Phase transitions in coupled two dimensional XY systems with spatial anisotropy

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We study phase transitions of coupled two dimensional XY systems with spatial anisotropy and \textit{U}(1) $\times \mathbb{Z}_2$ symmetry, motivated by spinless bosonic atoms trapped in square optical lattice on the metastable first excited \textit{p}--level orbitals with anisotropic hopping amplitudes. The phase transitions of the system are generally split into an Ising transition and an XY transition, but the sequence and the nature of the transitions depend on the ratio between the anisotropic couplings. In the isotropic limit the XY variables are expected to be disordered before the Ising variables when thermal or quantum fluctuations are turned on gradually. In the anisotropic limit with zero perpendicular hoppings, the finite temperature phase transition is a Kosterlitz-Thouless transition driven by proliferation of hybrid half vortices, and the zero temperature quantum phase transition is split into a bond order transition and a 3D XY transition, which can be driven by the condensation of either single vortices or half vortices. After the condensation of half vortices the resultant state is a Mott Insulator of paired bosons. A small perpendicular hopping $J_b$ leads to a 2D Ising transition at low temperature and a 2+1d quantum Ising transition with a small charging energy at zero temperature. Global phase diagrams for both classical and quantum phase transitions are drawn. The analytical results obtained in this work are expected to be checked both numerically and experimentally.

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Ever since the observation of the quantum phase transition between the Mott Insulator and the superfluid,\textsuperscript{1} the atomic systems trapped in optical lattices formed by laser beams have attracted a lot of attention. The potential formed by laser beams can usually be approximated by the harmonic potential. The single particle potential formed by laser beams can usually be approximated by the harmonic potential. The single particle ground state wavefunction within each well of the optical lattice has an approximate $s$--wave symmetry. The first excited states are three fold degenerate $p$--wave states. As discussed in reference\textsuperscript{2} and confirmed by recent experiments,\textsuperscript{3} although the $p$--wave states are not the ground states, the life time for these states can be much longer than the average tunnelling time between neighboring optical lattice sites. If all of the atoms are pumped from the ground state to the $p$--wave states, they will establish a metastable equilibrium which can survive for considerable time. In previous studies, various phases have been identified for this system, including a superfluid phase with one dimensional $\mathbb{Z}_2$ gauge symmetry\textsuperscript{4} on square and cubic optical lattices, a novel stripe phase on triangular lattice\textsuperscript{5}, a bond algebraic liquid phase\textsuperscript{6} and a crystalline orbital order on honeycomb lattice\textsuperscript{7}. Condensate of $p$--wave paired atoms has also been considered\textsuperscript{8},\textsuperscript{9}. Very recently, the long-life $p$--wave excited states have been realized experimentally, and the superfluid-like coherence between these $p$--band atoms has been successfully observed\textsuperscript{10}.

Orbital degeneracy also exists in materials. It is well-known that in transition metal oxides the $d$--level orbitals are usually partially filled, thus orbital dynamics plays an important role (for a recent review, see reference\textsuperscript{11}). It has been proposed that the quantum fluctuation of orbital occupancy can lead to many interesting physics like “orbital liquids”\textsuperscript{12}. However, in crystalline materials the quantum fluctuation which tends to disorder the orbital occupancy always competes with the Jahn-Teller effect which distorts the lattice and favors orbital ordered state (especially in the $e_g$ level), therefore quantum fluctuation is only substantially strong in certain materials with $t_{2g}$ level degeneracy (for instance, LaTiO$_3$\textsuperscript{13}). In optical lattices formed by laser beams there is no Jahn-Teller effect, thus it is expected that new and interesting physics driven by quantum fluctuations can emerge naturally in cold atom systems on high orbital levels in optical lattices.

The wave function of $p_x$ state $\phi_x(r) \sim x \exp(-ar^2)$ extends further in the $x$ than in the $y$ and $z$ directions, and so will preferentially hop to adjacent wells along the $x$--axis. Also, $p_y$ and $p_z$ particles tend to hop in $y$ and $z$ directions respectively. If the cubic symmetry of the lattice is broken down to the planar square symmetry (for instance the amplitude of laser beams propagating in the $z$ direction is stronger than those in the $x$ and $y$ directions), the first excited $p$--band state is two fold degenerate, with only $p_x$ and $p_y$ levels. Also, two $p_z$ particles can interact and convert to two $p_y$ particles, although single particle conversion is forbidden by the reflection symmetry of the square lattice. Thus the Hubbard type Hamiltonian describing the system can be written as

$$H = \sum_i t_{ab} b_{i,1}^\dagger b_{i,1,\bar{x}+\bar{z}} - t_{ab} b_{i,1,\bar{y}} b_{i,1,\bar{y}} + H.c.$$  

$$t_{a} b_{i,2}^\dagger b_{i,2,\bar{x}+\bar{y}} - t_{ab} b_{i,2,\bar{z}+\bar{x}} + H.c.$$  

