Interacting Bosonic Systems.

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 <u>unless</u>, $\bar{n} = N + \frac{1}{2}$ 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

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

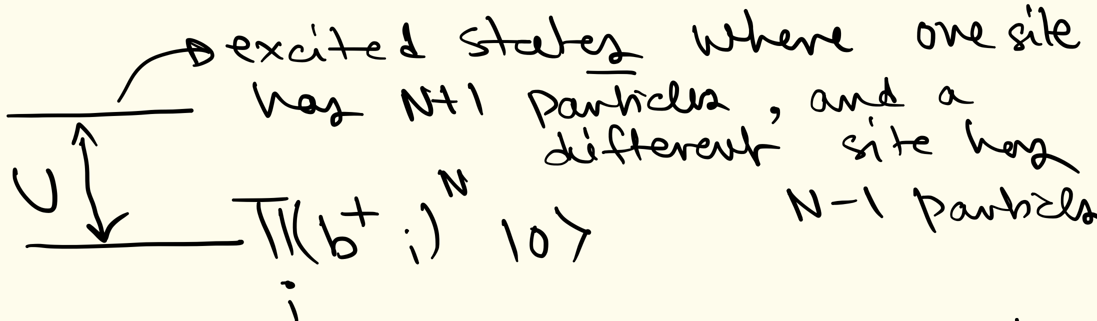
and

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

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 <u>insulator</u> 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,

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

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

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

$$\Rightarrow\ b^+_i\simeq\sqrt{\bar{n}}\,e^{i\varphi_i}$$

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

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

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

This is the superfluid phase.

Since φ_i doesn't fluctuate much,

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

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

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

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

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

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

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

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

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

Thus, the superfluid phase supports a phonon-like mode! $\Rightarrow$ the spectrum of superfluid is <u>gapless</u> 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)

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

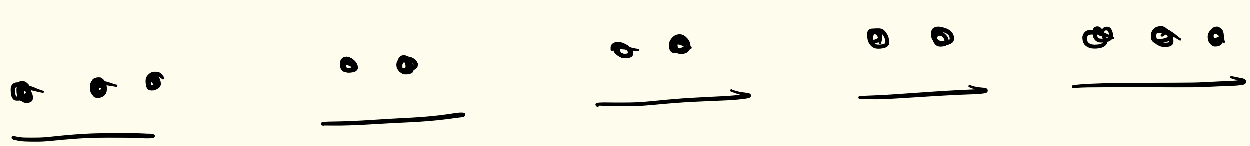
where P projects onto the $\Uparrow / \Downarrow$ subspace

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

An allowed configuration is

$i = 1 \quad 2 \quad 3 \quad 4 \quad 5$

$P\,(b^{+}_1 b_2 + b^{+}_2 b_1)\,P$ acting on the above state generates the following state that is still in the allowed Hilbert space:



In fact, in the spin-language

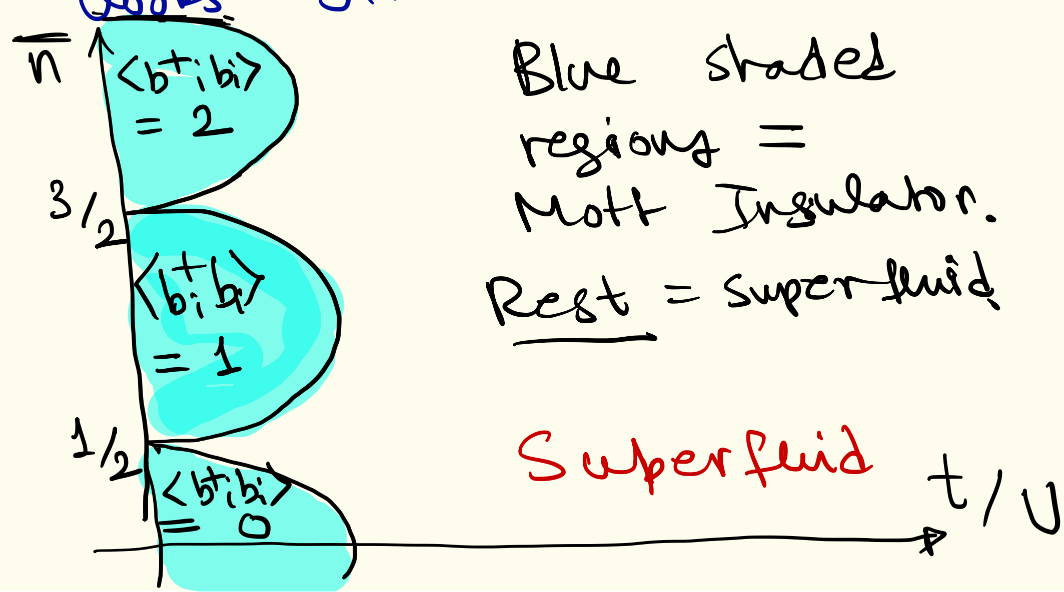
$$P\,(b^{+}_i b_j + h.c.)\,P = (S_i^{+} S_j^{-} + h.c.)$$

