Physics 212: Statistical mechanics II
Lecture XXI-XXII

For the past few lectures, we have been discussing some of the complex dynamical phenomena that can appear in classical statistical mechanics. In this final lecture, we turn to quantum systems where the dynamics and statics are both derived from the quantum-mechanical Hamiltonian. Our goal will be to show that in some cases there is a connection between quantum phase transitions at zero temperature, and classical phase transitions at finite temperature.

We previously gave an argument that, because of loss of phase coherence at sufficiently long times and distances, finite-temperature critical points were essentially unmodified (at least as far as universal, long-distance properties) by quantum mechanics. At zero temperature, this no longer holds: if a system has a transition between two ground states as a function of some parameter, then at this transition quantum effects will generally be very important.

We can divide such quantum phase transitions into two classes according to whether there is or is not a phase transition in the classical system at finite temperature. Experimentally, it is now possible in a number of systems to see signs of quantum critical behavior at low but nonzero temperature.

An example we discuss that is of relevance to some magnetic materials is the quantum or transverse-field Ising model. First consider the ordinary Ising model in one dimension,

$$H = -K \sum_i \sigma_i^z \sigma_{i+1}^z - h \sigma_i^x. \quad (1)$$

We can either think of the spins as classical Ising spins or as quantum spin-half variables, since even if the spins in the above are quantum spins, the above calculation gives the same result since we can go to the $z$ basis where all operators in the Hamiltonian are diagonal.

The quantum or transverse-field Ising model is just

$$H = -K \sum_i \sigma_i^z \sigma_{i+1}^z - h \sigma_i^x. \quad (2)$$

It turns out that having the magnetic field point in a different direction than the easy-axis of the spins dramatically changes the physics. It turns out that this “quantum Ising model” has a zero-temperature phase transition that is in the universality class of the classical 2D Ising model, which was solved by Onsager. The reason you may see textbooks writing $h = gK$ for the quantum Ising model is that, since the ground state is unchanged if we just multiply the entire Hamiltonian by a constant, we can think of the ground state as just a function of the dimensionless number $g$.

The classical Ising partition function in one dimension can be written as, with $M$ the number of spins,

$$Z = \sum_{\sigma_i^z} \prod_{i=1}^M T_1(\sigma_i^z, \sigma_{i+1}^z) T_2(\sigma_i^z) \quad (3)$$

where $T_1(\sigma_i^z, \sigma_j^z) = \exp(K \sigma_i^z \sigma_j^z)$, $T_2(\sigma_i^z) = \exp(h \sigma_i^z)$. (These give the same transfer matrix $T = T_1 T_2$ that was derived earlier in the course.) But this product is equivalent to a matrix product:
for periodic boundary conditions on the chain of spins,

\[ Z = \text{Tr}(T_1 T_2 T_1 T_2 \ldots) = \text{Tr}(T_1 T_2)^M. \]  

(4)

Using this it is easy to work through the full transfer-matrix solution of the classical limit, including, for example, the correlation between two spins in zero field:

\[ \langle \sigma_i^z \sigma_j^z \rangle = (\tanh K)^{|j-i|} \]  

(5)

which gives the result for the correlation length

\[ \xi^{-1} = -a^{-1} \log(\tanh K), \]  

(6)

where \( a \) is the lattice spacing. In the low-temperature limit \( K \gg 1, \xi \approx a e^{2K}/2 \). We will be interested in scaling properties when \( \xi \gg a \), as only then is the physics “universal” and independent of short-length-scale details.

Now we will show that the above model in its \textbf{scaling limit}, when the correlation length is much larger than a lattice spacing, can really be viewed as the quantum mechanics of a single Ising spin. We can write

\[ T_1 = e^K (1 + e^{-2K} \hat{\sigma}^x) \approx e^K (1 + (a/2\xi) \hat{\sigma}^x), \quad T_2 = \exp(a \hat{\sigma}^z (h/a)). \]  

(7)

We will first consider the case with \( h = 0 \) in the classical model. Consider the quantum partition function of a single spin,

\[ Z = \text{Tr} e^{-H_Q/kT}. \]  

(8)

We are going to show that the above expression for the partition function can be related to the classical model. Recall the following mathematical identity, which you probably saw in your single-variable quantum mechanics class:

\[ e^x = \lim_{n \to \infty} (1 + x/n)^n. \]  

