1 Superfluidity and Bose Einstein Condensate

1.2 Bose-Hubbard model: complete phase diagram

Before we investigate in more detail the properties of the superfluid phase, let’s see what the full phase diagram looks like. In the limit where $t \ll U$, the system looks very different. In particular, if we set $t = 0$, different lattice sites decouple from each other and the Hamiltonian becomes

$$H_{BH} = \frac{U}{2} \sum_i N_i(N_i - 1) - \mu \sum_i N_i = \sum_i \frac{U}{2} N_i^2 - (\frac{U}{2} + \mu) N_i = \sum_i \frac{U}{2} \left( N_i - \left(\frac{1}{2} + \frac{\mu}{U}\right)\right)^2 - \frac{(U/2 + \mu)^2}{2U}$$

Depending on the parameters $\mu$ and $U$, the ground state would host certain number of bosons on each lattice. When $\frac{\mu}{U} < 0$, $N_i = 0$ minimizes the energy and the ground state has no boson; when $0 < \frac{\mu}{U} < 1$, $N_i = 1$ and the ground state has one boson per site; generally, when $n < \frac{\mu}{U} < n + 1$, ($n > 0$), $N_i = n + 1$ and the ground state has $n + 1$ bosons per site.

Therefore, in this limit of the Bose Hubbard model, the bosons are completely immobile. Excitations on the ground states corresponds to adding or removing one boson from a lattice site, which costs energy of the amount $U \left( n + 1 - \frac{\mu}{U} \right)$ and $U \left( \frac{\mu}{U} - n \right)$. A finite amount of energy is needed (as long as $\frac{\mu}{U}$ is not exactly equal to an integer) to make an excitation in the system, therefore the system is gapped. If the bosons carry charge and we couple the system to a small electric field, as long as the electric field is small enough, we wouldn’t be able to make excitations in the system. Therefore, the system is an insulator. This insulating behavior is a result of the on-site interaction between the bosons and we call it the Mott insulator (similar to the Mott insulating phase for the fermions). When $\frac{\mu}{U}$ is exactly equal to an integer $n$, $N_i = n$ and $N_i = n + 1$ states have the same energy and this marks the transition point from one Mott insulating state to another.

Starting from one of the Mott insulating phases, if we turn on the hopping $t$ a little bit, because the system is gapped, we expect the system to stay in the same phase for some small but finite value of $t$. In particular, in the presence of hopping, the total boson number $\sum_i N_i$ is still a good quantum number of the Hamiltonian even though each individual $N_i$ no longer is. Within a finite region of small $t$, we expect the total boson number to remain the same as the $t = 0$ point. Of course, when $t$ is large enough, the system will go into the superfluid phase. Fig. 1.2 shows the structure of the total phase diagram with respect to parameters $\frac{\mu}{U}$, $\frac{t}{U}$. The phase diagram is composed of Mott insulating lobes corresponding to different boson density and the right hand side of the phase diagram is the superfluid phase. As the boson density in a Mott insulating lobe does not change with infinitesimal changes to the chemical potential $\mu$, the Mott insulating phase is said to be ‘incompressible’.

The Mott insulating phase is sharply distinct from the superfluid phase in terms of symmetry. The Hamiltonian of the Bose Hubbard model always has charge conservation symmetry, no matter what the parameters are. While the superfluid ground state spontaneously break this symmetry, the Mott insulating ground state does not. Because of this difference, to go from the superfluid phase to the Mott insulating phase or vice versa, one has to go across a phase transition.
(There was a question in class about why the lobes get smaller with increasing $\mu$. In the book “Quantum Phase Transitions” by Subir Sachdev, section 10.1 discussed a way to identify the location of the phase transition using the mean-field approximation of the model. You can read about it if interested.)

1.3 Superfluid phase: condensation

We said that the superfluid phase can describe a Bose-Einstein condensate which has a macroscopic number of bosons in the lowest energy single particle state. Let’s see how this is manifested in the mean field wave function. Consider the wave function with $\gamma = \rho_0$. That is, we have fixed the phase factor of the coherent state to be zero. The wave function then reads

$$\prod_i |\gamma = \rho_0\rangle = \left( e^{-\rho_0^2/2} \sum_{n_1=0}^{\infty} \frac{\rho_0^{n_1}}{\sqrt{n_1!}} |n_1\rangle \right) \left( e^{-\rho_0^2/2} \sum_{n_2=0}^{\infty} \frac{\rho_0^{n_2}}{\sqrt{n_2!}} |n_2\rangle \right) \ldots$$

If we expand it into components with a fixed number of bosons, we find that there is one component with no boson – the $|0\rangle$ state; with one boson, the wave function is (up to some prefactor)

$$|100\ldots + |010\ldots + |001\ldots + \ldots = (b_1^\dagger + b_2^\dagger + b_3^\dagger + \ldots)|0\rangle \propto b_{k=0}^\dagger |0\rangle$$

That is, the one boson component has one boson in the $k = 0$ state. With two bosons, the wave function is up to some prefactor

$$|110\ldots + |011\ldots + |101\ldots + \ldots + \frac{1}{\sqrt{2}}|200\ldots + \frac{1}{\sqrt{2}}|020\ldots + \frac{1}{\sqrt{2}}|002\ldots + \ldots \propto (b_1^\dagger + b_2^\dagger + b_3^\dagger + \ldots)(b_1^\dagger + b_2^\dagger + b_3^\dagger + \ldots)|0\rangle$$

