RESEARCH ARTICLE

Analytic calculation of high-order corrections to quantum phase transitions of ultracold Bose gases in bipartite superlattices

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We clarify some technical issues in the present generalized effective-potential Landau theory (GEPLT) to make the GEPLT more consistent and complete. Utilizing this clarified GEPLT, we analytically study the quantum phase transitions of ultracold Bose gases in bipartite superlattices at zero temperature. The corresponding quantum phase boundaries are analytically calculated up to the third-order hopping, which are in excellent agreement with the quantum Monte Carlo (QMC) simulations.

1 Introduction

The physics of ultracold Bose gases in optical lattices has been a hot topic during the last decade [1, 2]. Since the intensities and forms of interaction are highly controllable [2–7] for ultracold quantum gases, there is a great potential to simulate the physics of quantum many-body systems [8–10] that include a broad range of fields such as atomic physics, quantum chemistry, high energy physics, cosmology, and condensed matter physics.

As a famous example of simulation in condensed matter physics, the Bose–Hubbard model [11, 12] has been realized by loading ultracold bosonic atoms into the homogeneous simple cubic lattices [13]. In this system, ultracold bosonic atoms can experience a quantum phase transition from a Mott insulator (MI) to a superfluid (SF) when the ratio of the hopping amplitude t to the on-site interaction U goes above some critical value. The MI-SF transition can be detected directly in experiments via time-of-flight technique [13]. Recently, due to the development of experimental technologies and the deepening of theoretical studies, more and more attentions have been focused on complex systems which involve long-range interactions [14–18], multi-component gases

[19, 20], frustrations [21–23], and superlattice structures [24–28]. In such complex systems, there are some novel phases [29], including charge-density-wave (CDW) phase, supersolid phase [30], paired superfluid phase, super-counter-fluid phase [31] and so on. Phase diagrams of these complex systems are expected to be rather diverse and complex.

In order to study such plentiful phases in various optical superlattices systems, people have developed some numerical methods including QMC [32], exact diagonalization [32] as well as density-matrix renormalization group method [33, 34], and analytical methods including decoupled mean-field theory [35–38], multisite mean-field theory [39–42], the cell strong-coupling expansion [43, 44], the generalized Green's function method (GGFM) [45–47] as well as the GEPLT [47, 48]. Compared with the unbiased QMC results, it is found that the mean-filed theory underestimates the locations of the phase boundaries whereas the strong-coupling expansion method overestimates it. Based on the same perturbation treatment, both GGFM and GEPLT have the potential to obtain the more accurate locations of the boundaries of the second-order phase transition, but from a technical standpoint, the GEPLT is easy to obtain higher orders hopping corrections [47, 48]. However, the present GEPLT treatments [47, 48] have some technical issues that hinder its full application. These issues are required

to be fixed to demonstrate the power of GEPLT framework.

Although the phase boundaries of ultracold Bose gases in bipartite superlattices have been analytically calculated up to second-order hopping [48] and have also been numerically obtained [47] up to higher orders hopping via the process-chain approach with GEPLT, there still exist some subtle problems in their papers which need to be clarified. In Wang *et al.*'s work [48], the subtle problem is that when $\Delta\mu < 0.35U$ ($\Delta\mu$ is the difference of chemical potential for different sublattices), the full lobe of the MI phase (second-order result) can not be obtained. In Wei *et al.*'s work [47], there are two subtle problems. One is that there are no odd-order corrections for the critical t. The other is that when $\Delta\mu = 0$, the systems go back to the homogeneous systems, but the critical value of t [see Eq. (10) in Wei *et al.*'s work [47]] for bipartite systems is not the same with the results [see Eq. (11)] of the homogeneous systems. These subtle issues call for a more consistent and complete GEPLT treatment that includes high-order corrections.

In this paper, we will clarify these technical issues (see Section 2) and then propose a consistent and complete GEPLT to study the quantum phase transitions of ultracold Bose gases in bipartite superlattices. Using the corrected GEPLT, we get the quantum phase boundaries up to third-order hopping for ultracold Bose gases in square and cubic superlattices. Our analytical results are in good agreement with the QMC simulations and the relative deviation of our third-order results from the QMC results is less than 9% for square superlattices and 4% for cubic superlattices.