(9)

To prove this, note that expanding by the binomial formula gives the Taylor expansion for \( e^x \). The “Trotter product formula” is the generalization of this result to matrices, and applied to our problem and, introducing a small “imaginary time step” \( \Delta \tau \) equivalent to \( 1/n \), it gives

\[ e^{-H_Q/kT} = \left( e^{-H_Q} \right)^\beta = \lim_{\Delta \tau \to 0} (1 - H_Q \Delta \tau)^{\beta/\Delta \tau}. \]  

(10)

Now this will resemble our classical expansion if we can relate \( 1 - H_Q \Delta \tau \) to \( T_1 T_2 \). Defining

\[ H_Q = -h_x \sigma_x, \]  

(11)

where \( 2h_x \) gives the splitting of the energy levels of the quantum spin, we have

\[ 1 - \Delta \tau H_Q = 1 + h_x \Delta \tau \sigma_x. \]  

(12)

This will look similar to what we obtained above for \( T_1 T_2 \) provided that

\[ h_x \Delta \tau = e^{-2K} = \frac{a}{2\xi}, \]  

(13)
or \( h_x = \frac{a}{2\xi \Delta \tau} \). However, there is still a neglected overall factor:

\[
T_1 = e^K (1 - \Delta \tau H_Q). \tag{14}
\]

The simplest way to take care of this is by defining a new quantum Hamiltonian \( \tilde{H}_Q \) shifted by a constant energy:

\[
\text{Tr}(T_1)^M \approx (1 - H_Q \Delta \tau)^{\beta/\Delta \tau} e^{K \beta/\Delta \tau} = e^{-H_Q \beta} e^{K \beta/\Delta \tau} = e^{-\beta \tilde{H}_Q} \tag{15}
\]

where the second equality applies as \( \Delta \tau \to \infty \). Here

\[
\tilde{H}_Q = H_Q - \frac{K}{\Delta \tau} \tag{16}
\]

so the energy shift is actually large (but a constant in the energy is not very important), and the number of spins \( M = \beta/\Delta \tau \to \infty \). The above connection is valid in the limit \( \Delta \tau \to 0 \), which means that \( e^{-2K} \to 0 \) so \( K \) is large: the effective temperature in the classical model is small, so that the classical model has a large correlation length, whenever the mapping is valid. Note that the temperature in the quantum model may be large or small.

Before interpreting this result, let me give a slightly different derivation using the notation of Sachdev’s book on quantum phase transitions, and add a magnetic field on the quantum spin. We imagine again a lattice spacing \( a \) in the classical problem. The so-called scaling limit will be taken as \( a \to 0 \) and the quantity \( \tilde{h} = h/a \) finite, which is why we have formed this combination in the exponent of \( T_2 \) above.

Now we claim that the transfer matrix can be viewed as the “quantum evolution operator” for a \((2 \times 2)\) Hamiltonian \( H_Q \):

\[
T_1 T_2 \approx \exp(-a H_Q/c), \tag{17}
\]

where \( c \) is a finite constant (units of energy times distance). If \( \tilde{h} \) is set to unity, then \( c \) has units of velocity, and \( a/c \) is the same as \( \Delta \tau \) in the above derivation. This works provided that

\[
H_Q = E_0 - \frac{\Delta}{2} \hat{\sigma}^x - \tilde{h} \hat{\sigma}^z \tag{18}
\]

with \( E_0 = -cK/a, \Delta = \frac{\xi}{2} \). With \( \tilde{h} = 0 \), this is essentially the same result as derived above in different notation.

So, going back to the classical partition function above,

\[
Z = \text{Tr}(T_1 T_2)^M = \text{Tr} \exp(-H_Q/kT) \tag{19}
\]

with \( 1/kT = \beta = L_T = Ma/c \), where \( L_T \) is the “length” of the system in the imaginary time direction. Note that the use of the Trotter product formula is not really explicit in the above, but we implicitly used it in dividing up \( e^{-H_Q/kT} \) into many small exponentials, and assuming that we could expand each of these to first order without a large cumulative error.

