Berezinskii-Kosterlitz-Thouless transition of two-dimensional Bose gases in a synthetic magnetic field

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We study the field dependency of the Berezinskii-Kosterlitz-Thouless transition temperature $T_c(H)$ of Bose gases in a two-dimensional optical lattice in the synthetic magnetic field using the Metropolis Monte Carlo method. The system is described by the frustrated XY model and the critical temperature is determined through observing the disappearance of the central peak of the momentum distribution of the gas, which can be directly measured by the time-of-flight absorbing imaging in cold-atom experiments. $T_c(H)$ is found to exhibit a largest peak at the fraction of a flux quantum $f = \phi/\phi_0 = 1/2$ and a second-largest one at $f = 1/3$, in agreement with former studies on superconducting Josephson arrays. We also indicate that the synthetic magnetic field experiment can produce strong enough frustration for exploring the physics of the frustrated XY model.

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I. INTRODUCTION

It is well known that in two-dimensional (2D) systems with a continuous symmetry the conventional long-range order is prevented by thermal fluctuations at finite temperatures in the thermodynamic limit, and as a result no spontaneous continuous symmetry breaking takes place. However, these systems can undergo a transition through binding of vortex pairs to form a quasi-long-range order. This is the celebrated Berezinskii-Kosterlitz-Thouless (BKT) transition [1,2]. The 2D XY model is the prototype to elaborate on the BKT transition in theory. Experimentally, the BKT transition has been examined in various physical systems, including ^{4}He films [3], 2D superconductors [4] and superconducting Josephson-junction arrays (JJAs) [5,6], and observations agree well with theoretical predictions.

The study of JJAs greatly enriched the research of the BKT transition [6–9]. Experiments provided evidence that the BKT transition point T_c becomes a periodic function of the transverse magnetic field H once the field is introduced to JJAs [6]. Such a system can be described by the frustrated 2D XY model [7–9], and the physics of this model in JJAs has been the subject of intense research [10]. Theories also suggested that $T_c(H)$ is periodic in H, and one period corresponds to one flux quantum per unit cell of the array. Moreover, $T_c(H)$ exhibits complex structures at fractions of a flux quantum within a period. These abundant phenomena reflect the nontrivial energy spectrum of the model, known as the "Hofstadter butterfly" [11].

So far cold atoms have been regarded as ideal test beds for fundamental models of condensed-matter physics. It is of great interest to reexamine the BKT transition since the quasi-2D Bose gas has already been produced either in a single pancake traps or at the nodes of 1D optical lattice potentials [12]. Trombettoni *et al.* has raised a proposal to investigate the occurrence of BKT transitions in a 2D Bose-Einstein condensate [13]. In 2006, Hadzibabic *et al.* observed the BKT transition in atomic Bose gases experimentally [14]. They added the optical lattice in the z direction to construct a quasi-2D configuration, and the transition point was detected though the dislocations of interference patterns. Later new experiments identified this transition by the proliferation of vortex pairs [15] and a bimodal density distribution or coherent length [16].

The frustrated 2D XY model has been proposed in the rotating Bose-Einstein condensates with a corotating deep optical lattice by Kasamatsu [17]. However, experiments with rotating gases are usually difficult to add optical lattices and the rotating rate is limited. More recently, the technique of "synthetic" magnetic field has been developed to produce an effective "magnetic" field in cold atoms [18]. The effective Hamiltonian for a neutral atom in the synthetic field is like that of charged particles in the magnetic field. Thus, it stimulates us to investigate the behavior of BKT transition in the cold atomic Bose gases subject to the synthetic magnetic field. Comparing with former 2D experimental systems concerning on the superfluid density or sheet resistance to detect the superfluid transition, cold atoms can be manipulated more easily and precisely and thus it benefits the further investigation of the BKT transition.

In this paper, we start with the Bose-Hubbard model which describes a 2D Bose gas in a uniform magnetic field in a square optical lattice. This model can be mapped to the frustrated XY model. Then we study the BKT transition using the standard Metropolis Monte Carlo method. This method has been used by Trombettoni *et al.* to investigate the BKT transition in atomic Bose gases in a 2D optical lattice without magnetic field [13]. The transition point is determined through detecting the central peak of the expansion condensates after time-of-flight (TOF) expansion.

