Frustrated Quantum Magnetism with Bose Gases in Triangular Optical Lattices at Negative Absolute Temperatures

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We propose an experimental protocol to perform analog quantum simulation of frustrated antiferromagnetism with strong quantum fluctuations by using ultracold Bose gases in triangular optical lattices with isosceles anisotropy of hoppings. Specifically, we combine a phase-imprinting scheme with sudden sign inversion of the interatomic interaction and the trap potential to prepare a chiral superfluid state with a negative absolute temperature. In the framework of the time-dependent Gutzwiller approach, we compute the time evolution of the state subjected to a slow sweep of the hopping energy. We show that in this process the system simulates a state near equilibrium of the Bose-Hubbard model with sign-inverted hoppings. By means of the cluster mean-field method with a cluster size scaling, we quantitatively predict the quantum critical point of the superfluid-Mott insulator transition as a function of the spatial anisotropy parameter, which serves as a benchmark for quantum simulation.

Introduction.— Frustration is a key concept to understand various emergent phenomena in the modern many-body physics [1, 2]. When different interactions among particles strongly compete with each other, e.g., for a geometric reason, the system is “frustrated” in determining the true ground state. The study on the interplay of the frustration and strong quantum fluctuations has been one of the core challenges of quantum many-body physics, presenting many open problems in connection with nontrivial magnetic states including quantum spin liquids [3] and as a challenge for numerical techniques to handle highly entangled ground states [4, 5]. Quantum simulation with the use of ultracold atomic gases in optical lattices [6–8] has been discussed as a promising approach to make a critical breakthrough in this research area. However, the effort in realizing frustrated quantum systems with cold atoms has not yet paid off even though many theoretical proposals have been made [9–13].

One straightforward idea for creating frustration is the use of two-component ($\sigma = \uparrow, \downarrow$) Fermi gases [15–24] loaded into a nonbipartite (e.g., triangular [24] and kagome [25]) optical lattice. The second-order hopping process provides antiferromagnetic superexchange interactions between the (pseudo)spins $\sigma$ [24–27], which result in a frustrated situation because complete staggered spin configuration is not allowed by the lattice geometry. Although long-range magnetic correlation over a distance comparable to the system size has recently been observed in a square optical lattice [21], a further technical breakthrough is required to realize far lower temperatures to study frustrated quantum magnetism. Another interesting idea is a fast shaking of optical lattice, which can effectively invert the sign of the hopping integral from the natural one [28, 29]. For ultracold Bose gases with sign-inverted hopping, the relative local phase of Bose-Einstein condensates (BECs) tends to be $\pi$ on neighbor-
a phase-imprinting scheme combined with sudden sign inversion of the interaction and potential, which causes much less heating compared to the lattice shaking.

Supposing Bose gases in a triangular lattice, we simulate the dynamics along the protocol within the time-dependent Gutzwiller approach (TDGA) to demonstrate that quantum phases of the frustrated Bose-Hubbard model, including chiral superfluid (CSF), could indeed be realized. Moreover, considering general cases with isosceles-type anisotropy of hoppings, we give more quantitative analysis on the quantum phase transition between frustrated CSF and MI by means of the cluster mean-field plus scaling (CMF+S) method with two-dimensional (2D) density matrix renormalization group (DMRG) solver. This enables us to discuss the interplay of frustration and quantum fluctuations, which is a critical factor for producing various exotic frustrated states. The theoretical predictions provide a solid guidepost for future experiments to confirm that the interplay effects are properly captured in the quantum simulator.

We set $\hbar = 1$ except in the figures. See also the Supplementary Material (SM) for the technical details of the calculations.

**The Bose-Hubbard model on triangular lattice.**— A system of Bose gases in a deep optical lattice is described by the Bose-Hubbard model:

$$
\hat{H} = -\sum_{i,j} J_{ij} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \frac{V}{a^2} \sum_i |\mathbf{r}_i|^2 \hat{n}_i(1)
$$

with hopping integral $J_{ij}$ (for $i \neq j$), chemical potential $\mu$, onsite interaction $U$, harmonic trap potential $V |\mathbf{r}_i|^2 / a^2$, and lattice constant $a$. Here we consider a triangular optical lattice with spatially anisotropic hoppings of isosceles type, which can be created by tuning the intensity of one of the three lasers to be different from the others. The spatial anisotropy is parameterized by $J_{ij} = J_1$ for nearest neighbor (NN) sites $(i,j)$ in the $a_1 = (a,0)$ direction and $J_{ij} = J_2$ in the $a_2 = (-a/2, \sqrt{3}a/2)$ and $a_3 = (-a/2, -\sqrt{3}a/2)$ directions [Figs. 1(a) and 1(b)].

