Bose Hubbard Model

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1 Model

A general action for interacting lattice gas is

$$\begin{aligned} S\left[\psi^*, \psi\right] = & \int_0^{\hbar\beta} \mathrm{d}\tau \int \mathrm{d}\mathbf{x} \psi^*(\mathbf{x}, \tau) \left(\hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) \right) \psi(\mathbf{x}, \tau) \\ & + \frac{1}{2} \int_0^{\hbar\beta} \mathrm{d}\tau \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{x}' \psi^*(\mathbf{x}, \tau) \psi^*\left(\mathbf{x}', \tau\right) V\left(\mathbf{x} - \mathbf{x}'\right) \psi\left(\mathbf{x}', \tau\right) \psi(\mathbf{x}, \tau). \end{aligned} \tag{1}$$

Expanding in Wannier basis,

$$\psi(\mathbf{x}, \tau) = \sum_{\mathbf{n}, i} a_{\mathbf{n}, i}(\tau) w_{\mathbf{n}}\left(\mathbf{x} - \mathbf{x}_i\right), \tag{2}$$

we have

$$\begin{aligned} S\left[a^*, a\right] = & \int_0^{\hbar\beta} \mathrm{d}\tau \left\{ \sum_i a_i^*(\tau) \left(\hbar \frac{\partial}{\partial \tau} + \varepsilon_i - \mu \right) a_i(\tau) - \sum_{i \neq j} a_i^*(\tau) t_{i,j} a_j(\tau) \right\} \\ & + \int_0^{\hbar\beta} \mathrm{d}\tau \frac{U}{2} \sum_i a_i^*(\tau) a_i^*(\tau) a_i(\tau) a_i(\tau), \end{aligned} \tag{3}$$

with coefficients

$$\varepsilon_i = \int \mathrm{d}\mathbf{x} w_{\mathbf{0}}^*\left(\mathbf{x} - \mathbf{x}_i\right) \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) \right\} w_{\mathbf{0}}\left(\mathbf{x} - \mathbf{x}_i\right), \tag{4}$$

$$t_{i,j} = -\int \mathrm{d}\mathbf{x} w_{\mathbf{0}}^*\left(\mathbf{x} - \mathbf{x}_i\right) \left\{ -\frac{\hbar^2 \boldsymbol{\nabla}^2}{2m} + V^{\mathrm{ex}}(\mathbf{x}) \right\} w_{\mathbf{0}}\left(\mathbf{x} - \mathbf{x}_j\right), \tag{5}$$

$$U = \int \mathrm{d}\mathbf{x} \int \mathrm{d}\mathbf{x}' w_{\mathbf{0}}^*\left(\mathbf{x} - \mathbf{x}_i\right) w_{\mathbf{0}}^*\left(\mathbf{x}' - \mathbf{x}_i\right) V\left(\mathbf{x} - \mathbf{x}'\right) w_{\mathbf{0}}\left(\mathbf{x}' - \mathbf{x}_i\right) w_{\mathbf{0}}\left(\mathbf{x} - \mathbf{x}_i\right). \tag{6}$$

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The Hamiltonian for Boson is given by

$$\hat{H} = -t\sum_{\langle i,j\rangle}\hat{a}_i^\dagger\hat{a}_j + \sum_i\left(\varepsilon_i-\mu\right)\hat{a}_i^\dagger\hat{a}_i + \frac{U}{2}\sum_i\hat{a}_i^\dagger\hat{a}_i^\dagger\hat{a}_i\hat{a}_i, \tag{7}$$

and for Fermion

$$\hat{H} = -t_\alpha\sum_\alpha\sum_{\langle i,j\rangle}\hat{a}_{i,\alpha}^\dagger\hat{a}_{j,\alpha} + \sum_\alpha\sum_i\left(\varepsilon_{i,\alpha}-\mu_\alpha\right)\hat{a}_{i,\alpha}^\dagger\hat{a}_{i,\alpha} + U\sum_i\hat{a}_{i,\uparrow}^\dagger\hat{a}_{i,\downarrow}^\dagger\hat{a}_{i,\downarrow}\hat{a}_{i,\uparrow}. \tag{8}$$