$$+ g b_{i,1}^\dagger b_{i,2}^\dagger b_{i,1} b_{i,2} + H.c. + \cdots.$$  

Here $b_{i,1}$ and $b_{i,2}$ are annihilation operators for $p_x$ and $p_y$ atoms on site $i$ respectively. The ellipses above include the density-density repulsive interactions generated from $s$--wave scattering between atoms. In this Hamiltonian $t_{a} > t_{b} > 0$. If the boson operators are replaced...
by rotor operators through $b_{x,i} \sim (-1)^{i+x} \exp(-i\theta_x)$ and $b_{y,i} \sim (-1)^{i+y} \exp(-i\theta_y)$, the Hamiltonian becomes the coupled anisotropic XY model

$$H_c = \sum_i -J_0 \cos(\nabla_x \theta_{i,1}) - J_1 \cos(\nabla_y \theta_{i,1}) - J_0 \cos(\nabla_x \theta_{i,2}) - J_1 \cos(\nabla_y \theta_{i,2}) + \gamma \cos(2\theta_{i,1} - 2\theta_{i,2}).$$

In the above Hamiltonian $J_0 \sim t_x$ and $J_0 \sim t_y$ are generally unequal. Besides the classical model, we will also study the quantum version of this model by turning on the onsite repulsion energy between boson numbers $n_{i,\alpha}$, which is the canonical conjugate variable of $\theta_{i,\alpha}$:

$$H_q = H_c + \sum_{i,\alpha} u(n_{i,\alpha} - \bar{n})^2,$$

$\alpha = 1, 2$ denotes two orbital flavors, and $\bar{n}$ is the average filling of each orbital flavor on each site.

The pair conversion term in (1) breaks the particle conservation in each orbital flavor of bosons. If all the coefficients in (2) are finite, the symmetry of equation (2) is $U(1) \times \mathbb{Z}_2$. A $\mathbb{Z}_2$ variable $\sigma$ can be defined as $\theta_2 = \theta_1 + \pi\sigma/2$. The $U(1)$ phase of the system is $\chi = \theta_1 + \theta_2$. The ground state of Hamiltonian (2) is a superfluid with both $U(1)$ and $\mathbb{Z}_2$ symmetry broken. In the rest of the paper we are going to study the classical phase transitions between the superfluid and disordered phase at finite temperature, as well as the quantum phase transition between the superfluid and the Mott Insulator by tuning the repulsive charging energy $u$.

I. FINITE TEMPERATURE PHASE TRANSITIONS

A. isotropic limit: $J_0 = J_0$

In this section we study the finite temperature transition in model (2). In the isotropic limit with $J_0 = J_0$, the system becomes the isotropic coupled XY model.

$$H = \sum_{i,n,\rho} -J \cos(\nabla_n \theta_{i,\rho}) + \gamma \cos(2\theta_{i,1} - 2\theta_{i,2}).$$

In the absence of the pair conversion term $\gamma$, at low and finite temperature, the system has algebraic order of both $\exp(i\theta_1)$ and $\exp(i\theta_2)$, i.e. the correlation function $\langle \exp(i\theta_{1,x}) \rangle_{(x)} \exp(-i\theta_{2,y})$ falls off as a power law with distance. The coupling between the two XY variables are always relevant in the whole algebraic phase, which implies that no matter how weak $\gamma$ is, at large scale $\gamma$ is always renormalized strong, and at long enough length scale one can replace $\theta_2 = \theta_1 + \pi\sigma/2$, with $\sigma = \pm 1$. At this length scale, the effective Hamiltonian describing the coupled $U(1)$ and $\mathbb{Z}_2$ variables is

$$H_{eff} = \sum_{<i,j>} -J(1 + \sigma_i \sigma_j) \cos(\theta_i - \theta_j).$$

Now $\theta = \theta_1$, and $i$ and $j$ are positions of blocks after rescaling the lattice constant.

Many physical systems can be described by models (1) and (3). For instance, the $J_1 - J_2$ antiferromagnetic XY model on the square lattice with nearest neighbor interaction $J_1$ and next nearest neighbor interaction $J_2$ breaks up into two square sublattices in its ground states, each is ordered antiferromagnetically as long as $2J_2 > J_1$. Effective interaction generated by the second order spin wave perturbation theory favors parallel aligning between spins on the two sublattices, which breaks the $U(1) \times U(1)$ symmetry of the classical ground states down to $U(1) \times \mathbb{Z}_2$ symmetry. Another example is the fully frustrated XY spin model on square (or triangular) lattice. The classical ground states of the system break both the spin $U(1)$ symmetry and the $\mathbb{Z}_2$ symmetry of the chirality related to the rotation of spins around each unit square. An interesting fully frustrated model with $J_1 - J_2$ interactions was also studied.

