Bose Hubbard Model

Setting:-

Regular lattice in d-dimensions

$\downarrow$

lattice points are spaced regularly.

Original Hubbard Model : The degrees of freedom are spin-$\frac{1}{2}$ fermionic electrons

Bose Hubbard Model :- describes spinless bosons on a regular lattice

Exa:- These bosons could represent cooper pairs of electrons undergoing Josephson tunnelling between superconducting islands

or

Helium atoms moving on a substrate

Degrees of Freedom

$\hat{b}_i$:- annihilates bosons on the site i

$\hat{b}_i^+$:- Creates bosons on the site i

$$[\hat{b}_i, \hat{b}_i^+] = \delta_{ij}$$

Def:- Boson number operator

$$\hat{n}_{bi} = \hat{b}_i^+ \hat{b}_i$$

$\Downarrow$

Counts the number of bosons on site i

There can be arbitrary number of bosons on each site

$$\mathcal{H} = \oplus \, |\{m_j\}\rangle \quad \text{s.t} \quad \hat{n}_{bi} |\{m_j\}\rangle = m_j |\{m_j\}\rangle$$

Vaccuum state with no bosons : $| \{ m_j = 0 \} \rangle$

Hamiltonian

$$H_B = \underbrace{-\omega \sum_{\langle ij \rangle} \left(\hat{b}_i^{+} \hat{b}_j + \hat{b}_j^{+} \hat{b}_i \right)}_{} \underbrace{- \mu \sum_i \hat{n}_{bi}}_{} + \frac{U}{2} \sum_i \hat{n}_{bi} \left(\hat{n}_{bi} - 1 \right)$$

allows hopping of bosons from site i to site j

Exa :-

Site $\Leftrightarrow$ Superconducting grain

ω $\Leftrightarrow$ Josephson tunneling

bosons $\Leftrightarrow$ Cooper pairs.

Chemical potential of bosons

Change in μ $\Rightarrow$ Change in total number of bosons

$\mu = \left.\frac{\partial f}{\partial N}\right|$ $\rightarrow$ partial derivative of free energy w.r.t amount of the species, other species & temp. being constant.

fixed μ $\Rightarrow$ Grand Canonical Ensemble ($\mu V T$ Ensemble)

fixed N $\Rightarrow$ Canonical ensemble (NVT ensemble)

theoretically easy !

Results are interconvertible through legendre transformation !

$U > 0$:- On-site repulsion

Exa:- Charging energy of each superconducting grain

Bose Hubbard Model (H_B) and O(N) rotor Hamiltonian (H_R)

$$H_R = \frac{J\bar{g}}{2} \sum_i \hat{L}_i^2 - J \sum_{\langle i,j \rangle} \hat{n}_i \cdot \hat{n}_j$$

$\downarrow$

Claim:- It has O(N) Symmetry.

Similarly

H_B is invariant under global $U(1) \equiv O(2)$ transformation

$$\hat{b}_i \to \hat{b}_i e^{i\phi}$$

$$H_B = -\omega \sum_{\langle ij \rangle} \left(\hat{b}_i^+ \hat{b}_j + \hat{b}_j^+ \hat{b}_i \right) - \mu \sum_i \hat{n}_{bi} + \frac{U}{2} \sum_i \hat{n}_{bi} (\hat{n}_{bi} - 1)$$

$$\hat{b}_i \to \hat{b}_i e^{i\phi} \Rightarrow \hat{b}_i^+ \to \hat{b}_i^+ e^{-i\phi}$$

$\Rightarrow$ H_B is invariant under $U(1)$ phase transformation.

Quantum Rotor Model V/s Bose Hubbard Model

H_R	H_B	Remark.
J term	ω term	Both couple neighbouring sites in a manner that prefers a state that breaks the global symmetry.
Jg term	U term	Completely local and prefers states that are completely invariant under U(1) transformation.

