Quantum statistical mechanics

Now that we know how to operate with density matrices, we are ready to formulate a fully quantum mechanical version of equilibrium and non-equilibrium statistical mechanics

If a system of Hamiltonian H thermalizes to a temperature $\beta = 1/T$, then its state will be given by the Gibbs density matrix

$$\rho = \frac{e^{-\beta H}}{Z} \tag{1}$$

where

$$Z = \mathrm{tr}(e^{-\beta H}) \tag{2}$$

The expectation value of any observable is then

$$\langle A \rangle = \mathrm{tr}(A\rho) = \frac{\mathrm{tr}(A e^{-\beta H})}{\mathrm{tr}(e^{-\beta H})} \tag{3}$$

Written in this way, Eqs (1) - (3) are completely basis independent and provide an operator formulation for the equilibrium problem. This is quite useful because if we are dealing with a many-body system, the eigenenergies E_n will be quite complicated to list out. Of course, this doesn't mean our previous formulation no longer holds. For instance

$$U = \langle H \rangle = \mathrm{tr}(H\rho) = \sum_n E_n P_n$$

Feel free to choose $\mathrm{tr}(H\rho)$ or $E_n P_n$, whatever is more convenient for the problem at hand.

Some spin models we will deal with in this course

Spin models offer a really clean platform for understanding interacting systems and cool phenomena such as phase transitions, frustration and so on.

Consider a system of N spin 1/2 (qubit) particles, each described by Pauli operators σ_x^i, σ_y^i, σ_z^i, $i = 1, \dots N$. The simplest, although still incredibly interesting model is the Ising model, described by the Hamiltonian

$$H = \sum_{i,j} J_{ij} \, \sigma_z^i \sigma_z^j \tag{4}$$

where J_{ij} describes the coupling between spins i and j. The most common situation is when the spins are displaced in a regular lattice and only have nearest neighbor interactions.

For instance, in a 1D lattice we would have

$$H = J \sum_{i=1}^{N-1} \sigma_z^i \sigma_z^{i+1} \tag{5}$$

For general lattices, we usually write

$$H = J \sum_{\langle i,j \rangle} \sigma_z^i \sigma_z^j \tag{6}$$

where the symbol $\langle i,j \rangle$ means a sum over nearest neighbors.

The Ising model (4) is very special in that we already know all its eigenvalues and eigenvectors: they are simply the eigenvectors of all σ_z^i operators, which we define as

$$|\sigma\rangle := |\sigma_1, \dots, \sigma_N\rangle \qquad \sigma_i = \pm 1 \tag{7}$$

which are such that

$$\sigma_z^i |\sigma\rangle = \sigma_i |\sigma\rangle \tag{8}$$

Thus, applying (4) to (7) we get

$$H |\sigma\rangle = E(\sigma) |\sigma\rangle \tag{9}$$

where the eigenenergies are

$$E(\sigma) = \sum_{ij} J_{ij} \sigma_i \sigma_j \tag{10}$$

In total there are 2^N different eigenenergies, so listing them out becomes quite cumbersome even for moderately large N.

To compute the partition function (2), the obvious choice is to take the trace using the $|\sigma\rangle$ basis

$$Z = \mathrm{tr}(e^{-\beta H}) = \sum_{\{\sigma\}} \langle \sigma | e^{-\beta H} | \sigma \rangle = \sum_{\{\sigma\}} e^{-\beta E(\sigma)} \tag{11}$$

Here the notation $\{\sigma\}$ means a sum over all 2^N configurations of $(\sigma_1, \dots, \sigma_N)$. For instance if we had $N=2$ then we would have 4 terms in the sum

$$Z = e^{-\beta E(++)} + e^{-\beta E(+-)} + e^{-\beta E(-+)} + e^{-\beta E(--)} \tag{12}$$

This makes for an interesting point: even though we know all eigenvalues of H, it doesn't mean we can compute the partition function for arbitrary N. Indeed, for a 1D lattice the calculation is ok, for a 2D lattice it is quite hard and for a 3D lattice no one has found a solution yet.