Because in the superfluid phase both $U(1)$ and $\mathbb{Z}_2$ symmetry are broken while in the high temperature disordered phase both symmetries are restored, it is conceivable that at finite temperature there are an Ising transition with respect to $\sigma$ and a Kosterlitz-Thouless transition for $\theta$ driven by the proliferation of the vortices of $\theta$. A vortex of $\theta$ is also a hybrid vortex of $\theta_1$ and $\theta_2$. A lot of efforts have been devoted to study the sequence of the two transitions. Although it is still premature to make a conclusion, the most recent large size Monte-Carlo simulation suggests that there are two transitions at finite temperature, the Kosterlitz-Thouless transition is followed by an Ising transition at slightly higher temperature, with $\Delta T_c/T_c \sim 0.02$. Also, a theoretical argument based on the fact that the cluster percolation transition and the Ising transition coincide in the two dimensional classical Ising model indicates that the Ising transition should always occur at higher temperature than the Kosterlitz-Thouless transition. It is noticed that in Hamiltonian (6) the XY coupling across an Ising domain wall is zero, thus the algebraic order of $\exp(i\theta)$ can only exist in an infinite Ising domain. Because the density of infinite Ising domain vanishes to zero at the Ising critical point, the Kosterlitz-Thouless transition can only occur in the Ising ordered phase. Thus at the isotropic limit the Ising transition probably occurs at higher temperature than the XY transition.

B. anisotropic limit: $J_0 = 0$

In the anisotropic limit with $J_0 = 0$, the ground state is superfluid order in both $\theta_1$ and $\theta_2$ with a subextensive $\mathbb{Z}_2$ degeneracy: one can perform transformation $\theta_1 \rightarrow \theta_1 + \pi$ ($\theta_2 \rightarrow \theta_2 + \pi$) along any $y$ ($x$) row, the energy of the state is unchanged. Let us define Ising variable $\sigma$ as $\theta_2 = \theta_1 + \pi\sigma/2$, and define $\theta = \theta_1$ (although the $U(1)$ phase of the system is $\chi = \theta_1 + \theta_2$, it is more convenient to define $\theta = \theta_1$ to study the physics). It is noticed that
in the anisotropic limit, without the $\gamma$ term in (2) both $\theta_1$ and $\theta_2$ are disordered at finite temperature, therefore an infinitesimal $\gamma$ is not necessarily relevant. Hereafter we assume $\gamma$ is strong enough to guarantee that the two XY variables are perpendicular to each other in the temperature range we are interested in, for instance $\gamma > J_\sigma$. The effective classical Ising-XY coupled Hamiltonian reads

$$H = \sum_i -J \cos(\nabla \phi_i) - J \sigma_i \sigma_{i+\hat{y}} \cos(\nabla \phi_i).$$ \hspace{1cm} (6)$$

All the derivatives in the Hamiltonian are defined on the lattice. This model can be viewed as the XY variable $\theta$ coupled with an Ising gauge field background, and the Ising gauge field background might introduce frustration to the system. The lowest energy state can only be obtained if there is no frustration for $\theta$, i.e. the Ising gauge flux through each plaquette is zero. The nonfrustration criterion generates an effective coupling between the Ising variables as

$$H_{\text{ising}} = \sum_{\square} -K \sigma_1 \sigma_2 \sigma_3 \sigma_4. \hspace{1cm} (7)$$

In this Hamiltonian, the summation is over all the unit square, and $\sigma_i$, $i = 1, 2, 3, 4$ are Ising variables defined on four corners of each unit square. This model was first introduced in the context of $p \pm ip$ superconductor array. The ground state order parameter of this Ising Hamiltonian is the bond order $b_{i,\mu} = \sigma_i \sigma_{i+\mu}$, this bond order parameter takes nonzero expectation value along every row and column in the whole lattice at zero temperature. However, any infinitesimal thermal fluctuation will disorder the bond order.

The finite temperature transition is driven by the $U(1)$ defects and the $Z_2$ defects. Let us pick one ordered state from all the subextensive degenerate states with $\sigma = 1$ everywhere. The lowest energy $U(1)$ defect has been shown to be a hybrid half vortex with infinite straight $Z_2$ domain walls in both $x$ and $y$ directions without any string tension, which is also shown in Fig. 1. The straight infinite $Z_2$ domain walls violates the bond order $b_{i,\mu}$ along that row and column, but as the bond order disappears at any finite temperature, the hybrid half vortices deconfine at finite temperature.

The lowest energy $Z_2$ domain wall is shown in Fig. 2. At every corner of the $Z_2$ domain wall there is a hybrid half vortex attached. This implies that although the $Z_2$ domain wall has no string tension, the corners are interacting with each other through a logarithmic interaction. However, since the configuration entropy of the domain wall is linear with its length at finite temperature, the entropy always dominates the logarithmic interaction, thus the domain wall will proliferate at finite temperature.

