Interacting Bosonic Systems on Lattice

We will focus our attention on the following model :

$$H = -t\sum_{\langle ij\rangle}\left[b^{+}_{i}\, b_j + h.c.\right] + \sum_i U\,(n_i - \bar{n})^2$$

where $U > 0$, $n_i = b^{+}_{i}\, b_i$ and $\bar{n}$ is a fixed, positive real number.

Since the two terms in the Hamiltonian do not commute, it is useful to consider the two limits, $\frac{U}{t} \gg 1$ and $\frac{U}{t} \ll 1$. Recall our discussion of transverse field Ising model (where $H = \sum_i -J\sigma_i^z\, \sigma_j^z - h\sum \sigma_i^x$) where we used a similar approach.

① $U/t \gg 1$.

Let's set $t=0$ to begin with.
Then $H = U\sum_i (n_i - \bar{n})^2$. This Hamiltonian has a unique ground state unless,
$\bar{n} = N + \frac{1}{2}$ where N is an integer.

when $\bar{n} \neq N + \frac{1}{2}$, then the ground state is

$$|\psi\rangle = \prod_i (b^+_i)^N |0\rangle$$

where N is the integer closest to $\bar{n}$. for example, when $\bar{n} = 1.4$, then $N = 1$, when $\bar{n} = 1.51$, then $N = 2$ etc. On the other hand, when $\bar{n} = N + \frac{1}{2}$ for integer N, (e.g. when $\bar{n} = 1.5$), then the states

$$|\psi_1\rangle = \prod_i (b^+_i)^N |0\rangle$$

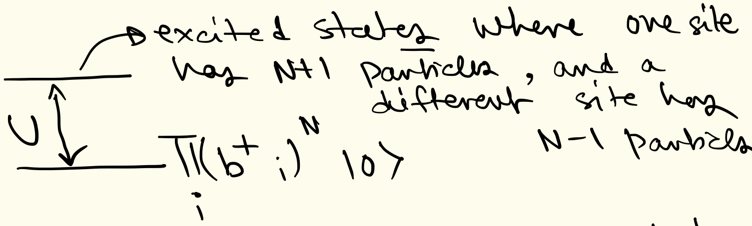
and

$$|\psi_2\rangle = \prod_i (b^+_i)^{N+1} |0\rangle$$

have exactly same energy.

The crucial question is : what happens when t is non-zero but small?

When $\bar{n} \neq N + \frac{1}{2}$ (N = integer), then the $t=0$ eigenspectrum looks like:



Since there is a unique ground state, the perturbation in t does not change the nature of ground state. Such a state with essentially fixed number of particles/site is called a

'Mott Insulator'. It is insulator because adding a particle to the system costs an energy U.

On the other hand, when $\bar{n} = N + \frac{1}{2}$, there are 2^N ground states because on each site there is two-fold degeneracy (as discussed above), and sites are decoupled.

Now it is not obvious if the perturbation in t dramatically changes the ground state or not. As we will discuss in a short while, the answer is that in this case, the Mott Insulator does not exist and one instead obtains a superfluid. But before we do that, an easier way to see the superfluid is to consider the opposite limit $t/U \gg 1$.

② $\frac{U}{t} \ll 1$.

For simplicity, in this limit, we will also assume that $\bar{n} \gg 1$.

Using the representation,

$$b^\dagger = \sqrt{n}\, e^{i\varphi}$$

where $[\varphi, n] = i$

the Hamiltonian becomes,

$$-t \sum_{\langle ij \rangle} \sqrt{n_i}\, e^{i(\varphi_i - \varphi_j)} \sqrt{n_j} + \sum_i U (n_i - \bar{n})^2$$

Since, $\bar{n} \gg 1$, one can write

$n_i = \bar{n} + \Delta n$ where $\langle \Delta n \rangle \ll \bar{n}$,

$$\Rightarrow \quad b_i^+ \simeq \sqrt{\bar{n}}\, e^{i\varphi_i}$$

$$\Rightarrow \quad H \simeq -2t\, \bar{n} \sum_{\langle ij \rangle} \cos(\varphi_i - \varphi_j) + U \sum_i (\Delta n_i)^2$$

if $t \gg U$, then one first minimizes the t term, $\Rightarrow$ $\varphi_i \cong \varphi \;\; \forall \; i$

$$\Rightarrow \quad \langle b^+_i \rangle \simeq \sqrt{\bar{n}}\, \langle e^{i\varphi_i} \rangle \neq 0$$

This is the superfluid phase.

