Lecture 20: Effective field theory for the Bose-Hubbard model

In the previous lecture, we have sketched the expected phase diagram of the Bose-Hubbard model, and introduced a mean-field treatment that can in principle calculate in a self-consistent way the value of the superfluid order parameter ψ. The next question we must ask is: What is the effective field theory that describes the low-energy properties of the phases and the phase transitions between them? This effective field theory would be the analog of the quantum rotor model, derived earlier as the effective field theory for the low-energy properties of quantum antiferromagnets.

Clearly, this field theory should be written in terms of a bosonic field ψ that represents, in some sense, the local superfluid order parameter as discussed in the previous lecture. This is the analog of focussing on the Néel-vector in the antiferromagnetic case. A convenient way to proceed is to begin with the imaginary-time path integral representation of the partition function corresponding to the Bose-Hubbard model Hamiltonian and introduce the order parameter field ψ discussed in the previous lecture via a Hubbard Stratanovich transformation.

Thus, we first write

$$\begin{aligned} Z_{BH} &= \int \mathcal{D}c_i(\tau)\mathcal{D}c_i^\dagger(\tau) \exp\left(-\int_0^{1/T} d\tau\, L_{BH}\right) , \\ L_{BH} &= \sum_i \left(c_i^\dagger \frac{dc_i}{d\tau} - \left[\mu + \frac{U}{2}\right] c_i^\dagger c_i + \frac{U}{2} c_i^\dagger c_i^\dagger c_i c_i\right) - w \sum_{\langle ij\rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i\right) . \end{aligned} \tag{1}$$

where we have departed from the convention used in the previous lectures and used the same label c for the coherent states as we have used for the annihilation operators, and we have introduced the standard convention of making an analogy of the functional in the exponent with the action of classical mechanics, *i.e.* the time integral of the system's Lagrangian (to be precise, this is not the usual action since we are working in imaginary time, but the analogy provides a convenient language that is commonly used).

Now, we "decouple" the hopping term by introducing an integral over an auxiliary field $\psi_i(\tau)$ via the so-called "Hubbard Stratanovich transforma-

tion", which gives the following alternate form for the action:

$$
\begin{aligned}
Z_{BH} &= \int \mathcal{D}c_i(\tau)\mathcal{D}c_i^\dagger(\tau)\mathcal{D}\psi_i(\tau)\mathcal{D}\psi_i^\dagger(\tau)\exp\left(-\int_0^{1/T} d\tau\, L'_{BH}\right) , \\
L'_{BH} &= \sum_i \left(c_i^\dagger \frac{dc_i}{d\tau} - \left[\mu + \frac{U}{2}\right] c_i^\dagger c_i + \frac{U}{2} c_i^\dagger c_i^\dagger c_i c_i - \psi_i c_i^\dagger - \psi_i^\dagger c_i \right) \\
&\quad + \sum_{i\,,j} \psi_i^\dagger w_{ij}^{-1} \psi_j \, ,
\end{aligned} \tag{2}
$$

Here w^{-1} denotes the inverse of the coupling matrix w_{ij} whose elements equal w if i and j are nearest neighbours and 0 otherwise, and the correctness of this alternate form can be easily checked by noting that we get back our original expression if we do the integral over the auxillary field ψ.

The main utility of this alternate form is that we can now imagine solving the single site problem exactly and expanding the result in powers of ψ_i. This would give us an action solely in terms of various powers of ψ_i and their time derivatives. The resulting expression can then be expanded in spatial gradients to finally arrive at the long-wavelength description we are interested in.

While it is possible in principle to carry this out explicitly (the coefficients of various powers of ψ will just be products of various Green functions of the single site Hamiltonian which is identical to the mean-field Hamiltonian discussed in the previous lecture), we will not do such a careful job here. For our purposes, it suffices to keep this general approach in mind, and directly write down the first few terms so obtained, without explicitly determining their coefficients in terms of the microscopic coupling constants. Thus, we write

$$
\begin{aligned}
Z &= \int \mathcal{D}\psi(\mathbf{x},\tau)\mathcal{D}\psi^\dagger(\mathbf{x},\tau)\exp\left(-\int_0^{1/T} d\tau \int d^d x\, \mathcal{L}\right) \\
\mathcal{L} &= K_1 \psi^\dagger \partial_\tau \psi + K_2 |\partial_\tau \psi|^2 + K_3 |\nabla \psi|^2 \\
&\quad + \tilde{r}|\psi|^2 + \frac{\tilde{u}}{3!}|\psi|^4 + \cdots \, ,
\end{aligned} \tag{3}
$$

