Lecture 21: Spin wave theory for quantum rotor model

In the last three lectures, we have introduced a simple model for a system of interacting bosons in a lattice potential, and developed caricatures for the superfluid and insulating states of this systems, as well as sketched the derivation of an effective theory that is designed to correctly reproduce the low-energy physics of both phases as well as the intervening superfluid-insulator transition. We have also discussed how this theory can be used to calculate observable quantities like the superfluid stiffness and the conductivity.

These developments are closely analogous to our earlier discussion of spin systems with antiferromagnetic exchange interactions, for which we derived an effective $O(3)$ quantum rotor Hamiltonian which is expected to correctly capture the low-energy physics of such quantum antiferromagnets, and discussed how experimentally relevant quantities such as NMR relaxation rates and inelastic neutron scattering cross-sections may be computed within such an effective theory.

In the next ten lectures or so (including this one), we will discuss the low-energy physics of both these effective theories in some detail. In each case, we will start by developing a systematic expansion about the ordered state in order to characterize the universal low-energy physics of the long-range ordered antiferromagnetic state and the superfluid state. Then we will identify instabilities that cause a breakdown of order, and develop so-called "renormalization group" ideas that help us understand how these instabilities eventually produce a disordered state in terms of the properties at the largest length-scales and lowest energy scales. In the bosonic case, the disordered state is a Mott-insulating state of the original Bose-Hubbard model, while in the case of quantum antiferromagnets, the disordered state is a quantum paramagnet in which quantum fluctuations succeed in destroying long-range antiferromagnetic order. As a by-product, we will also end up learning how to think about properties of a "critical point" separating the ordered and the disordered phases.

With this general orientation in mind, let us write down the effective Hamiltonian corresponding to the quantum rotor model:

$$H_{\rm rotor} = \sum_j \frac{\vec{L}_j^2}{2I} - J_{\rm eff} \sum_{\langle jk \rangle} \hat{n}_j \cdot \hat{n}_k \tag{1}$$

with moment of inertia I, nearest-neighbour exchange interactions J_{eff} and canonical commutation relations

$$[n_\alpha(j_1), L_\beta(j_2)] = i\delta_{j_1,j_2}\epsilon_{\alpha\beta\gamma}n_\gamma \tag{2}$$

In other words, $\vec{L}$, being the angular momentum of the rotor, *rotates* $\hat{n}$ which is the coordinate of the rotor.

If $I \to \infty$, then the first term has a negligible effect on the physics, and the problem becomes that of a classical system of unit vectors with aligning nearest neighbour interactions. Clearly, this orders by spontaneously choosing a common axis and aligning all the unit vectore $\hat{n}$ along that axis, since this is the configuration that gives the minimum exchange energy. Once I is finite, the kinetic energy of each rotor favours the $l = 0$ state individually for each rotor. Since the wavefunction of the $l = 0$ state of each rotor is uniform on the corresponding unit-sphere labeled by the rotor coordinate $\hat{n}$, the kinetic energy competes with this tendency of the exchange interaction to line up the rotors.

Therefore, our task in this lecture is to understand the stability of this ordered state to the effects of this kinetic energy term. The arguments and calculations we use to answer this question make up what is generically termed "spin-wave theory", since a crucial part of this analysis has to do with determining the nature of wave-like excitations of this ordered state. We begin by assuming that all the rotors line-up, except for small deviations, along a spontaneously chosen axis, which we take without loss of generality to be the z axis. From the equations of motion, we know that $\vec{L}_j$ is proportional to $\hat{n}_j \times \partial_t \hat{n}_j$, and is therefore expected to lie predominantly in the xy plane if all the $\hat{n}_j$ are nearly aligned with the $\hat{z}$ axis. Indeed, thinking in terms of small deviations from the perfectly aligned static configuration, we see that the x and y components of $\hat{n}$, and the x and y components of $\vec{L}$ are the leading effects of any departure from this static solution, while the z component of $\vec{L}$ is a *second-order effect.*

