Quantum Phases of Bose-Hubbard Model in Optical Superlattices

Bo-Lun Chen,¹ Su-Peng Kou,¹ Yunbo Zhang,² and Shu Chen³

¹Department of Physics, Beijing Normal University, Beijing 100875, P. R. China
²Institute of Theoretical Physics, Shanxi University, Taiyuan 030006, P. R. China
³Institute of Physics, Chinese Academy of Sciences, Beijing 100190, P. R. China

In this paper, we analyze the quantum phases of multiple component Bose-Hubbard model in optical superlattices, using a mean-field method, the decoupling approximation. We find that the phase diagrams exhibit complicated patterns and regions with various Charge Density Wave (CDW) for both one- and two- component cases. We also analyze the effective spin dynamics for the two-component case in strong-coupling region at unit filling, and show the possible existence of a Spin Density Wave (SDW) order.

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I. INTRODUCTION

The observation of Mott insulator – superfluid transition of ultracold bosons loaded in optical lattices has triggered huge amount of interest in quantum simulation. A lot of efforts have been made to investigate Bose-Hubbard Hamiltonian, both single and multiple components in cold atom systems (in double-wells, superlattices), using various techniques (projection wave-function, decoupling approximation, field theory, dynamical mean-field, etc.), aiming to achieve a comprehensible understanding of this many-body model.

Among these, multi-component Bose-Hubbard in optical superlattices attracts special attention due to its rich quantum phases and promising potential in emulating effective spin-spin interactions. Many works on this topic have revealed the existence of Mott insulator with integer and fractional fillings, correspond to various Charge Density Wave (CDW) and complex dynamical behaviors. People also reported topological phases and exotic localizations in disordered superlattices. Recently, to obtain a complete and thorough description of this model, several attempts have been made.

In this paper, we reinvestigate this problem by using a mean-field approach, the decoupling approximation. Working in the Mott insulating phase as an unperturbed ground state, and treating the hopping as perturbations, this method (though at mean-field level) can still give comparatively accurate results for phase transition, comparing with numerical simulations. Besides, since this method decouples the original Hamiltonian into a set of single-site Hamiltonian, it exhibits simple energy expressions for different filling situations in the Mott state. Therefore, we can analyze and write down all the possible filling configurations in a clear and evident manner. Then, we depict the corresponding phase boundaries for each filling condition, and gain a systematic description of possible quantum phases of this model. We further consider the effective spin dynamics at strong coupling limit and unit filling, and find both a ferromagnetic and an anti-ferromagnetic spin-wave excitation as the potential barrier between neighboring sites varies.

The paper is organized as follow: We first introduce the model in Sec. II, then deals with the single-component Bose-Hubbard model in Sec. III, which acts as a precedent of the two-component case that is discussed in Sec. IV. Both sections contain the mean-field calculations, the analysis of possible filling patterns and phase diagrams with corresponding illustrations. The spin dynamics is analyzed in the last subsection in Sec. IV. We give the conclusion in Sec. V.

II. MODELS

Our starting point is a two-component Bose-Hubbard model in a double-periodic superlattice,

\[ \hat{H} = - \sum_{\langle ij \rangle \sigma} (t_{ij} \hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + h.c.) + \frac{U}{2} \sum_{\sigma} \hat{n}_{i\sigma} (\hat{n}_{i\sigma} - 1) + V \sum \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \sum_{\sigma} (\mu_{\sigma} - \Delta) \hat{n}_{i\sigma}. \]  

(1)

Here \( \langle ij \rangle \) denotes the nearest-neighbor counting, \( t_{ij} \) is the hopping amplitude, \( U \) is the inter-species repulsion, \( V \) is the intra-species repulsion, \( \mu_{\sigma} \) is the chemical potential that restricts the particle number, \( \Delta \) is the energy bias on a given site, \( \hat{n}_{i\sigma} = \hat{a}_{i\sigma}^\dagger \hat{a}_{i\sigma} \) is the number operator for bosons with \( \sigma = \uparrow, \downarrow \) representing the two internal states of the trapped Bose Einstein Condensate (BEC).

For single-component Bose-Hubbard, the \((\text{pseudo})\)spin gets polarized so that \( \sigma \) takes a certain value; thus there is no intra-species interaction \( V \).

Generally speaking, the period of the superlattice can be set to be an arbitrary integer \( l \), as long as we require physical quantities are periodic functions, \( \psi_l = \psi_{l+l} \). For
written as, this mean-field scheme, we write the two bosonic opera-
pling approximation which was developed in Ref. \cite{4}. In
– superfluid (SF) transition, we apply an extended decou-
ament. The potential barrier is \( \Delta \). \((2)\) is denoted as the
parameter,

\[
\delta H = \sum_{i,j}(\hat{a}_i^\dagger \hat{a}_j + h.c.) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)
\]

\[ - \sum_i (\mu - \Delta_i) \hat{n}_i. \tag{3} \]