We first discuss the ground state for $V = 0$ within the site-decoupling Gutzwiller approach (GA). Under the assumption of the BEC order ($\langle \hat{b}_i \rangle \equiv \psi_i = \hat{\psi} e^{i \mathbf{q} \cdot \mathbf{r}_i + i \varphi}$ with momentum $\mathbf{q}$ and global phase $\varphi$, the kinetic energy of Eq. [1] is given by $-\sum_{i,j \neq i} \varepsilon_{\mathbf{q}} \hat{b}_i^\dagger \hat{b}_j \approx \varepsilon_{\mathbf{q}} \hat{\psi}^2 M$. Here, $\varepsilon_{\mathbf{q}} \equiv -2 J_1 \cos \mathbf{q} \cdot \mathbf{a}_1 + J_2 \cos \mathbf{q} \cdot \mathbf{a}_2 + J_2 \cos \mathbf{q} \cdot \mathbf{a}_3$ and $M$ is the number of lattice sites. For natural-sign hoppings $J_1, J_2 > 0$, the minimum kinetic energy is obtained at $\mathbf{q} = \mathbf{0}$, leading to a uniform SF state. The maximum of the kinetic energy is achieved at $\mathbf{q} = \pm \mathbf{Q}$ with

$$
\mathbf{Q} = \begin{cases} 
(2\pi/a,0) & \text{for } 0 \leq J_1/J_2 \leq 0.5, \\
(2 \arccos \left( \frac{J_2}{J_1} \right) / a,0) & \text{for } J_1/J_2 > 0.5.
\end{cases}
$$

![FIG. 1: (a) Typical potential landscape of isosceles triangular optical lattice created by three laser beams. (b) GA prediction of the local phase pattern in the frustrated case. (c) The order parameter $\psi$ as a function of $|U/J|$ for $\rho = 1$.](image)

Therefore, if sign-inverted hopping $(J_1,J_2 < 0)$ is prepared, a frustrated CSF state with finite BEC momentum $\mathbf{q} = \pm \mathbf{Q}$ is realized. The choice of $\mathbf{q} = \mathbf{Q}$ or $-\mathbf{Q}$ represents the degeneracy with respect to the chirality of vortex in unit triangles. Hereafter we suppose $\mathbf{q} = \mathbf{Q}$ to be spontaneously selected. In the equilateral case $(J_1 = J_2 = J)$, the momentum is $\mathbf{Q} = (4\pi/3a,0) \equiv \mathbf{Q}_K$. Therefore, the CSF state forms a “three-color” arrangement of the local phase $\langle \hat{\psi}_i \rangle = 0, 2\pi/3$, and $4\pi/3$ within a global phase shift) as shown in Fig. 1(b). This can be understood as a compromise solution for the frustration in the bond energy minimization. For generic $J_1/J_2 > 0.5$, the phase factor changes spatially with incommensurate pitch vector $\mathbf{Q}$. In the parameter range $0 \leq J_1/J_2 \leq 0.5$ and the 1D limit $J_1/J_2 \gg 1$, a “two-color” (0 and $\pi$) pattern is formed with no chiral degeneracy. The $J_1/J_2$ dependence of $\mathbf{Q}$ is analogous to the pitch vector of spin spiral states in spatially-anisotropic triangular antiferromagnets.

For large, repulsive interaction $U$, lattice bosons undergo a quantum phase transition to the MI state when the filling factor $\rho \equiv 1/M \sum_i \langle \hat{n}_i \rangle$ is an integer. Performing the GA decoupling $\hat{b}_i^\dagger \hat{b}_j \approx \hat{\psi}_i^* \hat{\psi}_j$ in Eq. [1], we calculate the order parameter $\hat{\psi}$ for $\rho = 1$ in the unfrustrated $(J_1,J_2 > 0; \mathbf{q} = \mathbf{0})$ and frustrated $(J_1,J_2 < 0; \mathbf{q} = \mathbf{Q})$ ground states [see Fig. 1(c)]. At $J_1 = J_2 = J$, the critical point at which $\hat{\psi}$ vanishes is given as $U_c^{(\text{GA})}/J = 17.5$ for the frustrated case, which is a half of $U_c^{(\text{GA})}/J = 35.0$ for the unfrustrated case. The strong reduction is attributed by the fact that the CSF state is less stable due to the frustrated local-phase arrangement in which the NN bonds are not fully satisfied in minimizing the local kinetic energy. For general values...
of the anisotropy $J_1/J_2$ and $\rho$, the critical point is given by $U_i^{(GA)} = -\varepsilon_Q/\sqrt{p+1}$ with $q = 0$ ($q = Q$) for the unfrustrated (frustrated) case. The ratio $|\varepsilon_Q/\varepsilon_0|$ equals to 1 only at $J_1/J_2 = 0$ or $J_1/J_2 \to \infty$, indicating that the reduction effect due to frustration exists even in the “two-color” region of $0 < J_1/J_2 \leq 0.5$.