where $S^{+} = S^{x} + i S^{y}$, $S^{-} = S^{x} - i S^{y}$

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

This is a ferromagnetic quantum spin model due to minus sign in front $\Rightarrow$ 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. All such ground states in the spin space 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

Mapping to Classical O(2) model at Integer filling

Above, in the superfluid phase, we approximated $-\cos(\nabla\theta) \sim \frac{(\nabla\theta)^2}{2}$. Based on our discussion of the BKT transition, this approximation must break down as one approaches the Mott phase as vortices become important. Lets first show that one can map the Bose-Hubbard model at integer filling in d-space dimensions to an O(2) rotor model in d+1 - dimensions.

$$H = U\sum_i n_i^2 - t\sum_{\langle ij\rangle}\cos(\theta_i - \theta_j) \quad \text{where}$$

we have set $\bar{n} = 0$ (if $\bar{n} = N \in \mathbb{Z}$, one can always redefine $n - \bar{n} \to n$).

Consider the partition fn

$$Z = \operatorname{Tr} e^{-\beta H}$$

$$= \left[e^{-d\tau H}\right]^N \qquad N\,d\tau = \beta$$

$$N \to \infty$$

$$= \int_{e^{i\theta(0)} = e^{i\theta(\beta)}} D\theta(\tau) \prod_{\tau=0}^{\beta} \langle\theta(\tau)| e^{-d\tau H} |\theta(\tau + d\tau)\rangle$$

Consider the matrix element $\langle \theta(\tau) | e^{-d\tau H} | \theta(\tau + d\beta) \rangle$.

$$= \langle \theta(\tau) | e^{d\tau \, t \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)} \; e^{-U d\tau n_i^2} | \theta(\tau + d\beta) \rangle$$

$$= e^{d\tau \, t \sum_{\langle ij \rangle} \cos(\theta_i(\tau) - \theta_j(\tau))}$$

$$\underbrace{\langle \theta(\tau) | e^{-d\tau \sum_i U n_i^2} | \theta(\tau + d\beta) \rangle}$$

$\hookrightarrow$ Lets consider this term separately for a single site i.

$$\langle \theta | e^{-d\tau U n^2} | \theta' \rangle$$

$$= \sum_{n \in \mathbb{Z}} \langle \theta | n \rangle \; e^{-d\tau U n^2} \; \langle n | \theta' \rangle$$

Note that $n \in \mathbb{Z}$, so it's a discrete sum and not an integral (unlike with variables x, p where both x, p eigenvalues $\in \mathbb{R}$). Recall this is related to the compactness of θ: $\theta \equiv \theta + 2\pi$.

