Statistical Mechanics - 2019-2 - Problem set 1

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Deadline: 24/09

This problem set is all about *spin*, from quantum to classical and back again.

1. **Spinzão:** there are many systems in nature which behave like macroscopic spins, which are not necessarily 1/2. One example are the so called single-molecule magnets, such as Mn_{12}. Recall that spin can in general take on either integer or half-integer values, $S = 1/2, 1, 3/2, 2, \ldots$. When a system has spin S it means that the spin components in any given direction can take on any value between S and $-S$ in integer steps:

$$s = S, S-1, \ldots, -S+1, -S. \tag{1}$$

When a spin S is placed in contact with a magnetic field h, the energy eigenvalues become

$$E_s = -hs, \tag{2}$$

where I chose simplified units such that h has dimensions of energy. The eigenvalues are thus equally spaced, with the ground-state being $s = S$ (spin fully aligned with the field).

(a) Compute the partition function[1], $Z = \sum_s e^{-\beta E_s}$.

(b) The magnetization is defined as

$$M = \langle s \rangle = \frac{1}{Z} \sum_{s=-S}^{S} s e^{-\beta E_s}, \tag{3}$$

Show that the magnetization can be computed as

$$M = -\frac{\partial F}{\partial h} = T \frac{\partial}{\partial h} \ln Z, \tag{4}$$

where $F = -T \ln Z$ is the Helmholtz free energy.

(c) Compute the magnetization and write it in terms of the Brillouin function

$$B_S(x) = \frac{2S+1}{2S} \coth\left(\frac{2S+1}{2S} x\right) - \frac{1}{2S} \coth\left(\frac{x}{2S}\right). \tag{5}$$

(d) Analyze your result. Explore the physics. Make plots. Check what happens in limiting cases (zero field, large field, zero temperature, large temperature, etc.).

(e) The classical limit is when the spin is not restricted to a discrete set of values, but can take on any value continuously between $-S$ and S. You can obtain this limit from the result of the previous exercise by taking $S \to \infty$. But this cannot be done naively; we don't really want $S = \infty$, since that is unphysical. We just want S large enough so

[1]The following result may be useful:

$$\sum_{n=0}^{L} x^n = \frac{1 - x^{L+1}}{1 - x}$$

For a derivation, see the appendix of Lecture note 1.

that the discreteness becomes unimportant. The correct way to do this is to pinpoint which quantities should increase with S (from a physical perspective). There are two in this problem: the magnetization and the energy. Thus, we have to take the limit $S \to \infty$, but keeping $m = M/S$ and hS finite. Show that in this limit one can write the magnetization in terms of the Langevin function

$$L(x) = \coth(x) - \frac{1}{x}. \tag{6}$$

2. **Classical spins:** Continuing from the previous exercise, one can also, from the start, formulate the problem for a classical spin, modeled as a vector $\boldsymbol{s} = (s_x, s_y, s_z)$ lying on a sphere of radius S (where S is an arbitrarily large number). Since the radius of the sphere is fixed, we can parametrize

$$s_x = S\,\sin\theta\cos\phi, \qquad s_y = S\,\sin\theta\sin\phi, \qquad s_z = S\,\cos\theta, \tag{7}$$

where $\theta \in [0, \pi)$ and $\phi \in [0, 2\pi]$ are the usual spherical angles. If the field is applied in the z direction, the energy (2) becomes

$$E(\theta, \phi) = -hs_z = -hS\,\cos\theta.$$

Moreover, sums now become integrals over the sphere. For instance, the partition function becomes

$$Z = \int e^{-\beta E(\theta,\phi)} \sin\theta \,\mathrm{d}\theta\,\mathrm{d}\phi \tag{8}$$

where $\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$ is the element of solid angle in the sphere.

(a) Compute the partition function.

(b) Compute the magnetization. Your results should match those of exercise 1(e).

(c) Suppose now that the energy of the system is given instead by

$$E(\theta, \phi) = -hS\,\cos\theta - \frac{kS}{2}\cos^2\theta, \tag{9}$$

where $k > 0$. This last term is sometimes called a *uniaxial anistropy*. It essentially pushes the system to lie within the z axis, irrespective of whether it is up or down (unlike the magnetic field which makes it point up). The magnetization now can no longer be computed analytically. Instead, let us focus on the case of low field, for which all quantities can be computed using series expansions. Show that for small h the magnetization has the form

$$M = \frac{S^2\mathcal{R}}{T}h, \tag{10}$$

where

$$\mathcal{R} = \frac{\int_{-1}^{1} \mathrm{d}z\; z^2 e^{\beta k S z^2/2}}{\int_{-1}^{1} \mathrm{d}z\; e^{\beta k S z^2/2}}. \tag{11}$$