What makes the Ising model (4) so special is that is a sum of commuting terms: z operators always commute among each other. There is currently a lot of interest in models with non-commuting parts. The most famous is called the transverse field Ising model (TFIM)

$$H = \sum_{ij} J_{ij} \, \sigma_z^i \sigma_z^j - h \sum_i \sigma_x^i \tag{13}$$

It is a "transverse" field because the last term contains a σ_x operator, instead of σ_z. This Hamiltonian is now a sum of non-commuting terms, so before we can even think about computing partition functions, we still need to find a way to diagonalize it. This model can be diagonalized exactly only in 1D. In 2D and 3D we still don't know how to do it.

I should point out that the choice of x and z in Eq (13) is arbitrary. Thus (13) is physically equivalent to

$$H = \sum_{ij} J_{ij} \, \sigma_x^i \sigma_x^{i+1} - h \sum_i \sigma_z^i \tag{14}$$

Classical and quantum phase transitions

Phase transitions are one of the coolest things in nature! It represents an abrupt change in the configuration of the system which occurs due the interactions between the particles in the system. Phase transitions are therefore collective effects, in the sense that they have nothing to do with the individual particles, but rather with how the particles interact with each other.

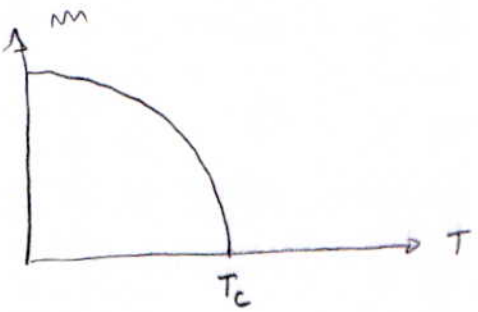
But more than being collective, phase transitions are above all else emergent properties. This terms has a very specific physical meaning. It refers to properties which appear (emerge) when the number of particles becomes very large (which is what we call the thermodynamic limit). Thus, an emergent property is a feature which is related to the mind boggling complexity of 10^{23} particles insanely interacting with other.

To give a kind of analogy, life is an emergent property. Quite definitely, life stems from chemical bonds between a bunch of atoms. But life is also much much more than that. We cannot understand life from the chemical reactions alone. For more neat discussions about this, have a look at Phillip Anderson's paper "More is different".

Spin systems offer a clean platform for studying phase transitions. The Ising model (4) has a phase transition for any dimension above 1. The transition is characterized by an <u>order parameter</u>, which in this case is the magnetization

$$\boxed{m = \frac{1}{N}\sum_{i=1}^{N} \langle \sigma_z^{\,i} \rangle} \qquad (15)$$

The order parameter is something which is non-zero in one phase but identically zero in another. Something like



The point where $m=0$ is called the critical point and T_c is the critical temperature. If $T > T_c$ then the system is said to be in a paramagnetic phase (PM) and if $T < T_c$ it is in a ferromagnetic phase (FM). We say that for $T < T_c$ the system develops an <u>spontaneous</u> <u>magnetization</u>.

To give an example, for the 2D Ising model, Onsager showed in 1948 that

$$\boxed{m = \left[1 - \frac{1}{\sinh^4(2J/T)} \right]^{1/8}} \qquad (16)$$

The critical point is when $m=0$ for the first time. The solution to

$$\sinh(x) = 1$$

is

$$x = \ln(1+\sqrt{2})$$

thus

$$\boxed{T_c = \frac{2J}{\ln(1+\sqrt{2})} = 2.26919\ J} \qquad (17)$$

these results were of enormous historical importance, as we will discuss below

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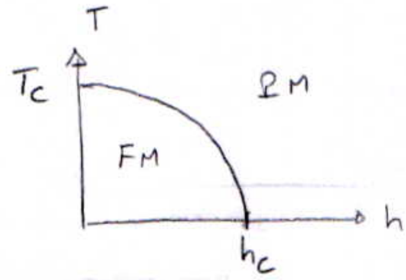
The phase transition of the Ising model is called a classical phase transition because it is related to the thermal fluctuations induced by the temperature T. The TFIM (13), on the other hand, presents a <u>quantum phase transition</u>, which occurs at zero temperature and is driven by quantum fluctuations instead.