II. THE MODEL

We consider a 2D Bose gas on a square optical lattice immersed in the synthetic magnetic field. The Hamiltonian is described by the frustrated Bose-Hubbard model [19],

$$\hat{H} = -K\sum_{\langle i,j\rangle}(\hat{\psi}_i^\dagger\hat{\psi}_j e^{iA_{ij}} + \text{H.c.}) + \frac{U}{2}\hat{N}_i(\hat{N}_i - 1), \quad (1)$$

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where the first term on the right side denotes the hopping energy and the summation is taken over all the nearest neighbors with K the hopping matrix element. $\hat{\psi}_i$ ($\hat{\psi}_i^\dagger$) is the field operator of bosons which annihilates (creates) a boson at site i. A_{ij} is the bond angle which can be calculated from the gauge potential of the synthetic magnetic field $\mathbf{A}(\mathbf{r})$, $A_{ij} = \frac{2\pi}{\phi_0}\int_i^j \mathbf{A}(\mathbf{r})d\mathbf{r}$, with ϕ_0 representing the flux quantum. So the number of fluxes through each plaquette is given by

$$f = \frac{1}{2\pi}(A_{ab} + A_{bc} + A_{cd} + A_{de}). \tag{2}$$

Apparently, f is proportional to the magnetic field H, $f = Ha^2/\phi_0$. a is the lattice constant and it is chosen to be unit hereinafter, $a = 1$. The second term of Eq. (1) refers to the on-site interaction with U being the interacting strength, and $\hat{N}_i$ is the particle number operator on site i.

Using the same procedure for reducing the Bose-Hubbard model to the quantum phase model [13], the frustrated Bose-Hubbard model in Eq. (1) can be mapped into the "frustrated" quantum phase model,

$$\hat{H} = \hat{H}_{FXY} - \frac{U}{2}\sum_j \frac{\partial^2}{\partial\theta_j^2}, \tag{3}$$

where H_{FXY} denotes the frustrated XY model,

$$\hat{H}_{FXY} = -J\sum_{\langle i,j\rangle}\cos(\theta_i - \theta_j - A_{ij}), \tag{4}$$

with $J = 2KN_0$. To fulfill this procedure, one can simply replace the field operator by the c-number wave function, $\hat{\psi}_i \to \psi_i = \sqrt{N_0}e^{i\theta_i}$, where N_0 is the average particle number of each site and θ_i is the corresponding phase on site i. This is reasonable since the system under consideration is a uniform system at sufficient low temperatures and thus it is in a quasicoherent state. The frustrated XY model was used to describe the superconducting Josephson arrays in transverse magnetic field by Teitel and Jayaprakash [7]. It can describe the thermodynamic behavior of the BECs stored in an optical lattice when $J \gg U$ and at temperatures $T \gg U/k_B$. On the other hand, since the mechanism of BKT transition, that is, the pairing of vortices, is due to topological long-range correlation, we can safely ignore the on-site interaction term at sufficient low temperatures.

We choose the Landau gauge for the synthetic magnetic field, which reads

$$\mathbf{A}(\mathbf{r}) = (0,\phi_0 f x); \tag{5}$$

therefore, $A_{ij} = 0$ for $i_x = j_x \pm 1, i_y = j_y$ and $A_{ij} = \mp 2\pi f x$ for $i_x = j_x, i_y = j_y \pm 1$. Obviously, the Hamiltonian in Eq. (4) is periodic in f with the period 1, so we just need to study the properties of the system in the interval $f \in [0,1]$. Here $f = 0$ corresponds to the unfrustrated case and $f = 1/2$ is the fully frustration condition.

