrt{\pi}$ .]

(c) Let  $n$  be a non-negative integer. Perform a similar  $u$ -substitution to find an expression for  $\int_0^\infty x^n e^{-x^2} dx$  in terms of the gamma function. From this, find  $\int_{-\infty}^\infty x^n e^{-x^2} dx$  in the two cases where  $n$  is even and  $n$  is odd.

Answer (highlight to reveal): [You should find that  $\int_0^\infty x^n e^{-x^2} dx = \frac{1}{2} \Gamma\left(\frac{n+1}{2}\right)$ ]

---

Next we expand to consider a  $d$ -dimensional space. Our task is to determine the “surface area” of a “sphere” in this space. In particular, in our  $d$ -dimensional space, we define the  $(d-1)$ -**sphere** to be the set of points a fixed radius from the origin. Let  $C_{d-1}$  to be the  $(d-1)$ -dimensional surface area of the unit  $(d-1)$ -sphere (that is, the sphere with radius 1). For example, when  $d = 2$ , the “surface area” (i.e. circumference) of the unit 1-sphere (the unit circle) is  $C_1 = 2\pi$ . When  $d = 3$ , the surface area of the unit 2-sphere (the unit sphere) is  $C_2 = 4\pi$ .

Consider the following  $D$ -dimensional Gaussian integral,<sup>5</sup>

$$\mathcal{I} \equiv \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \cdots \int_{-\infty}^{\infty} dx_d e^{-\sum_{i=1}^d x_i^2}.$$

We can change variables to higher-dimensional versions of spherical coordinates where the radial coordinate is defined by  $r^2 \equiv \sum x_i^2$ , where  $r$  ranges from 0 to  $\infty$ . The volume of a thin spherical shell of radius  $r$  and infinitesimal thickness  $dr$  in these coordinates becomes

$$dV = C_{d-1} r^{d-1} dr. \quad (3)$$

For example, in 3D the volume in spherical coordinates for a spherical shell of radius  $r$  and thickness  $dr$  is  $dV = C_2 r^2 dr = 4\pi r^2 dr$ . Therefore we can rewrite  $\mathcal{I}$  as a single integral,

$$\mathcal{I} = \int_0^{\infty} e^{-r^2} C_{d-1} r^{d-1} dr.$$

(d) Use the above expressions for  $\mathcal{I}$  and our previous results about Gaussian integrals to solve for  $C_{d-1}$ , the surface area of a  $(d-1)$ -dimensional unit sphere. What is the volume of a thin  $(d-1)$ -spherical shell of radius  $r$  and infinitesimal thickness  $dr$ ?

*Hint (highlight to reveal):* [Remember that for exponentials  $e^{\sum a_i} = \prod e^{a_i}$ .]

Ok, back to some physics. Suppose we have a monoatomic ideal gas of  $N$  particles with a fixed, known amount of internal energy  $U$ . The energy is the sum of all the kinetic energies of the  $N$  constituent particles. In terms of momenta,

$$U = \sum_{i=1}^N \sum_{a=1}^3 \frac{p_{i,a}^2}{2m},$$

where  $i$  indexes the  $N$  gas particles,  $a = \{1, 2, 3\}$  or  $a = \{x, y, z\}$  indexes the three components of momenta, and  $m$  is the mass of the particle. In **momentum space**, the  $3N$ -dimensional space of all possible momenta in our system, this equation defines a  $(3N-1)$ -sphere! (E.g. a 2-sphere of radius  $r$  can be defined by the equation  $r^2 = x^2 + y^2 + z^2$ .)

(e) Given energy  $U$ , what is the radius of the  $(3N-1)$ -sphere in momentum space? If we were to allow a very small  $\epsilon \ll U$  tolerance in our energy (so the energy is within  $\epsilon$  of  $U$ ), what would the associated tolerance in radius  $dr$  be? What is the volume of momentum space corresponding to energy  $U$  with tolerance  $\epsilon$ ?

*Hint (highlight to reveal):* [This last bit is basically an extension of your answer in part (d). For  $dr$ , don't forget your Taylor expansions (for real this time).]

Next suppose our ideal gas were contained in a box with a fixed, known volume  $V$ . The three parameters  $U, V, N$  determine the macrostate of our system. The question we want to ask is “what volume of **phase space** is consistent with this macrostate?” The phase space consists of  $6N$  dimensions (3 each for the spatial position of each particle and 3 each for the momentum of each particle). We will go over this in more detail in lecture but the basic result here is that our phase space volume is

$$(\text{Volume in phase space}) = V^N \cdot (\text{volume from part (e)}).$$

To “count microstates” we divide this volume by some natural phase space unit cell so that there is one state per cell. For various reasons that originate from quantum mechanics, the natural phase

<sup>5</sup>When we start getting lots of integration variables, it is customary to put the differential for the variable of integration immediately after the integral sign followed by the integrand as done here. It is the notational difference between  $\int f(x)dx$  and  $\int dx f(x)$  - both mean the same thing and can be used interchangeably.

space unit in a  $D$ -dimensional phase space is  $h^{D/2}$  (phase spaces are always even-dimensional). For *other* reasons that originate from quantum mechanics there is also an overcounting due to the identical nature of particles, so we divide our count by the number of permutations of the particles, leaving

$$\Omega(U, V, N) = \frac{1}{N!} \frac{(\text{Volume in phase space})}{h^{3N}}.$$

**(f) Extra Part (Not for Credit)** Check that your above work is right by showing

$$\Omega(U, V, N) = \frac{1}{N! \Gamma(\frac{3N}{2})} \left( \frac{2\pi m U}{h^2} \right)^{3N/2} V^N \frac{\epsilon}{U}. \quad (4)$$

As a second check, make sure this is in fact a dimensionless result, as we expect for a “number of states”.