2 The model and generalized effective-potential Landau theory

The systems with ultracold spinless bosonic atoms tapped in bipartite superlattices can be described by [35, 48]

$$\hat{H} = -t \sum_{i \in A, j \in B} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + \frac{U}{2} \sum_{i \in A, B} \hat{n}_i(\hat{n}_i - 1)$$
$$-(\mu + \Delta\mu) \sum_{i \in A} \hat{n}_i - \mu \sum_{i \in B} \hat{n}_i, \qquad (1)$$

where t is the nearest-neighbor hopping amplitude, U denotes the on-site repulsion, $\hat{a}_i^\dagger$ is the creation operator and $\Delta\mu$ is the difference of chemical potential for sublattice A and B. The square superlattices can be realized by choosing the trapping potential as [47, 50, 55]

$$V(\boldsymbol{r}) = -V_0 \left[\cos^2\left(\frac{2\pi x}{\lambda}\right) + \cos^2\left(\frac{2\pi y}{\lambda}\right) \right.$$
$$\left. + 2\cos\theta \cos\left(\frac{2\pi x}{\lambda}\right) \cos\left(\frac{2\pi y}{\lambda}\right) \right], \qquad (2)$$

where λ is the wavelength of laser, and θ ($0 < \cos\theta < 1$) is the phase difference between the counterpropagating laser beams. The corresponding sketch of square superlattice is shown in Fig. 1. The value of $\Delta\mu$ can be adjusted by changing the value of θ. Hereinafter, without loss of generality, we set $\Delta\mu > 0$.

Let us first investigate the diagonal part of the system, whose Hamiltonian $\hat{H}_0$ reads

$$\hat{H}_0 = \frac{U}{2} \sum_{i \in A, B} \hat{n}_i(\hat{n}_i - 1) - (\mu + \Delta\mu) \sum_{i \in A} \hat{n}_i - \mu \sum_{i \in B} \hat{n}_i. \quad (3)$$

The eigenvalue of $\hat{H}_0$ is E_{n_A, n_B} and the corresponding eigenstate is $|n_A, n_B\rangle$, where $n_{A(B)}$ denotes the filling factor of the sublattice $A(B)$. The eigen equation and E_{n_A, n_B} take the form

$$\hat{H}_0 |n_A, n_{n_B}\rangle = N_s E_{n_A, n_B} |n_A, n_{n_B}\rangle,$$
$$E_{n_A, n_B} = \frac{U}{2} n_A(n_A - 1) + \frac{U}{2} n_B(n_B - 1)$$
$$- (\mu + \Delta\mu)n_A - \mu n_B. \qquad (4)$$

The total number of lattice sites is $2N_s$ and N_s is the number of super unit cell. The ground states can be revealed via the game of throwing bosons into the superlattice. Bose atoms favor staying in sublattice A than sublattice B for positive $\Delta\mu$. The first N_s particles will fill up sublattice A, and then the second N_s bosons will fill up sublattice A or B that is determined by whether $E_{2,0}$ is larger than $E_{1,1}$ or not. The state $|n, n\rangle$ is called MI state and the state $|n_A, n_B\rangle$ with $n_A \neq n_B$ is called CDW state. In the case of $\Delta\mu \in [0, U)$, the second N_s bosons will fill up sublattice B, and the third N_s bosons will go to sublattice A and so on. Thus it is evident that $n_A - n_B$ is always 1 or 0 in this case. In the case of $\Delta\mu > U$, there is no MI state, because in the MI(n, n) state the chemical potential needs to satisfy the constraint $U(n-1) \leq \mu \leq Un - \Delta\mu$ obtained by solving the
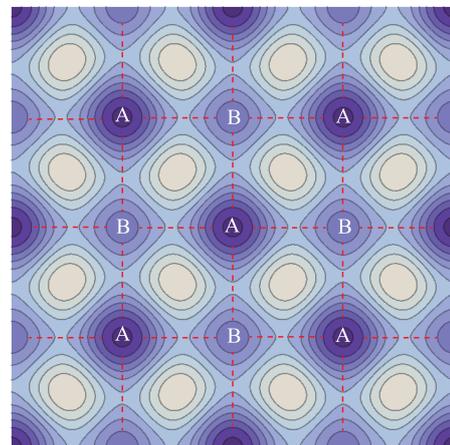

Fig. 1 The sketch of the square superlattice, the lattice sites A are $\Delta\mu$ deeper than lattice sites B.

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inequations $E_{n+1,n} \geq E_{n,n} \leq E_{n,n-1}$. This constraint is unsatisfied when $\Delta\mu > U$, thus there is only CDW state. Generally speaking, if $U(n-1) \leq \Delta\mu \leq Un$ with $n \geq 2$, the $n_A - n_B$ satisfies the constraint $1 \leq n_A - n_B \leq n$.

