Lecture 22: of Quantum rotor analysis of instability of Néel state to quantum and thermal fluctuations.

In the last lecture, we saw how one can expand about the fully ordered state of the quantum rotor model to obtain a description of the low-energy spectrum in terms of wave-like non-interacting magnon excitations with two polarizations $\alpha = x, y$ and dispersion relation

$$\omega(\vec{q}) = \sqrt{\frac{J_{\text{eff}}}{I}}\sqrt{2d - 2\cos(q_x a) - 2\cos(q_y a) - \cdots \text{ d terms}} \tag{1}$$

Each magnon excitation causes the rotors to deviate from perfect alignment along some spontaneously chosen axis, which we have taken without loss of generality to be the $\hat{z}$ axis. Now, the basic premise of our linearized theory is that these deviations from perfect alignment (the perfectly ordered state) are *small*. We used this assumption explicitly when we left out terms that were second-order in smallness in the equations of motion, and it was this omission that led us to the simple quadratic Hamiltonian $H_{\text{linearized}}$ for the magnons excitations. If we were to go beyond the linearized equations of motion, we would generate other terms that can be thought of as interactions between the magnons, and these can also be studied using a more elaborate version of the spinwave theory we have developed in the previous lecture.

Here we are concerned with a more basic question: Is our spinwave description consistent? In other words, if we calculate the mean value of $\vec{\phi}^2(j)$ at any site j in the ground state of $H_{\text{linearized}}$ at $T = 0$, or in the equilibrium ensemble defined by $e^{-H_{\text{linearized}}/k_B T}$ at nonzero temperature T, do we get an answer that is systematically small compared to 1? This is the question we will try and answer in this lecture. As we will see below, the answer to this question is somewhat delicate because $\omega(\vec{q}) \to 0$ as $|\vec{q}| \to 0$, and this means that $|\vec{q}| \to 0$ magnons are very easily excited by quantum and thermal fluctuations. Furthermore, since this property of $\omega(\vec{q})$ is a reflection of the general principle that breaking of a continuous symmetry leads to gapless excitations (these are "Goldstone modes" in the language of particle physics), the answer to this question also tells us whether a continuous symmetry can be broken in a given spatial dimension.

With this background, we turn now to a systematic calculation of $\langle \vec{\phi}^2 \rangle$ in the linearized theory, starting with the answer in the $T = 0$ ground state, and then extending the calculation to $T > 0$. We want to evaluate

$$\frac{1}{N_{\rm sites}} \sum_j \langle \vec{\phi}^2(j) \rangle_{\rm spinwave} \tag{2}$$

within spin-wave theory. To do this, we write each factor of $\vec{\phi}(j)$ in terms of its Fourier expansion, and express the Fourier coefficients in terms of creation and annihilation operators:

$$\begin{aligned}
\frac{1}{N_{\rm sites}} \sum_j \langle \vec{\phi}^2(j) \rangle_{\rm spinwave} &= \frac{1}{N_{\rm sites}} \sum_j \frac{1}{N_{\rm sites}^2} \sum_{\vec{q},\vec{q}_2} e^{i\vec{q}\cdot\vec{x}_j} e^{i\vec{q}_2\vec{x}_j} \langle \vec{\phi}(\vec{q}) \cdot \vec{\phi}(\vec{q}_2) \rangle_{\rm spin-wave} \\
&= \frac{1}{N_{\rm sites}^2} \sum_{\vec{q}} \langle |\vec{\phi}(\vec{q})|^2 \rangle_{\rm spinwave} \\
&= \frac{1}{N_{\rm sites}^2} \frac{N_{\rm sites}}{2I\omega(\vec{q})} \sum_{\vec{q},\alpha} \langle (a_\alpha(\vec{q}) + a_\alpha^\dagger(-\vec{q}))(a_\alpha(-\vec{q}) + a_\alpha^\dagger(\vec{q})) \rangle_{\rm spinwave} \\
&= \frac{1}{2N_{\rm sites}I} \sum_{\vec{q},\alpha} \frac{1}{\omega(\vec{q})} \langle n_\alpha(-\vec{q}) + n_\alpha(\vec{q}) + 1 \rangle_{\rm spinwave}
\end{aligned} \tag{3}$$

This is our master-formula. In the rest of this lecture we will carefully analyze the consequences of this result.

We begin by noting that as

$$N_{\rm sites} \to \infty , \tag{4}$$

we may write

$$\frac{1}{N_{\rm sites}} \sum_{\vec{q},\alpha} \;\to\; \sum_\alpha \int_{\rm BZ} \frac{d^d q}{(2\pi)^d} \tag{5}$$

where the integral is over the Brillouin zone corresponding to the d-dimensional hypercubic lattice. Furthermore, as will be clear in what follows, none of our conclusions will depend on the form of the upper cutoff in momentum space, and we will therefore freely replace the integral over the Brillouin zone by an integral over a ball of radius Λ centered at the origin of $\vec{q}$ space, with