Negative absolute temperature.— To experimentally create the frustrated quantum states, it is required to prepare sign-inverted hoppings $J_{ij} < 0$ with avoiding serious heating of the system. Below, we explain the details of the protocol through use of negative-temperature statistics.

Let us suppose an initial state in which $N$ particles are distributed in a triangular lattice and a harmonic potential, which realizes the SF ground state of the standard Bose-Hubbard model \cite{1} with $J_{ij} > 0$ and $U, V > 0$. See a typical example in Fig. 2(a) obtained within the GA \cite{31} for $N = 1400$, $J_1 = J_2 = J = 0.08U_0$, $U = U_0$, and $V = 0.001U_0$ (with $U_0 > 0$ being the energy unit). First, we suddenly change $U$ and $V$ to be attractive ($U < 0$) and anti-trapping ($V < 0$), and at the same time, achieve the maximum interaction and potential energies. In Ref. \cite{32} for square (unfrustrated) lattice, this has been performed simply with $U \to -U$ and $V \to -V$ by using the Feshbach resonance \cite{40} and blue-detuned lasers. In the present case with frustration, one requires special attention to achieve the maximum interaction and potential energies; the values of $U$ and $V$ have to be changed as $U \to -|\varepsilon_Q/\varepsilon_0|U$ and $V \to -|\varepsilon_Q/\varepsilon_0|V$ (e.g., $U \to -U/2$ and $V \to -V/2$ for $J_1 = J_2$) in order to adjust the energy scale in consideration of the reduction of the kinetic energy due to the frustration.

By making also the kinetic energy reach its maximum, one can realize a negative-temperature ground state (at $T \approx -0$) for $J_{ij} > 0$ and $U, V < 0$, which should be equivalent to the ground state (at $|T| \approx +0$) of the system with $J_{ij} < 0$ and $U, V > 0$ since the physics of the two systems obey the same factor $\exp[-H/E_B]$. To this end, here we suggest the use of the phase-imprinting techniques \cite{31,33}. When a single-particle energy difference $\delta E$ is introduced between two sites, the relative phase on the two sites starts to develop with $\exp[i\delta E]$ in time $t$. In a region deep inside the SF phase, the kinetic energy ($\propto \epsilon_q$) reaches the maximum when the BEC momentum takes $q = Q$ given in Eq. (2). One can transfer $q$ from 0 to $Q$ by introducing a temporary linear gradient potential $V_{\text{ext}} = \delta E \sum_n (x_n/a)\tilde{n}_i$ for appropriate time $\delta t = Q/a/\delta E$ [see Fig. 2(b)]. Such a temporary potential can be created, e.g., by a magnetic field gradient or by an extra 1D optical lattice satisfying $Q = Q_M$ or $Q = Q_K$ \cite{39}.

TDGA simulation.— In the framework of the TDGA \cite{39,47,48}, we simulate the time evolution of the initial state in Fig. 2(a) after suddenly performing the three operations shown in Fig. 2(b). In the simulation, we implement the phase imprinting on the initial state by the operation $\sum_n f^{(n)}(\langle n | \rightarrow \sum_n e^{i\varepsilon_Q x_n Q_i} \cdot f^{(n)}(\langle n |$ on the local wave function at every site $i$. Here, $f^{(n)}(\langle n |$ is the coefficient of the Fock basis $|n\rangle$. In addition, we perform the sudden changes of $U = U_0 \to -U_0/2$ and $V = 0.001U_0 \to -0.0005U_0$. After those three operations are performed at $t = 0$, we calculate the time evolution of the state fixing the value of $|U/J|$ for $0 < t \leq 200U_0^{-1}$ to see the stability of the created negative-temperature CSF state, and then slowly increasing $|U/J|$ for $t > 200U_0^{-1}$ through $J$ decreasing linearly with $J = 0.08U_0 - 0.0001(tU_0 - 200)U_0$ to observe the CSF-to-MI transition.

As shown in Fig. 2(c), the created negative-temperature state is predicted to be indeed dynamically stable for $0 < t \leq 200U_0^{-1}$. Note that the state collapses

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**Figure 2:** (a) Profiles of density (solid lines) and order parameter (dashed lines) in the harmonic trap along the cut of $y_i = a/\sqrt{3}$ in the initial state. (b) The three operations to make frustrated negative-temperature states (for $J_1 = J_2 = J$). The inset in the left panel illustrates a tilting of the optical lattice for the phase-imprinting. (c) Negative-temperature CSF states at time $t$. (d) Color plots for the local phase near the center of the trap at $t = 100U_0^{-1}$ (upper) and $700U_0^{-1}$ (lower).