This can be made precise by writing down the Hamilton equations of motion corresponding to H_{rotor} and systematically keeping only leading order deviations from the static state with all $\hat{n}$ lined up along the $\hat{z}$ axis. These equations read:

$$\begin{aligned} \frac{dn_x(j)}{dt} &= \frac{i}{2I}[\vec{L}^2(j), n_x(j)] \\ &= \frac{i}{2I}L_y[L_y, n_x] + \frac{i}{2I}[L_y, n_x]L_y + y \leftrightarrow z \end{aligned}$$

$$
\begin{aligned}
&= i\left(-i\frac{L_y n_z}{2I} - i\frac{n_z L_y}{2I} + i\frac{L_z n_y}{2I} + i\frac{n_y L_z}{2I}\right) \\
&= \frac{-1}{2I}\left(n_y L_z + L_z n_y - L_y n_z - n_z L_y\right) \\
&\approx \frac{1}{2I}\left(L_y n_z + n_z L_y\right) \\
&\approx \frac{L_y(j)}{I} \qquad (3)
\end{aligned}
$$

where we have dropped the site-label j in the intermediate steps to avoid notational clutter, but reinstated it in the final expression, which only contains terms that are first-order in smallness. Similarly, we obtain to linear order

$$
\frac{dn_y(j)}{dt} \approx -\frac{L_x(j)}{I} \qquad (4)
$$

To the same leading order, we have

$$
\frac{dn_z(j)}{dt} = 0 \qquad (5)
$$

Similarly, one can work out the leading order equations of motion for $L_x(j)$ and $L_y(j)$ (remember, $L_z(j)$ is only non-zero at second-order, and can therefore be consistently ignored in our discussion):

$$
\begin{aligned}
\frac{dL_x(j)}{dt} &= -J_{\text{eff}} \sum_{k\in j} n_y(k) n_z(j) + J_{\text{eff}} \sum_{k\in j} n_y(j) n_z(k) \\
\frac{dL_y(j)}{dt} &= -J_{\text{eff}} \sum_{k\in j} n_z(k) n_x(j) + J_{\text{eff}} \sum_{k\in j} n_z(j) n_x(k) \,. \qquad (6)
\end{aligned}
$$

In the above, the sum over $k \in j$ refers to all neighbours k of a given site j. Let us now parameterize the small deviations from the perfectly aligned state in terms of variables $\phi_x(j)$ and $\phi_y(j)$ by writing

$$
\begin{aligned}
n_x(j) &= \phi_x(j) \\
n_y(j) &= \phi_y(j) \\
n_z(j) &= \sqrt{1 - \phi_x^2(j) - \phi_y^2(j)} \\
&\approx 1 \qquad (7)
\end{aligned}
$$

where, in the last line, we have emphasized the fact that $n_z(j)$ plays no role in the linearized theory that only includes terms that are first order in the $\vec{\phi}(j)$. From the linearized equations derived above, it is clear that $-L_x(j)$ plays the role of the *linear momentum* that is canonically conjugate to $\phi_y(j)$ (with I playing the role of the mass), while $+L_y(j)$ plays the role of the linear momentum canonically conjugate to $\phi_x(j)$. Furthermore, as far as the linearized equations are concerned, L_z, the commutator of L_x with L_y, plays no role. Therefore, the linearized theory can be thought of as being a theory of two *independent canonically conjugate pairs*: $\phi_x(j)$ and its canonically conjugate momentum

$$\pi_x(j) \equiv L_y(j) \tag{8}$$

and $\phi_y(j)$ and its canonically conjugate momentum

$$\pi_y(j) \equiv -L_x(j) \tag{9}$$

with the only non-zero commutators being

$$[\phi_\alpha(i), \pi_\beta(j)] = \delta_{ij}\delta_{\alpha\beta} \tag{10}$$

In order to reproduce the linearized equations of motion, we must use these commutation relations in conjunction with the following Hamiltonian for the linearized theory:

$$H_{\text{linearized}} = \frac{1}{2I}\sum_j (\pi_x^2(j) + \pi_y^2(j)) + \frac{J_{\text{eff}}}{2}\sum_{\langle jk\rangle}(\vec{\phi}(j) - \vec{\phi}(k))^2 \tag{11}$$