2 Perturbative approach

2.1 Weak interaction limit

Transforming to momentum space, define

$$a_i(\tau) = \frac{1}{\sqrt{\hbar\beta N_\mathrm{s}}}\sum_{\mathbf{k},n}a_{\mathbf{k},n}\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{x}_i-\omega_n\tau)}, \tag{9}$$

and

$$\varepsilon_\mathbf{k} = -2t\sum_{j=1}^d\cos\left(k_j\lambda/2\right). \tag{10}$$

Note that $\lambda/2$ is the lattice spacing. Expanding the dispersion relation we have the effective mass $m^* = 2\hbar^2/t\lambda^2$, and that $m/m^* = t\pi^2/E_r$, with E_r the recoil energy.

If a huge number of atoms, say N_0, are condensed in the $\mathbf{0},0$ state, we can introduce the substitution

$$a_{\mathbf{0},0}^* \to \sqrt{\langle N_0\rangle\hbar\beta} + a_{\mathbf{0},0}^* \quad \text{and} \quad a_{\mathbf{0},0} \to \sqrt{\langle N_0\rangle\hbar\beta} + a_{\mathbf{0},0}. \tag{11}$$

The action to the quadratic order is given by

$$\begin{aligned} S\left[a^*,a\right] =& \hbar\beta\left(-zt-\mu+\frac{1}{2}Un_0\right)\langle N_0\rangle + \left(-zt-\mu+Un_0\right)\sqrt{\langle N_0\rangle\hbar\beta}\left(a_{\mathbf{0},0}^*+a_{\mathbf{0},0}\right) \\ &+ \sum_{\mathbf{k},n}\left(-\mathrm{i}\hbar\omega_n+\varepsilon_\mathbf{k}-\mu\right)a_{\mathbf{k},n}^*a_{\mathbf{k},n} + \frac{1}{2}Un_0\sum_{\mathbf{k},n}\left(a_{\mathbf{k},n}a_{-\mathbf{k},-n}+4a_{\mathbf{k},n}^*a_{\mathbf{k},n}+a_{-\mathbf{k},-n}^*a_{\mathbf{k},n}^*\right), \end{aligned} \tag{12}$$

with $n_0 = \langle N_0\rangle/N_s$ the number of condensed atoms per site. The linear term in the fluctuations being zero requires that $\mu = Un_0 - zt$, the action is therefore

$$\begin{aligned} S\left[a^*,a\right] =& -\frac{1}{2}\hbar\beta Un_0^2N_\mathrm{s} - \frac{1}{2}\hbar\beta\sum_\mathbf{k}\left(\bar{\varepsilon}_\mathbf{k}+Un_0\right) \\ &+ \frac{1}{2}\sum_{\mathbf{k},n}\left[a_{\mathbf{k},n}^*,a_{-\mathbf{k},-n}\right]\begin{bmatrix}\mathrm{i}\hbar\omega_n+\bar{\varepsilon}_\mathbf{k}+Un_0 & Un_0 \\ Un_0 & -\mathrm{i}\hbar\omega_n+\bar{\varepsilon}_\mathbf{k}+Un_0\end{bmatrix}\begin{bmatrix}a_{\mathbf{k},n} \\ a_{-\mathbf{k},-n}^*\end{bmatrix}, \end{aligned} \tag{13}$$

with $\bar{\varepsilon}_\mathbf{k} = \varepsilon_\mathbf{k} + zt$. Performing Bogolyubov transformation

$$\begin{bmatrix}b_{\mathbf{k},n} \\ b_{-\mathbf{k},-n}^*\end{bmatrix} = \begin{bmatrix}u_\mathbf{k} & v_\mathbf{k} \\ v_\mathbf{k}^* & u_\mathbf{k}^*\end{bmatrix}\begin{bmatrix}a_{\mathbf{k},n} \\ a_{-\mathbf{k},-n}^*\end{bmatrix} \tag{14}$$

with $|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1$, we have

$$S\left[b^*, b\right] = -\frac{1}{2}\hbar\beta U n_0^2 N_{\mathrm{s}} + \frac{1}{2}\hbar\beta \sum_{\mathbf{k}} \left(\hbar\omega_{\mathbf{k}} - \bar{\varepsilon}_{\mathbf{k}} - U n_0\right) + \sum_{\mathbf{k},n} \left(-\mathrm{i}\hbar\omega_n + \hbar\omega_{\mathbf{k}}\right) b^*_{\mathbf{k},n} b_{\mathbf{k},n} \tag{15}$$