To proceed, we investigate the BKT transition of the frustrated XY model in the context of cold atoms. After the system undergos the BKT transition at low temperatures, a peak appears in the center ($\mathbf{k} = 0$) of the lattice Fourier transform of ψ_j,

$$\tilde{\psi}_{\mathbf{k}} = \frac{1}{N_s}\sum_j \psi_j e^{-i\mathbf{k}\cdot\mathbf{r}_j}, \tag{6}$$

where N_s is the number of sites of the square lattice. The central peak in the momentum space describes the "quasicondensate" and it is analogous to the magnetization for a spin XY model; that is,

$$M = \langle|\tilde{\psi}_0|\rangle. \tag{7}$$

The ferromagnetic state of spin systems has the maximum magnetization with all spins pointing in the same direction. This corresponds to a global coherent phase of the Bose gas, which implies the true condensation (Bose-Einstein condensation) of the gas. However, the BKT superfluid state here is just the quasicondensed state with nonglobal coherent phases (the vortex pairs of coherent phases), which is the reason for the emergence of the central peak of momentum space [13].

In cold-atom experiments, the momentum distribution can be observed by the sudden release of the optical lattice. The absorption imaging is then taken after a TOF period t. The density profile of the image can be written as [12]

$$n(\mathbf{r}) = (M/\hbar t)^3|\tilde{\omega}(\mathbf{k})|^2 G(\mathbf{k}). \tag{8}$$

Here momentum $\mathbf{k}$ is related to position $\mathbf{r}$ by $\mathbf{k} = M\mathbf{r}/\hbar t$ under the assumption of ballistic expansion. $\tilde{\omega}(\mathbf{k})$ is the Fourier transform of the Wannier function and $G(\mathbf{k})$ is the Fourier transform of the single-particle density matrix defined by

$$G(\mathbf{k}) = \frac{1}{N_s}\sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)}\langle\hat{\psi}_i^\dagger\hat{\psi}_j\rangle. \tag{9}$$

For the quasicondensate state at low temperatures, there is a small condensate on each site of the optical lattice; thus, we can have $\langle\hat{\psi}_i^\dagger\hat{\psi}_j\rangle \approx \psi_i^*\psi_j$. Then the momentum space density matrix $G(\mathbf{k})$ can be written as

$$\begin{aligned} G(\mathbf{k}) &\approx \frac{1}{N_s}\sum_{i,j} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)}\psi_i^*\psi_j \\ &= N_s|\tilde{\psi}_{\mathbf{k}}|^2. \end{aligned} \tag{10}$$

$G(\mathbf{k})$ is closely related to momentum distribution, which can be observed experimentally using the TOF imaging. The disappearance of central peak in $G(\mathbf{k})$ ($\mathbf{k} = 0$) can be regarded as a criterion of the occurrence of BKT transition. Next, our Monte Carlo simulation will focus on the density profile of the density matrix and we will investigate the transition behavior under different frustration f, which is hopefully realized in cold-atom experiments.

Here we note that the frustrated XY model is U(1) gauge symmetry breaking in the superfluid state as the hopping term breaks the conservation of "charge." It means that physical quantities of a system described by the frustrated XY model can be gauge dependent, although observable quantities are usually gauge invariant in conventional systems. That is why the vector gauge potentials can be detected in the momentum distribution of the density matrix. Furthermore, the imaging of density of the expanding condensates in cold-atom experiments in fact measures the canonical momentum of the original model [19].

III. RESULTS AND DISCUSSIONS

We now employ the standard Metropolis Monte Carlo method with periodical boundary conditions to simulate the frustrated XY model. It has been used to investigate the BKT transition in Josephson arrays by Teitel and Jayaprakash [7]. This method is proved to always get believable results. The lattice sites are chosen as $L \times L = 40 \times 40$. For each temperature and frustration of the system we use 10^7 Monte Carlo steps.

Figure 1 illustrates the evolution of expansion image from the phase-coherent ground state to the noncoherent state. At sufficiently low temperatures the system is in a superfluid state and the density profile reveals regular sharp peaks at the momentum space lattices. That is due to the pairing of vortices. As the temperature increases the peaks begin to decay and at the transition point at about $Tc \approx 0.5J/k_B$ the sharp peaks go to zero [see Fig. 2(a) for the absolute value]. That is the signature of the BKT transition of 2D Bose gases. We can see that above the critical temperature there is disorder in the density profile of the momentum space and the system loses its coherent phase.