This linearized Hamiltonian leads to the following wave-equations for ϕ_x and ϕ_y, which are seen to follow by differentiating both sides of one of the Hamilton equations of motion again and invoking the other equation:

$$\begin{aligned}
\frac{d^2\phi_y(j)}{dt^2} &= -\frac{1}{I}\frac{dL_x(j)}{dt} \\
&= -\frac{J_{\text{eff}}}{I}\left(2d\phi_y(j) - \sum_{k\in j}\phi_y(k)\right) \\
\frac{d^2\phi_x(j)}{dt^2} &= \frac{1}{I}\frac{dL_y(j)}{dt} \\
&= -\frac{J_{\text{eff}}}{I}\left(2d\phi_x(j) - \sum_{k\in j}\phi_x(k)\right)
\end{aligned} \tag{12}$$

These are *wave-equations* characteristic of a system of coupled harmonic oscillators. The underlying decoupled harmonic oscillator eigenmodes can be exposed by working with Fourier transformed operators:

$$\begin{aligned} \pi_\alpha(\vec{q}) &= \sum_j e^{+i\vec{q}\cdot\vec{x}_j}\pi_\alpha(j) \\ \phi_\alpha(\vec{q}) &= \sum_j e^{-i\vec{q}\cdot\vec{x}_j}\phi_\alpha(j) \end{aligned} \tag{13}$$

where $\vec{x}_j$ is the coordinate of the site j on a d-dimensional hypercubic lattice with lattice spacing a. The commutation relations among these Fourier transformed operators follow from the original commutation relations among the ϕ and the π at each site:

$$\begin{aligned} [\phi_\alpha(\vec{q}), \pi_\beta(\vec{q}_2)] &= \sum_{kj} e^{-i\vec{q}\cdot\vec{x}_k} e^{i\vec{q}_2 x_j}[\phi_\alpha(k), \pi_\beta(j)] \\ &= i\delta_{\alpha\beta} N_{\text{sites}} \delta_{\vec{q},\vec{q}_2} \\ &= i\delta_{\alpha\beta}\delta^d(\vec{q}-\vec{q}_2) \text{ when } N_{\text{sites}} \to \infty \end{aligned} \tag{14}$$

It is easy to see that the linearized Hamiltonian can be written as a sum of independent harmonic oscillators, one for each $\vec{q}$, when expressed in terms of these Fourier transformed operators (please check this on your own):

$$H_{\text{linearized}} = \frac{1}{N_{\text{sites}}}\sum_{\vec{q}} \frac{1}{2I}\left(|\pi_x(\vec{q})|^2 + |\pi_y(\vec{q})|^2\right) + \frac{1}{N_{\text{sites}}}\sum_{\vec{q}} \frac{J_{\text{eff}}}{2} b^2(\vec{q})\left(|\phi_x(\vec{q})|^2 + |\phi_y(\vec{q})|^2\right) \tag{15}$$

with

$$b^2(\vec{q}) = (2d - 2\cos q_x a - 2\cos q_y a \cdots \text{ d cosines}) \tag{16}$$

Rescaling to bring it in standard form, we write

$$\begin{aligned} H_{\text{linearized}} &= \frac{1}{N_{\text{sites}}}\sum_{\vec{q}}\left(\frac{|\vec{\pi}(\vec{q})|^2}{2I} + \frac{1}{2}I\omega^2(\vec{q})|\vec{\phi}(\vec{q})|^2\right) \\ &\text{with } \omega^2(\vec{q}) = \frac{J_{\text{eff}}}{I}b^2(\vec{q}) \end{aligned} \tag{17}$$