Since φ_i doesn't fluctuate much,

$$-2t\bar{n}\cos(\varphi_i - \varphi_j) \simeq -2t\,\bar{n}\left[1 - \frac{(\varphi_i - \varphi_j)^2}{2}\right]$$

$$\Rightarrow H \simeq t\bar{n}\sum_{\langle ij\rangle}(\varphi_i-\varphi_j)^2 + U\sum_i(\Delta n_i)^2$$

This is essentially the same Hamiltonian as the one for coupled oscillators,

$$H \sim \sum_i \frac{p_i^2}{2m} + \frac{1}{2}m\omega_0^2\sum_{\langle ij\rangle}(x_i-x_j)^2$$

$$\Rightarrow H \simeq \sum_k \omega_k a^\dagger_k a_k$$

where $\omega_k \simeq \omega_0 k a$. ($a$ = lattice spacing)

What is ω_0? Comparing the harmonic oscillator problem and the boson problem,

$$\frac{1}{2m} = U \qquad \frac{1}{2}m\omega_0^2 = t\bar{n}$$

$$\Rightarrow \boxed{\omega_0 = \sqrt{2t\bar{n}\,2U} = 2\sqrt{t\bar{n}U}}$$

Thus, the superfluid phase supports a phonon-like mode! $\Rightarrow$ the spectrum of superfluid is gapless in strong contrast to the Mott insulator where it is gapped.

So far we have argued that when $\bar{n} \neq N + \frac{1}{2}$, at small t/U, one obtains a Mott Insulator while for any $\bar{n}$, at large $\frac{t}{U}$, one obtains a superfluid (we only showed this for $\bar{n} \gg 1$, but the conclusion turns out to be true even when $\bar{n} = O(1)$).

Now, we return to the question of $\bar{n} = N + \frac{1}{2}$ at small $\frac{t}{U}$.

As discussed above, at $t = 0$, there is a degeneracy of 2^N (in the grand canonical ensemble) corresponding to a two-state system at each site (the two states being $b^+_i b_i = N$ and $b^+_i b_i = N+1$). Therefore, the system behaves like a spin-$1/2$ spin system with $|N\rangle_i \equiv |\uparrow\rangle_i$ and $|N+1\rangle_i \equiv |\downarrow\rangle_i$, on each site i. With this setup, the perturbation theory in t/U is straightforward.

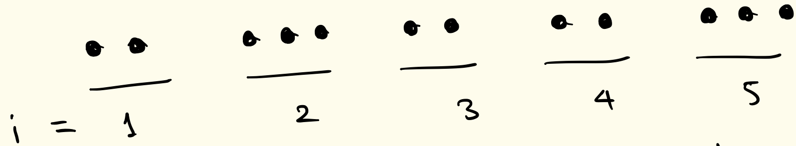
H_{eff} (i.e. H in the subspace of only two state $|\Uparrow\rangle_i, |\Downarrow\rangle_i$ on each site i)

$$= P - \sum_{ij} t\,(b^\dagger_i b_j + h.c.)\, P + \text{higher order terms}$$

where P projects onto the $\Uparrow / \Downarrow$ subspace

The main point to observe is that the leading term in H_{eff} is <u>not</u> identically zero. Consider e.g. when $N=2$:

An allowed configuration is



$P(b^\dagger_1 b_2 + b^\dagger_2 b_1)P$ acting on the above state generates the following state that is still in the allowed Hilbert space:

In fact, in the spin-language

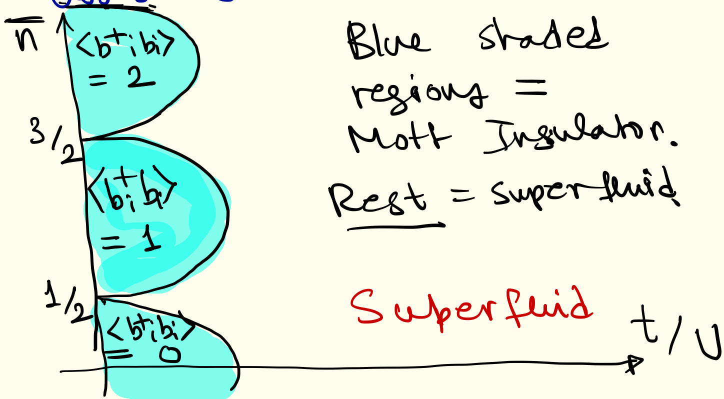
$$P(b^\dagger_i b_j + h.c.)P = (S_i^+ S_j^- + h.c.)$$

where $S^+ = S^x + iS^y$, $S^- = S^x - iS^y$

$$\Rightarrow \quad H_{eff} = -t \sum_{\langle ij \rangle} \left(S_i^+ S_j^- + h.c. \right)$$

This is a ferromagnetic quantum spin model due to minus sign in front $\Rightarrow$ the system orders ferromagnetically in the $x-y$ spin space. For example, one of the ground states is $|\psi\rangle = \prod_i |\rightarrow\rangle_i$ where $|\rightarrow\rangle_i$ denotes spin pointing along x-direction in the spin space. All such ground states break the spin rotation symmetry spontaneously $\Rightarrow \langle S_i^+ \rangle \neq 0$. This is exactly the superfluid phase, since $S_i^+ \sim b$.

Thus, when $\bar{n} = N + \frac{1}{2}$, one obtains a superfluid at infinitesimal t/U. The final phase diagram looks like:



Blue shaded regions = Mott Insulator.

Rest = superfluid