where Z differs from Z_{BH} by an overall ψ independent factor, related to the free energy of the single site Hamiltonian we have already analyzed in the previous section, and the constants K_1, K_2, K_3, $\tilde{r}$, and $\tilde{u}$ can in principle be

obtained in the manner outlined earlier. Here, we only note some restrictions that can be placed on their values. First of all, we expect that K_1, K_2, K_3 and $\tilde{u}$ are all positive while $\tilde{r}$ can have either sign. A more non-trivial constraint can be placed on these constants by demanding that our expression for $\int d^d x \mathcal{L}$ respect the invariance property of L'_{BH} under the following gauge transformation:

$$\begin{aligned} c_i &\rightarrow c_i e^{i\varphi_i(\tau)} , \\ \psi_i &\rightarrow \psi_i e^{i\varphi_i(\tau)} , \\ \mu &\rightarrow \mu + i\frac{\partial \varphi_i}{\partial \tau} . \end{aligned} \tag{4}$$

Requiring that the quadratic terms in ψ retain their form under an infinitesimal version of this transformation immediately gives us the important restriction

$$K_1 = -\frac{\partial \tilde{r}}{\partial \mu} . \tag{5}$$

This constraint has a very important consequence for our analysis: We wish to access the superfluid-insulator transition at fixed integer density. This critical point occurs at the tip of the corresponding Mott insulating lobe. Now, we expect that a small change in $\tilde{r}$ (keeping all the other couplings fixed at their critical values corresponding to the tip of the Mott insulating lobe) from it's critical value $\tilde{r}_c$ at the tip of the Mott insulating lobe will correspond to moving slightly *along the contour of constant integer density.* Since this contour has to come in horizontally at the transition (as we have just seen in the last section), we clearly must have

$$\frac{\partial \tilde{r}}{\partial \mu} = 0 . \tag{6}$$

This implies that $K_1 = 0$; in other words the effective theory for the universal properties of the transition at fixed integer density does not have a quadratic term with just one time derivative. Notice that the theory without this term now has the additional 'particle-hole symmetry' corresponding to $\psi \rightarrow \psi^\dagger$. This suggests another way of understanding this result: As the transition at integer density occurs precisely at the tip of the Mott insulating lobe, the energy gaps to particle-like and hole-like excitations asymptotically close to the critical point on the Mott insulating side of the transition are equal. This reflects the particle -hole symmetry that is present in the theory at

low-energies asymptotically close to the transition. The vanishing of K_1 is then required in order for $\mathcal{L}$ to also have this symmetry.

We may now rescale the remaining terms in $\mathcal{L}$ to rewrite it in more standard notation as

$$\mathcal{L} = |\partial_\tau \psi|^2 + c^2 |\nabla \psi|^2 + r|\psi|^2 + \frac{u}{3!}|\psi|^4 \, , \tag{7}$$

where we have left out the higher order terms as the long-wavelength, low-energy, universal scaling properties of the transition may all be computed from the Lagrangian density above.

If we now set $\psi = (\phi_1 + i\phi_2)/2^{1/2}$, where ϕ_1 and ϕ_2 are real fields, $\mathcal{L}$ becomes the Lagrangian density of the $O(2)$, version of the $O(3)$ rotor action that we derived as the low-energy description of quantum antiferromagnets. In making this identification, we are being cavalier about the distinction between a rotor with a fixed length, and a rotor whose length is controlled by non-linear terms in the action—the basic idea being that this distinction only affects some short-distance details and cannot influence the behaviour of the system at large length-scales and low energy scales. Thus, the effective field theory describing the universal properties of the system with fixed integer density in the vicinity of the superfluid-insulator transition is precisely the $O(2)$, ϕ^4 field theory.

In order to illustrate how this effective action may be used to calculate quantities of physical interest, let us introduce external electromagnetic fields into the Lagrangian density (7), so that we may discuss the response of the system to external fields. This is done by 'minimally' coupling to the external fields in the standard way. This represents the effect of the external electromagnetic fields on the particles and holes that are the elementary excitations of our low-energy effective Hamiltonian.

Since all our linear response analysis was of course formulated in real time, it is convenient to first write down the minimally coupled Lagrangian density in real time (as opposed to the imaginary time Lagrangian density we have been dealing with so far in our path integral formulation of quantum statistical mechanics). We therefore write

$$\mathcal{L} = |(\partial_t + iQU)\psi|^2 - c^2 |(\boldsymbol{\nabla} - iQ\mathbf{A})\psi|^2 - r|\psi|^2 - \frac{u}{3!}|\psi|^4 \, , \tag{8}$$

where Q is the quantum of charge carried by the particles or holes; naturally, when we use this theory to describe a superconductor-insulator transition,

we set $Q = 2e$, where e is the electronic charge, since the bosonic Cooper pairs have charge $2e$, while in the cold-atom context, Q is really the particle-number and not a charge, and the external vector and scalar potentials are merely a theoretical device that allows us to define a convenient diagnostic for the various phases of the system (the bosonic atoms that form a superfluid state are neutral atoms and do not couple to the real electromagnetic field except through induced dipole moments and other higher order effects).