Quantum phase transitions are therefore related to abrupt changes in the ground-state of a quantum system, which occurs due to a competition of different terms in a Hamiltonian. In the case of (13), the parameter that drives the transition is the transverse field h.

If $h=0$ we get the usual Ising model. But if h is infinitely large then the system (13) will polarize in the x direction so $\langle\sigma_z^i\rangle = 0$.

We can then draw a phase diagram in terms of T and h. It will look like this

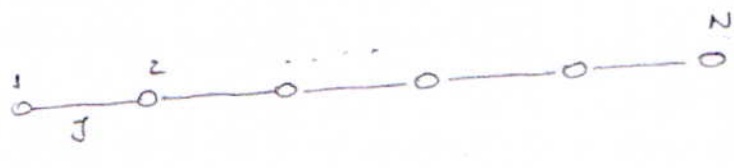


If $h=0$ we are on the classical Ising line and if $T=0$ we are on the quantum line. For non-zero h and T we get something in between.

A more thorough understanding of this interplay between quantum and classical phase transitions constitutes one of the most widely studied topics nowadays, with ramifications from condensed matter to high energy physics

Classical Ising model in 1D

Enough bla bla bla. Let's get our hands dirty. I want to illustrate to you know some of the challenges in dealing with many-body systems. We shall follow Ising's PhD thesis and compute the partition function for the classical Ising model in 1D:



The Hamiltonian we shall study is the same as (5), but we will also introduce a longitudinal field

$$H = -J \sum_{i=1}^{N} \sigma_z^i \sigma_z^{i+1} - h \sum_{i=1}^{N} \sigma_z^i \tag{18}$$

Here I also assume periodic boundary conditions (PBC), which means we define $\sigma_z^{N+1} = \sigma_z^1$, so there is also a term $\sigma_z^N \sigma_z^1$. This doesn't change the physics when N is large, but is convenient because it imposes translation invariance.

As discussed before, the Hamiltonian (18) is already diagonal in the computational basis, with energy eigenvalues

$$E(\sigma) = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - h \sum_{i=1}^{N} \sigma_i \tag{19}$$

where $\sigma_i = \pm 1$ are now c-numbers instead of operators.

Our goal now is to compute the partition function

$$Z = \sum_{\{\sigma\}} e^{-\beta E(\sigma)} \tag{20}$$

where the sum is over the 2^N possible spin configurations. This sum is not easy because the spins interact with other. If they didn't then the sum would factor and we would get $Z = Z_1^N$. But when they interact that no longer happens.

Let us write (20) as

$$Z = \sum_{\{\sigma\}} \exp\left\{ \beta J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} + \beta h \sum_i \sigma_i \right\} \tag{21}$$

Now I will write it in a sort of silly, but more symmetrical way

$$Z = \sum_{\{\sigma\}} \exp\left\{ \sum_{i=1}^{N} \left[\beta J \sigma_i \sigma_{i+1} + \frac{\beta h}{2} (\sigma_i + \sigma_{i+1}) \right] \right\} \tag{22}$$

I divide βh by 2 because we are summing each site twice.

Next we define the function

$$V(\sigma_1, \sigma_2) = e^{\beta J \sigma_1 \sigma_2 + \frac{\beta h}{2}(\sigma_1 + \sigma_2)} \tag{23}$$

so that Z may be written as

$$Z = \sum_{\{\sigma\}} V(\sigma_1, \sigma_2) V(\sigma_2, \sigma_3) \dots V(\sigma_{N-1}, \sigma_N) V(\sigma_N, \sigma_1) \tag{24}$$

