Quantum Phase Transitions

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May 2, 2000

Abstract

A quantum system can undergo a phase transition at zero temperature as some parameter of its Hamiltonian is varied. These quantum phase transitions are interesting because statics and dynamics are deeply correlated in quantum statistical mechanics. In this essay, the idea of studying quantum phase transitions through mapping quantum systems to classical systems is reviewed, with Josephson-junction arrays as an example.

1 Introduction

Is quantum mechanics relevant in understanding critical phenomena?

Quantum mechanics is important if temperature is lower than some characteristic energy of the system. But, what is the characteristic energy for critical phenomena? Let us consider a phase transition taking place at a nonzero temperature T_c. One of the important features of criticalities is the critical slowing down in which equilibration time τ_c diverges as we approach the critical point. The frequency $\omega_c = 1/\tau_c$ serves as the characteristic energy. So, quantum mechanics is important if

$$\omega_c \gg T_c \ . \tag{1}$$

However, since $T_c \neq 0$ and $\omega_c \to 0$ as the criticality is approached, we expect that quantum mechanics is not important in describing critical phenomena at nonzero temperature T_c. For instance, the critical phenomena of the superfluid lambda transition of ^{4}He can be described by doing classical statistical mechanics with an effective Hamiltonian even though the ordered phase has to be described by quantum mechanics.

In contrast, a quantum system can develop a phase transition as we vary the parameters of its Hamiltonian at zero temperature. Here quantum mechanics is certainly important because $T = 0$. This is called a quantum phase transition [1]. Tuning parameters playing the temperature's role in classical phase transitions might be the charging energy in Josephson-junction arrays, the magnetic field in quantum-Hall effects, or the disorder in metal-insulator transitions.

2 Statics and dynamics couple in quantum statistical mechanics

Let us consider a quantum mechanical system described by a Hamiltonian $\mathcal{H}$ at temperature $T = 1/\beta$. Later we will take the limit $\beta \to \infty$ to investigate zero-temperature phenomena. All the thermodynamic quantities can be obtained from the partition function

$$Z = \mathrm{Tr}\ e^{-\beta \mathcal{H}} \ . \tag{2}$$

One of the interesting features of quantum statistical mechanics is that dynamics and statics are deeply connected. In classical statistical mechanics, a Hamiltonian is usually split into two pieces of kinetic and potential energy

$$\mathcal{H}(p, q) = K(p) + U(q) \ , \tag{3}$$

where p and q represent multi-dimensional momenta and positions respectively. Hence the Boltzmann factor

$$e^{-\beta \mathcal{H}} = e^{-\beta K(p)} \ e^{-\beta U(q)} \tag{4}$$

is factorized into two pieces and the statics of the system can be studied separately from its dynamics. One example is our old friend *Ising model*,

$$\mathcal{H} = \sum_{\langle ij \rangle} J \ S_i S_j + H \sum_i S_i \ . \tag{5}$$

Where is dynamics? There is no dynamics in the Ising model. It is already factored out as in Eq. (4).

In quantum statistical mechanics, however, even if we have a Hamiltonian like Eq. (3), we cannot simply factorize the Boltzmann factor since p and q don't commute. So, statics and dynamics have to be coupled in quantum statistical mechanics. The connection between them is even deeper as we can see from the fact the Boltzmann factor $e^{-\beta \mathcal{H}}$ is equal to the time-evolution operator $e^{-i\mathcal{H}t}$ if we set $t = -i\beta$. Thus the partition function

$$Z = \sum_n \ \langle n | e^{-\beta \mathcal{H}} | n \rangle \tag{6}$$

looks exactly like a sum of transition amplitudes from state $|n\rangle$ to itself after time interval $-i\beta$ with respect to a basis $\{|n\rangle\}$.

3 Mapping of a quantum system to a classical system

By recognizing that the partition function is determined by the transition amplitudes in imaginary time, we can use the idea of *Feynman's path-integral* [5]. Inserting a sequence of sums over complete sets of intermediate states into Eq. (6), we get

$$Z = \sum_{n} \sum_{m_1} \cdots \sum_{m_N} \langle n|e^{-\Delta\mathcal{H}}|m_1\rangle\langle m_1|e^{-\Delta\mathcal{H}}|m_2\rangle \cdots \langle m_N|e^{-\Delta\mathcal{H}}|n\rangle, \tag{7}$$

where Δ is an imaginary time interval smaller than any time scale of interest and $N = \beta/\Delta$. If we consider the imaginary time axis as an additional spatial axis, Eq. (7) is in the form of a *classical* partition function written in terms of a transfer matrix. Therefore, a d-dimensional quantum system can be mapped to a $(d+1)$-dimensional classical system [3, 4]. But the size of the extra dimension is determined by the temperature β and becomes infinite as the zero-temperature limit is taken. So the corresponding classical system is infinite only at zero temperature.