From Fig. 1 and Fig. 2 one can notice that across a $Z_2$ domain wall along $x$ direction, $\theta_1 = \theta$ increases by $\pi$; while across a domain wall along $y$ direction $\theta_1$ is unchanged on average. On the contrary, $\theta_2$ gains a $\pi$-flip across a $Z_2$ domain wall along $y$ while no $\pi$-flip across $Z_2$ domain walls along $x$. Thus the $U(1)$ phase $\chi = \theta_1 + \theta_2$ is disordered after the proliferation of $Z_2$ domain walls, but since the superfluid stiffness is not affected by the $Z_2$ domain wall, $2\chi$ is still algebraically ordered.

There is another type of $Z_2$ defect, which is a $Z_2$ kink along one $x$ row (see Fig. 2). This kink defect only costs finite energy, and will also proliferate at finite temperature due to thermal fluctuation (very similar to the Ising kinks in one dimensional classical Ising model), which drives the disorder of $\theta$ along $x$ axis. Thus one can conclude that at small finite temperature $\exp(i\theta)$ has no algebraic order, while $\exp(2\theta)$ is algebraically ordered. The correlation length of $\theta$ along $x$ direction is similar to that of the one dimensional Ising model when $T \ll J$, $\xi \sim \exp(2J/T)$: while along $y$ direction the correlation length is zero.

Thus in the anisotropic limit with $J_b = 0$, the single finite temperature transition is a Kosterlitz-Thouless transition driven by the proliferation of hybrid half vortices shown in Fig. 1. It is well-known that the proliferation of half vortices leads to a universal stiffness jump at the transition, which is four times as large as the stiffness jump driven by the proliferation of single vortices:

$$\Delta \rho_s / T_c \sim 8 / \pi. \hspace{1cm} (8)$$

Here the stiffness is defined as the energy response to the same twisted boundary condition of both $\theta_1$ and $\theta_2$. Recently half vortex proliferation has also been predicted for the polar state in the two dimensional $s = 1$ spinor condensate.

The model (6) can be actually viewed as a “fixed gauge” version of the model with XY variables coupled with an Ising gauge field. Let us consider the following Hamiltonian

$$H_{\text{gauge}} = \sum_{<i,j>} -J s_{i,j} \cos(\phi_i - \phi_j). \hspace{1cm} (9)$$
FIG. 2: The $\mathbb{Z}_2$ defects. The top figure is the $\mathbb{Z}_2$ domain wall, with one hybrid half vortex attached to each corner. The green dashed line is the $\pi$ phase mismatch of $\theta_1$, and the red dashed line is the $\pi$ phase mismatch of $\theta_2$. The $\mathbb{Z}_2$ domain walls will proliferate at infinitesimal temperature. The bottom figure is the $\mathbb{Z}_2$ kink which also proliferates under thermal fluctuation.

$s_{i,j} = \pm 1$ is an Ising variable defined on the link between sites $i$ and $j$. It is well-known that this model has deconfined half vortices, and the finite temperature transition is accompanied with a universal stiffness jump $\Delta \rho_s/T_c \sim 8/\pi$. If now we define following gauge transformations: $\exp(i\beta_j) = \eta_j \exp(i\phi_j)$, $\eta_j = \prod_{j,j' = \pm 1,j < j'} s_{j,j'}$, $s_{i,i+1} = \eta_i \eta_{i,j} b_{i+1,i} \eta_{i,j}$, and $b_{i,j+1} = \sigma_i \sigma_{i+1} \eta_{i,j}$, the Hamiltonian \ref{eq:hamiltonian} becomes Hamiltonian \ref{eq:hamiltonian2}. Here $j_x$ and $j_y$ are $x$ and $y$ coordinates of site $j$. After the gauge transformation, an isolated half vortex with the $\pi$-mismatch string in the $y$ direction becomes a half vortex with the string in the $x$ direction.

C. $J_a > J_b > 0$, and phase diagram

Now if a small $J_b$ is turned up, after we introduce the Ising variable the Ising-XY Hamiltonian becomes

$$H = \sum_i -J(1 + \beta \sigma_i \sigma_{i+\hat{x}}) \cos(\theta_i - \theta_{i+\hat{x}}) - J(\sigma_i \sigma_{i+\hat{y}} + \beta) \cos(\theta_i - \theta_{i+\hat{y}}). \quad (10)$$

$\beta = J_b/J_a$. A small string tension proportional to $J_b$ is added to the $\mathbb{Z}_2$ domain wall in Fig. 2. The domain wall energy will compete with the configuration entropy of the domain wall, and the competition leads to a 2D Ising transition at temperature $T \sim J_b$ which separates an Ising ordered phase at low temperature and an Ising disordered phase at higher temperature. A similar Ising transition was found in another model with Hamiltonian