with

$$\begin{aligned} \hbar\omega_{\mathbf{k}} &= \sqrt{\bar{\varepsilon}_{\mathbf{k}}^2 + 2U n_0 \bar{\varepsilon}_{\mathbf{k}}}, \\ |v_{\mathbf{k}}|^2 = |u_{\mathbf{k}}|^2 - 1 &= \frac{1}{2}\left(\frac{\bar{\varepsilon}_{\mathbf{k}} + U n_0}{\hbar\omega_{\mathbf{k}}} - 1\right). \end{aligned} \tag{16}$$

Considering that the average filling $n = \sum_{\mathbf{k},n} \langle a^*_{\mathbf{k},n} a_{\mathbf{k},n}\rangle / \hbar\beta N_s$, we have

$$n = n_0 + \frac{1}{N_{\mathrm{s}}} \sum_{\mathbf{k}\neq 0} \left(\frac{\bar{\varepsilon}_{\mathbf{k}} + U n_0}{\hbar\omega_{\mathbf{k}}} \frac{1}{\mathrm{e}^{\beta\hbar\omega_{\mathbf{k}}} - 1} + \frac{\bar{\varepsilon}_{\mathbf{k}} + U n_0 - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}} \right). \tag{17}$$

Solving the equation above gives us the condensate fraction. This equation yields $n_0 = 0$ only at $U/t \to \infty$ in 2D and 3D while $n_0 = 0$ everywhere in 1D, therefore no superfluid-Mott transition is predicted.

2.2 Strong interaction limit

2.2.1 Ginzburg-Landau Theory

Performing Hubbard-Stratonovich transformation to decouple the hopping term yields an action

$$\begin{aligned} S\left[a^*, a, \psi^*, \psi\right] = &\int_0^{\hbar\beta} \mathrm{d}\tau \sum_i \left\{ a_i^*(\tau) \left(\hbar\frac{\partial}{\partial\tau} - \mu\right) a_i(\tau) + \frac{U}{2} a_i^*(\tau) a_i^*(\tau) a_i(\tau) a_i(\tau) \right\} \\ &+ \int_0^{\hbar\beta} \mathrm{d}\tau \sum_{i,j} \left\{ -t_{ij} \left(a_i^*(\tau)\psi_j(\tau) + \psi_i^*(\tau) a_j(\tau)\right) + t_{ij}\psi_i^*(\tau)\psi_j(\tau) \right\} \end{aligned} \tag{18}$$

Denoting the action with $t_{ij} = 0$ as $S^{(0)}\left[a^*, a\right]$, we have the effective action taking ψ as parameter

$$\begin{aligned} \exp\left\{-\frac{1}{\hbar} S^{\mathrm{eff}}\left[\psi^*, \psi\right]\right\} \equiv &\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \sum_{i,j} t_{ij}\psi_i^*(\tau)\psi_j(\tau)\right\} \\ &\times \int \mathrm{d}\left[a^*\right] \mathrm{d}[a] \exp\left\{-\frac{1}{\hbar} S^{(0)}\left[a^*, a\right]\right\} \\ &\times \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \left(-\sum_{i,j} t_{ij}\left(a_i^*(\tau)\psi_j(\tau) + \psi_i^*(\tau) a_j(\tau)\right)\right)\right\}. \end{aligned} \tag{19}$$

Note that this action is invariant under the followed gauge transformation,

$$\begin{aligned} a(\tau) &\to a(\tau)\mathrm{e}^{\mathrm{i}\theta(\tau)}, \\ a^*(\tau) &\to a^*(\tau)\mathrm{e}^{-\mathrm{i}\theta(\tau)}, \\ \psi(\tau) &\to \psi(\tau)\mathrm{e}^{\mathrm{i}\theta(\tau)}, \\ \psi^*(\tau) &\to \psi^*(\tau)\mathrm{e}^{-\mathrm{i}\theta(\tau)}, \\ \mu &\to \mu + \mathrm{i}\hbar\partial_\tau\theta(\tau). \end{aligned} \tag{20}$$