**Figure 3:** (a) Time evolution of the density fluctuation $\delta n^2(t)/\delta n^2(0)$ from the initial state (a) with and (b) without the three operations shown in Fig. 2(b) at $t = 0$. The time schedule for increasing $|U/J|$ is plotted together.
studies on frustrated quantum spins [14], to the present with 2D DMRG solver, which recently established in due to the lack of effective computational methods. Here, frustrated Bose gases in 2D lattices have been poorly studied of frustration and quantum fluctuations as a guideline mations (GA and TDGA) to predict the interplay effect V provide more quantitative estimation of the CSF-MI crit-

immediately within \( t \lesssim 2U_0^{-1} \) if the phase-imprinting is not performed \( [39] \). For \( t > 200U_0^{-1} \) with increasing \( |U/J| \), the MI plateau is gradually formed and \(|\psi_i|\) in the trap center decreases and eventually almost vanishes. Until the transition point, the three-color phase profile in the CSF state is properly kept within a global phase shift [Fig. 2(d)]. To show the transition process more clearly, we plot in Fig. 3(a) the time evolution of the density fluctuation \( \delta n_i^2 \equiv \langle n_i^2 \rangle - \langle n_i \rangle^2 \) averaged over the center sites within \(|r_i| \leq 10a\). The value of \( \delta n_i^2(t)/\delta n_i^2(0) \) decreases as \(|U/J| \) and almost vanishes at \(|U/J| \approx |U_{c(GA)}/J| \approx 17.5 \), which is consistent with the GA prediction of the critical point for the frustrated system. In the case of a box-shaped trap potential \([49, 50]\), which is modeled by \( V = 0 \) and the open boundary at \(|r_i| = 36a\), the transition is more sharply observed (the blue dashed line in Fig. 3(a) for \( N = 4692 \)). We also plot in Fig. 3(b) the unfrustrated case of the standard SF-MI transition as a reference, which shows \( \epsilon \) sharp difference from the frustrated case in the values of \(|U/J| \) of the transition region.

Quantitative analysis by CMF+S with DMRG.— We provide more quantitative estimation of the CSF-MI critical point for \( V = 0 \) beyond the site-decoupling approximations (GA and TDGA) to predict the interplay effect of frustration and quantum fluctuations as a guideline necessary for experiments. The quantum effects on frustrated Bose gases in 2D lattices have been poorly studied due to the lack of effective computational methods. Here, we generalize and apply the numerical CMF+S method with 2D DMRG solver, which recently established in studies on frustrated quantum spins \([14]\), to the present system. We consider the \( N_C \)-site cluster Hamiltonian on a triangular-shaped cluster [see the inset of Fig. 4(a) for \( N_C = 10 \)] under the mean-field boundary condition. We work in the twisted frame, \( \hat{b}_i \equiv e^{iQ \cdot r_i} \hat{b}_i \), with optimizing \( Q = (Q_x, 0) \) \([39]\). The CMF+S method permits the systematic inclusion of quantum intersite correlations by increasing \( N_C \), which connects between the GA (\( N_C = 1 \)) and exactly quantum (\( N_C \to \infty \)) results.

Figure 4(a) summarizes the \( N_C = 10, 15, 21 \) data and the CMF+S (\( N_C \to \infty \)) result for the \( \rho = 1 \) CSF-MI (SF-MI) critical point in the frustrated (unfrustrated) case with \( J_1, J_2 < 0 \) (\( J_1, J_2 > 0 \)). The value of \( U_c/|J_2| \) for the frustrated case exhibits a nonmonotonic behavior with a dip around \( J_1/J_2 \approx 0.8 \), while the unfrustrated one simply increases as the total hoppings \( J_1 + 2J_2 \) increases. This is indeed the frustration effect, which destabilizes the CSF state. Besides, the value of \( u_\epsilon \) is strongly reduced from the GA prediction \( U_c^{(GA)} \) due to the inclusion of the intersite quantum correlations. It should be noted that the relative difference \( (U_c^{(GA)} - U_c)/U_c^{(GA)} \) between the GA and CMF+S values is much larger for the frustrated case (∼40-50%) than the unfrustrated case (∼20%) as shown in Fig. 4(b). This indicates that the quantum effects are strongly enhanced by the interplay with frustration. Figure 4(c) shows that the BEC momentum \( Q_x \) in the CSF state is little affected by the inclusion of quantum correlations. The slight variance of \( Q_x \) from \( 4\pi/3 \) at \( J_2/J_1 = 1 \) is thought to be due to the finite cluster-size effect \([39]\).

