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

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We study the Berezinskii-Kosterlitz-Thouless transition of two-dimensional Bose gases in a synthetic magnetic field using the standard Metropolis Monte Carlo method. The system is described by the frustrated XY model and the critical temperature is calculated through the absence of central peak of the wave function in momentum space, which can be directly measured by the time-of-flight absorbing imaging in cold atoms experiments. The results of our work show agreement with former studies on superconducting Josephson arrays.

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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 temperature 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 \[1,2\]. Theoretically, the 2D XY model is the prototype to elaborate on the BKT transition. Experimentally, the BKT transition has been examined in various physical systems, including \[^{4}\text{He}\text{ films}[3,4,5]\], 2D superconductors \[4\] and superconducting Josephson-junction arrays (JJA) \[5\], and experimental works agree well with theoretical predictions.

The study of Josephson-junction arrays greatly enriched the research of the BKT transition \[5,6\]. Once a transverse magnetic field is introduced to JJA, the BKT transition point as a function of the field can be investigated \[3,4\]. Theoretically, such a system can be described by the frustrated 2D XY model \[7,8\]. Nevertheless, these systems reveal a complex energy spectrum, known as the “Hofstadter butterfly” \[10\], which gives rise to rich phenomena that are still of present research interest.

So far, cold atoms have been regarded as ideal test beds for fundamental models of condensed matter physics. It is of great interest to examine the BKT transition since cold atoms can be manipulated more easier and precisely and thus it benefits for further investigations.

II. THE MODEL

Consider a 2D Bose gas immersed into a uniform magnetic field in a square optical lattice. This model can be mapped to the frustrated XY model and the critical temperature is calculated through the absence of central peak of the expansion condensate after time-of-flight (TOF) expansion.

\[
\hat{H} = -K \sum_{\langle i,j \rangle} \left( \hat{\psi}_i^\dagger \hat{\psi}_je^{iA_{ij}} + h.c. \right) + \frac{U}{2} \hat{N}_i \left( \hat{N}_i - 1 \right),
\]

where the first term on the right side is the hopping energy with the summation over the nearest neighbor sites and \(K\) is the hopping matrix element. \(\hat{\psi}_i(\hat{\psi}_i^\dagger)\) is the field operator of bosons for annihilate(create) a boson at site.
i. $A_{ij}$ is a bond operator describing the magnetic field and around every plaquette we have:

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

Here $f = 2\phi_0/H_0a^2 = \frac{\phi_0}{\phi_0}$ is the uniform frustration with $\phi_0 = \hbar c/2e$ the flux quantum and we have chosen unit lattice constant $a = 1$. The second term of Eq. (1) refers to the on-site repulsive(attractive) interaction, according to the interacting strength $U > 0$($U < 0$), and $\hat{N}_i$ is the particle number operator on site $i$.

The system under consideration is a uniform system at sufficient low temperature, such that the system is density coherent with fluctuating phases. The field operator of bosons can be written as $\psi_i = \sqrt{N_0}e^{i\theta_i}$, where $N_0$ is the average particle number of each site and $\theta_i$ is the corresponding phase on site $i$. The mechanism of BKT transition, the pairing of vortices, is due to topological long-range correlation, thus we can safely ignore the on-site interaction term at sufficient low temperature. Upon these, the Eq. (1) can be mapped to the frustrated XY model:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \cos (\theta_i - \theta_j + A_{ij}).$$  \hspace{1cm} (3)

Here $J = 2KN_0$. This model was first used by Titel et al. to describe the superconducting Josephson arrays in transverse magnetic field [3].

We note here 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 is to say that in a conventional system described by the frustrated XY model physical quantities can be gauge dependent, however, all observable quantities should be gauge invariant. However this is not the case in the cold atoms experiment that the observable physical quantities, e.g., the momentum distribution of the wave function are gauge dependent. There is no paradox and on the other hand they are compatible in the case that the imaging of density of the expanding condensates in cold atoms experiment are in fact the canonical momentum of the original model [12]. This just reflects nothing but the exitance of vector gauge potential.

In the case of synthetic magnetic field we choose the Landau gauge, which is:

$$A = (0, 2\pi fx).$$  \hspace{1cm} (4)

Obviously the hamiltonian in Eq. (3) is periodic in $f$ with the period 1, thus we only need to study the properties of the system in the interval $f \in [0, 1]$. Here $f = 0$ corresponds to the unfrustrated case and $f = \frac{1}{2}$ is the fully frustrated condition.

The wave function of the system in the lattice space $\psi_i$ can be calculated using the Monte Carlo method. At low temperature the system undergo a superfluid transition and there will be a peak in the central of the wave function in the momentum space, which is fourier transformed as:

$$\tilde{\psi}_k = \frac{1}{N_s} \sum_j \psi_j e^{-ik\cdot r_j},$$  \hspace{1cm} (5)

where $N_s$ is the number of sites of the square lattice. The central peak of the momentum space describes the coherence of the phase of the condensates. It is analogous to the magnetization of a spin system, i.e.,

$$M = \langle \psi_0 \rangle.$$  \hspace{1cm} (6)

In cold atoms experiments, the observation of momentum distribution can be detected by the sudden release of the optical lattice. The absorption imaging is taken after a TOF period $t$. The density profile of the image can be written as [11]:

$$n(x) = (M/\hbar t)^3|\tilde{\psi}(k)|^2 G(k).$$  \hspace{1cm} (7)

Here momentum $k$ is related to position $x$ by $k = Mx/\hbar t$ under the assumption of ballistic expansion. $\tilde{\psi}(k)$ is the Fourier transform of the Wannier function and $G(k)$ is the momentum space density matrix and is defined by:

$$G(k) = \frac{1}{N_s} \sum_{i,j} e^{ik(r_i - r_j)} \langle \psi_i^\dagger \tilde{\psi}_j \rangle.$$  \hspace{1cm} (8)