It turns out that we are justified in approximating Eq. 4 by

$$\Omega(U, V, N) = \frac{1}{N! (\frac{3N}{2})!} \left( \frac{2\pi m U}{h^2} \right)^{3N/2} V^N = f(N) V^N U^{3N/2}, \quad (5)$$

which agrees with Eq. 2.40 in Schroeder.

**(g)** Use Stirling’s approximation on Eq. 5 to find an expression for the entropy  $S(U, V, N)$  of the ideal gas.

[Note: Don’t bother with the  $\sqrt{2\pi N}$  terms in the Stirling approximation.]

[Supplementary Part (Not for Credit): Use your answer to find the change in entropy keeping  $U$  and  $N$  constant while changing volumes from  $V_0$  to  $V_1$ .]

**(h)** Use your result for  $S(U, V, N)$  to find the temperature. Is this consistent with what you’d expect from equipartition?

[Supplementary Part (Not for Credit): You can also find  $P$  and  $\mu$ .]

## Problem 5.3 - DataHub - Ehrenfest’s Fleas

In this DataHub problem we will explore the *Ehrenfest dog flea* model. This model is an important one in the history of statistical physics and was proposed by the wife-husband physicist team of Tatyana and Paul Ehrenfest<sup>6</sup> and continues the time-honored tradition of using pets for thought experiments in physics. In the model, there are a fixed total number of  $N$  fleas infesting two dogs. The two dogs represent an “isolated system”, though the fleas can freely jump from one dog to the other. This is another example of a binary model system and the microstate will be specifying which dog each of the  $N$  fleas are on. The macrostate will be given by specifying  $N_1$ , the number of fleas on Dog 1. Dog 2 would necessarily be infested by the remaining  $N_2 = N - N_1$  fleas.

Note that the writeup in this problem uses  $g(N_1; N)$  to represent the number of microstates in the macrostate with  $N_1$  fleas on Dog 1 and  $N$  fleas total whereas we use  $\Omega(N_1; N)$ . The notation  $\mathcal{T}(x(t+1) | x(t))$  is to be read “the transition probability  $\mathcal{T}$  of finding the system in state  $x(t+1)$  at time step  $t+1$  given that the system was in the state  $x(t)$  at time step  $t$ .”

<sup>6</sup>They also co-authored the classic 1911 review “The Conceptual Foundations of the Statistical Approach to Mechanics”.

You do *not* need to do parts (d) or (e). Their answers are given below, though!  
[http://datahub.berkeley.edu/user-redirect/interact?account=ajh38&repo=phy112-001\\_spring\\_2023&branch=main&path=Sp23-112-Hw05-Python](http://datahub.berkeley.edu/user-redirect/interact?account=ajh38&repo=phy112-001_spring_2023&branch=main&path=Sp23-112-Hw05-Python)

---

**Answer for part (d)** If  $x(t+1)$  and  $x(t)$  differ in exactly one location (i.e. that particular flea has just jumped dogs), then  $\mathcal{T}(x(t+1) | x(t)) = 1/N$  (because each of the  $N$  fleas is equally likely to jump). Otherwise it is 0. Since  $\mathcal{T}$  is a transition matrix between microstates and there are  $2^N$  microstates total, this is a  $(2^N \times 2^N)$ -matrix which requires  $2^{2N}$  entries! Granted, most of these entries are 0, but that's still *far too big*. For  $N = 50$ , we would need  $2^{100}$  bits, equivalent to 158000 yottabytes (YB) (or, using the newly defined metric prefixes for  $10^{27}$  and  $10^{30}$ , 158 ronabytes (RB) or 0.158 quettabytes (QB)). We can make this more efficient using the sparseness of the matrix but still...

---

**Answer for part (e)** If we restrict ourselves to the *macrostate* transitions, this becomes significantly more tractable. Given  $N$  fleas, there are only  $N + 1$  possible values of  $N_A$  and we reduce the transition matrix to an  $((N + 1) \times (N + 1))$ -matrix. This only contains  $(N + 1)^2$  entries. Assuming each entry takes up 1 byte, the full matrix (ignoring efficiencies again) would only use up  $51^2$  bytes or 2.6 kB.

If we are in macrostate  $N_1$ , then a single jumping flea can either increase  $N_1$  by 1 (if the flea jumped from Dog 2 to Dog 1) or decrease  $N_1$  by 1 (if the flea jumped from Dog 1 to Dog 2). Thus,

$$\begin{aligned}\mathcal{T}(N_1(t+1) = N_1(t) - 1 | N_1(t)) &= N_1(t)/N, \\ \mathcal{T}(N_1(t+1) = N_1(t) + 1 | N_1(t)) &= N_2(t)/N = (N - N_1(t))/N, \\ \mathcal{T}(N_1(t+1) \neq N_1(t) \pm 1 | N_1(t)) &= 0.\end{aligned}$$

---

---

## Not for Credit - DataHub - Two Systems in Energy Equilibrium

I have added a second problem to the data hub, titled “*Two Systems in Energy Equilibrium*”. This is a Python-enhanced version of the paramagnet problem. Parts (a), (b), and (d) are basically versions of parts of Problem 5.1. The interesting bits are the plots in part (c) and (e) to explore the approach to equilibrium! Solutions to this will be released so even if you never get around to doing it you can see some of the results and how the solution was implemented.



*This content is protected and may not be shared, uploaded or distributed.*