Figure 2 shows the central peak G_0 $[G(k_x = 0, k_y = 0)/N_s]$ of the expansion image as a function of temperature T for four different fractional frustration $f = 1/2$, $2/5$, $1/3$, $1/5$, and the expansion image close to the ground state is illustrated in the insert. At $T = 0$ the peaks have maximal values where the system is in a superfluid state with paired vortices and nonzero M. As the temperature is rising, the peaks are reduced and the vortices begin to unpair. The central peak drops to zero at the critical point, as guided by the circle in the figure. For the fully frustrated case in Fig. 2(a), we can see the curve reveals different tendency as in Fig. 2(b) and Fig. 2(c) away from the transition temperature. The change of the bending direction approaching the transition point in the latter case comes from the relation: $M(T \to T^*) \sim (T - T_c)^{0.23}$ [20], where $M \propto \sqrt{G(0)}$ is the magnetization and T^* is a temperature near T_c where the power-law behavior holds best. The expansion images in Fig. 2(b) and Fig. 2(c) are the same as the unfrustrated system. We note that the ground state of the system is degenerate, while this cannot be directly revealed from the expansion image. However, we expect that it can be recognized using printing phase technology [19].

The critical temperatures T_c at different fractional frustration f are demonstrated in Fig. 3. There exist some peaks at some fractional magnetic fields. The largest peak is the fully frustrated case with $f = 1/2$, while the second largest is at $f = 1/3$. These results agree with former experimental and theoretical work on superconducting Josephson arrays [7]. We note that the structure of the diagram depends on the geometry of the lattice. For example, the second peak of the transition temperature for the triangular-lattice systems is at $f = 1/4$ instead [8,9].

Finally, we discuss the experimental realization of the system. The experiment on ^{87}Rb gas by Lin *et al.* produces a position-dependent vector potential with the slope $k_q = \partial(qA_y/\hbar k_L)/\partial(\hbar\delta/E_L) \approx 0.4$ in the interval $\hbar\delta/E_L \in [-5,5]$ for Raman coupling strength $\hbar\Omega_R = 8.20E_L$ [18]. Here $\hbar k_L = h/(\sqrt{2}\lambda)$ and $E_L = \hbar^2 k_L^2/2m$ are the units of momentum and energy, respectively, with $\lambda = 801.7$ nm being the wavelength of the Raman beams and m the mass of a single ^{87}Rb atom. Thus, an approximately uniform synthetic field is generated, $H = \partial A_y/\partial x = \delta' \partial A_y/\partial\delta$, where δ is the Raman detuning and δ' the gradient of it. To add an optical lattice with lattice constant a to the system, the Raman detuning gradient can then be expressed as a function of the frustration f,

$$\frac{\delta'}{2\pi} = \frac{E_L f}{\hbar k_L k_q a^2}. \tag{11}$$

Then we can get the Raman detuning gradient $\delta'/2\pi \approx 5.07 f/a^2$ kHz μm. If the lattice constant is chosen to be $a = 0.5$, 2.0, or 4.0 μm, the corresponding values of Raman detuning gradient for frustrations $f = 1/3, 1/2, 1$ are $\delta'/2\pi \approx$ 6.8, 10, 20 kHz μm^{-1}; 0.42, 0.63, 1.3 kHz μm^{-1}; or 0.11, 0.16, 0.32kHz μm^{-1}, respectively. The experiment by Lin *et al.* can generate a detuning gradient up to 0.40 kHz μm^{-1}; therefore, the lattice constant $a \sim 4$ μm is most appropriate for generating strong-enough frustration. For smaller a, it is necessary to increase the Raman detuning gradient.