To determine the phase boundary of Mott-insulator (MI)–
uperfluid (SF) transition, we apply an extended decou-
pling approximation which was developed in Ref. \cite{4}. In
this mean-field scheme, we write the two bosonic operators \( \hat{a}_i^\dagger \hat{a}_j \) as \( \hat{a}_i^\dagger \hat{a}_j \approx \left( \hat{a}_i^\dagger \right) \left( \hat{a}_j^\dagger \right) \left( \hat{a}_j \right) \left( \hat{a}_i \right) \). Then by
introducing a site-dependent (local and small) SF order
parameter, \( \psi_i \equiv \left\langle \hat{a}_i^\dagger \right\rangle \left\langle \hat{a}_i \right\rangle \), the hopping term can be
written as,

\[- \sum_{i,j}(t_{ij} \hat{a}_i^\dagger \hat{a}_j + h.c.) \approx -t \sum_{i,\delta} \left[ \psi_i (\hat{a}_{i+\delta} + \hat{a}_{i-\delta}) - \psi_{i+\delta} \right] \]

\[ + \psi_{i-\delta} (\hat{a}_i + \hat{a}_j) - \psi_{i+\delta} \psi_j \]

\[ = -2t \sum_i (\hat{a}_i^\dagger + \hat{a}_i - \psi_i) \sum_{\delta} \psi_{i+\delta} \]

\[ = -2zt \sum_i (\hat{a}_i^\dagger + \hat{a}_i - \psi_i) \psi_{i+1}, \tag{4} \]

where we assume that in the strong-coupling regime \((U, V \gg t_{ij}, t_{ji}) \approx t_{ij} \equiv t \) and denote \( \psi_i \approx \psi_{i+\delta} \equiv \psi_{i+1}, \delta \) is the position vector for the nearest neighbors,

\( z \) is the coordination number. We then decouple the ini-
tial Hamiltonian Eq. \((3)\) into \( N \) (nearly) independent parts\([\tilde{H}], \hat{H} = \sum_i^N \hat{H}_i, \) where

\[
\hat{H}_i = \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - (\mu - \Delta_i) \hat{n}_i 
\]

\[ - 2zt (\hat{a}_i^\dagger + \hat{a}_i - \psi_i) \psi_{i+1}. \tag{5} \]

As a result, we can concentrate in one super-cell as shown in
Fig. \((1)\) with reduced Hamiltonian

\[
\hat{H}_{sc} = (2zt)^{-1} \sum_{l=1}^2 \hat{H}_l
\]

\[ = \sum_{l=1}^2 \left( \frac{U}{2} \hat{n}_l (\hat{n}_l - 1) - (\bar{\mu} - \bar{\Delta}_l) \hat{n}_l 
\]

\[ - (\hat{a}_l^\dagger + \hat{a}_l - \psi_l) \psi_{l+1} \right] 
\]

\[ = \hat{H}_{sc}^{(0)} + \psi_2 \psi_1 \psi_{1}, \tag{6} \]

where the dimensionless quantities are \( \bar{U} \equiv U/2zt, \bar{\mu} \equiv \mu/2zt \) and \( \bar{\Delta}_l \equiv \Delta_l/2zt, \) the unperturbed Hamiltonian
\( \hat{H}_{sc}^{(0)} \) is

\[
\hat{H}_{sc}^{(0)} = \sum_{l=1}^2 \left( \frac{U}{2} \hat{n}_l (\hat{n}_l - 1) - \bar{\mu}_l \hat{n}_l \right) + 2\psi_2 \psi_1 \psi_{1} \tag{7} \]

with reduced chemical potential \( \bar{\mu}_l \equiv \bar{\mu} - \bar{\Delta}_l, \) while the
hopping-induced perturbations are

\[
\psi_{l+2} = \psi_l, l = 1, 2.
\]

The unperturbed energy is the energy of states that have
finite particle number (Mott state), namely,

\[
E_g^{(0)} = \min \{ E_n^{(0)} \}_{n=0,1,2,...}, \tag{9} \]

where \( g = g_1 + g_2 \) is the average particle number in one
super-cell, \( q_l \) is the particle number on a certain site \( l \) in
the super-cell. Up to the second order, this implies

\[
E_g^{(0)} = E_{g+1}^{(0)}, E_g^{(0)} < E_{g-1}^{(0)}, \tag{10} \]

thus there will be a constraint on the chemical potential
\( \bar{\mu}. \) (To be discussed later.)

In the Mott state and near the MI-SF transition, the on-site particle number is still well-defined, then the unperturbed energy (written in a dimensionless form) becomes

\[
E_{\{g_1;g_2\}}^{(0)} = \sum_{l=1}^2 \left( \frac{U}{2} g_l (g_l - 1) - \bar{\mu}_l g_l \right) + 2\psi_1 \psi_{2} \]

\[ = \frac{U}{2} (g_1^2 + g_2^2 - g) - \bar{\mu} g_1 + \bar{\Delta}_g \bar{g}_2 + 2\psi_1 \psi_{2}(11) \]

where we have used Eq. \((2)\).
Meanwhile, the perturbation term $\hat{V}$ results in an energy correction, we can calculate this second-order perturbation energy $E^{(2)}_g$ in a standard manner [3],