$H = \sum_{i,j} -J_b \cos(\nabla_i \theta) - J_a \cos(2 \nabla_i \theta)$

and $J_a \ll J_b$. The Ising transition in this model occurs at temperature $T \sim J_b$, and the proliferation of the Ising domain walls implies the deconfinement of half vortices. However, in our case, since every corner of the Ising domain wall is attached with a hybrid half vortex, the deconfinement of half vortices would imply the proliferation of straight infinite Ising domain walls, which cost infinite energy but the configuration entropy is still low. Another way to look at this confinement is that, with small $\beta$, the bond order operator $b_{i,j} = \sigma_i \sigma_{i+\hat{x}}$ always takes nonzero expectation value at any finite temperature, thus an infinite straight domain wall which destroys the bond order is not favored at any temperature. Thus even if the Ising domain wall proliferates at high temperature, the hybrid half vortices are still confined. The Kosterlitz-Thouless transition is still driven by the hybrid single vortices without any infinite $\mathbb{Z}_2$ domain wall, which leads to a universal stiffness jump $\Delta \rho_s/T_c \sim 2/\pi$. For the same reason, the $\mathbb{Z}_2$ kink defects are also always confined at finite temperature.

It is noticed that after the Ising variables are disordered, the XY variable $\exp(i\theta_1)$ and $\exp(i\theta_2)$ cannot be algebraically ordered on the whole $xy$ plane. Because of the symmetry between $\theta_1$ and $\theta_2$, the algebraic order of $\exp(i\theta_1)$ would imply the same type of order of $\exp(i\theta_2)$, which leads to the order (at least algebraic order) of Ising variable $\sigma \sim i \exp(i\theta_1 - i\theta_2)$. Also, since $\chi = \theta_1 + \theta_2$ always gains $\pi$-flip across the Ising domain wall, the $U(1)$ phase $\chi$ is also disordered after the Ising transition, while $2\chi$ is still ordered. The global finite temperature phase diagram is given by Fig. 3. When $J_b < J_a$, the Ising transition occurs at temperature $T \sim J_b$, which is lower than the Kosterlitz-Thouless XY transition. When $J_b$ is increasing, the Ising transition finally intersects with the XY transition and the sequence of the transitions are reversed close to the isotropic point $J_a = J_b$. The whole phase diagram is symmetric for interchanging $J_a$ and $J_b$.

Although the hybrid half vortices are always confined, as long as $J_b$ is small enough, the experimental observation should be similar to the anisotropic limit with $J_b = 0$. For instance, let us assume that the Kosterlitz-Thouless transition with $J_b = 0$ occurs at temperature $T_{\text{c0}}$, and the critical XY transition temperature with small $J_b$ is $T_{\text{c1}}$, then although there is no stiffness jump at $T_{\text{c0}}$, the slope of the stiffness change is expected to be very steep in the window $T_{\text{c0}} < T < T_{\text{c1}}$ (Fig. 4). The change of the critical temperature $(T_{\text{c1}} - T_{\text{c0}})/T_{\text{c0}}$ can be estimated as follows: With small $J_b$, although the hybrid half vortices are confined, the average distance between them is still large. Let us assume the average distance between the confined half vortices is $l_0$, which is much greater than the lattice constant. If the correlation length of the system is shorter than $l_0$, the system would behave as if there were deconfined hybrid half vortices. In the absence of $J_b$, the correlation length when $T > T_{\text{c0}}$ scales as $\xi \sim \exp(\sqrt{c/l})$, $t = T - T_{\text{c0}}$, and $c$ is a constant number. The scaling formula of the correlation length is significantly changed with the presence of $J_b$ only if $\xi$ given above is larger than $l_0$, i.e. $t < c/(\ln l_0)^2$. Thus the true Kosterlitz-Thouless transition driven by hybrid vortices at $T_{\text{c1}}$ can only occur within this small temperature.
tropy for the rectangular $\mathbb{Z}_2$ domain wall is about $\sim \ln L$. Thus the total free energy cost for this defect configuration is $F \sim J_b L - \left(C_1 J_a + C_2 T\right) \ln L$, which is minimized when $L = \left(C_1 J_a + C_2 T\right)/J_b$. Here $C_1$ and $C_2$ are nonuniversal numbers of order 1. Thus close to the XY critical point, the average distance between half vortices is $l_0 \sim J_a/J_b$. Combining the results in this paragraph and last paragraph, the change of the critical temperature due to $J_b$ and the slope of the stiffness change between $T_{c0}$ and $T_{c1}$ are

$$\frac{T_{c1} - T_{c0}}{T_{c0}} \sim \frac{1}{[\ln(J_a/J_b)]^2},$$

$$\frac{\Delta \rho_s}{\Delta T} \sim [\ln(J_a/J_b)]^2. \quad (11)$$

Thus when $J_b/J_a$ is small, the stiffness change still looks like a jump driven by half vortex proliferation. The stiffness change and jump plotted in Fig. 4 can be checked numerically.28

Experimentally the ratio $J_b/J_a$ can be tuned by changing the depth of the wells. Superfluid stiffness jump was observed in superfluid helium,27 and recently the Kosterlitz-Thouless transition has been observed in spinless atomic Bose-Einstein condensates.28 Our result about the stiffness change close to the XY transition is expected to be checked directly by future experiments.