Detection method.— The BEC momentum \( Q \) in the CSF state and the transition to the MI can be simply detected by time-of-flight (TOF) images of momentum distributions \([15]\). A more precise determination of the critical point can be made by extracting the condensate fraction from the TOF images \([52]\), by observing the critical velocity using a moving optical lattice \([53]\), or by measuring the density fluctuation \( \delta n^2 \) using the quantum-gas microscope \([18, 23]\). The frustrated CSF-MI transition is easily distinguishable from the standard SF-MI transition thanks to the sharp difference in the value of \( U_c/|J_2| \).

Conclusions.— We made a proposal and provided the necessary theoretical analysis for analog quantum simulation of frustrated quantum magnetism by using ultracold Bose gases in triangular optical lattices. We proposed an experimental protocol to create a frustrated quantum state at negative absolute temperature by performing a phase imprinting together with sudden inversion of the interatomic interaction and the trap potential. Simulating the time evolution, we demonstrated that a dynamically-stable superfluid state with chiral symmetry breaking was indeed realized, and underwent the quantum transition to the MI as the hopping amplitude decreased. Moreover, we performed state-of-the-art numerical calculations on the quantum critical point as a function of the spatial hopping anisotropy, which predicted a significant interplay of frustration and quantum
fluctuations.

It has been expected that adding long-range interatomic interaction to the present system may give rise to an exotic chiral MI state [34], which is essentially equivalent to the so-called “chiral liquid” expected in a spin-1 frustrated magnet [35]. Besides, our protocol for direct creation of a frustrated quantum state is advantageous for preparing the phases that are not neighboring to the MI phase, such as quantum spin liquids expected for ρ = half integers [36, 37]. Thus the present study gives a crucial guidepost for cold-atom quantum simulations of those exotic quantum frustrated physics.

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Supplementary Material for “Frustrated Quantum Magnetism with Bose Gases in Triangular Optical Lattices at Negative Absolute Temperatures”

In this Supplementary Material, we provide more details on the preparation of triangular optical lattice with spatially-anisotropic hoppings, the phase imprinting with an extra 1D optical lattice, and the calculation techniques used in the main text.

### Triangular optical lattice with spatially-anisotropic hoppings

A triangular optical lattice can be created by superposing three laser beams that intersect in the x-y plane with wave vectors \( k_1 = k_L(1, 0) \), \( k_2 = k_L(-1/2, -\sqrt{3}/2) \), and \( k_3 = k_L(-1/2, \sqrt{3}/2) \) and equal frequency \( \omega_L \). All beams are linearly polarized orthogonal to the plane and each has field strength \( E_i (i = 1, 2, 3) \). The total electric field is given by

\[
E(r, t) = \sum_{i=1}^{3} E_i \cos(k_i \cdot r - \omega_L t + \phi_i) e_z. \tag{S1}
\]

The dipole potential generated by the electric field is proportional to its squared amplitude,

\[
V(r) \propto |E_{\text{tot}}(r, t)|^2 = \frac{E_1^2 + E_2^2 + E_3^2}{2} + E_2 E_3 \cos(b_2 \cdot r - \phi_{23}) + E_1 E_3 \cos((b_1 - b_2) \cdot r + \phi_{13}) + E_1 E_2 \cos(b_1 \cdot r + \phi_{12}) + A(t), \tag{S2}
\]

where \( b_1 = k_1 - k_2, b_2 = k_3 - k_2, \phi_{ij} = \phi_i - \phi_j \), and \( A(t) \) represents the terms dependent on time \( t \). Since the frequency of light is quite large, only the time-averaged value of \( |E_{\text{tot}}|^2 \) can affect atoms. All the terms in \( A(t) \) oscillate at frequency \( 2\omega_L \), and thus can be dropped. Finally, we obtain a periodic dipole potential

\[
V(r) = -V_1 \cos(b_2 \cdot r - \phi_{23}) - V_2 \cos((b_1 - b_2) \cdot r + \phi_{13}) - V_3 \cos(b_1 \cdot r + \phi_{12}) + \text{const.,} \tag{S3}
\]