In the case of $\Delta\mu < U$ or $\Delta\mu > U$, the systems belong to different types, i.e., existence or nonexistence of the MI state. In the next section, we will study the phase boundaries of bipartite superlattices with three representative points $\Delta\mu = 0.1U$, $0.5U$, $1.5U$ to reveal this difference. In Wang *et al.*'s work [48], they have presented the QMC result for $\Delta\mu = 0.5U$, thus we can calculate the phase diagrams at this point to check the corrected GEPLT. The reason for choosing the case of $\Delta\mu = 0.1U$ is that in Wang *et al.*'s framework [48], they declare that when $\Delta\mu < 0.35U$, the full lobe of the second-order corrected phase boundary of the MI phase can not be obtained by GEPLT. The reason why Wang *et al.* failed to obtain this full MI lobe is that they make a tiny mistake for getting phase boundary equation, in which the negative radicand of the square root [see Eq. (27) in Wang *et al.*'s work [48]] is included when $\Delta\mu < 0.35U$. It is very subtle in obtaining the phase boundary equations by using GEPLT. We will clarify this problem at below.

Before clarifying this subtle problem, we would like to give a short review of GEPLT introduced by Wang *et al* [48]. We add two components external current vector $\boldsymbol{J} = (J_A, J_B)^T$ into the above bipartite superlattice Bose–Hubbard Hamiltonian as follows:

$$\hat{H}(\boldsymbol{J}, \boldsymbol{J}^\dagger) = \hat{H} + \sum_{i \in A}(J_A \hat{a}_i^\dagger + J_A^* \hat{a}_i)$$
$$+ \sum_{i \in B}(J_B \hat{a}_i^\dagger + J_B^* \hat{a}_i). \qquad (5)$$

By treating the hopping amplitude t, the external current $\boldsymbol{J}$ and $\boldsymbol{J}^\dagger$ as perturbations, the free energy of systems with external current can be written as

$$F(\boldsymbol{J}, \boldsymbol{J}^\dagger, t) = N_s(F_0(t) + \boldsymbol{J}^\dagger C_2(t)\boldsymbol{J} + \boldsymbol{J}^\dagger \boldsymbol{J}^\dagger C_4(t)\boldsymbol{J}\boldsymbol{J} + \cdots) \qquad (6)$$

at zero temperature, where the expansion coefficient $C_2(t)$ is a second-order tensor which reads

$$C_2(t) = \begin{pmatrix} c_{2AA} & c_{2AB} \\ c_{2BA} & c_{2BB} \end{pmatrix}$$
$$= \sum_{n=0}^{\infty} \begin{pmatrix} \alpha_{2AA}^{(2n)}(-t)^{2n} & \alpha_{2AB}^{(2n+1)}(-t)^{2n+1} \\ \alpha_{2BA}^{(2n+1)}(-t)^{2n+1} & \alpha_{2BB}^{(2n)}(-t)^{2n} \end{pmatrix}. \qquad (7)$$

It is obvious that c_{2AB} is equal to c_{2BA}, for they describe Hermitian processes. Because the ground state of nonperturbation part is MI or CDW state, the free energy $F(\boldsymbol{J}, \boldsymbol{J}^\dagger, t)$ is only constituted by pairing of the external current $\boldsymbol{J}$ and $\boldsymbol{J}^\dagger$.

Due to the bipartite lattice structure of systems, the order parameter can be defined as two components vector

$\Psi = (\psi_A, \psi_B)$, where $\psi_A = \langle \hat{a}_i \rangle$ for $i \in A$ and $\psi_B = \langle \hat{a}_i \rangle$ for $i \in B$. It is easy to find that order parameter reads $\psi_{A/B} = \frac{1}{N_s} \frac{\partial F(\boldsymbol{J}, \boldsymbol{J}^\dagger, t)}{\partial J_{A/B}^*}$. After Legendre transformation, we have the effective potential

$$\Gamma(\Psi, \Psi^\dagger, t) = \frac{1}{N_s} F(\boldsymbol{J}, \boldsymbol{J}^\dagger, t) - \Psi \boldsymbol{J}^\dagger - \Psi^\dagger \boldsymbol{J}, \qquad (8)$$

composed of free energy $F(\boldsymbol{J}, \boldsymbol{J}^\dagger, t)$. Thus, the external current can be calculated from the effective potential $\Gamma(\Psi, \Psi^\dagger, t)$ by $J_{A/B} = -\frac{\partial \Gamma(\Psi, \Psi^\dagger, t)}{\partial \psi_{A/B}^*}$. Moreover, the effective potential $\Gamma(\Psi, \Psi^\dagger, t)$ can be rewritten as a function of Ψ and $\Psi^\dagger$

$$\Gamma(\Psi, \Psi^\dagger, t) = F_0(t) + \Psi^\dagger A_2(t)\Psi + \Psi^\dagger \Psi^\dagger A_4(t)\Psi\Psi + \cdots, \qquad (9)$$

where the expansion coefficient matrix $A_2(t)$ is the inverse of $-C_2(t)$ [48]. According to Landau theory, the phase boundaries of this systems can be obtained by setting

$$\det A_2(t) = \frac{-1}{c_{2AA}c_{2BB} - c_{2AB}c_{2BA}} = 0. \qquad (10)$$

Hence, the critical value of t can be determined by the radius of convergence of series $c_{2AA}c_{2BB} - c_{2AB}c_{2BA}$.

