Staggered quantum phases of dipolar bosons at finite temperatures

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The extended Bose-Hubbard model with correlated tunneling exhibits staggered superfluid and supersolid quantum phases. We study finite-temperature phase transitions of quantum phases of dipolar bosons in a two-dimensional optical lattice using Gutzwiller mean-field and quantum Monte Carlo approaches. When nearest-neighbor repulsion is comparable to the on-site interaction, we find that the two topologically distinct superfluids are separated by a normal-fluid phase, while at stronger off-site interactions, density-modulated insulating quantum phases appear. We estimate the critical temperature of the staggered-superfluid to normal-fluid transition and show that this transition is of the Kosterlitz-Thouless type. Finally, we elucidate the coexistence of staggered quantum phases in the presence of an external trapping potential. Our study paves the way to observe novel staggered quantum phases in dipolar optical lattice experiments.

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I. INTRODUCTION

Ultracold atomic gases trapped in an optical lattice provide a powerful tool to simulate the low-energy behavior of the effective Hamiltonians of condensed-matter models [1–4]. Excellent experimental control over model parameters led to the observation of the Mott-insulator (MI) to superfluid (SF) phase transition [5], realization of the Hofstadter model [6], and various novel phenomena in many-body physics [7]. This setup can also be used to investigate effects that are not possible in conventional solid-state physics, such as tuning the interparticle interaction strength [8] and generating very strong effective magnetic fields [9]. The Bose-Hubbard model (BHM) describes interatomic interactions at a lattice site. However, other interaction processes also affect the properties of strongly correlated materials. In particular, the bond-charge interaction of the extended Hubbard model [10] has been invoked to explain various phenomena, including high-temperature superconductivity [11–13]. Due to the lack of precise control over the interaction strengths, as well as the complexity of materials, interaction-induced phenomena cannot be probed in condensed-matter physics.

The unique features of ultracold atoms and optical lattices create an ideal platform to study complex phenomena due to interparticle-particle interactions [4,14]. For long-range interacting atomic gases, the introduction of nearest-neighbor (NN) interaction induces charge-density-wave (CDW) and supersolid (SS) ground states, which spontaneously break the translational symmetry of the lattice [15,16]. At higher average atomic densities, the on-site interaction results in higher-order tunneling processes. One such effect is density-induced tunneling (DIT), which is analogous to the bond-charge

interaction of fermions. This considerably affects the properties of soft-core dipolar bosons. Theoretical investigations have shown the influence of DIT on MI-SF quantum phase transitions [17–19], Bose-Fermi multicomponent mixtures [20–24], band structures [18], nonequilibrium dynamics [25], and the emergence of staggered quantum phases [26-29]. Density-induced tunneling was observed in recent quantum gas experiments [25,30]. The ramp of the lattice potential and the heating mechanism during time-of-flight measurements contribute to thermal fluctuations in experiments. The excited states in the system affect the parameter region of quantum phases, and a normal-fluid (NF) state appears in the system at finite temperatures. Several previous studies discussed the role of finite temperature in the homogeneous system for the MI-SF transition of the BHM [31–37] and the CDW-SS transition of the extended BHM [38-40]. Moreover, the effects of the trapping potential on the coexistence of uniform and density-modulated phases have also been examined for short-[35,41,42] and long-range many-body systems [38,43,44]. Since experiments are performed at finite temperatures, it is imperative to consider the role of thermal fluctuations in determining the thermal and insulating regions [45,46]. Moreover, the effects of finite temperatures on the staggered superfluidity of strongly correlated quantum many-body systems remain unanswered.

In the present work, we investigate the finite-temperature phase diagram of a homogeneous two-dimensional extended Bose-Hubbard model with correlated hopping. In particular, we focus on higher average number densities where interaction-induced processes lead to staggered quantum phases. Our results show the role of thermal fluctuations resulting in a NF state which intervenes in two different kinds of superfluidity, one due to single-particle hopping and one due to DIT. In order to have experimental relevance, we examine both the finite-size effects and the phase coexistence caused by the trapping potential. The thermal phase transition

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of the staggered superfluidity follows the Kosterlitz-Thouless (KT) transition. We discuss the combined effects of trapping and finite temperature and identify the parameter regime of staggered superfluidity.

This paper is organized as follows. In Sec. II we introduce the model Hamiltonian for isotropic dipolar bosons and describe the approaches used in the present work. We discuss the finite-temperature phase diagrams for weak and strong off-site interactions in the presence of correlated tunneling in Sec. III. In Sec. IV we further examine the finite-size effects of staggered quantum phases using the quantum Monte Carlo (QMC) approach. The coexistence of staggered quantum phases at finite temperatures in an external harmonic trapping potential is discussed in Sec. V. Finally, we conclude in Sec. VI.

II. HAMILTONIAN AND METHODS

A. Extended Bose-Hubbard model with correlated hopping

We consider spinless bosons confined to a two-dimensional square optical lattice. The atoms can hop between nearest-neighbor sites of the lattice and experience on-site repulsion. The dipolar interaction considered here is isotropic in nature, and as a minimal model, the atoms of nearest-neighbor sites interact repulsively. The model Hamiltonian reads [30]

$$\hat{H} = -t \sum_{\langle i,j \rangle} (\hat{b}_i^{\dagger} \hat{b}_j + \text{H.c.}) + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$$

$$+ \sum_{\langle i,j \rangle} [V \, \hat{n}_i \hat{n}_j - t' \, \hat{b}_i^{\dagger} (\hat{n}_i + \hat{n}_j) \hat{b}_j] - \mu \sum_i \hat{n}_i. \quad (1)$$

The bosonic operator \hat{b}_i^{\dagger} (\hat{b}_i) creates (annihilates) an atom at the ith lattice site, and $\hat{n}_i = \hat{b}_i^{\dagger} \hat{b}_i$ is the corresponding number operator. The first term describes the kinetic energy, with t being the hopping strength between nearest-neighbor sites i and j on a square lattice with periodic boundary conditions. The second term represents the on-site repulsive interaction between atoms with strength U. The third term is the dipolar interaction, which includes the nearest-neighbor repulsive interaction V and density-induced tunneling with strength t', depending on the density of atoms at each site. The last term, μ , denotes the chemical potential which controls the atomic density in the grand-canonical ensemble.