where \( V_1, V_2, \) and \( V_3 \) are proportional to \( E_2 E_3, E_1 E_3, \) and \( E_1 E_2 \), respectively. A variation of the phases \( \phi_i \) of the laser beams yield only a global shift of the lattice in position. The primitive lattice vectors \( a_1 \) and \( a_2 \) are given so that \( a_i \cdot b_j = 2\pi \delta_{ij} \). In the main text, we define \( a_3 = -a_1 - a_2 \) for convenience. For red-detuned lasers with \( V_i > 0 \), the potential minima form a geometrically equilateral triangular lattice in lattice constant: \( a = |a_i| = 4\pi/3k_L = 2\lambda_L/3 \) with \( \lambda_L \) being the laser wavelength. The spatial anisotropy in the hopping amplitudes can be introduced by the difference in \( V_1, V_2, \) and \( V_3 \) through tuning the laser intensities \( E_1, E_2, \) and \( E_3 \). For example, the set of the field strengths with the relation of \( E_1 = 1.6E_2 = 1.6E_3 (1.6V_1 = V_2 = V_3) \) yields the potential landscape shown in Fig. 1(a), which gives anisotropy of “isosceles-type” in the nearest-neighbor hopping amplitudes.

### Tilting triangular optical lattice with an additional 1D optical lattice

To perform the phase-imprinting process in the protocol proposed in the main text, one has to introduce a single-particle energy difference \( \delta E \) between adjacent two sites. This could be directly implemented by a magnetic field gradient, which introduces an extra linear gradient potential. Here, let us also provide another way to perform the phase-imprinting process for preparing the commensurate \( Q = Q_M = (2\pi/a, 0) \) (two-color) and \( Q = Q_K = (4\pi/3a, 0) \) (three-color) states by the use of an additional 1D optical lattice. We suppose that a potential of 1D optical lattice is created with additional laser beams in the \( a_1 \) direction:

\[
V_{\text{1D}}(x) = V' \cos^2(k'_L x + \phi') \tag{S4}
\]

with amplitude \( V' \), wave vector \( k'_L = 2\pi/\lambda'_L \), and phase \( \phi' \). Here, let us set \( \phi_i = 0 (i = 1, 2, 3) \) for the triangular optical lattice without loss of generality.

Let us first consider the range of \( 0 \leq J_1/J_2 \leq 0.5 \) (\( V_1 \gg V_2 = V_3 \)), in which the configuration of the local phase factor is expected to form the two-sublattice (say A and B) structure with the pitch vector \( Q = Q_M \) as illustrated in Fig. 1(b). For creating the local phase configuration by the phase imprinting, it is required to introduce a temporary single-particle energy difference \( \delta E \) only between the two-sublattice groups of sites for time \( \delta t = 2\pi/\delta E \). This can
be achieved by using an additional 1D optical lattice of magic wavelength defined by $\lambda'_L = 4\lambda_L/3$ and phase shift $\phi' = 0$ or $\pi/2 \pmod \pi$. Figure S1(a) shows an example of the total potential $V(r) + V_{1D}(x)$ with the parameters $2V_1 = V_2 = V_3 = V'$ and $\phi' = 0$. Note that the two options in $\phi'$ correspond to the exchange of A and B.

In a similar way, using a 1D periodic potential with $\lambda'_L = 2\lambda_L$, one can also implement a temporary energy difference $\delta E$ between the three-sublattice groups of sites, say A, B, and C. The additional lasers are shined for time $\delta t = 4\pi/3\delta E$ to imprint the three-color phase configuration illustrated in Fig. 1(b) to the initial SF state. Figure S1(b) shows an example of the total potential $V(r) + V_{1D}(x)$ with the parameters $V_1 = V_2 = V_3 = V'$ and $\phi' = \pi/12$. Note that the phase shift $\phi'$ has six options, $(2n - 1)\pi/12 \ (n = 1, 2, \cdots, 6)$, reflecting the possible permutation of A, B, and C.

The GA analysis for finite-momentum BEC states

Within the site-decoupling mean-field approximation, known as the GA, the effective local Hamiltonian at site $i$ is given by

$$\hat{H}_i^{GA} = -\sum_{j \neq i} J_{ij} \left( \psi_j \hat{b}_j^\dagger + \psi_j^* \hat{b}_j - \psi_i \psi_j^* \right) - \mu \hat{n}_i + \frac{U}{2} \hat{n}_i(\hat{n}_i - 1) + \frac{V}{\alpha^2} |r_i|^2 \hat{n}_i,$$

