Directional Ordering of Fluctuations in a Two-Dimensional Compass Model

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In the Mott insulating phase of the transition metal oxides, the effective orbital-orbital interaction is directional both in orbital space and in real space. We discuss a classical realization of directional coupling in two dimensions. Despite extensive degeneracy of the ground state, the model exhibits partial orbital ordering in the form of directional ordering of fluctuations at low temperatures stabilized by an entropy gap. Transition to the disordered phase is shown to be in the Ising universality class through exact mapping and multicanonical Monte Carlo simulations.

Recently, there has been growing interest in the effects of orbital degeneracy in the physics of transition metal oxide (TMO) insulators [1,2]. In these systems, the dominating energy scales for d electrons on the TM ions are the on-site Coulomb repulsion (which freezes out the charge degrees of freedom), the Hund's rule coupling, and the crystal field due to the surrounding oxygen ions. The latter two together determine the degeneracies and degrees of freedom of spin and orbital on each transition metal ion. Spins and orbitals on neighboring TM ions can then be coupled through the superexchange mechanism. In the case of orbitals, they are also coupled through the phonon-mediated cooperative Jahn-Teller mechanism [1]. These couplings determine the low temperature properties of these systems.

Because orbital coupling is intrinsically directional [3], orbital ordering brings up some unusual questions. Especially interesting is when the coupling along a given bond direction is Ising-like, but with different Ising axes along different bond directions [4]. The Hamiltonian for orbitals is then given by

$$H = -J\sum_{\langle ij \rangle} \boldsymbol{\tau}_i \cdot \hat{\mathbf{n}}_{ij} \boldsymbol{\tau}_j \cdot \hat{\mathbf{n}}_{ij}, \qquad (1)$$

where τ is an isospin operator representing the orbital degree of freedom, and $\hat{\mathbf{n}}_{ij}$ is a unit vector. For example, for e_g orbitals in Perovskite structures, $\hat{\mathbf{n}}_{ij}$ for the three different bond directions are coplanar and oriented relative to each other by 120°, giving rise to the so-called 120° model [4–6]. This model is also applicable to t_{2g} orbitals on the three bonds of a honeycomb lattice as in planes of V_2O_3 [7,8]. On the other hand, for t_{2g} orbitals on Perovskite structures (e.g., LaTiO$_3$ [9]), the relevant model is the compass model [1,4,10] with $\hat{\mathbf{n}}_{ij} = \hat{x}, \hat{y}, \hat{z}$ for the three bond directions. The compass model may also feature as part of the spin-spin coupling of t_{2g} orbitals when spin-orbit interaction is taken into account [11]. A common feature of both the compass model and the 120° model is the competition between bonds in different directions, with the resulting frustration leading to macroscopic degeneracy of the classical ground state.

In this Letter, we report analytical and numerical results on a classical version of (1) in two dimensions (2D). The highly anisotropic coupling gives rise to interesting interplay between one- and two-dimensional ordering, between continuous and discrete spin physics, and between slow and fast modes. Our main result is that at low $T > 0$, there is no conventional ordering [12], but there is, nevertheless, long-ranged order (LRO) in the form of a directional ordering in fluctuations. This ordering corresponds to a partial breaking of the fourfold symmetry and is stabilized by entropy. In this phase, the system exhibits spontaneous dimension reduction by essentially decoupling into one-dimensional (1D) chains running either horizontally or vertically along the bonds. Through exact mapping and extensive Monte Carlo simulations, we show that this ordering transition belongs to the Ising universality class. We then discuss generalizations of these results to the quantum case and in three dimensions, as well as their implications with respect to orbital ordering.

Consider the classical compass model on a square lattice of $N = L \times L$ sites,

$$H = -J\sum_i (S_{ix}S_{i+\hat{x},x} + S_{iy}S_{i+\hat{y},y}), \qquad (2)$$

where $\mathbf{S}_i = (\cos\theta_i, \sin\theta_i)$ represents either a real spin or an orbital isospin. On the square lattice, the sign of J can be gauged away, so we take $J > 0$. Along each row (column), we have a simple Ising model (IM) with quantization axis along $\hat{x}$ ($\hat{y}$). Hamiltonian (2) has two types of discrete symmetry. (I) There is a global fourfold rotation symmetry corresponding to simultaneously rotating the spins and lattice by multiples of 90°. (II) In addition, it is also invariant under the 1D spin flip transformation $S_{ix} \rightarrow -S_{ix}$, $S_{iy} \rightarrow S_{iy}$ for all i on any one row and $S_{ix} \rightarrow S_{ix}$,

$S_{iy} \rightarrow -S_{iy}$ for all i on any one column. Since symmetry (I) is two-dimensional, we expect that it may be broken at finite T, while the 1D nature of symmetry (II) should imply no symmetry breaking except possibly at $T = 0$. We see, indeed, that this is the case, but the physics leading to it and their consequences are not trivially deduced from such symmetry considerations.