Then we estimate the magnitude of the transition temperature $T_c \sim J/k_B = 2KN_0/k_B$. According to the variational estimate [13], the hopping matrix element K is relevant to the depth of the potential at each cite, V_0, which reads

$$K = e^{-\frac{\pi^2\sqrt{s}}{4}} \left[\pi^2 s \left(\frac{1}{4} - \frac{1}{\pi^2\sqrt{s}} \right) - s \right] E_r, \tag{12}$$

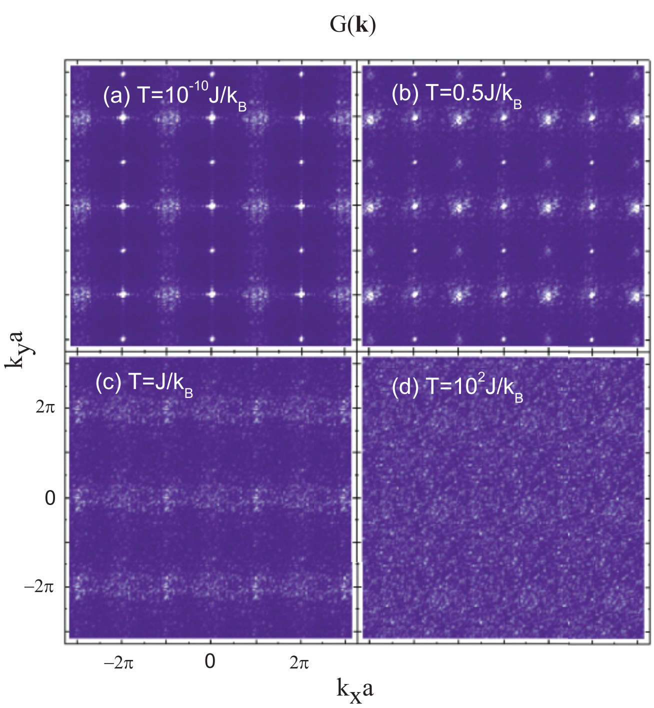

FIG. 1. (Color online) Illustration of the expansion image of the system at different temperatures T for the fully frustrated case ($f = 1/2$). The lattice constant is chosen to be $a = 1$. The BKT transition takes place at about $T = 0.5J/k_B$, where the peaks decay to nearly zero in (b). The color represents the relative magnitude of the density which increases from purple to white.

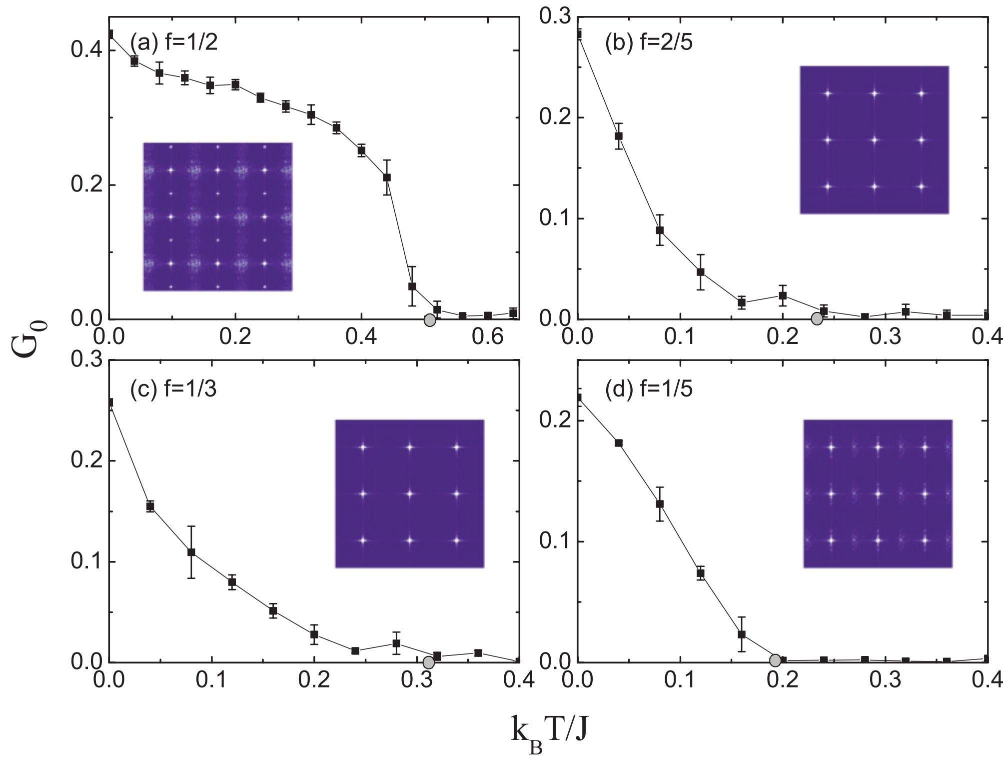

FIG. 2. (Color online) The central peak G_0 $[G(k_x = 0, k_y = 0)/N_s]$ of expansion image as a function of temperature T for four different fractional frustrations f =1/2, 2/5, 1/3, 1/5. The square points are numerical results with the error bar obtained using the standard deviation. The circle in each figure guides the estimated critical transition temperature. The insert shows the corresponding expansion image close to the ground state.