3. **Lipkin-Meshkov-Glick model, part 1:** Quantum mechanically, a system of spin S can be characterized by three operators S_x, S_y and S_z satisfying the canonical commutation relations

$$[S_x, S_y] = iS_z, \tag{12}$$

(and cyclic permutations). We usually choose to work on the basis where S_z is diagonal. Its eigenvalues and eigenvectors will then have the form

$$S_z|s\rangle = s|s\rangle, \qquad s = S, S-1, \ldots, -S+1, -S, \tag{13}$$

which are essentially the eigenvalues we used in problem 1. In this basis the operators S_x and S_y are not diagonal. Defining $S_\pm = S_x \pm iS_y$, it can be shown (you can check any quantum mechanics book) that

$$S_+|s\rangle = \sqrt{(S-s)(S+s+1)}|s+1\rangle, \tag{14}$$

$$S_-|s\rangle = \sqrt{(S+s)(S-s+1)}|s-1\rangle. \tag{15}$$

With these expressions, we can now construct the matrix elements of S_x and S_y.

(a) Construct the spin matrices S_x, S_y and S_z for spin 1.

(b) Consider now the Lipkin-Meshkov-Glick (LMG) model, described by the Hamiltonian

$$H = -hS_z - \frac{k}{2S} S_x^2, \tag{16}$$

where $k > 0$ is a constant. Notice the similarity with Eq. (9). The 2nd term is also a uniaxial anistropy, but applied instead at the x direction. This model is non-trivial because there are two competing terms in the Hamiltonian and these terms do not commute. Compute the partition function of the Hamiltonian (16) for the case of spin 1.

(c) Study the heat capacity. The formulas may be ugly, but making plots are easy. You can set the energy scale so that $k = 1$, which leaves you with only h and T as parameters.

(d) Study the entropy.

(e) Compute the magnetization in the z direction, $M = \langle S_z \rangle$.

4. **Spin coherent states:** It is possible to connect quantum with classical spins using the notion of spin coherent states, which are defined as

$$|\theta, \phi\rangle = e^{-i\phi S_z} e^{-i\theta S_y} |s = S\rangle, \tag{17}$$

where $|s = S\rangle$ means the highest spin state of S_z. The operator $e^{-i\theta S_y}$ does a rotation around the y axis by an angle θ, whereas $e^{-i\phi S_z}$ rotates by ϕ around z. Thus, the state (17) essentially means we start in the north pole, rotate by θ around y and then by ϕ around z. This is exactly how you get to a point (θ, ϕ) [as in Eq. (7)] in the unit sphere.

Show that the average of the spin operators in the spin-coherent state (17) read

$$\langle S_x \rangle = S \sin\theta \cos\phi, \qquad \langle S_y \rangle = S \sin\theta \sin\phi, \qquad \langle S_z \rangle = S \cos\theta, \tag{18}$$

which is exactly the same structure as Eq. (7), even though this holds for arbitrary S. To prove this you will need the BCH formula

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \ldots \tag{19}$$

Spin coherent states are therefore the closest one can get to classical physics when dealing with quantum mechanical spins. They are the key for understanding the transition from quantum to classical as S increases. If you want to know more, a good reference is J. M. Radcliffe, "Some properties of coherent spin states," *J. Phys. A.* **4**, 313–323 (1971).

5. **Lipkin-Meshkov-Glick model, part 2:** Consider again the LMG model (16). This model saw a revival of popularity around 10 years ago because, in the limit $S \to \infty$, it presents a quantum phase transition. In fact, the LMG model can be viewed as a mean-field version of the transverse field Ising model (this sentence probably didn't make any sense now, but I promise until the end of the semester it will!). A quantum phase transition is an abrupt transition in the ground-state of the model as one changes a parameter in the Hamiltonian. It is thus a $T = 0$ effect: it is independent of thermal fluctuations and depends only on the quantum fluctuations of the ground-state.

   For arbitrary S the ground-state of Eq. (16) will be very complicated [if you want, you can compute it numerically using the matrix elements in Eqs. (14) and (15)]. But as $S \to \infty$, it can be shown that the ground-state becomes closer and closer to a spin coherent state (17), for some value of θ and ϕ. Consider then the average of H in (17),

$$E(\theta, \phi) = \langle \theta, \phi | H | \theta, \phi \rangle. \tag{20}$$

   In the limit of $S \to \infty$ one may show that the dominant terms have the form

$$E(\theta, \phi) = -hS \cos\theta - \frac{kS}{2} \sin^2\theta \cos^2\phi. \tag{21}$$

   The ground-state will be the minimum of $E(\theta, \phi)$ as a function of θ and ϕ. Show that this minimum has an abrupt transition as a function of the magnetic field h. This problem is entirely at $T = 0$. It refers only to the ground-state. Determine the critical field h_c where this happens. Analyze the magnetization in the z direction, $M = \langle S_z \rangle = S \cos\theta$ as a function of h.

We will come back to the LMG model later on, but if you want to learn more about it, a paper which I like is `arXiv0805.4078`.