To illustrate this point, let us consider a d-dimensional *Josephson-junction array.* A Josephson-junction is a tunneling junction connecting two superconducting metallic grains. If the coupling among the grains is big enough, Cooper pairs are able to move freely from grain to grain. Then the system is in a superconducting state. In contrast, if the charging energy which it costs to move an excess Cooper pair onto a grain is big enough, Cooper pairs are stuck on individual grains and the system is an insulator.

The degrees of freedom are the phases of the complex superconducting order parameters on the metallic grains and the Hamiltonian is

$$\mathcal{H} = \frac{C}{2} \sum_{i} V_i^2 - E_J \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j) \ . \tag{8}$$

Here θ_i is the operator representing the phase on the i-th site of the d-dimensional lattice, and $V_i = -i(2e/C)(\partial/\partial\theta_i)$ is the conjugate operator of θ_i. The two terms of the Hamiltonian represent competition between the charging energy $E_C = (2e)^2/C$

and the coupling energy E_J. When E_J is much bigger than E_C, the second term is important and the ground state is determined by minimizing it. So the ground state is characterized by the fact that all the θ_i's have the same value (ordered state). On the other hand, when E_C is much bigger than E_J, the first term is more important and the ground state is one of the "momentum" eigenstates in which θ_i's can have any values (disordered state). So we expect that there might be a phase transition between those two extremal states.

Using the idea of mapping a quantum system to a classical system, it can be shown [6] that a d-dimensional Josephson-junction array can be mapped to a $(d+1)$-dimensional classical XY *model* [2] with the Hamiltonian

$$\mathcal{H} = \frac{1}{K}\sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \ , \tag{9}$$

where $K \sim \sqrt{E_C/E_J}$ and θ_i is a c-number on site i of the $(d+1)$-dimensional lattice. In this case the obtained classical system happens to have an isotropic interaction, but in general it can have a different coupling constant along the extra temporal direction from that along the original spatial directions.

4 Quantum critical points

Now that we mapped our quantum system to a classical system, we can use the classical system to analyze the quantum system. (Also, we can study a quantum system by doing Monte Carlo or molecular dynamics simulations of the appropriate $(d+1)$-dimensional classical system.)

It is known that a classical XY model undergoes phase transition at some critical temperature K_c. Spins are not aligned at high temperatures and they are aligned at low temperatures. As we decrease the temperature from infinity to zero, the system changes from a disordered(paramagnetic) state to an ordered(ferromagnetic) state at the critical temperature K_c. Recall that a Josephson-junction array can be mapped to a classical XY model and that K is completely determined by the ratio of the charging energy and Josephson coupling. K is not a real temperature any longer. The real temperature affects only the size of the extra temporal dimension. Thus it follows that a Josephson-juction array must undergo a phase transition as the ratio of the two coupling constants is varied. When E_C is much larger than E_J, K is large and the system must be in a disordered state (insulator). And when E_C is much smaller than E_J, K is small and the system must be in an ordered state (superconductor). The critical point should be given by the critical temperature of the classical XY model.

For classical systems, correlation lengths diverge at critical points. Thus the correlation lengths of the corresponding quantum systems must diverge too. As mentioned before, the interaction along the extra temporal direction can be different from that along the spatial direction in general. So we have two different kinds of correlation length : ξ along the spatial direction, and ξ_τ along the extra temporal direction. The asymptotic forms near the critical point

$$\xi \sim |K - K_c|^{-\nu} \tag{10}$$

$$\xi_\tau \sim \xi^z \tag{11}$$

define the critical exponents ν and z. For a Josephson-junction array, the dynamical exponent z is equal to 1 because the corresponding classical system happens to have the same interaction on the extra temporal direction as on the spatial direction.

5 Nonzero temperature and finite-size scaling

So far, we were assuming $T = 0$. Thus the size of the extra dimension was infinite and the corresponding classical system was truly $(d+1)$-dimensional. (Recall that only infinite systems can develop phase transitions at nonzero temperature.) However, since all the experiments are being done at nonzero temperatures, we are forced to study nonzero-temperature phenomena.

Let us consider 2-dimensional Josephson-junction arrays for example. At $T = 0$, a 2D Josephson-junction array is mapped to a 3D XY model of infinite size and the transition between the superconducting state and the insulating state is described by the order-disorder transition in the 3D XY model which also describes the lambda transition in liquid helium. However at low but nonzero T(If we increase T too much, the mapping from Josephson-junction array to XY model breaks down, that is to say, quantum mechanics becomes unimportant as temperature gets higher than some characteristic energy.), a 2D Josephson-junction array is mapped to a quasi-3D XY model which has finite length L_τ in the extra dimension. So it is effectively a 2D XY model and undergoes the Kosterlitz-Thouless transition which is in a different universality class than that of the 3D XY model. It has a different set of critical exponents not to mention a different transition temperature K_c.

As we can see from the above example, a nonzero temperature changes the dimension of the classical system and hence changes the universality class. As we approach zero temperature, crossover between the two different critical phenomena is expected. And we can study it through the finite-size scaling of the corresponding classical system [7].

References

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