II. QUANTUM PHASE TRANSITIONS

Now let us study the quantum phase transition at zero temperature by tuning the ratio between the repulsion energy $u$ and the hopping energy $J$, and we will focus on the simplest case with integer average filling $\bar{n}$, i.e. the system has particle-hole symmetry, more general quantum phase transitions will be discussed in another separate work.29 The Mott insulator phase at $\bar{n} = 1$ has been studied in reference, which is a featureless Mott state with one $p_x$ particle and one $p_y$ particle per site. In the Mott insulator phase neither $U(1)$ nor $\mathbb{Z}_2$ symmetry is broken. This quantum problem can be mapped to a classical problem in 3 dimensional space. In the isotropic case with $J_a = J_b = J$, the corresponding three dimensional model is simply model (1) with spatial couplings in all three directions. In three dimensional space, although the argument based on the percolation of clusters20 is no longer applicable (because the density of infinite Ising domains is always finite in 3D Ising model), the $U(1)$ transition is still expected to occur at lower temperature than the Ising transition, since the order of $\theta_1$ and $\theta_2$ implies the order of $\sigma \sim \exp[i(\theta_1 - \theta_2)]$. Thus when $u/J$ is tuned from small to large, the quantum XY transition (belonging to the 3D XY universality class) will occur before the quantum Ising transition (belonging to the 3D Ising universality class). However, the separation between the two transitions is expected to be very tiny (smaller than the two dimensional case), because a mean

![Diagram](image-url)
field Ginzburg-Landau theory for coupled XY spin systems with the same coupling for two XY spins always gives rise to one single transition, and the mean field result is expected to be more accurate in three dimensional systems than in two dimensional systems.

In the anisotropic limit with $J_b = 0$, although the Ising bond order disappears with infinitesimal temperature, it does survive from small quantum fluctuation. Now the effective Hamiltonian describing the Ising variables can be written as

$$H = \sum_\square -K\sigma^1_i\sigma^2_j\sigma^3_k\sigma^4_l - \sum_\square h\sigma^z_i,$$  \hspace{1cm} (12)

and $K \sim J$, $h \sim u$. The bond order $\langle b_{i,j}\rangle$ is nonzero with small $h/K$, because infinite order of perturbation of $h/K$ is necessary in order to mix two classical ground states. It was conjectured that the model (12) has a quantum phase transition at $J = h$ which separates a bond ordered phase and a disordered phase\(^\text{22}\), and later on the nature of the quantum phase transition was studied based on an exact mapping to fermionic degrees of freedom\(^\text{23}\). In the bond ordered phase, the hybrid half vortices are confined. The XY transition is driven by the hybrid single vortex condensation if it occurs in the bond ordered phase, otherwise it is driven by the condensation of hybrid half vortices.

If the XY transition occurs in the bond disordered phase, in the dual formalism this transition can be described by Hamiltonian $H = \sum_{\mu} -t\cos(\nabla_* \phi - \frac{1}{2} \sigma^1_{1,\mu} - \frac{1}{2} \sigma^2_{2,\mu})$, $\phi$ is the phase angle of the annihilation operator of hybrid half vortex, and the fluxes of $a_{1,\mu}$ and $a_{2,\mu}$ are the boson densities $n_1$ and $n_2$ respectively. The condensate of the vortices is the Mott Insulator in the original boson language. One can see that after the condensation of hybrid half vortices, an excitation in the condensate is a vortex of $\phi$, which always involves two boson numbers $n_1 + n_2 = \oint a_1 \cdot d\ell + \oint a_2 \cdot d\ell = 2n_x$, $n_x$ is the number of the vortices. Thus the condensate of hybrid half vortices is a Mott Insulator of paired bosons. The possible phase diagrams are shown in Fig. 5.