Expanding the effective action within the gauge invariance condition yields

$$\begin{aligned}S^{\mathrm{eff}}\left[\psi^*,\psi\right] =& S[0,0]+\int_0^{\hbar\beta}\mathrm{d}\tau\left\{\sum_{i,j}t_{ij}\psi_i^*(\tau)\psi_j(\tau)+\sum_i\left(u\psi_i^*(\tau)\partial_\tau\psi_i(\tau)\right.\right.\\ &\left.\left.+v|\partial_\tau\psi_i(\tau)|^2+a|\psi_i(\tau)|^2+b|\psi_i(\tau)|^4+O\left(|\psi|^6,\psi^*\partial_\tau^3\psi\right)\right)\right\}.\end{aligned} \tag{21}$$

The coefficients satisfy the relations due to gauge invariance

$$\frac{\partial a}{\partial\mu}+u=0, \tag{22}$$

$$\hbar\frac{\partial u}{\partial\mu}-2v=0. \tag{23}$$

To the continuous limit the effective action becomes

$$\begin{aligned}S^{\mathrm{eff}}\left[\psi^*,\psi\right]=S[0,0]+\int_0^{\hbar\beta}\mathrm{d}\tau\int\mathrm{d}^d\mathbf{x}\left\{u\psi^*(\mathbf{x},\tau)\partial_\tau\psi(\mathbf{x},\tau)+v|\partial_\tau\psi(\mathbf{x},\tau)|^2+w|\nabla\psi(\mathbf{x},\tau)|^2\right.\\ \left.+(a+zt)|\psi(\mathbf{x},\tau)|^2+b|\psi(\mathbf{x},\tau)|^4+O\left(|\psi|^6,\psi^*\partial_\tau^3\psi,|\nabla^2\psi|^2\right)\right\}.\end{aligned} \tag{24}$$

We now have an effective Ginzburg-Landau theory. From the action we can see that if $u\neq 0$, the model is in the universality class of the $T=0$ Bose-Einstein condensation, while if $u=0$, the action is Lorentz invariant and falls into the universality class of the XY model in $d+1$ dimensions. The condition for $u=0$ will be discussed later.

2.2.2 Phase transition

We are going to reveal the phase transition from the effective action derived previously.

The phase transition is determined by the condition $a=0$ Calculate the effective Hamiltonian perturatively to the quadratic term,

$$\begin{aligned}S^{(2)}\left[\psi^*,\psi\right]=-\frac{1}{2\hbar}\left\langle\left(\int_0^{\hbar\beta}\mathrm{d}\tau\sum_{i,j}t_{ij}\left(a_i^*(\tau)\psi_j(\tau)+\psi_i^*(\tau)a_j(\tau)\right)\right)^2\right\rangle_0\\ +\int_0^{\hbar\beta}\mathrm{d}\tau\sum_{i,j}t_{ij}\psi_i^*(\tau)\psi_j(\tau).\end{aligned} \tag{25}$$

Considering the unperturbed energy and transforming to momentum space, we fianlly have

$$S^{(2)}\left[\psi^*,\psi\right]=-\hbar\sum_{\mathbf{k},n}\psi_{\mathbf{k},n}^*G^{-1}\left(\mathbf{k},\mathrm{i}\omega_n\right)\psi_{\mathbf{k},n}, \tag{26}$$

where the inverse Green's function obeys

$$\hbar G^{-1}\left(\mathbf{k},\mathrm{i}\omega_n\right)=\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{k}}^2\left(\frac{g+1}{-\mathrm{i}\hbar\omega_n-\mu+gU}+\frac{g}{\mathrm{i}\hbar\omega_n+\mu-(g-1)U}\right). \tag{27}$$

The energies of quasiparticle and quasihole excitations can be revealed from the zeros of the inverse Green's function with an analytic continuation from $\mathrm{i}\omega_n$ to ω.

$$\hbar\omega_{\mathbf{k}}^{\mathrm{qp,qh}}=-\mu+\frac{U}{2}(2g-1)+\frac{\varepsilon_{\mathbf{k}}}{2}\pm\frac{1}{2}\sqrt{\varepsilon_{\mathbf{k}}^2+2(2g+1)U\varepsilon_{\mathbf{k}}+U^2}. \tag{28}$$