Note that the energy \( \Delta \) in this new notation is the gap between the two states of the single spin Hamiltonian in zero applied field:

\[
E = E_0 \pm \sqrt{(\Delta/2)^2 + \tilde{h}^2}. \tag{20}
\]

3
The gap is just (in the right units) the inverse of the correlation length in the classical model, which turns out to be a quite general property. So two important relations in this quantum-classical (QC) mapping are that the inverse temperature $\beta$ in the quantum model becomes the system size in the classical model, and the gap $\Delta$ in the quantum model becomes the inverse correlation length in the classical model. Points where the classical model has infinite temporal correlation length are points where the quantum model has zero energy gap. In this simple 1D model, the infinite temporal correlation length occurs only at zero temperature, but if the effective classical model for a quantum system were more than one-dimensional, it might have a phase transition.

This QC mapping is very powerful but not very intuitive at first glance. So far we have shown that the partition function of a quantum spin at low temperature is like that of a classical system of “length” $L_\tau = \beta$ in the continuum limit $a \to 0$.

In a similar way, coupling a chain of spins becomes, via the above QC mapping, a 2D classical Ising model. Before we go into the details of what this tells us about the quantum model, we show that the 1D quantum Ising model has an exact self-duality that is even simpler than that in the 2D classical Ising model. Suppose that we define new operators on the bonds of the original chain: let $s_i$ be the new spin-half degree of freedom on the bond between spins $\sigma_i$ and $\sigma_j$ of the original chain

$$s^z_i = \prod_{j<i} \sigma^x_j, \quad s^x_i = \sigma^z_i \sigma^z_{i+1}. \quad \text{(21)}$$

Then, using the fact that $(\sigma_i^h)^2 = 1$, it is easy to show that the original Hamiltonian is transformed into

$$H = -h \sum_i s^z_i s^z_{i+1} - K s^x_i. \quad \text{(22)}$$

The form of the Hamiltonian is the same, but the roles of $K$ and $h$ are reversed! One also has to check that the newly defined $s$ operators satisfy the same commutation relations as the operators in the original model; indeed they do. The duality of the 1D quantum Ising model is even simpler than that of the 2D classical Ising model: if there is a single phase transition, it must lie at $K = h$.

Now let’s see what we can understand about this 1D quantum Ising model using the QC mapping. It becomes a 2D Ising model with anisotropic couplings: the coupling in the imaginary-time direction is determined by the magnetic field in the quantum model,

$$h \Delta \tau = e^{-2K}. \quad \text{(23)}$$

Recall that as before $h$ and $K$ (in the quantum model) have units of energy, while $K_\tau$ and $K_x$ in the classical model are dimensionless. The classical coupling in the spatial direction is simpler, and differs from the quantum coupling only by a factor $\Delta \tau$ (exercise):

$$K \Delta \tau = K_x. \quad \text{(24)}$$

In the limit $\Delta \tau \to 0$ in which the QC mapping is valid, $K_\tau$ is large while $K_x$ is small. However, the exact critical line of the anisotropic 2D Ising model is known via the Kramers-Wannier duality: it is

$$\sinh 2K_x \sinh 2K_y = 1. \quad \text{(25)}$$

Under the limits we need for the QC mapping, this becomes

$$\frac{2K \Delta \tau}{2h \Delta \tau} = 1 \quad \text{(26)}$$
and we confirm that the critical point is at $K = h$ in the quantum model.

There is a good discussion in Cardy of the following problem: when one has a system that has both a classical phase transition at finite temperature, and a quantum phase transition at the $T = 0$ end of the classical phase transition line, when are the exponents of the quantum case observed? A simple argument can be made by comparing the correlation length $\xi$ with the size of the additional imaginary time dimension (proportional to inverse temperature). When the correlation length is longer (close to the critical point at finite temperature), the finiteness of the extra dimension is apparent, and the classical exponents are observed; when the correlation length is shorter than the size of the extra dimension (as is always true at zero temperature), then the quantum exponents are observed.

A question you might think about that does not seem to have a simple answer is whether there a signal of a truly quantum phase transition, i.e., one that cannot be related to a classical critical point via the above QC mapping. More precisely, there are quantum models where all the simple tricks to generate a classical version in one higher dimension yield models with imaginary Boltzmann weights, which makes obtaining either a numerical or analytical understanding much more difficult.