We may now rewrite this in terms of the more familiar fields $\phi_{1\,,\,2}$ to obtain

$$\mathcal{L} = \frac{1}{2}\left(\partial_t \phi_\alpha - QU\epsilon^{\alpha\beta}\phi_\beta\right)^2 - \frac{c^2}{2}\left(\boldsymbol{\nabla}\phi_\alpha + Q\mathbf{A}\epsilon^{\alpha\beta}\phi_\beta\right)^2 - \frac{r}{2}\phi_\alpha^2 - \frac{u}{4!}\left(\phi_\alpha^2\right)^2 \ , \quad (9)$$

where $\epsilon^{\alpha\beta}$ is the totally antisymmetric tensor with $\epsilon^{12} = +1$, and repeated $O(2)$ indices are summed over. The current operator can now be written down by following the usual prescription:

$$\mathbf{J}(\mathbf{x}, t) = \frac{\delta \mathcal{S}}{\delta \mathbf{A}(\mathbf{x}, t)} \ , \quad (10)$$

where $\mathcal{S} = \int dt \int d^d x \mathcal{L}$ is the action corresponding to the Lagrangian density $\mathcal{L}$. In our case, this gives

$$\mathbf{J}(\mathbf{x}, t) = -Qc^2\left(\boldsymbol{\nabla}\phi_\alpha \epsilon^{\alpha\beta}\phi_\beta + Q\mathbf{A}\phi_\alpha^2\right) \ , \quad (11)$$

where repeated indices are again summed over.

Let us now specialize to a situation in which the scalar potential is zero. Furthermore, let us assume that the vector potential is slowly varying in space. Below, we will be more careful about what precisely we mean by this. For now, we simply note that

$$\mathbf{A}(\mathbf{x}, t) \ = \ \mathrm{Re}(\mathbf{A}(\mathbf{q}, \omega) e^{i\mathbf{q}\cdot\mathbf{x} - i\omega t}) \quad (12)$$

where q, the magnitude of $\mathbf{q}$ is assumed small.

In studying the current response of the system to a slowly varying external vector potential, it is conventional to focus on two distinct limits, each with a different physical meaning. The first of these is related to the stiffness or rigidity that emerges when a continuous symmetry is spontaneously broken. Thinking of bosonic action as the path integral representation of a $O(2)$ spin system, this is identical to the "spin-stiffness" we discussed in our

introductory lectures as being one of the hallmarks of a broken symmetry state of a spin system. This limit is best discussed in imaginary time: If we consider the system in the presence of a uniform external vector potential $\mathbf{A}(\tau)$ (we are now working in imaginary time) pointing along the x axis, it is apparent from the gradient term in the Lagrangian density that turning on this vector potential is equivalent to imposing a twist in the orientation of ϕ of magnitude $QA(\tau)$ per unit length (where A is the magnitude of $\mathbf{A}$) as we move along the x direction on the time slice labeled by τ.

If we take the external vector potential to be *static*, *i.e.* independent of imaginary time, then this is a familiar situation in the context of classical spin systems (as mentioned earlier, the imaginary time action we consider is essentially a coarse grained version of the xy model in $d+1$ dimensions). Therefore, the change in the free energy density, $\delta\mathcal{F}$, that results from the imposition of a small twisting potential is related to the 'stiffness' ρ_s of the system as we discussed in our introductory lectures on broken symmetry and related issues:

$$\delta\mathcal{F} = \frac{1}{2}\rho_s(QA)^2 \tag{13}$$

to leading order in A, the magnitude of the external vector potential.

Let us now be a bit more precise about what we mean by "uniform" and "static". The precise limit that probes the stiffness is one in which the frequency $\omega_n = 2\pi nT$ is set to zero by working with $n = 0$ (periodicity in the imaginary time direction of course constraints allowed frequencies to have this form), and $q_\parallel$, the component of the momentum parallel to the vector potential is also set to zero, while the transverse component $q_\perp$ is *sent to zero later*. To understand this limit, we note that in this limit, the magnetic field obtained from this vector potential will be a non-zero constant, and the stiffness of the system is nothing but its ability to create internal currents that try and cancel out this magnetic flux, giving rise to the Meissner effect in superconductors, familiar from your elementary solid-state physics classes. Indeed, the stiffness we are talking about here is, up to a proportionality constant, the superfluid density of the system.