If a small $J_b$ is turned on, a quantum Ising transition belonging to the 3D Ising universality class is expected to occur at $u \sim J_b$, and after the transition $\chi = \theta_1 + \theta_2$ is disordered while $2\chi$ is ordered. It was shown in reference\(^\text{10}\) that, if an Ising system is coupled with superfluid, the universality class of the Ising transition is unchanged if the superfluid has particle hole symmetry, which is satisfied in the case we are discussing. As in the finite temperature case, with small $J_b$, hybrid half vortices are always confined, and the XY transition is driven by hybrid single vortices condensation. After the quantum Ising transition, the bond order-disorder transition no longer exists, because the bond order parameter $\langle b_{i,j}\rangle = \sigma^1_i\sigma^2_i\sigma^3_j\sigma^4_j$ always takes nonzero expectation values, hence the kink defect in Fig. 2 will never proliferate. The confinement of half vortices and $\mathbb{Z}_2$ kinks can also be understood after we map the system to a 3D classical problem, now a deconfined hybrid half vortex and a deconfined kink become defect lines (world lines of half vortex and kink) along the $z$ direction, and the energy of these defect lines in the 3D space-time always dominate the entropy. For instance, Let us imagine a single vortex with vorticity $+2$ be split into four half vortices at $(0,0,0)$, the four half vortices evolve in the 3D space time and recombine into a single vortex at $(0,0,z)$ (Fig. 6). In any $xy$ plane between $(0,0,0)$ and $(0,0,z)$ the four half vortices are at four corners of a rectangle. The 3 dimensional volume enclosed by the world lines is an isolated Ising domain. The energy cost of this Ising domain is proportional to its boundary area, while the entropy is linear with the length of the half vortex world lines (for instance, the shape of the whole Ising domain is fully determined by world lines $A$ and $C$ in Fig. 6), i.e. the entropy is dominated by the energy and hybrid-half vortices never deconfine. The confinement of $\mathbb{Z}_2$ kinks can be understood similarly.

Therefore we conclude that after the quantum Ising transition both $\mathbb{Z}_2$ variable $\sigma = \exp(i\theta_1 - i\theta_2)$ and $U(1)$ phase $\chi = \theta_1 + \theta_2$ are disordered, while $2\chi$ is still ordered. The topology of the phase diagram at zero temperature is the same as the finite temperature phase diagram (Fig. 3). The analytical results and phase diagram Fig. 5 will be valid.
be checked numerically in another work\textsuperscript{33}.

\section{Conclusion, Experiments and Other Physical Systems}

The phases and phase transitions studied in this work can be detected experimentally by measuring the momentum distribution function $n_k$ and measuring the momentum density correlation $\langle n_k n_{k'} \rangle$. In real experimental systems $J_b$ is always nonzero, let us assume $J_b$ is small and take the quantum phase transition phase diagram as an example (case $d$ in Fig. 6). In the phase where both $\sigma$ and $\theta$ are ordered, the momentum distribution at small momentum is

$$
\langle n_k \rangle \sim \sum_{\vec{G}} N k_2^2 \delta^2(\vec{k} - (\pi, 0) - \vec{G}) + N k_2^2 \delta^2(\vec{k} - (0, \pi) - \vec{G}) + 2N k_2 k_0 \delta^2(\vec{k} - (\pi, \pi) - \vec{G}).
$$

$\vec{G}$ is the basis of the reciprocal lattice. After the Ising transition at $u \sim J_b$, the sharp coherence of $\theta_1$ and $\theta_2$ is erased, the best way to characterize the system is through the momentum density correlation function $\langle n_k n_{k'} \rangle$ has also been proposed as a tool of measuring the many body effect of cold atom systems\textsuperscript{22}, and this technique has been successfully implemented to detect crystalline density order\textsuperscript{22}. Although $\theta_1$ and $\theta_2$ are not ordered after the Ising transitions, $2\theta_1$ and $2\theta_2$ are still ordered. Thus sharp coherence peaks still exist in the momentum density correlation functions

$$
\langle n_k n_{k'} \rangle \sim \langle n_k \rangle \langle n_{k'} \rangle + \delta^2(\vec{k} - \vec{k'}) \langle n_k \rangle
$$

although one has to subtract the effect of the first two terms of this formula from the signal. The peaks in the correlation function disappear after the XY transitions. Thus by making use of both single particle momentum distribution function and momentum density correlation function one can detect the phase transitions studied in this work.

In conclusion, we studied the phase transitions of the coupled anisotropic XY models. Both the classical and quantum phase transitions are split into an XY transition and an Ising transition, the global phase diagrams were drawn. The results obtained in this work can be checked numerically and hopefully by future experiments on $p-$band cold atom systems. Throughout the paper we assumed that the cubic symmetry is broken down to the square lattice symmetry and only $p_x$ and $p_y$ orbital levels are considered. If the optical lattice has perfect cubic symmetry, then all three $p-$wave states should be taken into account. However, the pair conversion term between all three $p-$wave states $\gamma\{\cos[2(\theta_1 - \theta_2)] + \cos[2(\theta_1 - \theta_3)] + \cos[2(\theta_3 - \theta_1)]\}$ is frustrating when $\gamma > 0$, the three terms cannot be minimized simultaneously, which makes the problem more complicated.