Wang *et al.* make an easy mistake on obtaining the phase boundaries via $\det A_2(t) = 0$. In the case of $\Delta\mu = 0$, the phase boundaries of superlattice systems calculated by Wang *et al.* go back to the phase boundaries of the homogeneous systems which have been calculated by dos Santos *et al.* via effective-potential Landau theory [51]. Unfortunately, the results obtained by dos Santos *et al.* are incorrect and thus Wang *et al.* make the same mistake with dos Santos *et al.* The arguments for dos Santos *et al.*'s mistake are presented as below.

dos Santos *et al.* presented a powerful method [51] (effective-potential Landau theory) to determine the location of second-order phase transition boundaries for high-dimensional single-component bose systems, such as square and cubic lattice as well as triangular, hexagonal and Kagomé lattice [49], but they make an easy mistake on the details for obtaining the phase boundary equations. In dos Santos *et al.*'s work [51], if the equation $\frac{1}{c_2(t)} = (\alpha_2^{(0)})^{-1}(1 + x + x^2 + \cdots)$ (see Ref. [51]) is tenable that implicates $x \ll 1$, where $x = (\alpha_2^{(0)})^{-1}(\alpha_2^{(1)}t - \alpha_2^{(2)}t^2 + \alpha_2^{(3)}t^3 + \cdots)$ and $c_2(t) = \sum_{n}^{\infty} \alpha_2^{(n)}(-t)^n = \alpha_2^{(0)}(1 - x)$. Here, $\alpha_2^{(n)}$ is the perturbative coefficient for homogeneous systems and the corresponding perturbative coefficient for bipartite lattice systems reads $\alpha_{2ij}^{(n)}$. These perturbative coefficients can be calculated by the Rayleigh-Schrodinger perturbation expansion via

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diagrammatic representations, which have been gracefully and detailedly introduced [48, 49, 51]. Thus, we do not give the detail for calculating these coefficients $\alpha_{2ij}^{(n)}$ ($\alpha_2^{(n)}$), but we would like to present the first four orders of diagrammatic expressions of $\alpha_{2ij}^{(n)}$ ($\alpha_2^{(n)}$), which are shown in the Fig. 2 (in homogeneous systems, the sites A and B are equivalent, thus there are $\alpha_{2ij}^{(n)} = \alpha_2^{(n)}$ for $i \in A, B$ and $j \in A, B$). The $c_2(t)$ is the coefficient of the free energy with a pair of current $|J|^2$ [51], which includes all-order hopping corrections. According to Landau theory, the phase boundaries can be obtained by solving the equation $1/c_2(t) = 0$ [51] that means the $c_2(t) \to \infty$ on the phase boundaries. Since the value of coefficient $\alpha_2^{(0)}$ is finite [see Eq. (30a) in Ref. [51]], it is easy to know that on the phase boundaries x will be diverging and this property is inconsistent with $x \ll 1$. So, it's not the right way [solving the equation $1/c_2(t) = 0$ by the series expanding $1/c_2(t)$] to obtain the phase boundaries in dos Santos *et al.*'s work [51]. The correct phase boundaries [49, 52, 53] are given by

$$t_c^{(n)} = -\frac{\alpha_2^{(n-1)}}{\alpha_2^{(n)}}, \tag{11}$$

which is the radius of convergence of $c_2(t)$ determined by the d'Alembert's ratio test.

In the above-mentioned arguments, we have clarified the minor mistake made by dos Santos *et al.* and Wang *et al.* to determine the phase boundaries of the homogeneous systems and bipartite superlattices systems respectively. At below, we will show the right way to handle this subtle problem. Since $c_{2AA}c_{2BB}$ can be rewritten as $(a + bt^2 + ct^4 + \cdots)^2$, the series $c_{2AA}c_{2BB} - c_{2AB}c_{2BA}$ (only even-order hopping) can read as a product of two series, where each series include the all-order hopping. Up to the fourth-order hopping, the series $c_{2AA}c_{2BB} - c_{2AB}c_{2BA}$ reads