The low temperature properties of (2) are further complicated by an additional O(2) degeneracy. Apart from a constant term, Eq. (2) can be written as

$$H = \frac{J}{2} \sum_i [(\cos\theta_i - \cos\theta_{i+\hat{x}})^2 + (\sin\theta_i - \sin\theta_{i+\hat{y}})^2]. \quad (3)$$

Clearly $\theta_i \equiv 0$ is a ground state, as are the $D = 2 \times 2^L$ states obtained from it by the symmetry operations (I) and (II). However, Eq. (3) shows that the ground state energy is invariant under arbitrary global rotation of $\theta_i \equiv 0$ to $\theta_i \equiv \theta$. Unlike the isotropic XY model, where this invariance holds for each bond, here the energy loss from the horizontal bonds are compensated by energy gain in the vertical bonds. Thus, the ground state exhibits an O(2) degeneracy not related to the symmetries of H. We see that this "accidental" degeneracy is lifted at finite temperatures by entropy due to slow mode fluctuations.

Upon a redefinition of the spins through symmetry (II), any of the ground states mentioned above can be recast as $\theta_i \equiv \theta$. To study slow mode physics, we start with the spin-wave or harmonic approximation. Expanding (3) to the second order in $\varphi_i = \theta_i - \theta$, we obtain the spin-wave Hamiltonian in Fourier form, $H_{\mathrm{SW}} = J \sum_k \epsilon_k(\theta)|\varphi_k|^2$. For general θ, the spin-wave spectrum $\epsilon_k(\theta) = (1 - \cos k_x)\sin^2\theta + (1 - \cos k_y)\cos^2\theta$ is an anisotropic 2D one, with zero modes at $k_x = k_y = 0$. However, for special ordering directions $\theta = 0$, $\pi/2$, π, and $3\pi/2$, the spectrum becomes 1D-like, independent of either k_x ($\theta = 0$, π) or k_y ($\theta = \pi/2$, $3\pi/2$), and the density of states of gapless excitations is 1D rather than 2D. The high density of low lying states suggests an entropic mechanism to stabilize these four directions at $T > 0$.

To put the discussion on a firmer footing, we employed a self-consistent harmonic approximation for the ordered phase at $\theta = 0$. Based on the Bogolyubov-Peierls theorem [13,14], $F \leq F_0 - \langle H_0 \rangle_0 + \langle H \rangle_0$, we compute the variational free energy using a trial Hamiltonian $H_0 = J \sum a_k |\varphi_k|^2$. Minimizing the free energy, we obtain

$$a_k = m + \gamma_x(1 - \cos k_x) + \gamma_y(1 - \cos k_y), \quad (4)$$

where m is the self-consistent spin-wave gap, and γ_x and γ_y are the self-consistent stiffnesses.

At low temperatures, a 1D spectrum with $\gamma_x(T) = 0$, $\gamma_y(T) = 1 - O(T^{2/3})$, and $m(T) = \frac{1}{2} T^{2/3} + O(T)$ is obtained. Anharmonic effects are incorporated into a shift of these parameters at finite T from their bare spin-wave values. Most significantly we see that a gap m is generated, which suppresses the diverging 1D fluctuations in

the spin-wave analysis, and stabilizes the ordering along one of the four special directions.

To address whether there is ordering into one of the D degenerate ground states, we need to consider the effects of fast modes or, more precisely, abrupt spin flips. For this purpose, the continuous nature of the spins should not be crucial, so we discretize the compass model into a "four-state Potts compass model (PCM)" with the same symmetry as (2), given by

$$H_{\mathrm{P}} = -J \sum (n_{i\sigma} n_{i+\hat{x},\sigma} \sigma_i \sigma_{i+\hat{x}} + n_{i\tau} n_{i+\hat{y},\tau} \tau_i \tau_{i+\hat{y}}), \quad (5)$$

where on each site we have "occupation numbers" $n_{i\sigma} = 0, 1$ and $n_{i\tau} = 1 - n_{i\sigma}$. If $n_{i\sigma} = 1$, then there is an additional internal degree of freedom $\sigma = \pm 1$, and similarly for $n_{i\tau}$ and τ. The correlation of these internal degrees of freedom with the occupation numbers together with the constraint in the latter couple these various variables.

The partition function of the PCM takes the form $Z_{\mathrm{P}} = \mathrm{Tr}_{\{n_{i\sigma}\}} \mathrm{Tr}'_{\{\sigma_i, \tau_i\}} \exp(-\beta H_{\mathrm{P}})$, where Tr' indicates that for a given configuration of $\{n_{i\sigma}\}$ the trace over $\sigma(\tau)$ should be on only those sites with $n_{i\sigma} = 1(0)$. On the other hand, we note that if, for example, $n_{i\sigma} = 0$, then H_{P} is independent of σ_i, and tracing over $\sigma_i = \pm 1$ simply gives a superfluous factor of 2. Thus, Tr' can be replaced by the unrestricted Tr to give $Z_{\mathrm{P}} = 2^{-N} \mathrm{Tr}_{\{n_{i\sigma}\}} \mathrm{Tr}_{\{\sigma_i, \tau_i\}} \exp(-\beta H_{\mathrm{P}})$. The trace over σ and τ can now be easily done using a transfer matrix since H_{P} consists of decoupled 1D chains as far as σ and τ are concerned, resulting in $Z_{\mathrm{P}} = \mathrm{Tr}_{\{n_{i\sigma}\}} \exp(-\beta H_{\mathrm{eff}})$, where

$$H_{\mathrm{eff}} = -T \ln[\cosh(\beta J)] \sum_i (n_{i\sigma} n_{i+\hat{x},\sigma} + n_{i\tau} n_{i+\hat{y},\tau})$$
$$- T \ln[1 + \tanh^L(\beta J)] \left[\sum_\alpha C_\alpha + \sum_\gamma D_\gamma \right]. \quad (6)$$