B. Methods

To study the properties of the system at finite temperatures, we first use the Gutzwiller mean-field approach [47–51]. In the mean-field approximation, the bosonic annihilation operator is decomposed as $\hat{b}_i = \langle \hat{b}_i \rangle + \delta \hat{b}_i$, where $\langle \hat{b}_i \rangle \equiv \phi_i$ is the mean field, also referred to as the superfluid order parameter, and $\delta \hat{b}_i$ is the fluctuation operator. A similar decomposition for the creation operator can be defined. Using this approximation, the Hamiltonian decouples the sites, and all the off-site contributions are incorporated through the mean field. The many-body Gutzwiller wave function is

$$|\Psi_{\rm GW}\rangle = \prod_{i} |\psi_{i}\rangle = \prod_{i} \sum_{n}^{n_{\rm max}} c_{n}^{i} |n_{i}\rangle,$$
 (2)

where $|n_i\rangle$ is the occupation basis state with n atoms at the ith site, we introduce a cutoff n_{\max} on the maximum number of bosons per site, and c_n^i are the complex coefficients for state $|\psi_i\rangle$. $|\Psi_{\rm GW}\rangle$ is normalized by the corresponding complex coefficients c_n^i . At zero temperature, the SF order parameter is a measure of the off-diagonal long-range order or long-range phase coherence $\phi_i \equiv \langle \Psi_{\rm GW} | \hat{b}_i | \Psi_{\rm GW} \rangle = \sum_n \sqrt{n} c_{n-1}^{*i} c_n^i$. It is finite for the SF phase and zero for the incompressible phase. The average density ρ is given by $\sum_i n_i / L^2$, where L is the system size. The atomic density at the ith lattice site is $n_i \equiv \langle \Psi_{\rm GW} | \hat{n}_i | \Psi_{\rm GW} \rangle = \sum_n n |c_n^i|^2$. The density-assisted correlation or DIT order parameter is

$$\eta_i = \langle \Psi_{\text{GW}} | \hat{n}_i \hat{b}_i | \Psi_{\text{GW}} \rangle = \sum_n \sqrt{n} (n-1) c_{n-1}^{*i} c_n^i,$$
(3)

which is finite for phases with finite SF order parameter.

At finite temperatures, the presence of thermal fluctuations significantly modifies the phase transitions of the system [38,52–54]. The order parameters defining the superfluidity and density-dependent transport properties are given by their thermal averages. We retain the entire energy spectrum E_i^l and eigenstates $|\psi\rangle_i^l$ obtained from the diagonalization of the mean-field Hamiltonian. Then, the partition function of the system is $Z = \sum_l e^{-\beta E^l}$, where $\beta = (k_B T)^{-1}$ is the inverse of thermal energy at temperature T. The thermal average of the order parameters is

$$\langle \phi_i \rangle = \frac{1}{Z} \sum_{l} {}^{l}_{i} \langle \psi | \hat{b}_i e^{-\beta E^l} | \psi \rangle_i^l, \qquad (4a)$$

$$\langle \eta_i \rangle = \frac{1}{Z} \sum_{l} {}^{l}_{i} \langle \psi | \hat{n}_i \hat{b}_i e^{-\beta E^l} | \psi \rangle_i^l, \qquad (4b)$$

where $\langle \cdots \rangle$ represents the thermal averaging of the observable. Additionally, the average local occupancy at finite T is defined as

$$\langle \hat{n}_i \rangle = \frac{1}{Z} \sum_{l} {}^{l}_{i} \langle \psi | \hat{n}_i e^{-\beta E^l} | \psi \rangle^l_i, \qquad (5)$$

from which the average density at finite T is $\rho = \sum_{i} \langle \hat{n}_i \rangle / L^2$. The introduction of finite T leads to the appearance of the NF phase. The NF phase is a compressible phase, and it can be distinguished from other insulating MI and CDW phases by inspecting the compressibility [35,45]. The compressibility, which is the measure of local-density variance, is $\kappa = \sum_{i} (\langle \hat{n}_{i}^{2} \rangle - \langle \hat{n}_{i} \rangle^{2})/L^{2}$. At finite T, due to the presence of thermal fluctuations, the insulating phases appear with nearly integer site occupancy, whereas the NF phase has real occupancy. Ideally, κ is zero for insulating MI and CDW phases, while it is nonzero for the NF phase. In the mean-field approach, the crossover between the insulating MI or CDW phase and the NF phase is determined by the value of κ . Here, we identify the NF phase by $\kappa > 10^{-5}$ [35,55] and $\phi = \eta = 0$. The zero SF order parameter also distinguishes the NF phase from other compressible phases. Furthermore, the single-particle correlation and structure factor, which are

the measures of off-diagonal and diagonal long-range order, for momentum wave vector ${\bf k}$ are

$$M(\mathbf{k}) = \frac{1}{L^2} \sum_{j,j'} e^{i\mathbf{k}\cdot(\mathbf{r}_j - \mathbf{r}_{j'})} \langle \hat{b}_j^{\dagger} \hat{b}_{j'} \rangle, \tag{6a}$$

$$S(\mathbf{k}) = \frac{1}{L^2} \sum_{i,j'} e^{i\mathbf{k} \cdot (\mathbf{r}_j - \mathbf{r}_{j'})} \langle \hat{n}_j \hat{n}_{j'} \rangle.$$
 (6b)

Complementary to the Gutzwiller mean-field approach, we also employ the quantum Monte Carlo method to study the finite-temperature phase diagrams of the model. In principle, at finite T, QMC is numerically exact and subject only to the finite-size effect and statistical error if the infamous sign problem is absent [56]. Unfortunately, in our extended BHM \hat{H} , a negative value of the DIT t' competes with the single-particle hopping t (t > 0), so that the overall effective hopping matrix elements,

$$\langle n_i + 1, n_j - 1 | -t \hat{b}_i^{\dagger} \hat{b}_j - t' \hat{b}_i^{\dagger} (\hat{n}_i + \hat{n}_j) \hat{b}_j | n_i, n_j \rangle$$

= $[-t - t' (n_i + n_j - 1)] \sqrt{n_i + 1} \sqrt{n_j},$ (7)

can be either positive or negative, depending on the neighboring local particle densities n_i and n_j . This leads to possible opposite signs in the QMC simulation that cannot be removed with some simple transformation. In that case, the statistical uncertainty tends to diverge at low enough temperatures. Nevertheless, for most of the parameter regime and temperature range we investigate in this work, the average sign is not close to zero; therefore, the sign problem is manageable, and we can provide reliable observable measurements.