We may now define creation and annihilation operators for each $\vec{q}$ to write the Hamiltonian explicitly as a sum of independent oscillator Hamiltonians at each $\vec{q}$:

$$\begin{aligned} a_\alpha(\vec{q}) &= \frac{1}{\sqrt{2N_{\text{sites}}}}\left(\sqrt{I\omega(\vec{q})}\phi_\alpha(\vec{q}) + i\frac{\pi_\alpha(-\vec{q})}{\sqrt{I\omega(\vec{q})}}\right) \\ a_\alpha^\dagger(\vec{q}) &= \frac{1}{\sqrt{2N_{\text{sites}}}}\left(\sqrt{I\omega(\vec{q})}\phi_\alpha(-\vec{q}) - i\frac{\pi_\alpha(\vec{q})}{\sqrt{I\omega(\vec{q})}}\right) \end{aligned} \tag{18}$$

Since $\omega(\vec{q}) = \omega(-\vec{q})$, these definitions imply the following canonical commutation relations:

$$[a_\alpha(\vec{q}), a_\beta^\dagger(\vec{q}_2)] = \delta_{\vec{q}\vec{q}_2}\delta_{\alpha\beta} \tag{19}$$

Thus, each $(a_\alpha(\vec{q}), a_\alpha^\dagger(\vec{q}))$ gives an independent set of creation and annihilation operators, one for each $\vec{q}$ and α. The corresponding number operators

$$n_\alpha(\vec{q}) = a_\alpha^\dagger(\vec{q})a_\alpha(\vec{q}) \tag{20}$$

keep track of the number of quanta of the corresponding harmonic oscillator mode, and can be thought of as counting the number of spin-wave particles (sometimes called magnons) propogating with *polarization* α in momentum eigenstate $\vec{q}$. In terms of these number operators, the linearized Hamiltonian reads:

$$H_{\text{linearized}} = \sum_{\vec{q},\alpha}\omega(\vec{q})\left(n_\alpha(\vec{q}) + \frac{1}{2}\right) \tag{21}$$

Clearly, the ground state of the linearized theory is the vacuum for all magnons, *i.e.*

$$n_\alpha(\vec{q}) = 0 \tag{22}$$

for all $\vec{q}$ and $\alpha = x, y$, and each magnon excitation ($n_\alpha(\vec{q}) \rightarrow n_\alpha(\vec{q}) + 1$) corresponds to an excitation energy of $\omega(\vec{q})$ (in all our analysis, $\hbar$ has been set to zero at the very outset). Clearly the vacuum state corresponds to the perfectly aligned state with all $\hat{n}(j)$ pointing along the $\hat{z}$ direction

What does it mean to excite one of these magnons? From the equations of motion, it is clear that these quanta correspond to wave-like modes propogating at wavevector $\vec{q}$ and oscillating in time at frequency $\omega(\vec{q})$. These modes disturb the perfect alignment of all $\hat{n}(j)$ along the $\hat{z}$ axis. Magnons with polarization $\alpha = x$ correspond to waves with $\hat{n}$ oscillating in the xz plane with corresponding angular momentum along the $\pm\hat{y}$ direction, while those with polarization $\alpha = y$ correspond to waves with $\hat{n}$ oscillating in the yz plane with corresponding angular momentum along the $\pm\hat{x}$ direction.

These magnon excitations of our rotor model are like phonons in a solid, or photons in a microwave cavity. Any external perturbation that couples energetically to the system can *create* these magnons. Like phonons or photons, the total number of magnons is therefore not conserved, and as a result, they obey Bose statistics with chemical potential μ set to 0. In the next lecture, we will see these facts emerge from a more formal analysis, and we will look more closely at the internal consistency of the assumptions that went into this linearized theory for the spectrum of low-lying states above the ordered ground state with long-range order for the $\hat{n}(j)$.