$$
\begin{aligned}
&c_{2AA}c_{2BB} - c_{2AB}c_{2BA} \\
&= \left[a + \alpha_{2AB}^{(1)}t + bt^2 + \alpha_{2AB}^{(3)}t^3 + ct^4 + \cdots \right] \\
&\quad \times \left[a - \alpha_{2AB}^{(1)}t + bt^2 - \alpha_{2AB}^{(3)}t^3 + ct^4 - \cdots \right],
\end{aligned} \tag{12}
$$

where the coefficient a, b, and c read

$$
a = \left(\alpha_{2AA}^{(0)}\alpha_{2BB}^{(0)} \right)^{1/2}, \quad b = \frac{\alpha_{2AA}^{(0)}\alpha_{2BB}^{(2)} + \alpha_{2AA}^{(2)}\alpha_{2BB}^{(0)}}{2a},
$$
$$
c = \frac{\alpha_{2AA}^{(0)}\alpha_{2BB}^{(4)} + \alpha_{2AA}^{(4)}\alpha_{2BB}^{(0)} + \alpha_{2AA}^{(2)}\alpha_{2BB}^{(2)} - b^2}{2a}. \tag{13}
$$

Here, the expanding coefficient a, b and c can be obtained by directly comparing coefficients of each power of t for series $c_{2AA}c_{2BB}$ and $(a + bt^2 + ct^4 + \cdots)^2$. Since $(\alpha_{2AA}^{(0)}\alpha_{2BB}^{(0)})^{1/2}$, $\alpha_{2AB}^{(1)}$, $\alpha_{2AA}^{(0)}\alpha_{2BB}^{(2)} + \alpha_{2AA}^{(2)}\alpha_{2BB}^{(0)}$ and $\alpha_{2AB}^{(3)}$ are all positive, this series can be rewritten
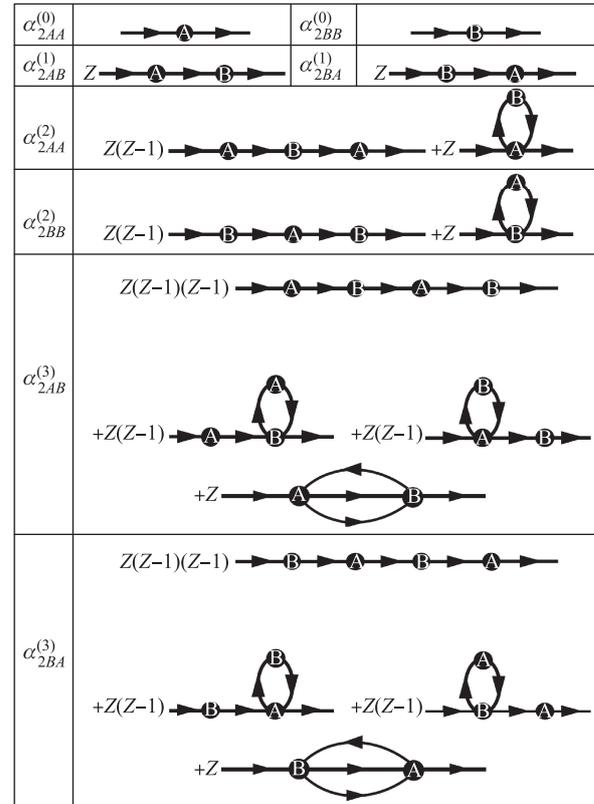

Fig. 2 The diagrams of the coefficients $\alpha_{2ij}^{(n)}$ for bipartite sublattice systems, where Z is the coordination number of the systems.

as $c_{2AA}c_{2BB} - c_{2AB}c_{2BA} = (\sum_{n=0}^{\infty} a_n t^n)(\sum_{n=0}^{\infty} |a_n| t^n)$, where $\sum_{n=0}^{\infty} a_n t^n$ reads

$$\sum_{n=0}^{\infty} a_n t^n = \left[a - \alpha_{2AB}^{(1)}t + bt^2 - \alpha_{2AB}^{(3)}t^3 + ct^4 \cdots \right]. \tag{14}$$

Importantly, the series $\sum_{n=0}^{\infty} |a_n| t^n$ include all-order hopping processes that is very obvious when $\Delta\mu = 0$ (when $\Delta\mu = 0$, $\sum_{n=0}^{\infty} |a_n| t^n = -\sum_{n=0}^{\infty} \alpha_2^{(n)}(-t)^n$, here $\alpha_{2AA}^{(0)} < 0$ and $\alpha_{2BB}^{(0)} < 0$). Moreover, power series $\sum_{n=0}^{\infty} a_n t^n$ and $\sum_{n=0}^{\infty} |a_n| t^n$ have the same radius of convergence $r = \lim_{n\to\infty} |a_n|/|a_{n+1}|$ determined by d'Alembert's ratio test. Thus, the radius of convergence of $c_{2AA}c_{2BB} - c_{2AB}c_{2BA}$ is only determined by the series $\sum_{n=0}^{\infty} |a_n| t^n$.