We adopt the well-established stochastic series-expansion approach with a directed loop algorithm to simulate the model Hamiltonian \hat{H} [57,58]. As usual, the superfluidity is measured via the fluctuation of the winding numbers W_x and W_y . This is given by the number of times the off-diagonal operator list is wound around the lattice [59–61]

$$\rho_s = \frac{1}{2\beta} (\langle W_x^2 \rangle + \langle W_y^2 \rangle). \tag{8}$$

On the other hand, the computation of the off-diagonal order parameter $M(\mathbf{k})$ requires the measurement of the matrix elements $\langle \hat{b}_j^{\dagger} \hat{b}_{j'} \rangle$, which can be carried out directly during the loop update [62]. While the compressibility κ is related to the density variance, which in turn is affected by the average sign of each measurement, it is problematic to calculate κ when opposite signs arise in the simulation. Therefore, in our QMC calculations, instead of measuring the compressibility κ , we identify the boundary between the MI and NF phases by observing the saturation of the particle occupancy as the temperature is reduced. In general, we restrict the maximum particle occupancy to 6 and set the lattice size L=36.

III. FINITE-TEMPERATURE PHASE DIAGRAMS

The competition between various terms in the model Hamiltonian leads to different phases at zero temperature. For V = t' = 0, the competition between the kinetic and on-site interaction energy leads to two quantum phases of the BHM [63,64]. Most of the phase diagram consists of a Bose-Einstein condensed superfluid phase which possesses

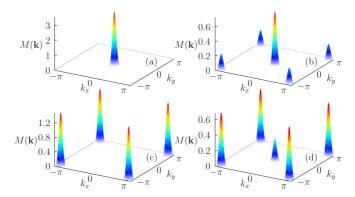


FIG. 1. Examples of the momentum distributions of $M(\mathbf{k})$ for the compressible phases of dipolar bosons in two-dimensional optical lattices. (a) SF phase: the off-diagonal long-range order associated with superfluidity results in a sharp peak in $M(\mathbf{k})$ at the center of the Brillouin zone. (b) SS phase: the nearest-neighbor interaction leads to a supersolid compressible phase which exhibits a sharp peak in $M(\mathbf{k})$ at the center (due to the superfluid nature) and smaller peaks at the corners of the Brillouin zone (due to the long-range diagonal order). (c) SSF and (d) SSS phases: in both cases the largest peaks move to the corners of the Brillouin zone.

off-diagonal long-range order and is phase coherent. The momentum distribution of the single-particle correlation $M(\mathbf{k})$ for the SF phase is shown in Fig. 1(a), which shows a sharp peak in $M(\mathbf{k})$ at $\mathbf{k} = (0, 0)$. This indicates a finite superfluid stiffness (or SF order parameter) $\rho_s \neq 0$ ($\phi \neq 0$). For integer mean atomic densities and strong repulsion, the Mottinsulator phase appears in the lobe structures in the t- μ plane of a homogeneous system. The size of the insulating lobes decreases with increasing μ as the corresponding larger meandensity favors superfluidity in the system. The MI phase is an incompressible phase with $M(\mathbf{k}) = \rho_s = 0$. At finite temperatures, the interplay of the quantum and thermal fluctuations results in a third, NF phase [32,35,65-67]. This phase has zero ρ_s even though the local atomic occupancy is incommensurate. In the finite-temperature phase diagrams, there is no broken symmetry between the insulating and NF phases; hence, the transition across these phases exhibits a smooth crossover which is signaled by the change in the compressibility. Around the tip of the lobes, due to the prevailing role of quantum fluctuations, the mean-field and quantum Monte Carlo approaches predict different phases [45,68]. This is due to the limitation of the mean-field theory, in which, once the SF order parameter ϕ is zero, the hopping terms do not play any role. And this underestimates the temperature-induced NF state around the tips of the insulating lobes.

The introduction of an off-site nearest-neighbor interaction $V \neq 0$ offers the possibility to stabilize quantum phases with spatial ordering, which is identified by the structure factor at finite momentum, for example, for checkerboard compressible phases $S(\pi,\pi) \neq 0$. This leads to two new phases, the charge-density-wave solid phase with integer or half-integer mean densities and the supersolid phase, which breaks two continuous symmetries, the phase invariance of the superfluidity and translational invariance, to form crystalline order [15,16,38,69,70]. These two broken symmetries result in a sharp peak in $M(\mathbf{k})$ at the center and four smaller

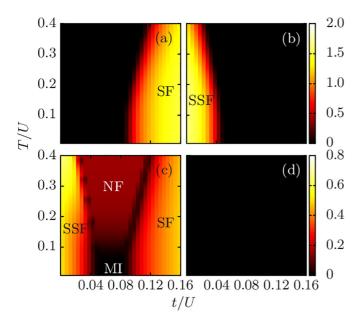


FIG. 2. The thermal-averaged Fourier transform of the single-particle correlation $M(\mathbf{k})$ at (a) $\mathbf{k} = (0,0)$ and (b) $\mathbf{k} = (\pi,\pi)$, (c) compressibility κ , and (d) the structure factor $S(\pi,\pi)$ as a function of hopping and temperature at weak NN interaction V=0.24. These are obtained using finite-temperature Gutzwiller mean-field theory in the grand-canonical ensemble. Here, $\mu=3.5$ is considered. Different kinds of superfluidity are separated by MI at lower T and NF at higher T. Here, the maximum occupancy of bosons per site $n_{\max}=10$ is assumed. The system size is L=36.

peaks at finite \mathbf{k} in the two-dimensional Brillouin zone, as shown in Fig. 1(b). Furthermore, recent theoretical studies reported that the presence of density-induced tunneling ($t' \neq 0$) at sufficiently higher densities leads to the existence of staggered-superfluid (SSF) and staggered-supersolid (SSS) phases [27–29]. The emergence of staggered quantum phases is attributed to the destructive interference between single-particle hopping and DIT. The momentum distributions $M(\mathbf{k})$ of the staggered phases reveal four sharp peaks at finite \mathbf{k} and $M(\pi,\pi) > M(0,0)$ [Figs. 1(c) and 1(d)]. Here, we numerically determine the finite-temperature phase diagrams of isotropic dipolar bosons with correlated tunnelings. In particular, we choose a higher average atomic density or chemical potential to examine the effects of DIT under the influence of thermal fluctuations.