(S5)

as the result of the decoupling $\hat{b}_j^\dagger \hat{b}_j \approx \psi_j \hat{b}_j^\dagger + \psi_j^* \hat{b}_j - \psi_i \psi_j^* \psi_i$ in the original Hamiltonian (1). The results displayed in Fig. 1(c) are calculated under the assumption of finite-momentum BEC, $\psi_i = \tilde{\psi}_i e^{i q \cdot r_i + \varphi}$, for $V = 0$. In this case, one has only to consider a certain single site $i$, e.g., the site at the origin $r_i = 0$, and $\varphi = 0$ without loss of generality. Equation (S5) becomes

$$\hat{H}_i^{GA} = \varepsilon_q \tilde{\psi} \left( \hat{b}_i^\dagger + \hat{b}_i - \tilde{\psi} \right) - \mu \tilde{n}_i + \frac{U}{2} \tilde{n}_i(\tilde{n}_i - 1),$$

(S6)

for the origin site $i$. As explained in the main text, the minimization of the kinetic energy gives $q = 0$ for $J_1, J_2 > 0$ and $q = Q$ given in Eq. (2) for $J_1, J_2 < 0$. The Hamiltonian $\hat{H}_i^{GA}$ can be easily diagonalized on the Fock state basis for the local wave function, $|\Psi_i\rangle = \sum_{n=0}^{n_{\text{max}}} f_i^{(n)} |n_i\rangle$, in which the maximum one-site occupation number $n_{\text{max}}$ must be sufficiently large (we take $n_{\text{max}} = 10$). The order parameter is obtained from $\tilde{\psi} = \sum_n \sqrt{n} f_i^{(n-1)} f_i^{(n)}$ with eigenvector $f_i^{(n)}$ in a self-consistent way.

In the presence of the trap potential $V \neq 0$, the mean field $\psi_i$ can no longer be assumed to have spatially uniform amplitude. Therefore, one have to deal with Eq. (S5) on the entire lattice sites each of which is connected to the six neighboring sites through the mean fields $\{\psi_{i \pm \alpha n} \ | n = 1, 2, 3\}$. To prepare the initial state shown in Fig. 2(a), we solve the set of self-consistent equations $\psi_i = \sum_n \sqrt{n} f_i^{(n-1)} f_i^{(n)}$ for all sites within a cutoff length $l_c$ from the trap center. We take $l_c = 36a$. 

FIG. S1: Potential landscapes of triangular optical lattice without and with an additional 1D periodic potential for (a) $2V_1 = V_2 = V_3 = V'$ and $\phi' = 0$ and (b) $V_1 = V_2 = V_3 = V'$ and $\phi' = \pi/12$. The right panels for each are the cuts along $r = r(1,0)$ and $r = r(1/2, \sqrt{3}/2)$.
FIG. S2: (a) Profiles of density (solid lines) and order parameter (dashed lines) in the harmonic trap along the cut of \( y_i = a/\sqrt{3} \) at \( t = 0 \) (initial state), \( 2U_0^{-1} \), and \( 7U_0^{-1} \) when the phase imprinting is not performed at \( t = 0 \). The lines of the density profiles for the three values of \( t \) are almost overlapped. (b) The evolution of the density fluctuation \( \delta n^2 \) of the initial state with and without the phase imprinting in a short-time region of Fig. 3(a).

The TDGA equation in a trap potential

The TDGA equation is given by

\[
\frac{i}{\partial t} |\Psi_i(t)\rangle = \hat{H}_{GA}^i(\{\psi_j(t)\}) |\Psi_i(t)\rangle \quad \text{with} \quad \psi_j(t) \equiv \langle \Psi_j(t) | \hat{b}_j | \Psi_j(t) \rangle
\]

for each site \( i \). We numerically solve the equations for all sites (within \( |r_i| \leq l_c \)) in parallel. In Figs. 2(c) and 3(a), we show the time evolution of the initial state in Fig. 2(a) after the sudden changes \( U \rightarrow -U/2 \) and \( V \rightarrow -V/2 \) at \( t = 0 \) as well as the phase-imprinting \( |\Psi_i\rangle \equiv \sum_n f_i^{(n)} |n\rangle \rightarrow \sum_n e^{i n Q \cdot r_i} f_i^{(n)} |n\rangle \). In Fig. S2, as a reference for the comparison, we present the results in the case with the same settings but without the phase-imprinting operation. It can be seen in the case without the phase-imprinting that the order parameter decreases within a short time, although the density profile is kept. The density fluctuation \( \delta n^2 \) rapidly increases and then exhibits an irregular oscillation. These results indicate that the state immediately collapses due to the dynamical instability, which is attributed to the fact that the conditions for the negative-temperature ground state — the maximum kinetic, interaction, and potential energies — are not satisfied.