For density coherent states at low temperature, the system forms a quasi-condensate where on each site of the lattice there is a small condensate and we can have $\langle \psi_i^\dagger \psi_j \rangle \approx \psi_i^\dagger \psi_j$. Thus the momentum space density matrix $G(k)$ can be written as:

$$G(k) \approx \frac{1}{N_s} \sum_{i,j} e^{ik(r_i - r_j)} \psi_i^\dagger \psi_j = N_s \cdot |\tilde{\psi}_k|^2.$$  \hspace{1cm} (9)

In this case, the momentum space wave function is related to the density matrix and then can be observed experimentally using the TOF imaging. In the following we will do the Monte Carlo simulation and investigate the transition behavior under different frustration $f$, which can be directed realized in cold atoms experiments.

III. RESULTS AND DISCUSSIONS

We now use 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 Titel. 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.

Fig. [H] illustrates the evolution of expansion image from phase coherent ground state to the non-coherent state.
At sufficient low temperature 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 increasing the peaks begin to decay and at the transition point at about $T_c \approx 0.5J/k_B$ the sharp peaks go to zero. That’s the signature of BKT transition of 2D Bose gases. We can see that above the critical temperature there is disordered in the density profile of the momentum space and the system loses its coherent phase.

In Fig. 2 we show the central peak $G_0(G(k_x = 0, k_y = 0))$ of expansion image as a function of temperature $T$ for four different fractional frustration $f$. 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 growing, the peaks are reduced and the vortices begin to unpair. The central peak drops to zero at the critical point and the transition temperature is guided by the circle. The inserts illustrate the ground state image for different frustration. For the fully frustrated case in Fig. 2a we can see the curve reveals different tendency as in Fig. 2b and Fig. 2c. The expansion images in the latter case are the same as the non-frustration system. We note that ground state has $1/f$ degenerate states while this can not be directly revealed from the expansion image. However, they can be recognized using printing phase technology [17].

We show the critical temperature $T_c$ at different fractional frustration $f$ in Fig. 3. It reveals a unanalytical behavior of the transition temperature. We can see that there are peaks in some fractional magnetic field. The largest peak is the fully frustrated case in $f = \frac{1}{2}$ while the second largest is in $f = \frac{1}{4}$, which agrees 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 a triangular structure the experimental and theoretical works reveal a second peak for the transition temperature in $f = \frac{1}{4}$ instead [8, 9].

FIG. 2: The central peak $G_0(G(k_x = 0, k_y = 0))$ of expansion image as a function of temperature $T$ for four different fractional frustration $f$. The insert is the corresponding image close to the ground state. The square points are the numerical results with the error bar the standard deviation and the circle in each figure guides the critical transition temperature.

FIG. 3: Transition temperature $T_c$ of 2D BKT transition for different fractional frustration $f$. The critical point is corresponding to the absence of the central as illustrated in Fig. 2.
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 central peak of the density matrix in momentum space, which can be detected in cold atoms by TOF expansion imaging. We have got the overall phase diagram of BKT transition for different fractional frustration. The obtained results agree with former experimental and theoretical work on superconducting Josephson arrays [7]. Our results suggest that cold atoms can be used as an ideal system to explore the physics of the frustrated 2D systems.

Note added: After this paper was almost finished, a preprint by Y. Nakano, K. Kasamatsu, and T. Matsui appeared on the arXiv.org [18]. These authors have studied the finite-temperature phase structures of hard-core bosons in a two-dimensional optical lattice subject to an effective magnetic field based on the extensive Monte Carlo simulations.

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[1] V. L. Berezinskii, Sov. Phys. JETP 34, 610 (1972);
[2] J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973);
[3] D. J. Bishop and J. D. Reppy, Phys. Rev. Lett. 40, 1727 (1978);
[4] M. R. Beasley, J. E. Mooij, and T. P. Orlando, Phys. Rev. Lett. 42, 1165 (1979).
[5] D. J. Resnick, J. C. Garland, J. T. Boyd, S. Shoemaker, and R. S. Newrock, Phys. Rev. Lett. 47, 1542 (1981).
[6] R. F. Voss, and R. W. Webb, Phys. Rev. B 25, 3446 (1982).
[7] S. Teitel and C. Jayaprakash, Phys. Rev. B 27, 598 (1983); S. Teitel and C. Jayaprakash, Phys. Rev. Lett. 51, 1999 (1983).
[8] W. Y. Shih and D. Stroud, Phys. Rev. B 28, 6575 (1983).
[9] R. K. Brown and J. C. Garland, Phys. Rev. B 33, 7827 (1986).
[10] D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976).
[11] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[12] A. Trombettoni, A. Smerzi, and P. Sodano, New J. Phys. 7, 57 (2005).
[13] Z. Hadzibabic, P. Krüger, M. Cheneau, B. Battelier, and J. Dalibard, Nature 441, 1118 (2006).
[14] V. Schweikhard, S. Tung, and E. A. Cornell, Phys. Rev. Lett. 99, 030401 (2007).
[15] P. Cladé, C. Ryu, A. Ramanathan, K. Helmerson, and W. D. Philips, Phys. Rev. Lett. 102, 170401 (2009).
[16] Y. J. Lin, R. L. Compton, K. Jiménez-García, J. V. Porto, and I. B. Spielman, Nature 462, 628 (2009).
[17] G. Möller and N. R. Cooper, Phys. Rev. A 82, 063625 (2010).
[18] Y. Nakano, K. Kasamatsu, and T. Matsui, arXiv: 1112.0145 (2011).