In Fig. 2, we show the mean-field values of the single-particle correlation $M(\mathbf{k})$, the compressibility κ , and the structure factor $S(\pi,\pi)$ as a function of hopping and temperature. The truncation in the Fock space $n_{\text{max}}=10$ is chosen such that the phases reported in the present work do not depend on it. In our calculations, U sets the unit of energy scale, U=1, and periodic boundary conditions are assumed. We first consider $\mu=3.5$, V=0.24, and t'=-0.02, where previous studies show the existence of the staggered quantum phases at T=0 in square lattices [29]. In the T=0 limit, a MI(2) phase appears in between two topologically distinct superfluid states. There exists a SSF phase for lower t, i.e., $t \sim |t'|$. This is confirmed by $M(0,0) < M(\pi,\pi)$, finite compressibility, and zero density-density correlation

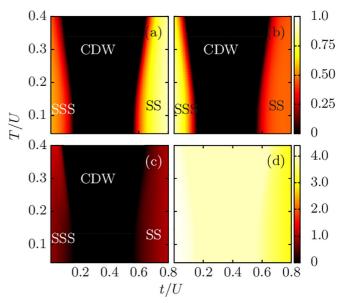


FIG. 3. Shown here are various observables at strong NN interaction (V=1) in the hopping t-temperature T plane. The top row shows the Fourier transform of the single-particle correlation $M(\mathbf{k})$ at (a) $\mathbf{k}=(0,0)$ and (b) $\mathbf{k}=(\pi,\pi)$. In the bottom row (c) the compressibility κ and (d) structure factor at $\mathbf{k}=(\pi,\pi)$ are plotted. The chemical potential μ is chosen such that the effect of DIT introduces staggered phases. The normal and staggered supersolid phases are separated by an incompressible CDW phase for the temperature limit considered. Here, the maximum occupancy per lattice site $n_{\text{max}}=10$ and system size L=36 are considered.

 $[S(\pi,\pi)=0]$. However, at larger t, single-particle hoppingdriven normal superfluidity emerges. The thermal fluctuations melt both superfluid regions and widen the NF parameter space at higher temperatures, as expected. For lower hopping strengths, the value of $M(\pi, \pi)$ decreases with temperature, which suggests a shrinking of the novel staggered superfluidity regime [Fig. 2(b)]. We further present the finitetemperature phase diagram at higher off-site NN interaction, V = 1. It is pertinent to note that the DIT scales with NN interaction; hence, we consider here t' = -0.1. The quantitative variations in the single-particle correlation $M(\mathbf{k})$ at $\mathbf{k} = (0,0)$ [Fig. 3(a)] and (π,π) [Fig. 3(b)] suggest that the SSS phase is present at lower t and the normal SS phase is present at larger t. The two compressible phases are separated by a phase with zero correlations and compressibility [Fig. 3(c)] but finite structure factor $S(\pi, \pi) = 4$ [Fig. 3(d)]. This intervening phase is identified as CDW(4,0), which is also confirmed by the density contrast at two consecutive sites. As T increases, the CDW is robust to the thermal fluctuations and remains stable up to the maximum temperature range considered. However, at higher temperatures T > 0.4, we expect the incompressible CDW phase and compressible SS and SSS phases to melt into the normal-fluid state.

In Fig. 4 we present the QMC results showing the typical phase transitions of the SSF-NF (SSS-CDW) with V = 0.24 (V = 1) at finite temperature T = 0.2. Consistent with Fig. 2 with small NN interaction V = 0.24 [Fig. 4(a)], the single-particle correlation $M(\pi, \pi)$ is finite, while M(0, 0) vanishes at small t, which signals the SSF phase as the DIT t' dominates

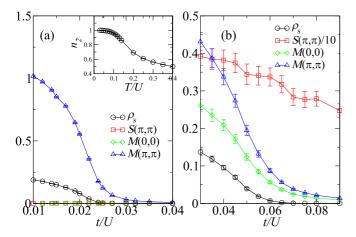


FIG. 4. The order parameters obtained with QMC as a function of t/U at T/U = 0.2 for (a) V = 0.24, t' = -0.02 and (b) V = 1, t' = -0.1, showing the SSF-NF and SSS-CDW phase transitions, respectively. The inset in (a) shows the crossover from MI(2) to NF as the double occupancy n_2 decreases from its saturation value.

the dynamics. When the domination of t' ends at $t \sim 0.025$, the superfluid coherence is destroyed, and the system becomes a NF. Similarly, in the case of strong NN interaction V=1 [Fig. 4(b)], the superfluidity order is destroyed as t/U increases, except now the diagonal long-range order remains intact, which indicates a continuous phase transition from SSS to CDW(4,0), again in agreement with the mean-field results shown in Fig. 3. Here, the staggered character of the supersolid phase is verified by $M(0,0) < M(\pi,\pi)$.

Based on various observables using the mean-field and QMC simulations, we present the finite-temperature phase diagrams in Fig. 5. In the phase diagram for weak NN interaction [Fig. 5(a)], we find interesting features that the phase

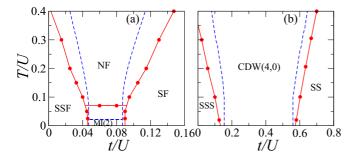


FIG. 5. The finite-temperature phase diagram at $\mu=3.5$ obtained using quantum Monte Carlo (solid lines) and Gutzwiller mean-field (dashed lines) approaches. At finite temperatures, (a) for NN interaction comparable to the on-site interaction (V=0.24), the compressible normal SF phase makes a transition to the SSF (as t decreases) with an intervening NF phase. (b) When V is strong (V=1), a quantum phase transition between two types of supersolids occurs with an intervening CDW phase. The QMC corrects the prediction of the staggered phase regime using mean-field theory, which overestimates the parameter space of compressible superfluid (supersolid) phases due to the poor resolution of atomic correlation between the lattice sites. The phase boundaries are obtained for L=36.