$$E^{(2)}_g = E^{(2)}_{\{g_1, g_2\}} = \psi_1^2 \sum_{n_1 \neq n_2, g_1 \neq g_2} \frac{|\langle n_1, n_2 | \hat{V} | g_1, g_2 \rangle|^2}{E^{(0)}_{\{g_1, g_2\}} - E^{(0)}_{\{n_1, n_2\}}} + \psi_2^2 \sum_{n_1 \neq n_2, g_1 \neq g_2} \frac{|\langle n_1, n_2 | \hat{V} | g_1, g_2 \rangle|^2}{E^{(0)}_{\{g_1, g_2\}} - E^{(0)}_{\{n_1, n_2\}}}, \quad (12)$$

where the summation over $\{n_1, n_2\}$ has only the following terms, $\{n_1, n_2\} = \{g_1 \pm 1; g_2\}, \{g_1; g_2 \pm 1\}$, due to the simple form of $\hat{V}_t$. After straightforward calculations, we find

$$E^{(2)}_{\{g_1, g_2\}} = \psi_2^2 \left[ \frac{g_1 + 1}{-U g_1 + \bar{\mu}} + \frac{g_1}{U (g_1 - 1) - \bar{\mu}} \right] + \psi_1^2 \left[ -\frac{g_2 + 1}{-U g_2 + \bar{\mu}} + \frac{g_2}{U (g_2 - 1) - \bar{\mu}} \right] + \frac{\psi_1^2}{U (g_1 - 1) - \bar{\mu}} \left( -U g_1 + \bar{\mu} \right) + \frac{\psi_2^2}{U (g_2 - 1) - \bar{\mu}} \left( -U g_2 + \bar{\mu} \right). \quad (13)$$

Therefore, the total energy of a super-cell is $E = E^{(0)}_g + E^{(2)}_g + \cdots$ can be expanded into a power series of the SF order parameter $\psi_1$ and $\psi_2$ (Landau expansion),

$$E(\psi_1, \psi_2) = a_0 + a_2 \psi_1^2 + b_2 \psi_2^2 + c_2 \psi_1 \psi_2 + \mathcal{O}(\psi_1^4, \psi_2^4), \quad (14)$$

where we presume all coefficients of fourth-order and above are positive, stabilizing the system. The coefficients are

$$a_0 = \frac{\bar{U}}{2} (g_1^2 + g_2^2 - g - \bar{\mu} g + \Delta g),$$

$$a_2 = \frac{U^{(2)} (g_1 - 1) - \bar{\mu} + \Delta}{(-U g_2 + \bar{\mu} - \Delta)} \bar{\Delta}, \quad (15a)$$

$$b_2 = \frac{U^{(2)} (g_1 - 1) - \bar{\mu}}{(-U g_1 + \bar{\mu}) - c_2 = 2. \quad (15c)$$

Clearly, $E(\psi_1 = 0, \psi_2 = 0)$ is a local extremum, and represents the MI state. As the interaction $U$, the biased potential $\Delta$ and the particle number (chemical potential $\bar{\mu}$) changes to a critical point, the extremum $E(0, 0)$ becomes an instability point, thus a phase transition to SF state occurs. To express this idea explicitly, we should compare $\partial_{\psi_1}^2 E_{\{0,0\}}$, $\partial_{\psi_2}^2 E_{\{0,0\}}$ and $\partial_{\psi_1} \partial_{\psi_2} E_{\{0,0\}}$. The critical condition is $\bar{\Delta}^2 E_{\{0,0\}} \partial_{\psi_1} \partial_{\psi_2} E_{\{0,0\}} = (\partial_{\psi_1} \partial_{\psi_2} E_{\{0,0\}})^2$, i.e., $4a_2 b_2 = c_2^2$, or equivalently,

$$1 = \frac{(\bar{\mu} + \bar{U}) (\bar{\mu} - \bar{\Delta}) + \bar{\Delta}}{(U (g_1 - 1) - \bar{\mu}) (U (g_2 - 1) - \bar{\mu} + \Delta)(-U g_2 + \bar{\mu} - \Delta)}. \quad (16)$$

Simplify it, we obtain the phase boundary,

$$\bar{t}_c = \frac{1}{2} \sqrt{\frac{(g_1 - 1 - \bar{\mu}) (g_2 - 1 - \bar{\mu} + \Delta)(-g_2 + \bar{\mu} - \Delta)}{(\bar{\mu} + 1)(\bar{\mu} - \Delta + 1)}}, \quad (17)$$

where $\bar{t}_c \equiv zt/\bar{U}$, $\bar{\mu} \equiv \mu/\bar{U}$, and $\bar{\Delta} \equiv \Delta/\bar{U}$.

Before we come to the phase diagram, let us make some remarks on our approximation method. As pointed out in Ref. [11], the decoupling scheme works well in the vicinity of Mott state. The hopping effect induces a weak and local superfluid $\psi_t$, serving as a perturbation over the Mott state. Consequently, although this technique can determine the phase boundary conveniently, it cannot extrapolate correct physics in deep superfluid phase. Besides, from Eqs. (6, 7, 8) and the introduction of many dimensionless quantities we know that the MI-SF transition is universal, i.e., it occurs in similar manners in different dimensions; and this approximation gets better accuracy in higher dimensions.