Similar problems can be studied for atoms on even higher orbital levels. For instance, in cubic lattice the $d-$level state on each well is split into a three fold degenerate level, the $e_g$ level. Within the $e_g$ level, the $d_{x^2-y^2}$ state extends further and isotropically in the $xy$ plane, while the $d_{3z^2-r^2}$ level extends in the $z$ direction. Thus in the isotropic limit the problem becomes the coupled isotropic XY model in three dimensional space, and as discussed in section III, the 3D Ising transition is expected to occur at higher temperature than the 3D XY transition. On the contrary, in the anisotropic limit with extreme directional hoppings, the finite temperature model can be written as

$$
H = \sum_i \sum_{\mu=x,y} -J \cos(\nabla_\mu \theta_1) - J \cos(\nabla_z \theta_1, \theta_2) + \gamma \cos(2\theta_1 - 2\theta_2).
$$

If the Ising variable is introduced through $\theta_2 = \theta_1 + \sigma \pi/2$, the Ising-XY model becomes

$$
H = \sum_i \sum_{\mu=x,y} -J \cos(\nabla_\mu \theta_1) - J \sigma_i \sigma_{i+z} \cos(\nabla_z \theta_i).
$$

Again the nonfrustration criterion generates an effective classical Ising Hamiltonian

$$
H = \sum_i -J \sigma_i \sigma_{i+z} \sigma_{i+z} \sigma_{i+z}
$$

If we define bond operator $b_i = \sigma_i \sigma_{i+z}$, the model becomes decoupled 2D classical Ising model for new Ising.
variable \( b_i \). Thus in the anisotropic limit there are again two transitions at finite temperature, one is the 3D XY transition, and the other is a 2D Ising transition.

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1. M. Greiner and et. al., Nature 415, 39 (2002).
2. A. Isacsson and S. M. Girvin, Phys. Rev. A 72, 053604 (2005).
3. W. V. Liu and C. Wu, Phys. Rev. A 74, 013607 (2006).
4. C. Wu, W. V. Liu, J. Moore, and S. DasSarma, Phys. Rev. Lett 97, 190406 (2006).
5. C. Xu and M. P. A. Fisher, Phys. Rev. B 75, 104428 (2007).
6. C. Wu, D. Bergman, L. Balents, and S. D. Sarma, arXiv:cond-mat/0701788 (2007).
7. A. B. Kuklov, Phys. Rev. Lett 97, 110405 (2006).
8. T. Mueller, S. Foelling, A. Widera, and I. Bloch, arXiv:0704.2856 (2007).
9. G. Khaliullin, Prog. Theor. Phys. Suppl 160, 155 (2005).
10. G. Khaliullin and S. Maekawa, Phys. Rev. Lett 85, 3950 (2000).
11. B. Keimer and et. al., Phys. Rev. Lett 85, 3946 (2000).
12. C. L. Henley, Phys. Rev. Lett 62, 2056 (1989).
13. P. Chandra, P. Coleman, and A. I. Larkin, Phys. Rev. Lett 64, 88 (1990).
14. D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, Phys. Rev. Lett 52, 433 (1984).
15. D. H. Lee, R. G. Caffisch, J. D. Joannopoulos, and F. Y. Wu, Phys. Rev. B 29, 2680 (1984).
16. G. Franzese, V. Cataudella, S. E. Korshunov, and R. Fazio, Phys. Rev. B 62, R9287 (2000).
17. J. Lee, E. Granato, and J. M. Kosterlitz, Phys. Rev. B 44, 4819 (1991).
18. E. Granato, J. M. Kosterlitz, J. Lee, and M. P. Nightingale, Phys. Rev. Lett 66, 1090 (1991).
19. M. Hasenbusch, A. Pelissetto, and E. Vicari, J. of Stat. Mech p. P12002 (2005).
20. S. E. Korshunov, Phys. Rev. Lett 88, 167007 (2002).
21. A. Coniglio, C. R. Nappi, F. Peruggi, and L. Russo, J. of Phys. A 10, 205 (1977).
22. J. E. Moore and D.-H. Lee, Phys. Rev. B 69, 104511 (2004).
23. C. Xu and J. E. Moore, Phys. Rev. Lett 93, 047003 (2004).
24. S. Mukerjee, C. Xu, and J. E. Moore, Phys. Rev. Lett 97, 120406 (2006).
25. D. H. Lee and G. Grinstein, Phys. Rev. Lett 55, 541 (1985).
26. C. Xu and S. Mukerjee, in progress (2007).
27. D. J. Bishop and J. D. Reppy, Phys. Rev. Lett 40, 1727 (1978).
28. Z. Hadzibabic, P. Kruger, and et. al., Nature 441, 1118 (2006).
29. C. Xu, in progress (2007).
30. H.-D. Chen, C. Fang, J. Hu, and H. Yao, Phys. Rev. B 75, 144401 (2007).
31. E. Frey and L. Balents, Phys. Rev. B 55, 1050 (1997).
32. E. Altman, E. Demler, and M. D. Lukin, Phys. Rev. A 70, 013603 (2004).
33. S. Folling, F. Gerbier, A. Widera, and et. al., Nature 434, 481 (2005).