boundaries of the staggered superfluid and normal superfluid have opposite slopes on either side of the insulating (or NF) phase. This means that when the single-particle hopping t increases, the critical temperature of SSF reduces to zero at a critical t and the system becomes a MI(2) solid. As t increases to another critical t, the normal SF stabilizes, with its critical temperature increasing with t. This opposite dependence of the critical temperature on both sides of the insulating regime on the hopping t can be understood by the competing roles of t and t'. As shown in Eq. (8), the effective hopping of bosons depends on the occupation of neighboring sites and the competing values of t and t'. For the MI(2) phase, all sites are doubly occupied, and the effective hopping vanishes if $t \sim$ -3t', i.e., is near the middle of the MI(2) phase with $t \sim 0.06$ in our case of weak NN interaction where t' = -0.02. For t < 0.06, the effective hopping becomes negative and results in the SSF phase. The SSF phase, however, becomes less stable when t increases as the quantum coherence deteriorates, resulting in a lower critical temperature. In contrast, when increasing t > 0.06 from the MI(2) phase, the effective hopping is more positive and leads to a more stable SF and higher critical temperature. Therefore, the opposite dependence of the phase boundaries of SSF and SF on the hopping t is a clear demonstration of the interplay of the hopping terms t and t'. A similar mechanism also occurs for strong NN interaction [Fig. 5(b)], where t' = -0.1 and zero effective hopping appears at $t \sim 0.3$, again near the middle of the insulating CDW(4,0) phase. The only difference here is that the strong interaction leads to the diagonal long-range ordering in the whole phase diagram and the CDW survives even in the hightemperature regime in the diagram and hence the NF phase is not observed. Nevertheless, using the mean-field approach, we find that at high enough temperatures ($T/U \sim 0.636$), thermal fluctuations will eventually destroy the insulating CDW phase and the system becomes NF.

Although both the results of mean-field and QMC simulations provide the same feature of phase boundaries as mentioned above, there are quantitative differences between the two approaches. Previous studies have shown the importance of the QMC phase boundaries at finite temperatures [35,45,71]. The main difference can be seen in Fig. 5, where the mean field overestimates the staggered and normal superfluid regions due to poor intersite correlations. For example, at $\mu = 3.5$ the mean-field method shows SSF for t = 0.03and T = 0.3, while the QMC predicts the NF state. The critical hopping for the phase boundary separating SSF and NF obtained with QMC is lower, and the deviations from the mean-field boundaries are prominent at higher temperatures. On the other hand, the critical value of t for the NF-SF transition is larger for QMC. It is important to note that the mean-field theory predicts larger SSS and SS domains due to the absence of intersite atomic correlations; however, these predictions are corrected by QMC calculations [see Fig. 5(b)].

IV. FINITE-SIZE SCALING ANALYSIS

A natural question that arises about the thermal transition from staggered superfluid or supersolid to normal-fluid or solid is whether it can be described by the Kosterlitz-Thouless transition as in the usual superfluid thermal phase

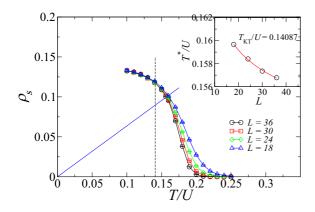


FIG. 6. Finite-size scaling of the superfluidity ρ_s as a function of T for V=0.24, t=0.025, and $\mu=3.5$. The dashed line represents the fitted $T_{\rm KT}$. The blue line shows $\rho_s=\frac{2}{\pi}T$, and its intersection with $\rho_s(T)$ for various L gives $T^*(L)$, which shows the excellent logarithmic dependence (inset) expected for the KT transition (see the text).

transitions [72]. An instructive way to test the nature of the transition is via the finite-size scaling analysis, which we will describe here. In the thermodynamics limit, the superfluidity shows a universal jump at the KT transition temperature $T_{\rm KT}$ where $\rho_s(T_{\rm KT}) = 2T_{\rm KT}/\pi$, which, however, is subjected to the logarithmic correction $\rho_s(T_{\rm KT}, L) = \rho_s(T_{\rm KT}, \infty)\{1 +$ $1/[2 \ln(L/L_0)]$ for finite size L [73,74]. The constant value L_0 and the transition temperature $T_{\rm KT}$ can be fitted by measuring the superfluidity of different system sizes L, as shown in Fig. 6. The temperatures T^* extracted from the interaction points $\rho_s(T^*) = \frac{2}{\pi}T^*$ for various system sizes L exhibit good agreement with the logarithmic correction $T^*(L) = T_{KT}\{1 +$ $1/[2\ln(L/L_0)]$ (inset) expected for the KT transition. In a normal SF, it is clear that the thermal fluctuations lead to the unbinding of vortex and antivortex pairs via the KT transition [75]. Our result suggests that the same mechanism is unaffected by shifting the condensation momentum from (0,0) to (π, π) such that the staggered ordering of the superfluidity does not alter the nature of the thermal phase transition.

V. STAGGERED PHASES IN A TRAPPING POTENTIAL

We now consider the effects of realistic confinement on the staggered quantum phase transitions. The staggered phases result from the destructive interference between single-particle tunneling and DIT. In recent years, density-induced higherorder processes have led to several novel phases, such as the interaction-driven mixing of orbitals [76] and correlated pairtunneling leading to a twisted superfluid phase [77]. Here, we discuss the parameter regime which can provide the staggered quantum phases in the presence of a magneto-optical trap in cold-atom experiments. We add a spatially varying chemical potential to the offset energy term of the model Hamiltonian [Eq. (1)]. The trapping potential is assumed to be the harmonic potential $\epsilon_i = \Omega i^2$, where Ω sets the strength of the potential. In this external confinement the local chemical potential of the system changes as $\tilde{\mu} = \mu - \epsilon_i$. Coexistence of quantum phases occurs within the trapped system as a result of a change in $\tilde{\mu}$ within the trap. We have kept fixed the NN interaction

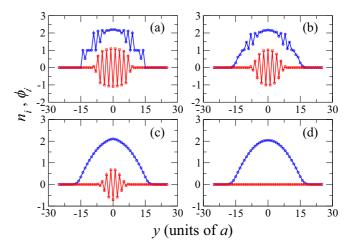


FIG. 7. The average number occupancy and SF order parameter for an L=50 square lattice along a one-dimensional cut at x=0 within a confining potential. The density-distribution (blue circles) and order parameter (red squares) profiles are shown for different temperatures: (a) T=0.05, (b) T=0.2, (c) T=0.3, and (d) T=0.35. With an increase in T, the staggered variations of ϕ_i decrease, which indicates a staggered-to-normal phase transition. The staggered quantum phases vanishes due to thermal fluctuations at $T\approx0.35$. The other parameters chosen are t=0.025, $\mu=3.5$, and V=0.24, and temperatures are in units of U. Here, y is in units of the lattice constant a.

 $V=0.24, \, \mu=1,$ and $\Omega=0.015.$ The latter ensures that the trapped atomic density vanishes at the edge of the lattice.