The CMF+S analysis with 2D DMRG solver for bosons

In the CMF+S analysis, we consider the \( N_C \)-site cluster Hamiltonian

\[
\hat{H}_C = -\sum_{i,j \in C} J_{ij} e^{i q \cdot (r_j - r_i)} \hat{b}_i \hat{b}_j + \frac{U}{2} \sum_{i \in C} \hat{n}_i (\hat{n}_i - 1) \\
-\bar{\psi} \sum_{i \in \partial C} \left( \sum_{j \notin C} J_{ij} e^{i q \cdot (r_j - r_i)} \hat{b}_i \hat{b}_j + \text{H.c.} \right)
\]

on a triangular-shaped cluster of \( N_C = 10, 15, 21 \) sites. The mean-field boundary condition on the cluster-edge sites \( \partial C \) is implemented by the third term, and the twisted frame, \( \hat{b}_i \equiv e^{i q \cdot r_i} \hat{b}_i \), is adopted. The cluster Hamiltonian (S8) is treated with 2D DMRG solver. Here we take the maximum one-site occupation \( n_{\text{max}} = 4 \), which is confirmed to be sufficient for the discussion near the \( \rho = 1 \) SF-MI (CSF-MI) transition. For large-size clusters and especially for the large Hilbert space of bosons, the exact diagonalization is practically not realistic as a solver for the cluster problem. Therefore, we employ the DMRG on the equivalent 1D chain model with long-range hoppings and mean fields (see Fig. S3). The DMRG calculation is performed in the standard way but with the mean-field terms in Eq. (S8) \[2\]. The dimension of the truncated matrix product states kept in the present DMRG calculations is typically \( \sim 10^3 \) to obtain numerically precise results. In order to solve

\[
\bar{\psi} = \frac{1}{N_C} \sum_{i \in C} \langle \hat{b}_i \rangle \hat{H}_C(\bar{\psi})
\]

(S9)
FIG. S3: The mapping of the 2D cluster problem with the mean-field boundary onto an equivalent 1D chain with long-range interactions and mean fields.

FIG. S4: Typical behavior of the provisional critical point $U^*_c/|J_2|$ as a function of the given momentum $q = (q_x, 0)$ for $J_1/J_2 = 0.7$ and $N_C = 21$.

in a self-consistent way, we iteratively perform the DMRG calculations until convergence.

Note that when we put a real number $\bar{\psi}$ as an input for $\tilde{H}_C(\bar{\psi})$ in the fixed global gauge, the output $(1/N_C) \sum_{i \in C} \langle \tilde{b}_i \rangle \tilde{H}_C(\bar{\psi})$ includes a small but finite imaginary component ($\lesssim 4\%$ for $N_C = 21$). This is due to a finite-size effect; the order with uniform amplitude $\bar{\psi}$ and spiral phase twist $\exp[i\mathbf{q} \cdot \mathbf{r}_i]$ is not fully commensurate with the shape of the finite-size clusters with the mean-field boundary. We just ignore the small imaginary component in the calculations for each $N_C$ since it decreases as $N_C$ and is expected to vanish at the limit of $N_C \to \infty$.

The optimization of the spiral twist $\mathbf{q}$ is performed in the following way: For different values of $\mathbf{q} = (q_x, 0)$, the “provisional” critical point $U^*_c/|J_2|$ (at which $\bar{\psi} = 0^+$) is numerically determined [Fig. S4]. The maximum value of $U^*_c(q_x)/|J_2|$ and $(q_x, 0)$ at which it occurs were adopted as the CMF+S prediction of the critical point $U^*_c/|J_2|$ and the BEC momentum $Q$ at the critical point, respectively. The slight variance of $Q_x$ from $4\pi/3$ at $J_1/J_2 = 1$ [see Fig. 4(c)] is thought to stem from the same finite cluster-size effect mentioned above.

The CMF+S curves in Fig. 4(a) are obtained from the size scaling of the phase boundaries for $N_C = 10, 15, 21$. Figure (S5) shows the extrapolation of the $N_C = 10, 15, 21$ data to $N_C \to \infty$ ($\lambda \to 1$) for several values of $J_1/J_2$ with a linear function of the scaling parameter $\lambda \equiv N_B/3 N_C$ [3, 4]. Here, $N_B$ is the number of NN bonds treated exactly in the cluster ($N_B = 18, 30, 45$ for $N_C = 10, 15, 21$, respectively). The error bars estimated from the variation in the linear fittings for different pairs of the $N_C = 10, 15, 21$ data are smaller than the symbol size in Fig. 4(a).

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FIG. S5: Cluster-size scalings of the SF-MI (CSF-MI) critical points for the (a) unfrustrated \( (J_1, J_2 > 0) \) and (b) frustrated \( (J_1, J_2 < 0) \) cases. The extrapolated \( (\lambda \to 1) \) values are plotted as a function of \( J_1/J_2 \) in Fig. 3(a) of the main text.