B. Phase Diagrams

To depict the phase diagram, we can plot the phase boundary surface, Eq. (17) in the $\bar{\mu}$-$\bar{\Delta}$-$\bar{t}$ coordinate system. Before that, we need to take a closer look at the unperturbed groundstate to find appropriate constraints on the chemical potential $\bar{\mu}$.

As we mentioned, assuming the average filling in a supercell is $g = g_1 + g_2 \equiv \{g_1; g_2\}$, a natural question arises: what is the most energetically favorable filling factor $\{g_1; g_2\}$ for a given $g$? A straightforward solution to this question is to compare two arbitrary filling configurations $\{k_1; k_2\}$ and $\{m_1; m_2\}$ with $k_1 + k_2 = m_1 + m_2 = g$; namely, to compare their unperturbed en-
energy, \( \Delta E = E_{\{k_1,k_2\}}^{(0)} - E_{\{m_1,m_2\}}^{(0)} \). By using Eq. (11), this energy difference is

\[
\bar{\Delta}E = (k_2 + m_2 - \Delta)(k_2 - m_2) + (k_2 - m_2) \hat{\Delta}
\]  

(18)

with \( \bar{\Delta}E = \Delta E / U \), \( k_2, m_2 = 0, 1, \ldots, g \), respectively. Therefore, for a given potential bias \( \Delta \equiv \Delta / U \) and filling number \( g \), we can determine the groundstate configuration \( \{g_1; g_2\} \) which has the largest differences \( \bar{\Delta}E \) with respect to all other configurations.

More intuitively, we can simply draw the energy levels in the two sites of a supercell with a given reduced potential bias \( \hat{\Delta} \), and then fill atoms from the lowest level to higher levels one by one, up to \( g \). This filling sequence naturally costs the least energy, thus the resulting configuration is just the groundstate filling \( \{g_1; g_2\} \) (see Appendix).

As a result, for a given groundstate \( \{g_1; g_2\} \), from Eq. (10) we obtain the constraint on chemical potential \( \bar{\hat{\mu}} \).

For the most imbalanced case \( \{g; 0\} \), \( \bar{\hat{\mu}} \in (g - 1, g) \). For other cases, the calculations are simple but tedious. The results are listed in the following table. (\( p \in \text{even} \).)

| \( \Delta \) | \( g \in \text{even} \) | \( g \in \text{odd} \) |
|---|---|---|
| \((p - 1, p)\)| \( \bar{\hat{\mu}} \in (\frac{1}{2} [g + (p - 2)] + \frac{1}{2} (g - p) + \Delta) \) | \( \bar{\hat{\mu}} \in (\frac{1}{2} [g - (p + 1)] + \Delta, \frac{1}{2} [g + (p - 1)]) \) |
| \((p, p + 1)\)| \( \bar{\hat{\mu}} \in (\frac{1}{2} [g - (p + 2)] + \Delta, \frac{1}{2} (g + p)) \) | \( \bar{\hat{\mu}} \in (\frac{1}{2} [g + (p - 1)], \frac{1}{2} [g - (p + 1)] + \Delta) \) |

FIG. 2: (color online) The phase diagram for one-component case. Regions under the lopes are Mott insulating phase (MI), regions above those lopes are superfluid phase.

With these restrictions in hand, we now plot the phase diagram for one-component Bose-Hubbard model in superlattices, as shown in Figs. (2) and (3). It can be seen that in strong-coupling regions \( (t \ll U, \text{under the lobes}) \) with given potential bias \( \Delta \), the system is in Mott phase. As \( U \) decreases, phase transitions occur, the system goes into superfluid phase that is above the lobes. On the other hand, when \( \Delta \) changes, the phase boundaries and allowed Mott states change correspondingly.

For clarity, we denote the groundstate filling configuration at different parameter regions in Fig. (3). In regions to the left of the black solid line, parameters are chosen such that in Mott phase particles in a supercell must reside in the deep site (site 1), thus forms crystalline structure that has a doubled period of the original optical lattice. To illustrate the effect of increasing potential bias, we draw the phase boundaries along the vertical black dashed lines with fixed chemical potential \( \mu \), and along the oblique black dashed lines with fixed particle
and decoupled Hamiltonian is

$$
\hat{H}_1 = \frac{U}{2} \sum_{\sigma} (\hat{n}_{i\sigma} - 1) V \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \sum_{\sigma} (\mu_{\sigma} - \Delta_{\sigma}) \hat{n}_{i\sigma} - 2zt \sum_{\sigma} (\hat{a}_{i\sigma}^\dagger + \hat{a}_{i\sigma} - \psi_{i\sigma}) \psi_{i+1,\sigma},
$$

and decoupled Hamiltonian is

$$
\hat{H}_1 = \frac{U}{2} \sum_{\sigma} (\hat{n}_{i\sigma} - 1) + V \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \sum_{\sigma} (\mu_{\sigma} - \Delta_{\sigma}) \hat{n}_{i\sigma} - 2zt \sum_{\sigma} (\hat{a}_{i\sigma}^\dagger + \hat{a}_{i\sigma} - \psi_{i\sigma}) \psi_{i+1,\sigma}.
$$