On the other hand, it is not suitable to fix the radius of convergence by directly handling $c_{2AA}c_{2BB} - c_{2AB}c_{2BA} = \sum_{n=0}^{\infty} d_n(t^2)^n$, which include only even-order term of t. The coefficient $d_n(t^2)^n$ fails to describe the $2n$-th order hopping process. To see this, let us consider $\Delta\mu = 0$. It is clear that $d_1 = 2\alpha_2^{(0)}\alpha_2^{(2)} - (\alpha_2^{(1)})^2$ does not correspond to second-order hopping process, since terms $\alpha_2^{(0)}\alpha_2^{(2)}$ and $(\alpha_2^{(1)})^2$ are not included in second-order hopping process and do not cor-

respond to any physical hopping process ($\alpha_2^{(2)}$ represents the real second-order hopping process). Thus, we can not directly calculate the radius of convergence by $r_d = \lim_{n\to\infty} |d_n|/|d_{n+1}|$. Because Wei *et al.* [47] use the wrong radius of convergence r_d, there are two physical problems in Wei *et al.*'s [47] work. One is that there are no odd-order correction terms of critical t. The other is that if we set $\Delta\mu = 0$, the systems go back to the homogeneous systems, but the phase boundary equations of bipartite systems [see Eq. (10) in Wei *et al.*'s work [47]] are not same with the phase boundary equations of the homogeneous systems. In homogeneous systems, the correct n-th order critical value of $t^{(n)}$ [see Eq. (11)] is determined by coefficients $\alpha_2^{(n-1)}$ and $\alpha_2^{(n)}$ which includes the $(n-1)$-th order and n-th order hopping process, respectively. But in Wei *et al.*'s work [47], the $2n$-th order critical value of $t^{(2n)}$ is calculated by d_{n-1} and d_n which does not correspond to $2(n-1)$-th order and $2n$-th order hopping process, respectively. Moreover, the correct n-th order critical value of $t^{(n)}$ is relevant to the odd-order hopping process but the critical value of $t^{(2n)}$ given by Wei *et al.* is not correlated with odd-order hopping process. Those are the reasons why the critical value of t given by Wei *et al.* is not the same with the homogeneous result.

So far, all technical issues in the present GEPLT have been clarified. Based on d'Alembert's ratio test, the correct phase boundaries of bipartite superlattice systems are given by

$$t_c^{(1)} = \frac{\sqrt{\alpha_{2AA}^{(0)}\alpha_{2BB}^{(0)}}}{\alpha_{2AB}^{(1)}}, \tag{15}$$

$$t_c^{(2)} = \frac{2\sqrt{\alpha_{2AA}^{(0)}\alpha_{2BB}^{(0)}}\alpha_{2AB}^{(1)}}{\alpha_{2AA}^{(0)}\alpha_{2BB}^{(2)} + \alpha_{2BB}^{(0)}\alpha_{2AA}^{(2)}}, \tag{16}$$

$$t_c^{(3)} = \frac{\alpha_{2AA}^{(0)}\alpha_{2BB}^{(2)} + \alpha_{2BB}^{(0)}\alpha_{2AA}^{(2)}}{2\sqrt{\alpha_{2AA}^{(0)}\alpha_{2BB}^{(0)}}\alpha_{2AB}^{(3)}}, \tag{17}$$

which are the radius of convergence of $\sum_{n=0}^{\infty} |a_n| t^n$. Here $t_c^{(n)}$ is the n-th order phase boundary and the first-order result is the same as the mean-field result [45, 54] (by setting the nearest-neighbor interaction $V = 0$ and $\mu_A = \mu + \Delta\mu$ in Refs. [45, 54]). When $\Delta\mu = 0$, the Eqs. (15)–(17) of phase boundaries are consistent with the Eq. (11) of phase boundaries of the homogeneous systems [49, 52, 53]. It is an independent check that proves our results.