Therefore, the total condensate wave function is a superposition of components with different number of bosons. Within each component, there are $n$ bosons all in the same $k = 0$ single particle state. If we look at each component in real space, then it is a superposition of all possible configurations with $n$ bosons. The relative weight between different components are tuned by the parameter $\rho$ to make sure that on average, the condensate has a boson density

$$\left( \prod_i \langle \gamma = \rho_0 \rangle \right) \frac{1}{N} \sum_i b_i^\dagger b_i \left( \prod_i |\gamma = \rho_0\rangle \right) = \rho_0^2$$

where $N$ is the total number of lattice sites.
Although the condensate wave function does not have a fixed particle number, usually we can ignore this fact to some extent. This is because the fluctuation of the particle number is small. To characterize this, we can calculate the variance of total particle number $\Delta N$:

\[
(\Delta N_{tot})^2 = \langle (\sum N_i)^2 \rangle - \langle \sum N_i \rangle^2 = \sum_{i \neq j} \langle N_i N_j \rangle + \sum_i \langle N_i^2 \rangle - \langle \sum N_i \rangle^2 = N(N-1)\rho_0^4 + N\rho_0^2(\rho_0^2 + 1) - N^2\rho_0^4
\]

Therefore, $\Delta N_{tot} \sim \sqrt{N}\rho_0$. On the other hand, $N_{tot} \sim N\rho_0^2$. Therefore, when $N$ is large, the variance (fluctuation of total particle number) is negligible compared to the total particle number.

### 1.4 Superfluid phase: long range correlation

The idea of symmetry breaking is actually a tricky one in quantum mechanics. Consider the mean field ground states of the superfluid phase discussed above $\prod_i |\gamma_i = \rho_0 e^{i\phi_0}\rangle$. It is true that $\phi_0$ can change to a different $\phi_1$ if we apply the global symmetry operator $e^{i(\phi_1-\phi_0)}\sum_k N_k$, so that each one of these wave functions is not $U(1)$ symmetric. However, we can make a linear superposition of all such wave functions to restore symmetry. That is, a wave function of the form

\[
|\psi_{sym}\rangle = \int d\phi \prod_i |\gamma_i = \rho_0 e^{i\phi}\rangle
\]

is actually invariant under the $U(1)$ symmetry transformation and also a legitimate ground state! (after proper normalization) In particular, if we try to measure an order parameter – an operator that transform nontrivially under the global symmetry – and use that as an indication of symmetry breaking, we would find that it is zero on the symmetric state. For example, we can take the order parameter to be $b$ which transforms under symmetry as $V_{\alpha} b V_{\alpha}^\dagger = e^{-i\alpha} b$. If we calculate its expectation value on $\prod_i |\gamma_i = \rho_0 e^{i\phi_0}\rangle$, we find it to be $\rho_0 e^{i\phi_0}$ indicating symmetry breaking. However, if we calculate its expectation value on $|\psi_{sym}\rangle$, we will have to average over the phases $\phi$ and the expectation value becomes zero. In fact, this always has to be the case as long as the order parameter transform in a nontrivial way under the symmetry because

\[
\langle \psi | O | \psi \rangle = \langle (\psi | U^\dagger(g)) O (U(g) | \psi \rangle \rangle = \langle \psi | (U^\dagger(g)OU(g)) | \psi \rangle = e^{i\alpha(g)} \langle \psi | O | \psi \rangle
\]

How do we tell then that in the superfluid phase the symmetry is spontaneously broken while in the Mott insulating phase the symmetry is not broken? One way to see that these two phases are definitely different is from their ground state degeneracy: the Mott insulator phase has a unique ground state while the superfluid phase has a very large ground state degeneracy, which can be lifted by local perturbations to the Hamiltonian but only by an amount that is exponentially small in system size. To have a more quantitative way to characterize spontaneous symmetry breaking, we can do either of the following things:

1. Take any state from the ground space and calculate the correlator $C_{ij} = \langle b_i^\dagger b_j \rangle$. We can see that for the superfluid ground state, $C_{ij} = \rho_0^2$ is a nonzero constant while for the Mott insulator ground state, $C_{ij} = 0$. This distinguishes between the two phases. At a generic point in the superfluid phase, we would expect $C_{ij}$ to approach a constant nonzero value when the distance between $i$ and $j$ ($|i-j|$) is large; at a generic point in the Mott insulator phase, we would expect $C_{ij}$ to decay to zero in an exponential way $e^{-|i-j|/\xi}$. 


2. If we do want to use the expectation value of the order parameter as an indication of symmetry breaking, we can still do so but be very careful that we need to pick states with short range correlation as measured by the CONNECTED correlator. That is, we need to pick states for which the connected correlator of any two operators \( \langle \psi | O_i^\dagger O_j | \psi \rangle - \langle \psi | O_i^\dagger | \psi \rangle \langle \psi | O_j | \psi \rangle \) goes to zero as \( |i - j| \to \infty \). We can check that this is true in the state \( \prod_i | \gamma_i = \rho_0 e^{i \phi_0} \rangle \) but not true in the symmetrized version \( | \psi_{\text{sym}} \rangle = \int d\phi \prod_i | \gamma_i = \rho_0 e^{i \phi} \rangle \). So if we pick states with short range connected correlation, the expectation value of the order parameter can be used as an indication of symmetry breaking.