Using $\langle \theta | n \rangle = e^{-in\theta}$.

$$\Rightarrow \langle \theta | e^{-d\tau U n^2} | \theta' \rangle$$

$$= \sum_n e^{-d\tau U n^2 + i n (\theta' - \theta)}$$

Now we can use the Poisson resummation formula to simplify the sum:

$$\sum_{n \in \mathbb{Z}} f(n) = \sum_{k \in \mathbb{Z}} \hat{f}(k) \quad \text{where}$$

$\hat{f}$ is the Fourier transform of $f(n)$, i.e.

$$\hat{f}(k) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i k x}\, dx$$

In our problem,

$$f(x) = e^{-d\tau\, U x^2 + i x(\theta' - \theta)}$$

$$\Rightarrow \hat{f}(k) = \int_{-\infty}^{\infty} dn\, e^{-d\tau\, U x^2 + i x(\theta'-\theta) - 2\pi i k x}$$

This is a Gaussian integral, we can do it using saddle point: $-2Ux\,d\tau + i(\theta' - \theta - 2\pi k) = 0$

$$\Rightarrow x = i(\theta' - \theta - 2\pi k)/2U d\tau$$

$$\Rightarrow \hat{f}(k) \sim e^{-\frac{1}{4U d\tau}(\theta' - \theta - 2\pi k)^2}$$

$$\Rightarrow \langle \theta | e^{-d\tau U n^2} | \theta' \rangle \sim \sum_k e^{-\frac{1}{4U d\tau}(\theta' - \theta - 2\pi k)^2}$$

But this precisely the approximation to the cosine fn we discussed earlier.

$$\Rightarrow \quad \langle \theta | \, e^{-d\tau\, U n^2} \, | \theta' \rangle$$

$$= \quad e^{\frac{1}{2U d\tau} \cos(\theta - \theta')}$$

Putting everything together,

$$Z = \int d\theta \prod_{\tau=0}^{\beta} e^{d\tau \, t \sum_{\langle ij \rangle} \cos(\theta_i(\tau) - \theta_j(\tau))} \; e^{\frac{\cos[\theta_i(\tau) - \theta_i(\tau + d\tau)]}{2U d\tau}}$$

Again appealing to universality, the anisotropy in space-time is not expected any role for universal properties, and one may write.

$$Z = \int d\theta \; e^{J \sum_{\langle r r' \rangle} \cos(\theta_r - \theta_{r'})}$$

where $r \equiv (x, \tau)$ is a space-time coordinate in $d+1$ dimensions.

Using this mapping, we can now map our interacting boson phase diagram to that of the O(N) model:

$$\text{Superfluid} \longleftrightarrow \langle e^{i\theta} \rangle \neq 0$$

$$\text{Mott phase} \longleftrightarrow \langle e^{i\theta} \rangle = 0$$

(condensate of vortices)

Superfluid – Mott phase transition at <u>integer</u> <u>filling</u> = Wilson-Fisher fixed point for the O(2) model in d+1-dimensions

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Mapping to O(N) model at non-integral filling.

When $H = -t \sum_{\langle ij \rangle} (b^\dagger_i b_j + h.c.) + U \sum_i (n_i - \bar{n})^2$ with $\bar{n} \notin \mathbb{Z}$, the above derivation is not valid. Let's repeate the calculation and see where lies the difference.

$$\langle \theta | \, e^{-U(n-\bar{n})^2 d\tau} \, | \theta' \rangle$$

$$= \sum_{n \in \mathbb{Z}} e^{i n (\theta' - \theta) - U d\tau (n - \bar{n})^2}$$

$$= \sum_{n} e^{in(\theta' - \theta) - U d\tau \, n^2 + 2 U d\tau \, n \bar{n}}$$

(upto a constant factor)

$$= \quad e^{in(\theta' - \theta - i 2 U d\tau \bar{n}) - U d\tau \, n^2}$$

One may again use Poisson resummation

$$= \sum_{k} e^{-\frac{1}{4 U d\tau} (\theta' - \theta - i 2 U d\tau \bar{n} - 2\pi k)^2} .$$

$$\simeq \quad e^{\frac{1}{2 U d\tau} \cos(\theta' - \theta - i \, 2 U \, d\tau \, \bar{n})}$$

$$= \quad e^{\frac{1}{2 U d\tau} \cos((\partial_\tau \theta) \, d\tau - i \, 2 U \, d\tau \, \bar{n})}$$

$$\simeq \quad e^{\frac{1}{2 U d\tau} \{ \cos[(\partial_\tau \theta) \, d\tau] - \sin[(\partial_\tau \theta) d\tau] \sin(-i 2 U d\tau \, \bar{n}) \}}$$

$$= \quad e^{\frac{1}{2 U d\tau} \cos[(\partial_\tau \theta) d\tau]} \quad e^{i \bar{n} \, \partial_\tau \theta \, d\tau}$$