Λ chosen to best match the overall volume of the Brillouin zone. We will denote the latter by

$$\int^{\Lambda} \frac{d^d q}{(2\pi)^d} \tag{6}$$

Consider first the magnitude of the mean-square fluctuations at $T = 0$. At $T = 0$, the system is in the ground state, which is characterized by

$$n_{\alpha}(\vec{q}) \;=\; 0 \tag{7}$$

for all α and $\vec{q}$. Therefore we have

$$\frac{1}{N_{\mathrm{sites}}} \sum_j \langle \vec{\phi}^2(j) \rangle_{\mathrm{spinwave}} \;=\; \frac{1}{2I} \sum_{\alpha} \int_{\mathrm{BZ}} \frac{d^d q}{(2\pi)^d} \frac{1}{\omega(\vec{q})} \tag{8}$$

We now use the explicit form of $\omega(\vec{q})$ to rewrite this as

$$\frac{1}{N_{\mathrm{sites}}} \sum_j \langle \vec{\phi}^2(j) \rangle_{\mathrm{spinwave}} \;=\; \frac{1}{\sqrt{J_{\mathrm{eff}} I}} \int_{\mathrm{BZ}} \frac{d^d q}{(2\pi)^d} \frac{1}{\sqrt{2d - 2\cos(q_x a) - 2\cos(q_y a) - \cdots \text{ d terms}}} \tag{9}$$

If the integrand is convergent, our answer for the mean-square deviations from perfect ordering is going to be a very small number because of the overall prefactor of $1/\sqrt{J_{\mathrm{eff}} I}$. This is because $\sqrt{J_{\mathrm{eff}} I}$ is large by construction—indeed, our spinwave analysis of the previous chapter was an attempt to study the stability of the ordered state that is expected to obtain in this regime. Thus, if the integrand is indeed convergent, we can end our discussion right here, and conclude that the quantum rotor model supports an ordered state for large values of $\sqrt{J_{\mathrm{eff}} I}$, whose low-energy properties can be consistently described by spinwave theory.

However, and this is key, the integrand is *not* always convergent. The source of potential difficulty is the vanishing of $\omega(\vec{q})$ linearly as $\sim |\vec{q}|$ when $\vec{q} \to 0$. Since the convergence difficulties arise near the origin in $\vec{q}$ space, the shape of the Brillouin zone, and the detailed form of $\omega(\vec{q})$ away from $\vec{q} = 0$ are not germane to any discussion of this issue. Therefore, we replace $\omega(\vec{q})$ by its small $|\vec{q}|$ form, and replace the integral over the Brillouin zone by that over a ball of radius Λ centered at the origin, and study the behaviour of the integral

$$\int^{\Lambda} \frac{d^d q}{(2\pi)^d} \frac{1}{|\vec{q}|} \tag{10}$$

Clearly, this integral diverges for $d = 1$, but converges for $d \geq 2$. Our conclusion therefore is that our assumption of a long-range ordered state in which the $\hat{n}$ spontaneously break $O(3)$ rotational invariance is perfectly valid in spatial dimensions $d \geq 2$ at $T = 0$ for large enough $J_{\text{eff}} I$, but such an ordered state with spontaneously broken $O(3)$ symmetry cannot exist even at $T = 0$ no matter how large one makes $J_{\text{eff}} I$ in $d = 1$. Since this arises due to the divergent contributions of the zero-point motion, one may say that quantum fluctuations destroy any tendency to long-range order even at $T = 0$ (the most favourable case) in $d = 1$.

Once we state our conclusion in this way, we are immediately led to ask: What about the effect of thermal fluctuations? To answer this, we go back to our master-formula and evaluate it at $T > 0$. At nonzero temperature, the magnon occupation numbers $n_\alpha(\vec{q})$ clearly follow Bose-Einstein statistics with chemical potential $\mu = 0$. Therefore, we have the result

$$\frac{1}{N_{\text{sites}}} \sum_j \langle \vec{\phi}^2(j) \rangle_{\text{spinwave}} = \frac{1}{I} \int_{\text{BZ}} \frac{d^d q}{(2\pi)^d} \frac{1}{\omega(\vec{q})} \left(1 + \frac{2}{e^{\omega(\vec{q})/T} - 1} \right) \tag{11}$$

Again, if the integral is convergent, one can immediately conclude that spin-wave theory is consistent and an ordered phase can exist for large enough values of J_{eff} and I. And again, the integral is not always convergent. Indeed, the strongest divergence now comes from the effects of thermal fluctuations, since the Bose function contributes an additional factor of $1/\omega(\vec{q})$ to the integrand in the limit of small $\vec{q}$.

In other words, at issue now is the convergence of the integral

$$\int^{\Lambda} \frac{d^d q}{(2\pi)^d} \frac{1}{|\vec{q}|^2} \tag{12}$$

Clearly, this diverges in $d = 1$ *and* in $d = 2$, and is only convergent for $d \geq 3$. Therefore, we conclude that thermal fluctuations preclude the possibility of spontaneously breaking the $O(3)$ symmetry at $T > 0$ for dimensions $d = 1$ and $d = 2$, but are not strong enough to destroy long-range order for $d \geq 3$. The case of two spatial dimensions, $d = 2$, is thus very special. Quantum antiferromagnets in two spatial dimensions can exhibit long-range Néel order in their ground state, but heating the system to any nonzero temperature, no matter how small, must destroy the long range order!