The effective Hamiltonian in one supercell $\hat{H}_{sc}$ can still be written into two parts, $\hat{H}_{sc} = (2zt)^{-1} \sum_{l=1}^2 \hat{H}_l = \hat{H}_{sc}^{(0)} + \hat{V}$, where the unperturbed part is

$$
\hat{H}_{sc}^{(0)} = \sum_{l=1,\sigma} \left( \frac{U}{2} \hat{n}_{l\sigma} (\hat{n}_{l\sigma} - 1) - \mu_{l\sigma} \hat{n}_{l\sigma} + \psi_{l\sigma} \psi_{l+1,\sigma} \right)
$$

$$
+ V \sum_{l=1} \hat{n}_{l\uparrow} \hat{n}_{l\downarrow}
$$

with $\mu_{l\sigma} \equiv \bar{\mu}_{\sigma} - \Delta_l$ and $\bar{V} \equiv V/2zt$; while the perturbation is

$$
\hat{V} = - \sum_{l=1,\sigma} (\hat{a}_{l\sigma}^\dagger + \hat{a}_{l\sigma}) \psi_{l+1,\sigma} = \sum_{l=1,\sigma} \hat{V}_{l\sigma} \psi_{l+1,\sigma}
$$

(21)

with $\hat{V}_{l\sigma} \equiv - (\hat{a}_{l\sigma}^\dagger + \hat{a}_{l\sigma})$.

Similar to the one-component case, the unperturbed energy for a supercell with $g$ atoms is $E_g^{(0)} \equiv E_{\{g_{\uparrow},g_{\downarrow};g_2\}}^{(0)} = \min\{E_g^{(0)}\}_{g=1,2,...}$, which means $E_g^{(0)} < E_g^{(0)}$. Thus, the zero-order energy is

$$
E_{g_{\uparrow},g_{\downarrow};g_2}^{(0)} = \frac{U}{2} (g_{\uparrow}^2 + g_{\downarrow}^2 + g_2^2) + \bar{V} (g_{\uparrow}g_{\downarrow} + g_{\downarrow}g_2 + g_2g_{\uparrow}) - (\bar{\mu}_g - \bar{\mu}_1 g_1) + \bar{\Delta} g_2 + 2 (\psi_{\uparrow} g_1 + \psi_{\downarrow} g_2),
$$

(23)

and the second-order perturbation energy is

$$
E_{g_{\uparrow},g_{\downarrow};g_2}^{(2)} = \frac{E_{g_{\uparrow},g_{\downarrow};g_2}^{(2)}}{E_{g_{\uparrow},g_{\downarrow};g_2}^{(0)}} = \sum_{n \neq g} \frac{|\langle n | \hat{V} | g \rangle|^2}{E_n^{(0)} - E_0^{(0)}}
$$

$$
= E_{g_{\uparrow},g_{\downarrow};g_2}^{(2)} + E_{g_{\uparrow},g_{\downarrow};g_2}^{(2)} + E_{g_{\uparrow},g_{\downarrow};g_2}^{(2)} + E_{g_{\uparrow},g_{\downarrow};g_2}^{(2)},
$$

(24)

where $\bar{\sigma} \equiv -\sigma$
Hence, the Landau expansion takes the form

\[ E = a_0 + a_{2\uparrow} \psi_{1\uparrow}^2 + a_{2\downarrow} \psi_{1\downarrow}^2 + b_{2\uparrow} \psi_{2\uparrow}^2 + b_{2\downarrow} \psi_{2\downarrow}^2 + c_{2\uparrow} \psi_{1\uparrow} \psi_{2\uparrow} + c_{2\downarrow} \psi_{1\downarrow} \psi_{2\downarrow} + O (\psi^4) . \]

The coefficients are

\[ a_0 = \frac{U}{2} (g_{1\uparrow}^2 + g_{1\downarrow}^2 + g_{2\uparrow}^2 + g_{2\downarrow}^2 - g) + \Delta g_2 + \bar{V} (g_{1\uparrow}g_{1\downarrow} + g_{2\uparrow}g_{2\downarrow}) - (\mu_{1\uparrow} g_{1\uparrow} + \mu_{1\downarrow} g_{1\downarrow}), \]

\[ a_{2\sigma} = \frac{g_{2\sigma} + 1}{U (g_{2\sigma} - 1) + \bar{V} g_{2\sigma} - \mu_{1\sigma} + \Delta}, \]

\[ b_{2\sigma} = \frac{g_{1\sigma} + 1}{U (g_{1\sigma} - 1) + \bar{V} g_{1\sigma} - \mu_{1\sigma} + \Delta}, \]

(26a)

(26b)

(26c)