3 Quantum phase diagram

Before showing the phase diagrams of these systems, we would like to discuss the property of SF phase in bipartite

superlattice. When $t \gg U$, the eigenstates of systems can be written as $|\Psi\rangle \sim \prod_i [\exp\{\sqrt{n_i}\hat{a}_i^\dagger\}|0\rangle_i]$ [2], where n_i denotes the condensate density on the site i. Using this wave function, we can get free energy of each super unit cell, which takes the form

$$
\begin{aligned}
E &\sim -2Zt\sqrt{n_A}\sqrt{n_B} - (\mu + \Delta\mu)n_A \\
&\quad + \frac{U}{2}n_A(n_A - 1) - \mu n_B + \frac{U}{2}n_B(n_B - 1) \\
&\sim \overline{n}[-2t - 2\mu - \Delta\mu + U(\overline{n} - 1)] \\
&\quad + \frac{Zt(\delta n)^2}{\overline{n}} - \Delta\mu\delta n + U(\delta n)^2,
\end{aligned}
\tag{18}
$$

where $n_A = \overline{n} + \delta n$ and $n_B = \overline{n} - \delta n$ is the density on sublattice A and B, $\overline{n}$ is the average density and δn is the density fluctuation. In the final step of Eq. (18), we use the condition $\delta n/\overline{n} \ll 1$. Remarkably, we can find that the free energy has a minimum at density fluctuation $\delta n = \frac{\Delta\mu}{2Zt/\overline{n}+2U}$ which is in good agreement with the experiential result [55] [See Fig. 1(d) in Ref. [55]]. This means that homogeneous SF phase will not appear in these systems for any finite value of $\Delta\mu$ and there is only anisotropic superfluid (ASF). In Wei *et al.*'s work [47], there always are extra peaks at $(\pm\pi, \pm\pi)$ in time-
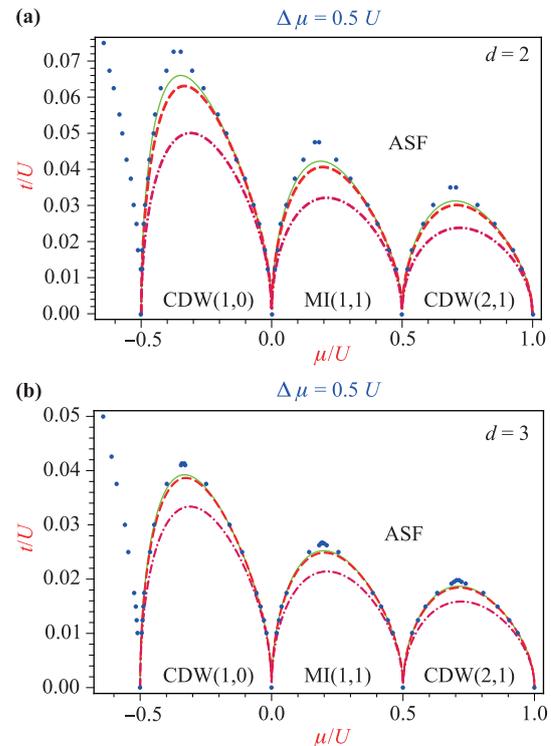

Fig. 3 The phase diagram of ultracold Bose gases in square ($d = 2$) **(a)**, cubic ($d = 3$) **(b)** bipartite superlattice for the case of $\Delta\mu = 0.5U$. The green solid line is the third-order calculation, the red dashed line is the second-order result, and the pink dot-dashed line is the first-order (mean-field) result. The blue dots line is the QMC result [48].

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of-flight pictures in SF phase for bipartite superlattice systems. These extra peaks reflect the inhomogeneity of the SF phase that is in accord with our argument. Using Eqs. (15)–(17), we can get the first, second and third order phase boundaries of CDW(MI)-ASF quantum phase transition for ultracold Bose gases in square and cubic superlattice systems. From Fig. 3, we easily find our analytical result accord with the QMC result [48] very well at $\Delta\mu = 0.5U$. The relative deviation of our third-order results from the QMC results is less than 9% for square superlattices and 4% for cubic superlattices. Furthermore, using these new phase boundaries Eqs. (15)–(17), we can show the phase boundaries at $\Delta\mu = 0.1U < 0.35U$ (see Fig. 4), but it can not be obtained in Wang *et al.*'s work [48]. Comparing Fig. 3 and Fig. 4, it is clear that the region of MI(1,1) expands with decreasing $\Delta\mu$ while the region of CDW(1,0) or CDW(2,1) shrinks correspondingly, which are as expected (the region of CDW(1,0) shrinks with decreasing $\Delta\mu$, which is in excellent qualitative agreement with the experimental result [55] (see Fig. 2 in Ref. [55])). In the case of $\Delta\mu > U$, there is no MI state in systems. Taking $\Delta\mu = 1.5U$ as an example, we show its phase boundaries in Fig. 5.