To illustrate the competition among different phases we have selected the cases T = 0.05, 0.2, 0.3, and 0.35. Using the mean-field approach, we compute the local atomic distributions and the SF order parameter in the trap. We plot the density and order parameter profiles for L = 50 in Fig. 7. In particular, the plots are shown as a vertical cut at x = 0of the trapped square lattice, to observe the effects of the trapping potential. First, we start considering T=0.05, where the observed effects are similar to the zero-temperature case. From Fig. 7(a), we find a homogeneous atomic distribution n_i at the center of the trap while the SF order parameter modulates between the same number and an alternating sign. These properties characterize the SSF at the center of the trap. In addition, the SSF phase is surrounded by a density modulation with a staggered order parameter distribution indicating the parameter domain of the SSS. It is important to note that the SS phase also exhibits modulations in n_i and ϕ_i but the variation in ϕ_i between two real numbers does not change sign. In contrast, the staggered phase changes sign with the same (different) magnitude of the real numbers for SSF (SSS). Thus, the presence of the harmonic potential exhibits the coexistence of two staggered quantum phases, SSF and SSS. At the edges of the trap, the superfluidity vanishes (as identified by $\phi_i = 0$), and the insulating (MI and CDW) or normal state surrounds the staggered phases.

We further show the effects of thermal fluctuations at finite temperatures on the stability of staggered phases. From Fig. 7(b) we observe the reduction in the regime with the modulation of ϕ_i at T = 0.2; however, the constant density at

the center and the crystalline nature of the phase near the trap center still persist. This shows that the melting of staggered quantum phases begins from the edges, and it is more pronounced at T=0.3 [Fig. 7(c)]. At even higher temperatures, the staggered superfluidity vanishes, and the normal-fluid state occupies the trap due to the prevailing role of thermal fluctuations. The temperature corresponding to $T\approx0.3$ is in the few-nanokelvin regime for the extended Bose-Hubbard model with DIT for ¹⁶⁸Er atoms [30]. Hence, the combined effects of the NN interaction as a genuine consequence of long-range interaction and interaction-driven DIT can lead to many-body staggered quantum phases in optical lattice experiments.

VI. CONCLUSION

We have studied the finite-temperature phase diagrams of soft-core dipolar bosons with density-induced tunneling in a square lattice potential. At weak dipolar interaction, the normal state intervenes between two topologically distinct superfluid states, while at strong interaction the staggered and normal supersolid phases appear on either side of the insulating density-wave solid state. Both the mean-field calculation and quantum Monte Carlo simulation show that the critical temperature of the staggered superfluid phase decreases with

single-particle tunneling, while that of the normal superfluid increases, which results from the interplay of DIT and singleparticle tunneling. We have further shown, by using finite-size scaling of the superfluid density, that the thermal phase transition of the staggered superfluidity is the KT type, just like that of normal superfluids. This result suggests that the staggering of the superfluid phase does not alter the symmetry-breaking process of the off-diagonal long-range order. Finally, we revealed the coexistence of quantum phases in the presence of an external trapping potential at finite temperatures. In quantum gas experiments, thermal fluctuations play a decisive role in the emergence of quantum phases. Recent experimental advances in the observation of density-induced tunneling and the superfluidity and phase transitions discussed in the present work may provide a way to realize staggered superfluids in ultracold dipolar experiments.

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- [1] M. Lewenstein, A. Sanpera, V. Ahufinger, B. Damski, A. Sen(De), and U. Sen, Ultracold atomic gases in optical lattices: Mimicking condensed matter physics and beyond, Adv. Phys. 56, 243 (2007).
- [2] I. Bloch, J. Dalibard, and W. Zwerger, Many-body physics with ultracold gases, Rev. Mod. Phys. 80, 885 (2008).
- [3] I. Bloch, J. Dalibard, and S. Nascimbène, Quantum simulations with ultracold quantum gases, Nat. Phys. **8**, 267 (2012).
- [4] C. Gross and I. Bloch, Quantum simulations with ultracold atoms in optical lattices, Science **357**, 995 (2017).
- [5] M. Greiner, O. Mandel, T. Esslinger, T. W. Hansch, and I. Bloch, Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms, Nature (London) 415, 39 (2002).
- [6] M. Aidelsburger, M. Atala, M. Lohse, J. T. Barreiro, B. Paredes, and I. Bloch, Realization of the Hofstadter Hamiltonian with Ultracold Atoms in Optical Lattices, Phys. Rev. Lett. 111, 185301 (2013).
- [7] F. Schäfer, T. Fukuhara, S. Sugawa, Y. Takasu, and Y. Takahashi, Tools for quantum simulation with ultracold atoms in optical lattices, Nat. Rev. Phys. 2, 411 (2020).
- [8] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga, Feshbach resonances in ultracold gases, Rev. Mod. Phys. 82, 1225 (2010).
- [9] M. Aidelsburger, S. Nascimbene, and N. Goldman, Artificial gauge fields in materials and engineered systems, C. R. Phys. 19, 394 (2018).
- [10] D. M. Luz and R. R. dos Santos, Bond-charge interaction in the extended Hubbard chain, Phys. Rev. B **54**, 1302 (1996).
- [11] J. Hirsch, Bond-charge repulsion and hole superconductivity, Phys. C (Amsterdam, Neth.) 158, 326 (1989).