To express the superfluid density in terms of correlation functions of the system, it is convenient to work with the imaginary time path integral representation of the partition function $Z$and take two derivates of $-k_BT\log(Z)$

to give:

$$\rho_s = c^2\{T\sum_{\epsilon_m}\int\frac{d^dk}{(2\pi)^d}\langle\phi_\alpha(\mathbf{k},\epsilon_m)\phi_\alpha(-\mathbf{k},-\epsilon_m)\rangle - c^2\langle\Xi(q_\perp\to 0,q_\parallel=0,\omega_n=0)\Xi(q_\perp\to 0,q_\parallel=0,\omega_n=0)\rangle_c\}\ ; \tag{14}$$

here the subscript c on the correlation function of Ξ indicates that we only keep the connected terms, $\omega_n = 2\pi nT$, the sum in the first term is over frequencies $\epsilon_m = 2\pi mT$, and $\Xi(\mathbf{x},\tau)$ is defined as

$$\Xi(\mathbf{x},\tau) = \left(\boldsymbol{\nabla}\phi_\alpha(\mathbf{x},\tau)\epsilon^{\alpha\beta}\phi_\beta(\mathbf{x},\tau)\right)_\parallel\ , \tag{15}$$

where the subscript indicates the component parallel to A.

The second limit is the one appropriate for the discussion of transport properties: We now wish to study the current the system can carry in a transport experiment when acted on by a time-varying electric field. We therefore revert to real-time and note that the external electric field in this situation can be written as

$$\mathbf{E}(\mathbf{q}) = -\frac{\partial\mathbf{A}(\mathbf{q})}{\partial t}\ . \tag{16}$$

For a transport experiment, the appropriate limit is one in which $q_\parallel$ and $q_\perp$ are both set to zero at the outset, and the frequency *sent to zero later* if we wish to model the d.c. transport.

Now, the uniform conductivity tensor at non-zero temperature T is defined as

$$\sigma(t,t',T) = \frac{\delta\langle\mathbf{J}\rangle(t)}{\delta\mathbf{E}(t')}_{\mathbf{E}=0} \tag{17}$$

Using the expression for $\mathbf{E}$ in terms of $\mathbf{A}$, we then have

$$\sigma(\omega,T) = \frac{1}{i\omega}\frac{\delta\langle\mathbf{J}\rangle(\omega)}{\delta\mathbf{A}(\omega)}_{\mathbf{A}=0}\ ; \tag{18}$$

here it is understood that the current $\mathbf{J}$ is parallel to the vector potential $\mathbf{A}$ due to the isotropy of our theory. One may now use the standard linear response theory formalism we have already studied in previous lectures to derive an expression for the conductivity at frequency ω in terms of a retarded correlation function. I leave this to you as an exercise to work out.

Here, we prefer to highlight a different approach: In this alternate path integral approach, one works with the imaginary-time path integral and derives an expression for the imaginary frequency conductivity $\sigma(\omega_n, T)$:

$$\begin{aligned}\sigma(\omega_n, T) &= \frac{c^2 Q^2}{\omega_n}\{T\sum_{\epsilon_m}\int \frac{d^d k}{(2\pi)^d}\langle\phi_\alpha(\mathbf{k},\epsilon_m)\phi_\alpha(-\mathbf{k},-\epsilon_m)\rangle \\ &\quad - c^2\langle\Xi(q_\perp=0,q_\parallel=0,\omega_n)\Xi(q_\perp=0,q_\parallel=0,-\omega_n)\rangle_c\}\ ;\end{aligned} \tag{19}$$

here we have used the same notation as in our earlier expression for the superfluid stiffness. At this point, you may wonder: How does one obtain the real-frequency conductivity from this expression at the imaginary frequencies $i\omega_n$? To answer this, you should go back to the discussion of analyticity properties of response functions in the complex ω plane (in our earlier lectures on linear response theory), and convince yourself that the correct procedure is to take the above result at positive ω_n, *i.e.* in the upper-half plane, and continue down to the real-axis. Although this is true in principle, the analytical continuation of approximate or numerical results for the imaginary frequency conductivity is fraught with difficulty, and requires us to have at least a rough idea of what the answer should look like. It is therefore common to constrain the end-result of analytical continuation with sum-rules and Kramers-Kronig relations whenever applicable.

This concludes our discussion of the effective field theory for the low-energy properties of the Bose-Hubbard model.