To derive the stability condition, we need to consider the following derivative at the point \( E_0 \equiv E (\psi_{1\uparrow} = 0, \psi_{1\downarrow} = 0, \psi_{2\uparrow} = 0, \psi_{2\downarrow} = 0): \)

\[ D = \begin{vmatrix} \frac{\partial^2 E_0}{\partial \psi_{1\uparrow}^2} & \frac{\partial^2 E_0}{\partial \psi_{1\uparrow} \partial \psi_{1\downarrow}} & \frac{\partial^2 E_0}{\partial \psi_{1\uparrow} \partial \psi_{2\uparrow}} & \frac{\partial^2 E_0}{\partial \psi_{1\uparrow} \partial \psi_{2\downarrow}} & \frac{\partial^2 E_0}{\partial \psi_{1\downarrow} \partial \psi_{2\uparrow}} & \frac{\partial^2 E_0}{\partial \psi_{1\downarrow} \partial \psi_{2\downarrow}} \\ \frac{\partial^2 E_0}{\partial \psi_{2\uparrow} \partial \psi_{2\uparrow}} & \frac{\partial^2 E_0}{\partial \psi_{2\uparrow} \partial \psi_{2\downarrow}} & \frac{\partial^2 E_0}{\partial \psi_{2\downarrow} \partial \psi_{2\uparrow}} & \frac{\partial^2 E_0}{\partial \psi_{2\downarrow} \partial \psi_{2\downarrow}} \end{vmatrix} = \begin{vmatrix} 2a_{2\uparrow} & c_{2\uparrow} & 0 \\ 0 & 2a_{2\downarrow} & c_{2\downarrow} \\ c_{2\uparrow} & 0 & 2b_{2\uparrow} \\ 0 & c_{2\downarrow} & 0 & 2b_{2\downarrow} \end{vmatrix} \]

\[ = c_{2\uparrow}^2 c_{2\downarrow}^2 - 4a_{2\uparrow} b_{2\uparrow} c_{2\downarrow}^2 - 4a_{2\downarrow} b_{2\downarrow} c_{2\downarrow}^2 + 16a_{2\uparrow} b_{2\uparrow} b_{2\downarrow}. \]

When \( D = 0 \), the insulating phase is no longer stable, thus a phase transition takes place. This critical condition can be written as \( 4a_{2\uparrow} b_{2\uparrow} = c_{2\uparrow}^2 \) or \( 4a_{2\downarrow} b_{2\downarrow} = c_{2\downarrow}^2 \). (Either one being satisfied will destabilize the system.) As a result, there exists two phase boundaries, each one

\[ \tilde{t}_{\sigma} = \frac{1}{2} \sqrt{\frac{[(g_{1\sigma} - 1) - \bar{\mu}_{\sigma} + \bar{V} g_{1\sigma}](-g_{1\sigma} + \bar{\mu}_{\sigma} - \bar{V} g_{1\sigma})[(g_{2\sigma} - 1) - \bar{\mu}_{\sigma} + \Delta + \bar{V} g_{2\sigma}](-g_{2\sigma} + \bar{\mu}_{\sigma} - \bar{V} g_{2\sigma}) - (\bar{\mu}_{\sigma} + 1 - \bar{V} g_{1\sigma})(\bar{\mu}_{\sigma} + 1 - \Delta - \bar{V} g_{2\sigma})}. \]

(27)

B. Phase diagrams

Similar to the single component case, we first determine the unperturbed groundstate and the range of the chemical potential, then depict the critical curve Eq. [27]. As \( \bar{V} \equiv V/U \) varies, there exists various filling configurations for the Mott state (unperturbed state). For the sake of clarity, we focus on the case \( \bar{V} = 1 \), which is most accessible in current experiments.

When the inter-species and intra-species repulsions

\[ \Delta = \begin{array}{c|c|c|c} \hline \Delta & g \in \text{even} & g \in \text{odd} \\ \hline (p - 1, p) & \bar{\mu}_{\sigma} \in \left( \frac{1}{2} (g + (p - 2)), \frac{1}{2} (g + p) \right) & \bar{\mu}_{\sigma} \in \left( \frac{1}{2} [g - (p + 1)] + \Delta, \frac{1}{2} [g + (p - 1)] \right) \\ (p, p + 1) & \bar{\mu}_{\sigma} \in \left( \frac{1}{2} [g - (p - 2)] + \Delta, \frac{1}{2} (g + p) \right) & \bar{\mu}_{\sigma} \in \left( \frac{1}{2} [g - (p + 1)], \frac{1}{2} [g - (p + 1)] + \Delta \right) \\ \hline \end{array} \]

With these, we plot the phase diagram for spin-\( \uparrow \) atoms in Figs. 5 and 6. The global structure of these dia-
grams are similar to the one-component case, but there exist many small lobes hiding in a large lobe, as shown in Fig. 6. They are the phase boundaries of various filling patterns in the Mott phase. The details are listed in Fig. 5, where the sequence reflects the actual position of lobes in Figs. 5. For example, \( \{1,0;0,1\} \) is written above \( \{0,1;1,0\} \), this means that in the 3D phase diagram, the lobe of filling \( \{1,0;0,1\} \) is also located beyond the lobe of \( \{0,1;1,0\} \). The illustrate these multiple lobes more clearly, in Fig. 7 we draw the cross-sections of the 3D phase diagram, \( \Delta = 0 \) (a) and \( \Delta = U \) (b). The structures of other cross-sections are similar to these two. Every lobes from bottom to top corresponds to a filling configuration in Fig. 6. From them, we find that there may exist weak superfluid (WSF) regions between two lobes that have the same particle number \( g \). In WSF regions, one spin species becomes superfluid while the other type remains insulating.