where $s = V_0/E_r$ and $E_r = \hbar^2\pi^2/2ma^2$ is the recoil energy. If we choose $s = 18$ and $N_0 = 170$, as suggested in Ref. [13], we have $K/E_r \approx 0.0006$ and then $J = 2KN_0 \approx 3.2 \times 10^{-24}$, 2.0×10^{-25}, and 5.0×10^{-26} erg for $a = 0.5, 2.0,$ and $4.0\ \mu$m, respectively, and the critical temperatures are $T_c \sim 23, 1.5,$ and 0.4 nK, correspondingly. The critical temperatures are quite low and hard to attain. However, one can obtain higher critical temperatures by increasing the average particle number at each site N_0 or reducing depth of the lattice potential in the real experiment at a given lattice constant.

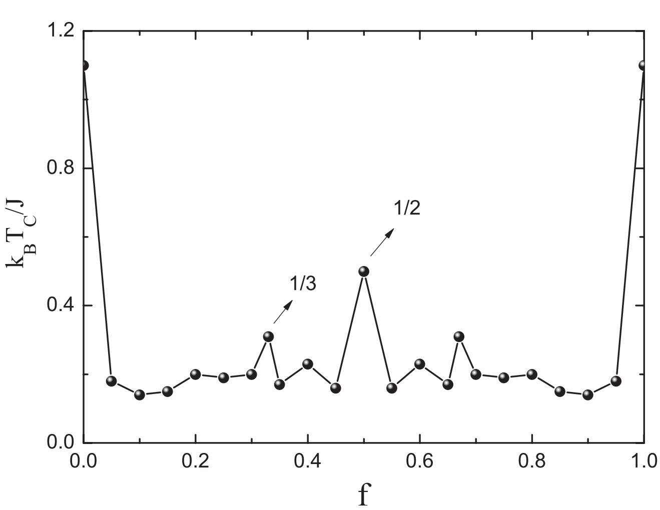

FIG. 3. Transition temperature T_c of 2D BKT transition for different fractional frustration f. The critical point corresponds to the absence of the central as illustrated in Fig. 2. There is a peak for the fully frustrated case ($f = 1/2$) and a second peak at $f = 1/3$.

IV. CONCLUSIONS

In conclusion, we have studied the BKT transition of 2D Bose gases in the synthetic magnetic field using the standard Metropolis Monte Carlo method. The critical transition temperature is decided by the absence of the central peak of the density matrix in momentum space, which can be detected in cold atoms by TOF expansion imaging. We have obtained the transition temperature as a function of the field which is represented by the fraction of a flux quantum per plaquette f. We have observed the largest peak of the temperature in the fully frustrated case, $f = 1/2$, and the second-largest one at $f = 1/3$. These results agree with former studies on superconducting Josephson arrays. We have also estimated that the frustrations $f = 1/3, 1/2,$ and 1 are attainable in the present synthetic magnetic field experiment.

Note added. Recently, two preprints appeared on the arXiv.org. One preprint by Y. Nakano, K. Kasamatsu, and T. Matsui studied the finite-temperature phase structures of hard-core bosons in a 2D optical lattice subject to effective magnetic field based on the extensive Monte Carlo simulations [21]. The ground-state energy per site as a function of the field is studied. The second preprint by Allard *et al.*

reported experimentally study the disorder effect on trapped quasi-2D ^{87}Rb clouds in the vicinity of the BKT transition through measurements of momentum distributions [22]. This implies that our proposal of investigating the BKT transition of cold atoms in synthetic magnetic field is realizable in experiments.

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