This formula clearly shows why the sum in Z doesn't factor out into a product of terms. However, it also introduces a neat idea on how we may compute the sum. Suppose we interpret the function $V(\sigma_1, \sigma_2)$ as the entries of a 2×2 matrix, which we call the transfer matrix

$$V = \begin{pmatrix} V(++) & V(+-) \\ V(-+) & V(--) \end{pmatrix} = \begin{pmatrix} e^{\beta J + \beta h} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta h} \end{pmatrix} \qquad (25)$$

Then (24) is looking like some type of matrix product. Actually it looks like trace. The trace of a matrix A is

$$tr(A) = \sum_i A_{ii}$$

and the trace of A^2 is

$$tr(A^2) = \sum_i (A^2)_{ii} = \sum_{ij} A_{ij} A_{ji}$$

and A^3

$$tr(A^3) = \sum_{ijk} A_{ij} A_{jk} A_{ki}$$

and so on. We see that this is precisely the structure appearing in (24). In fact even the last term $V(\sigma_N, \sigma_1)$ fits in perfectly. Thus, we conclude that

$$\boxed{Z = tr(V^N)} \qquad (26)$$

This expression is now easy to compute, as V is just a 2×2 matrix.

The eigenvalues of V are

$$\lambda_{\pm} = e^{\beta J}\cosh(\beta h) \pm \sqrt{e^{-2\beta J} + e^{2\beta J}\sinh^2(\beta h)} \tag{27}$$

But the trace is the sum of eigenvalues and the eigenvalues of V^N are simply λ_+^N and λ_-^N. Hence we get

$$Z = \lambda_+^N + \lambda_-^N \tag{28}$$

It is also useful to note that

$$\begin{aligned} tr(V) &= \lambda_+ + \lambda_- = 2e^{\beta J}\cosh(\beta h) \\ \det(V) &= \lambda_+ \lambda_- = 2\sinh(2\beta J) \end{aligned} \tag{29}$$

Thus both are clearly positive. Moreover from (27) we have $\lambda_+ > \lambda_-$. Hence, let us write Z as

$$Z = \lambda_+^N \left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N \right] \tag{30}$$

then $\lambda_-/\lambda_+ < 1$ so when N gets large then extra term will become smaller and smaller. In the thermodynamic limit, $N \to \infty$, we then get

$$\boxed{Z = \lambda_+^N} \tag{31}$$

And we are done! All that is left is to have fun with pretty plots

The free energy will be

$$\boxed{F = -T \ln Z = -NT \ln \left\{ e^{\beta J} \cosh(\beta h) + \sqrt{e^{-2\beta J} + e^{2\beta J} \sinh^2 \beta h} \right\}} \quad (32)$$

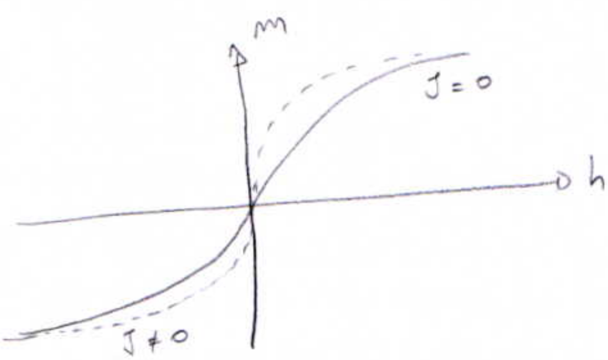
The free energy is clearly extensive, as expected. From this we get the magnetization

$$\boxed{m = -\frac{1}{N} \frac{\partial F}{\partial h} = \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}} \quad (33)$$

If $J=0$ we get

$$m = \tanh(\beta h) \quad (34)$$

which is a result we already found before. The result (33) looks a lot like (34), but a bit more stiff



But when $h \to 0$ we always have $m = 0$, except if $T \equiv 0$. Thus the Ising model in 1D has no phase transition, except at $T = 0$.

This is precisely what Ising conclude in this PhD thesis. But then he erroneously conclude that this would also happen for other dimensions. And that turns out not to be true. The Ising model does have a phase transition in 2D and 3D, so 1D is actually the exception.