Of course, since our conclusions are based on the fact that the assumption that the system is long-range ordered leads to inconsistent results in low dimensions, one may wonder if there is some way to reach the same conclusions in a rigorous way. The answer to this question is yes. In the next lecture, we will in fact obtain the same results in a mathematically sound way—this is the well-known Mermin-Wagner theorem which says that a continuous symmetry cannot be broken in $d = 2$ or lower at non-zero temperature, and cannot be broken even at $T = 0$ in dimension $d = 1$.

Leaving that to the next lecture, let us turn to the question: What is the ultimate fate of the system if $J_{\rm eff}$ and I are large, but quantum and thermal fluctuations destroy long-range order? The full answer to this question is very difficult, since one is in a parameter regime in which the system locally likes ordered arrangements of $\hat{n}$, but long-wavelength fluctuations destroy this short-range order. Indeed, we will spend nearly four lectures understanding how this happens using the renormalizaton group approach.

Here, we answer a simpler question: What happens if $J_{\rm eff}$ and I are both very *small*? In this opposite limit $\sqrt{IJ} \ll 1$, the kinetic energy of each rotor will dominate. Therefore, to zeroth order, we just have each rotor in the total angular momentum $l = 0$ state, *i.e.*

$$l_j = 0.\forall j \tag{13}$$

The wavefunction of this state for each rotor is of course uniformly spread out over the corresponding unit sphere. In other words, each $\hat{n}_j$ is fluctuating wildly, independent of even its nearest neighbours.

This is a quantum paramagnet, in which quantum effects (the kinetic energy of the rotors) have overwhelmed the tendency of the rotors to align. What are the lowest lying excitations in this limiting case? Clearly, the first excited level is $3N_{\rm sites}$-fold degenerate, since one can take any one site $j = j_0$, and promote the corresponding rotor to any one of the $l = 1$ triplet states. In this limit, the excitation energy is $1/I$, *i.e.* very large. This large gap indicates that this state is stable to corrections due to the nonzero value of $J_{\rm eff}$. To leading, order, it is easy to see that the exchange term

$$-J_{\rm eff} \sum_{\langle jk \rangle} \hat{n}_j \cdot \hat{n}_k \ , \tag{14}$$

when projected into the manifold of these $3N_{\rm sites}$ degenerate excited states as required by our standard prescription of first-order degenerate perturbation theory, makes the triplet at $j = j_0$ *hop* with amplitude proportional to $J_{\rm eff}$ to each of its neighbours.

In other words, if we think of the site j_0 as hosting a triplet particle, which is a gapped version of the gapless spinwave excitations found in the ordered state, then this particle has no kinetic energy in the absence of the exchange coupling. And the leading effect of the exchange coupling is to allow this triplet particle to hop to neighbouring sites with amplitude proportional to J_{eff}. Higher order terms in this perturbation series lead to further neighbour hopping terms as well as two-particle interaction terms in the Hamiltonian for these triplet magnons, while the ground state remains a singlet with extremely short-ranged correlations for the $\hat{n}_j$. All of this can be worked out quite explicitly using elementary perturbation theory, and I urge you to do this as a homework exercise.

Here, I turn instead to a discussion of what we have learnt from all of the foregoing about the original quantum antiferromagnet: Our basic conclusion is that quantum antiferromagnets with short range Néel order can have two phases. One phase, which is the quantum paramagnetic phase, can exist in any dimension and has a featureless singlet ground state with a triplet of gapped magnon excitations. The other phase has long-range Néel order with a *doublet* of gapless spinwave excitations that are linearly dispersing near the antiferromagnetic wavevector (which translates to linear dispersion in the rotor model near $\vec{q} = 0$). However, the long-range Néel ordered phase cannot exist in $d = 1$ even at $T = 0$, and cannot exist in $d = 2$ for $T > 0$.

Of course, all of this has been actaully worked out for the quantum rotor model studied here. And this model is a faithful description of the low energy physics of the original quantum antiferromagnet only if Berry phases play no role. As we have argued earlier, Berry phases do not play a role in $d \geq 2$ in the Néel ordered phase, nor do they play a role for integer values of spin in $d = 1$. Therefore, our conclusions above, which are based on the quantum rotor description, are valid in these cases for the original quantum antiferromagnet. However, for half-integer spins in $d = 1$, Berry phases play a crucial role, and the physics is therefore quite different (and beyond the scope of this lecture course). In addition, when Néel order is destroyed by quantum fluctuations in spin $S = 1/2$ antiferromagnets in $d \geq 2$, Berry phases do play a role in determining the detailed spatial structure of correlations in the quantum disordered phase, as well as in determining the nature of the transition between the Néel ordered and quantum paramagnetic states, so some of our conclusions need modifications in these cases. This is again a subject that goes beyond the scope of these lectures. Here, we only note that conclusions drawn on the basis of results for the quantum rotor model hold whenever there is an integer spin per unit cell.