\textbf{C. Spin dynamics in biased superlattices}

In addition to the phase transitions that we describe above, in the Mott insulating phase, the two-component BEC trapped biased superlattices can exhibit spin dynamics and SDW-like patterns at different filling configurations.

At unit filling, Hubbard model [Eq. (1)] can be transformed into a Heisenberg-type model, via a canonical transformation and a second-order perturbation over \( t \),

\[ \hat{H}_{\text{eff}} = -J \sum_{\langle ij \rangle} (\hat{S}_i^x \hat{S}_j^y + \hat{S}_i^y \hat{S}_j^x) + (J_s - J) \sum_{\langle ij \rangle} \hat{S}_i^z \hat{S}_j^z, \]

where the (pseudo) spin operator is defined as usual, \( \hat{S}_i^\alpha = \frac{1}{2} \sum_{\mu \nu} \hat{a}_i^\dagger \sigma^\alpha_{\mu \nu} \hat{a}_i^\nu \) with \( \sigma^\alpha \) the Pauli matrix, \( \alpha = x, y, z \). The effective exchange energy is

\[ J = \frac{4t^2V}{V^2 - \Delta^2}, \quad J_s = \frac{8t^2U}{U^2 - \Delta^2}. \]
When $V \ll U$ and $V \gg U$, $J = 0$, then $\hat{H}_{\text{eff}} = -J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j$, which is an Ising model. There is no spin wave excitations in this case.

When $V = U$, $J_s = 2J$, then $\hat{H}_{\text{eff}} = -J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j$, which is a Heisenberg model. For ferromagnetic case ($\Delta < U$, $J > 0$), we define Holstein-Primakoff (HP) transformation as

$$\hat{S}^+ = \sqrt{2S - \hat{c}^\dagger \hat{c}} \hat{c}, \quad \hat{S}^- = \hat{c}^\dagger \sqrt{2S - \hat{c}^\dagger \hat{c}}, \quad \hat{S}^z = S - \hat{c}^\dagger \hat{c},$$

(30)

where bosonic operator $\hat{c}^\dagger (\hat{c})$ creates (annihilates) spin deviations, $S^\pm = S^x \pm i S^y$, $S$ is the total spin. For low excited states, spin deviation is small, thus $\sqrt{2S - \hat{c}^\dagger \hat{c}} \approx \sqrt{2S}$; applying this transformation up to second order, the ferromagnetic Heisenberg Hamiltonian becomes

$$\hat{H}_{\text{eff}} = -J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j = E_0 + 2zJS \sum_{i} \hat{c}_i^\dagger \hat{c}_i - JS \sum_{\langle ij \rangle} (\hat{c}_i^\dagger \hat{c}_j + \text{h.c.})$$

(31)

Here the ground state energy is $E_0 = -NzJS^2$ with $N$ the number of lattice site. This Hamiltonian is easy to diagonalize, the excitation energy in square lattice (in arbitrary dimensions) is

$$\epsilon_k = 2JS [z - \sum_{\delta} \cos (k \cdot \delta)] \approx JS \sum_{\delta} (k \cdot \delta)^2 = 2JS k^2,$$

(32)

Here, we set the lattice spacing to unity.

For anti-ferromagnetic case $\Delta \gtrsim U$, $J < 0$, the single-occupied state is metastable and it would decay to a triplet groundstate which satisfies the Libe-Mattis theorem. However, this metastable state can be prepared and probed in an experiment-accessible time interval, if the band width of a single particle $t$ is much smaller than its band gap $\Delta E = \Delta - U$, $t \ll \Delta E$. Under this circumstance, we can perform the HP transformation in $A$-$B$ sublattices and find the long-wave excitation in square lattices is

$$\epsilon_k = 2z |J| S \sqrt{1 - \gamma_k^2} \approx \sqrt{2z} |J| S k,$$

(33)

where $\gamma_k = z^{-1} \sum_{\delta} \cos (k \cdot \delta)$.

V. CONCLUSIONS

In this paper, using a decoupling approximation, we analyze the possible phase diagrams of one-and two-component Bose-Hubbard models in optical superlattices in the mean-field level. As the potential bias $\Delta$ of the superlattice, the atomic repulsion $U$ and hopping $t$, the filling configuration and chemical potential $\mu$ varies, we discover complex phases in different parameter regions. For one-component case, there exists Mott states with CDW order and corresponding MI-SF transitions. For two-component case, besides the CDW in Mott state, there also exists weak SF regions where one spin component holds the CDW order while the other component becoming superfluid. In addition, the spin imbalance for a certain filling configuration (see Appendix) implies the existence of an SDW-like order in the Mott state. We also calculate spin dynamics of the two-component model at unit filling. The results explicit different low-energy dispersions for different $\Delta/U$. The features can be tested via many accessible probing techniques in current experiments with single-site resolution.