- [12] F. H. L. Essler, V. E. Korepin, and K. Schoutens, New Exactly Solvable Model of Strongly Correlated Electrons Motivated by High-*t_c* Superconductivity, Phys. Rev. Lett. **68**, 2960 (1992).
- [13] J. Appel, M. Grodzicki, and F. Paulsen, Bond-charge repulsion and hole superconductivity in the atomic representation of the CuO₂ plane, Phys. Rev. B 47, 2812 (1993).
- [14] I. Bloch, Ultracold quantum gases in optical lattices, Nat. Phys. 1, 23 (2005).
- [15] T. Lahaye, C. Menotti, L. Santos, M. Lewenstein, and T. Pfau, The physics of dipolar bosonic quantum gases, Rep. Prog. Phys. 72, 126401 (2009).
- [16] M. A. Baranov, M. Dalmonte, G. Pupillo, and P. Zoller, Condensed matter theory of dipolar quantum gases, Chem. Rev. 112, 5012 (2012).
- [17] M. J. Mark, E. Haller, K. Lauber, J. G. Danzl, A. J. Daley, and H.-C. Nägerl, Precision Measurements on a Tunable Mott Insulator of Ultracold Atoms, Phys. Rev. Lett. 107, 175301 (2011).
- [18] D.-S. Lühmann, O. Jürgensen, and K. Sengstock, Multi-orbital and density-induced tunneling of bosons in optical lattices, New J. Phys. **14**, 033021 (2012).
- [19] S. Pilati and M. Troyer, Bosonic Superfluid-Insulator Transition in Continuous Space, Phys. Rev. Lett. 108, 155301 (2012).
- [20] S. Ospelkaus, C. Ospelkaus, O. Wille, M. Succo, P. Ernst, K. Sengstock, and K. Bongs, Localization of Bosonic Atoms by Fermionic Impurities in a Three-Dimensional Optical Lattice, Phys. Rev. Lett. 96, 180403 (2006).
- [21] K. Günter, T. Stöferle, H. Moritz, M. Köhl, and T. Esslinger, Bose-Fermi Mixtures in a Three-Dimensional Optical Lattice, Phys. Rev. Lett. **96**, 180402 (2006).

- [22] T. Best, S. Will, U. Schneider, L. Hackermüller, D. van Oosten, I. Bloch, and D.-S. Lühmann, Role of Interactions in ⁸⁷Rb - ⁴⁰K Bose-Fermi Mixtures in a 3D Optical Lattice, Phys. Rev. Lett. 102, 030408 (2009).
- [23] O. Jürgensen, K. Sengstock, and D.-S. Lühmann, Density-induced processes in quantum gas mixtures in optical lattices, Phys. Rev. A **86**, 043623 (2012).
- [24] D.-S. Lühmann, K. Bongs, K. Sengstock, and D. Pfannkuche, Self-Trapping of Bosons and Fermions in Optical Lattices, Phys. Rev. Lett. 101, 050402 (2008).
- [25] O. Jürgensen, F. Meinert, M. J. Mark, H.-C. Nägerl, and D.-S. Lühmann, Observation of Density-Induced Tunneling, Phys. Rev. Lett. 113, 193003 (2014).
- [26] D.-S. Lühmann, Twisted superfluid phase in the extended onedimensional Bose-Hubbard model, Phys. Rev. A 94, 011603(R) (2016)
- [27] D. Johnstone, N. Westerberg, C. W. Duncan, and P. Öhberg, Staggered ground states in an optical lattice, Phys. Rev. A 100, 043614 (2019).
- [28] R. Kraus, K. Biedroń, J. Zakrzewski, and G. Morigi, Super-fluid phases induced by dipolar interactions, Phys. Rev. B 101, 174505 (2020).
- [29] K. Suthar, R. Kraus, H. Sable, D. Angom, G. Morigi, and J. Zakrzewski, Staggered superfluid phases of dipolar bosons in two-dimensional square lattices, Phys. Rev. B 102, 214503 (2020).
- [30] S. Baier, M. J. Mark, D. Petter, K. Aikawa, L. Chomaz, Z. Cai, M. Baranov, P. Zoller, and F. Ferlaino, Extended Bose-Hubbard models with ultracold magnetic atoms, Science 352, 201 (2016).
- [31] I. B. Spielman, W. D. Phillips, and J. V. Porto, Mott-Insulator Transition in a Two-Dimensional Atomic Bose Gas, Phys. Rev. Lett. **98**, 080404 (2007).
- [32] B. Capogrosso-Sansone, Ş. G. Söyler, N. Prokof'ev, and B. Svistunov, Monte Carlo study of the two-dimensional Bose-Hubbard model, Phys. Rev. A 77, 015602 (2008).
- [33] M. Rigol, G. G. Batrouni, V. G. Rousseau, and R. T. Scalettar, State diagrams for harmonically trapped bosons in optical lattices, Phys. Rev. A **79**, 053605 (2009).
- [34] K. Jiménez-García, R. L. Compton, Y.-J. Lin, W. D. Phillips, J. V. Porto, and I. B. Spielman, Phases of a Two-Dimensional Bose Gas in an Optical Lattice, Phys. Rev. Lett. 105, 110401 (2010).
- [35] K. W. Mahmud, E. N. Duchon, Y. Kato, N. Kawashima, R. T. Scalettar, and N. Trivedi, Finite-temperature study of bosons in a two-dimensional optical lattice, Phys. Rev. B 84, 054302 (2011).
- [36] A. S. Sajna, T. P. Polak, R. Micnas, and P. Rożek, Ground-state and finite-temperature properties of correlated ultracold bosons on optical lattices, Phys. Rev. A 92, 013602 (2015).
- [37] M. O. C. Pires and E. J. V. de Passos, Superfluid to normal fluid phase transition in the Bose gas trapped in two-dimensional optical lattices at finite temperature, Braz. J. Phys. 47, 1 (2017).
- [38] K. Suthar, H. Sable, R. Bai, S. Bandyopadhyay, S. Pal, and D. Angom, Supersolid phase of the extended Bose-Hubbard model with an artificial gauge field, Phys. Rev. A **102**, 013320 (2020).
- [39] R. Bai, D. Gaur, H. Sable, S. Bandyopadhyay, K. Suthar, and D. Angom, Segregated quantum phases of dipolar bosonic mixtures in two-dimensional optical lattices, Phys. Rev. A 102, 043309 (2020).