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direction. Therefore,

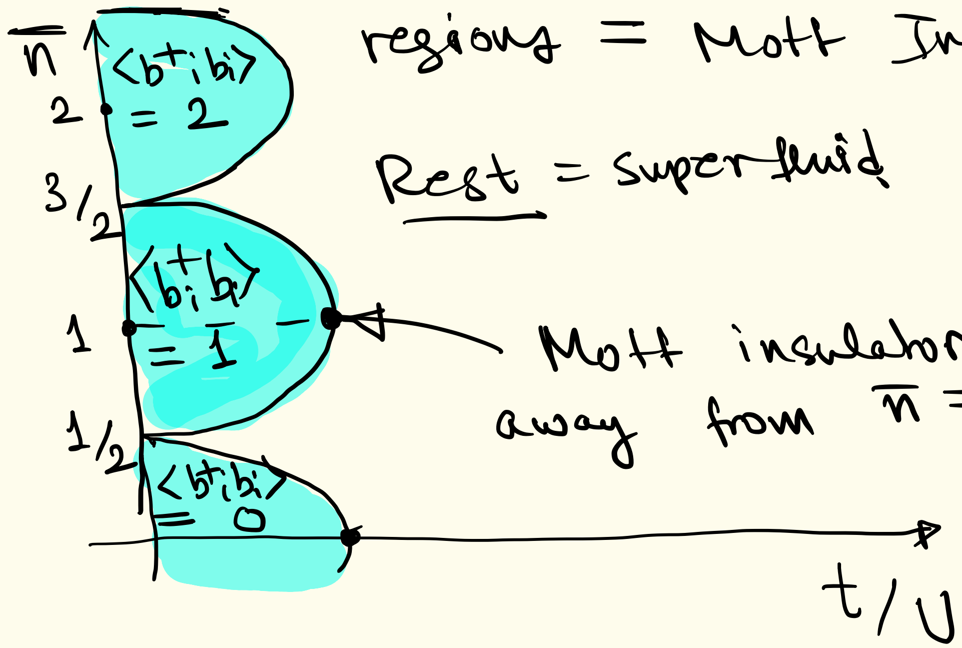
$Z =$

$$= \int D\theta \, \exp\Big[\int \frac{\sum_i}{2U\, d\tau} \cos(\partial_\tau \theta_i \, d\tau) + 2\pi i \bar{n} \sum_i n_{v,i}$$

$$+ \; t \sum_{\langle ij \rangle} \int d\tau \; \cos(\theta_i(\tau) - \theta_j(\tau)) \Big]$$

where $n_{v,i}$ is the vorticity in the time direction on site 'i'.

Therefore, $\bar{n} \neq \mathbb{Z}$ leads to quantum interference effects related to vorticity in the time direction. Since path integral fluctuates a lot in the presence of the vorticity, one expects that this imaginary term enhances superfluidity since vortices are suppressed due to phase cancellation. This is a heuristic way to understand the shape of phase boundaries.



Blue shaded regions = Mott Insulator.

Rest = superfluid

Mott insulator less stable away from $\bar{n}$ = integer

Quantum phase transition when $\bar{n} \neq$ integer.

The easiest way to proceed is to work with coherent-state path integral for bosons in the grand canonical ensemble:

$$Z = \int db\, Db^* \; \exp(-S)$$

$$S = \int_0^\beta d\tau \left[\sum_i b^*_i \frac{\partial b_i}{\partial \tau} - \mu \sum_i b^*_i b_i + U \sum_i (b^*_i b_i)^2 - t \sum_{\langle ij \rangle} (b^*_i b_j + c.c.) \right]$$

Where b = complex number.