Moreover, high-order corrections for different dimensional systems ($d = 2, 3$) are investigated. As shown in
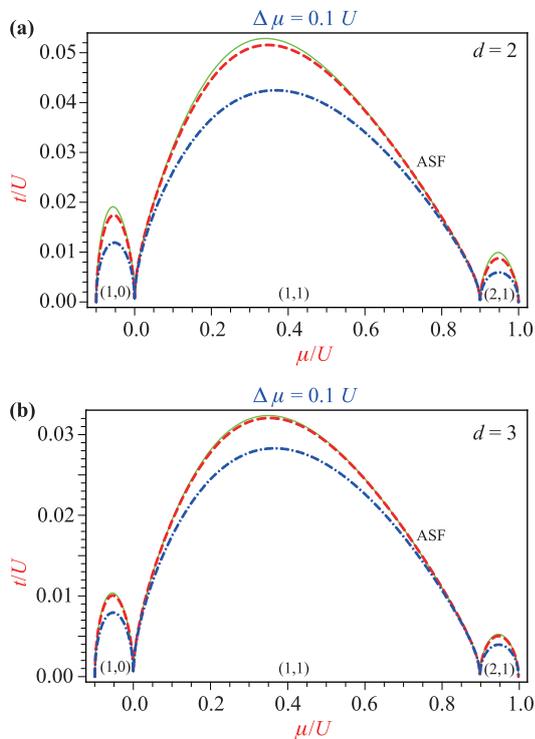

Fig. 4 The phase diagram of ultracold Bose gases in square **(a)** and cubic **(b)** superlattice for the case of $\Delta\mu = 0.1U$. The green solid line is the third-order calculation, the red dashed line is the second-order result, and the blue dot-dashed line is the first-order (mean-field) result.
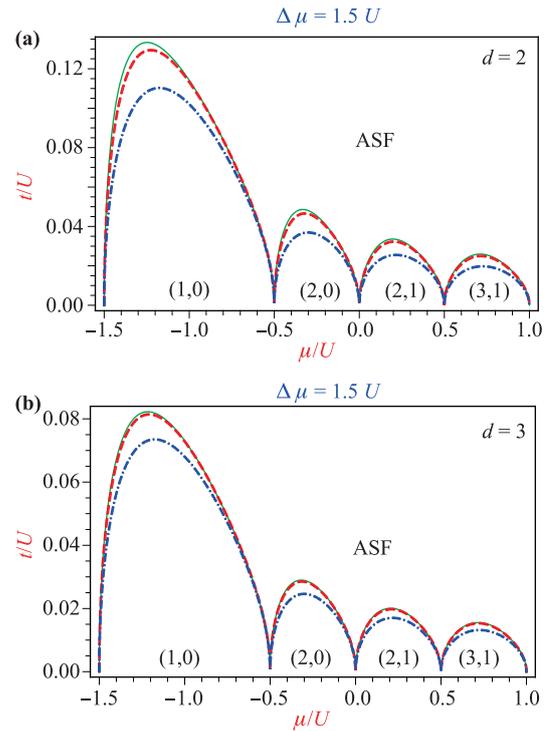

Fig. 5 The phase diagram of ultracold Bose gases in square **(a)** and cubic **(b)** superlattices systems at $\Delta\mu = 1.5U$. The green solid line is the third-order calculation, the red dashed line is the second-order result, and the blue dot-dashed line is the first-order (mean-field) result.

Figs. 3–5, higher-order corrections are smaller in $d = 3$ (cubic superlattice) than that in $d = 2$ (square superlattice) systems. This phenomenon is due to the fact that the effect of quantum fluctuation is smaller in higher dimensionality.

4 Summary

In this paper, we clarify a tiny and easy mistake made by Wang *et al.* [48] and Wei *et al.* [47] when they use GEPLT to study the phase boundaries of square and cubic superlattice systems respectively. After clarifying these technical issues, GEPLT becomes more consistent and complete, valid for all value of $\Delta\mu$. Specially, the critical t obtained by corrected GEPLT coincides with the result of homogeneous systems [49] when $\Delta\mu = 0$. Using the corrected phase boundary equations, we have presented the quantum phase boundaries up to third-order hopping for ultracold Bose gases in square and cubic superlattices. Our analytical results ($\Delta\mu = 0.5U$) are in excellent agreement with the QMC simulations and the relative deviation of our third-order results from the QMC results is less than 9% for square superlattices and

4% for cubic superlattices. Comparing Fig. 3 and Fig. 4, the region of CDW$(1,0)$ shrinks with decreasing $\Delta\mu$, which is in good qualitative agreement with the experimental result [55] (see Fig. 2 in Ref. [55]). Furthermore, we emphasize that homogeneous SF phase does not appear when $\Delta\mu \neq 0$ and only ASF phase exists in such superlattice systems. The corresponding superfluid density fluctuation $\delta n = \frac{\Delta\mu}{2Zt/\bar{n}+2U}$ decreases with increasing interaction U, which is in good qualitative agreement with the experimental result [55].

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