- [40] H.-J. Chen, Y.-Q. Yu, D.-C. Zheng, and R. Liao, Extended Bose-Hubbard model with cavity-mediated infinite-range interactions at finite temperatures, Sci. Rep. 10, 9076 (2020).
- [41] G. Ceccarelli and C. Torrero, Scaling behavior of trapped bosonic particles in two dimensions at finite temperature, Phys. Rev. A **85**, 053637 (2012).
- [42] M. Gupta, H. R. Krishnamurthy, and J. K. Freericks, Strong-coupling expansion for ultracold bosons in an optical lattice at finite temperatures in the presence of superfluidity, Phys. Rev. A 88, 053636 (2013).
- [43] R. Landig, L. Hruby, N. Dogra, M. Landini, R. Mottl, T. Donner, and T. Esslinger, Quantum phases from competing short- and long-range interactions in an optical lattice, Nature (London) 532, 476 (2016).
- [44] C. Lagoin, U. Bhattacharya, T. Grass, R. W. Chhajlany, T. Salamon, K. Baldwin, L. Pfeiffer, M. Lewenstein, M. Holzmann, and F. Dubin, Extended Bose-Hubbard model with dipolar excitons, Nature (London) 609, 485 (2022).
- [45] L. de Forges de Parny, F. Hébert, V. G. Rousseau, and G. G. Batrouni, Finite temperature phase diagram of spin-1/2 bosons in two-dimensional optical lattice, Eur. Phys. J. B 85, 169 (2012).
- [46] L. de Forges de Parny and V. G. Rousseau, Quantum and thermal phase transitions in a Bosonic atom-molecule mixture in a two-dimensional optical lattice, Phys. Rev. A 95, 013606 (2017).
- [47] M. C. Gutzwiller, Effect of Correlation on the Ferromagnetism of Transition Metals, Phys. Rev. Lett. 10, 159 (1963).
- [48] D. S. Rokhsar and B. G. Kotliar, Gutzwiller projection for bosons, Phys. Rev. B 44, 10328 (1991).
- [49] W. Krauth, M. Caffarel, and J.-P. Bouchaud, Gutzwiller wave function for a model of strongly interacting bosons, Phys. Rev. B 45, 3137 (1992).
- [50] K. Sheshadri, H. R. Krishnamurthy, R. Pandit, and T. V. Ramakrishnan, Superfluid and insulating phases in an interacting-boson model: Mean-field theory and the RPA, Europhys. Lett. 22, 257 (1993).
- [51] R. Bai, S. Bandyopadhyay, S. Pal, K. Suthar, and D. Angom, Bosonic quantum Hall states in single-layer two-dimensional optical lattices, Phys. Rev. A 98, 023606 (2018).
- [52] K. V. Krutitsky, Ultracold bosons with short-range interaction in regular optical lattices, Phys. Rep. 607, 1 (2016).
- [53] S. Pal, R. Bai, S. Bandyopadhyay, K. Suthar, and D. Angom, Enhancement of the Bose glass phase in the presence of an artificial gauge field, Phys. Rev. A 99, 053610 (2019).
- [54] K. Suthar, P. Kaur, S. Gautam, and D. Angom, Spin-orbit-coupling-driven superfluid states in optical lattices at zero and finite temperatures, Phys. Rev. A **104**, 043320 (2021).
- [55] P. Buonsante and A. Vezzani, Phase diagram for ultracold bosons in optical lattices and superlattices, Phys. Rev. A 70, 033608 (2004).
- [56] L. Pollet, Recent developments in quantum Monte Carlo simulations with applications for cold gases, Rep. Prog. Phys. 75, 094501 (2012).
- [57] A. W. Sandvik, Stochastic series expansion method with operator-loop update, Phys. Rev. B 59, R14157 (1999).
- [58] O. F. Syljuåsen and A. W. Sandvik, Quantum Monte Carlo with directed loops, Phys. Rev. E 66, 046701 (2002).

- [59] A. W. Sandvik, Finite-size scaling of the ground-state parameters of the two-dimensional Heisenberg model, Phys. Rev. B 56, 11678 (1997).
- [60] E. L. Pollock and D. M. Ceperley, Path-integral computation of superfluid densities, Phys. Rev. B 36, 8343 (1987).
- [61] D. M. Ceperley and E. L. Pollock, Path-integral simulation of the superfluid transition in two-dimensional ⁴He, Phys. Rev. B 39, 2084 (1989).
- [62] A. Dorneich and M. Troyer, Accessing the dynamics of large many-particle systems using the stochastic series expansion, Phys. Rev. E **64**, 066701 (2001).
- [63] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Boson localization and the superfluid-insulator transition, Phys. Rev. B 40, 546 (1989).
- [64] D. Jaksch, C. Bruder, J. I. Cirac, C. W. Gardiner, and P. Zoller, Cold Bosonic Atoms in Optical Lattices, Phys. Rev. Lett. 81, 3108 (1998).
- [65] F. Gerbier, Boson Mott Insulators at Finite Temperatures, Phys. Rev. Lett. 99, 120405 (2007).
- [66] K.-K. Ng, Thermal phase transitions of supersolids in the extended Bose-Hubbard model, Phys. Rev. B **82**, 184505 (2010).
- [67] K.-K. Ng and M.-F. Yang, Thermal phase transitions in the attractive extended Bose-Hubbard model with three-body constraint, Phys. Rev. B 83, 100511(R) (2011).
- [68] D.-S. Lühmann, Cluster Gutzwiller method for bosonic lattice systems, Phys. Rev. A 87, 043619 (2013).

- [69] K.-K. Ng and Y.-C. Chen, Supersolid phases in the bosonic extended Hubbard model, Phys. Rev. B 77, 052506 (2008).
- [70] S. Bandyopadhyay, R. Bai, S. Pal, K. Suthar, R. Nath, and D. Angom, Quantum phases of canted dipolar bosons in a two-dimensional square optical lattice, Phys. Rev. A 100, 053623 (2019).
- [71] T. Flottat, L. de Forges de Parny, F. Hébert, V. G. Rousseau, and G. G. Batrouni, Phase diagram of bosons in a two-dimensional optical lattice with infinite-range cavity-mediated interactions, Phys. Rev. B 95, 144501 (2017).
- [72] G. Schmid, S. Todo, M. Troyer, and A. Dorneich, Finite-Temperature Phase Diagram of Hard-Core Bosons in Two Dimensions, Phys. Rev. Lett. 88, 167208 (2002).
- [73] H. Weber and P. Minnhagen, Monte Carlo determination of the critical temperature for the two-dimensional XY model, Phys. Rev. B 37, 5986 (1988).
- [74] Y.-D. Hsieh, Y.-J. Kao, and A. W. Sandvik, Finite-size scaling method for the Berezinskii–Kosterlitz–Thouless transition, J. Stat. Mech. (2013) P09001.
- [75] J. M. Kosterlitz and D. J. Thouless, Ordering, metastability and phase transitions in two-dimensional systems, J. Phys. C 6, 1181 (1973).
- [76] P. Soltan-Panahi, D.-S. Lühmann, J. Struck, P. Windpassinger, and K. Sengstock, Quantum phase transition to unconventional multi-orbital superfluidity in optical lattices, Nat. Phys. 8, 71 (2012).
- [77] O. Jürgensen, K. Sengstock, and D.-S. Lühmann, Twisted complex superfluids in optical lattices, Sci. Rep. 5, 12912 (2015).