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APPENDIX A: FILLING CONFIGURATION FOR ONE-COMPONENT CASE

The groundstate filling configurations $\{g_1; g_2\}$ for different $g$ (total number of particles in a supercell) and $\Delta \equiv \Delta/U$ are listed in the following table. Here, $p$ is an even number, $p - 1 \geq 0$, reflecting the ratio between potential bias $\Delta$ and inter-atomic repulsion $U$. The notation $\{g_1; g_2\}$ means that there are $g_1$ particles in the left (deep) site and $g_2$ particles in the right (shallow) site in a supercell.

| $\Delta$ | $g \in \text{even}$ | $g \in \text{odd}$ |
|----------|-------------------|-------------------|
| $(p - 1, p)$ | $\left\{ \frac{g + l}{2}, \frac{g - l}{2} \right\}$, if $g \leq p$ | $\left\{ \frac{g + l}{2} + \left( \frac{g}{2} - 1 \right), \frac{g - l}{2} - \left( \frac{g}{2} - 1 \right) \right\}$, if $g \leq p - 1$ |
| $(p, p + 1)$ | $\left\{ \frac{g + l}{2}, \frac{g - l}{2} \right\}$, if $g \leq p$ | $\left\{ \frac{g + l}{2} + \left( \frac{g}{2} - 1 \right), \frac{g - l}{2} - \left( \frac{g}{2} - 1 \right) \right\}$, if $g \leq p + 1$ |

APPENDIX B: FILLING CONFIGURATION FOR TWO-COMPONENT CASE

The filling configurations $\{g_{11}; g_{12}; g_{21}, g_{22}\}$ for two-component case is listed in the following tables. Here, $p$ is still an even number that set the value of $\Delta, k, l, q$.
are integers that take values in certain intervals. The notation \(\{g_{11}, g_{1 \uparrow}; g_{2 \uparrow}, g_{2 \downarrow}\}\) means that there are \(g_{11}\) spin-\(\uparrow\) atoms and \(g_{1 \uparrow}\) spin-\(\downarrow\) atoms in the left (deep) site, \(g_{2 \uparrow}\) spin-\(\uparrow\) atoms and \(g_{2 \downarrow}\) spin-\(\downarrow\) atoms in the right (shallow) site in a supercell.

| \(\Delta\) | \(g \in \text{even}\) |
|-----------|------------------|
| \((p-1,p)\) | \(\{\frac{p}{2} + k - l - q, \frac{p}{2} - k + \frac{q}{2} - \frac{l}{2} - q\}\) |
| \((p,p+1)\) | \(\{\frac{p}{2} + k - l - q, \frac{p}{2} - k + \frac{q}{2} - \frac{l}{2} - q\}\) |

| \(\Delta\) | \(g \in \text{odd}\) |
|-----------|------------------|
| \((p-1,p)\) | \(\{\frac{2p+1}{2} + (k - l) - q, (\frac{p}{2} - 1) - (k - l) + q; l + q, \frac{2p+1}{2} - (\frac{p}{2} - 1) - (l + q)\}\) |
| \((p,p+1)\) | \(\{\frac{2p+1}{2} + k - l - q, \frac{p}{2} - (k - l) + q; l + q, \frac{2p+1}{2} - \frac{p}{2} - l\}\) |

We can also define the spin imbalance \((m_1 = g_{1 \uparrow} - g_{1 \downarrow}, m_2 = g_{2 \uparrow} - g_{2 \downarrow})\) for a given filling pattern, the results are listed in the following table.

| \(\Delta\) | \(g \in \text{even}\) | \(g \in \text{odd}\) |
|-----------|------------------|------------------|
| \((p-1,p)\) | \(m_1 = \frac{3p}{2} - \frac{k}{2} + 2(k - l - q), m_2 = 2(l + q) - (\frac{q}{2} - \frac{k}{2})\) | \(m_1 = \frac{3p+1}{2} - \frac{k}{2} + 2(k - l - q), m_2 = 2(l + q) - (\frac{q}{2} - \frac{k}{2})\) |
| \((p,p+1)\) | \(m_1 = \frac{3p}{2} - \frac{k}{2} + 2(k - l - q), m_2 = 2(l + q) - (\frac{q}{2} - \frac{k}{2})\) | \(m_1 = \frac{3p+1}{2} - \frac{k}{2} + 2(k - l - q), m_2 = 2(l + q) - (\frac{q}{2} - \frac{k}{2})\) |

For filling configuration \(\{g;0\}\), we combine both filling pattern and spin imbalance in the following.

| \(\Delta\) | \(g \in \text{even}\) | \(g \in \text{odd}\) |
|-----------|------------------|------------------|
| \((p-1,p)\) | \(\{\frac{p}{2} + k, \frac{2}{2} - k; 0, 0\}, g \leq p, k \in [0, \frac{p}{2}]\), \(m_1 = 2k, m_2 = 0\) | \(\{\frac{p}{2} + k, \frac{2}{2} - k; 0, 0\}, g \leq p - 1, k \in [0, \frac{p}{2}]\), \(m_1 = 2k + 1, m_2 = 0\) |
| \((p,p+1)\) | \(\{\frac{p}{2} + k, \frac{2}{2} - k; 0, 0\}, g \leq p, k \in [0, \frac{p}{2}]\), \(m_1 = 2k, m_2 = 0\) | \(\{\frac{p}{2} + k, \frac{2}{2} - k; 0, 0\}, g \leq p + 1, k \in [0, \frac{p}{2}]\), \(m_1 = 2k + 1, m_2 = 0\) |

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