Nos.

$$|\Psi_{SF}\rangle = \frac{1}{\sqrt{N}}\left(\frac{1}{\sqrt{N_{sites}}}\sum_i b_i^\dagger\right)^{N_{atom}} |0\rangle$$

$$|\Psi_{Mott}\rangle = \prod_i b_i^\dagger |0\rangle$$

Under $b_i \to b_i e^{i\phi}$ both $|\Psi\rangle_{SF}$ & $|\Psi_{Mott}\rangle$ just acquire a global phase.

Phase 1 : $U(1)$ Symmetry is broken

Phase 2 : $U(1)$ Symmetry is unbroken

Phase transition occurs as a function of $\left(\frac{\omega}{U}\right)$.

Let us analyze the two regimes

(i) $\omega << U$

$$H = \frac{U}{2}\sum_i n_i(n_i-1) - \mu\sum_i n_i$$

$n=0 \qquad E=0$

$n=1 \qquad E=-\mu$

$n=2 \qquad E=-2\mu+U$

$\vdots$

$n \qquad E_n = -n\mu + \frac{U}{2}n(n-1)$

$N_b = \sum_i n_{bi}$ $\quad\quad$ $\hat{n}_{bi} = \hat{b}_i^+ \hat{b}_i$

Claim:- $[\hat{N}_b, H_B] = 0.$

Proof:- $\hat{n}_{bi} = \hat{b}_i^+ \hat{b}_i$

$\hat{N}_b = \sum_i \hat{b}_i^+ \hat{b}_i$

We know that $[A+B+C, D] = [A,D] + [B,D] + [C,D]$

$$A = \omega \sum_{\langle i,j \rangle} (\hat{b}_i^+ \hat{b}_j + \hat{b}_j^+ \hat{b}_i)$$

$$D = \sum_i \hat{b}_i^+ \hat{b}_i$$

$$\left[\sum_{\langle i,j \rangle} \hat{b}_i^+ \hat{b}_j + \hat{b}_j^+ \hat{b}_i , \sum_i \hat{b}_i^+ \hat{b}_i \right]$$

$$= N^2(N-1) - N^2(N-1)$$

$$= 0$$

$$B = -\mu \sum_i \hat{n}_{bi}$$

$$[B, A] = 0$$

$$[C, A] = 0$$

thus, $[\hat{N}_b, H_B] = 0.$

Since

$$[\hat{N}_b, \hat{H}] = 0$$

We have the conservation of total number of bosons.

→ μ term in H_B does not break global $U(1)$ Symmetry for any value of μ.

Exercise:- $\hat{N}_b$ is the generator of $U(1)$ transformation.

Mean Field theory

Goal :- to model the properties of H_B by the best possible sum of single site Hamiltonians

$$H_{MF} = \sum_i \left\{ -\mu \hat{n}_{bi} + \frac{U}{2} \hat{n}_{bi} \cdot (\hat{n}_{bi} - 1) \right\} - \psi_B^* \hat{b}_i - \psi_B \hat{b}_i^\dagger$$

How do we come up with such a prescription at first instance?

→ ψ_B is a field which describes the influence of neighbouring sites (on site i)

→ No longer symmetric under global $U(1)$ transformation.

→ For $\psi_B \neq 0$, $[\hat{M}, \hat{n}_B] \neq 0$

⇒ total number of particles is not conserved.

$\psi_B \neq 0$:- Broken symmetry phase

$\psi_B = 0$:- Symmetric phase

Claim:- The state that breaks the U(1) symmetry will have nonzero $\underbrace{\text{stiffness}}_{}$ to rotations of the order parameter.

$\Updownarrow$ Superfluid density characterizing a superfluid ground state of bosons

Verify by reading rotor model

Since the mean field Hamiltonian is the same on each site, ground state does not spontaneously break translational symmetry of the lattice. This is however possible, but will remove it to avoid complications.

Why? How?

Finding the