In the last two terms of H_{eff}, $C_\alpha = \prod_i n_{i\sigma} n_{i+\hat{x},\sigma}$, for all sites i in the row α, while $D_\gamma = \prod_j n_{j\tau} n_{j+\hat{y},\tau}$, for all sites j in the column γ. At any $T > 0$, these two terms are finite-sized terms that vanish in the thermodynamic limit $L \rightarrow \infty$. Ignoring them, we may rewrite H_{eff} in terms of $n_{i\sigma,\tau} = \frac{1}{2}(1 \mp \mu_i)$ as

$$H_{\mathrm{eff}} = -2N\tilde{J} - \tilde{J} \sum_i (\mu_i \mu_{i+\hat{x}} + \mu_i \mu_{i+\hat{y}}). \quad (7)$$

The four-state PCM is thus mapped exactly into the 2D Ising model (2DIM). The coupling constants of the two models are related by $\tilde{J} = T \ln[\cosh(J/T)]/4$. From the 2DIM exact $\tilde{T}_c = 2\tilde{J}/\ln(1 + \sqrt{2})$, we conclude that the PCM has LRO for all $T < T_c = 0.4084J$. What is the nature of this LRO? First, note that because the trace over σ and τ are for decoupled chains, $\langle \sigma_i \rangle$ and $\langle \tau_i \rangle \equiv 0$ for all $T > 0$. Instead, the 2DIM uniform ordering of $\langle \mu_i \rangle$ corresponds to $\langle n_\sigma \rangle - \langle n_\tau \rangle \neq 0$. In other words, the ordering is not a conventional ordering with the spins sponta-

neously pointing along one of the four possible states, but of them having stronger fluctuations in two of the four states, henceforth called directional ordering of fluctuations. In this phase, the Z_4 symmetry of the compass model is only partially broken into $Z_2 \times Z_2$. While at $T = 0$, the ground state has macroscopic degeneracy, the free energy has only two degenerate minima at $T = 0_+$.

Based on symmetry considerations and on our entropy stabilization arguments earlier, we expect the above conclusions to hold also for the continuous compass model except for the value of T_c. To confirm this and to rule out a preemptive first order transition, we perform Monte Carlo simulations. However, such simulations are complicated by the strong size dependence that originates from the finite-sized terms in Eq. (6) under the periodic boundary condition when the 1D correlation length ξ_{1D} exceeds the linear system size L at sufficiently low temperature. To eliminate this effect, we adopted a "bond fluctuating" boundary condition. A multicanonical Monte Carlo scheme [15] is used to sample the degenerate low energy states. Details will be published elsewhere.

Figure 1(a) shows the average of the directional order parameter $q = N^{-1}\sum_i(S_{ix}^2 - S_{iy}^2) = N^{-1}\sum_i \cos 2\theta_i$ against T for $L = 8, 12, 16, 24, 32,$ and 48. The existence of an ordered state at low temperatures is evident from the data. To locate the transition point, we computed the Binder cumulant $B = 1 - \langle q^4 \rangle /(3\langle q^2 \rangle^2)$ for various system sizes, as shown in Fig. 1(b). At $T = T_c$ the value of B should be size independent and universal; hence, we estimate $T_c/J = 0.147 \pm 0.001$. The value of B at the crossing point for large system sizes also agrees reasonably well with the 2DIM result $B_c = 0.610\,69 \ldots$ [16].

Figure 2 shows the specific heat data for the six different sizes up to $L = 48$. A weak divergence near the T_c value determined above is clearly seen. The inset shows the same data in the critical region after subtraction of a background linear function, plotted using the scaled variables according to the finite-size scaling form derived in Ref. [17]. Apart from the smallest size at $L = 8$, the data collapse is quite satisfactory.

The simulation data show quite convincingly that directional ordering exists at low temperatures with a nonzero value of the directional order parameter q. The transition to the disordered phase is an ordinary continuous transition of the Ising universality class, just as in the PCM. The transition temperature of the continuous compass model, on the other hand, is considerably lower than that of the PCM. We attribute this to the softening of domain wall energy in the continuous model. Indeed, the free energy gap between the favored orientation and other states does not remain constant, but, in fact, vanishes as $T^{2/3}$ at low T.

We next discuss the implications of our results to orbital ordering, taking the spin in the Hamiltonian to represent the orbital isospin. For TMO, the relevant S are then $1/2$ and 1 for double and triple orbital degeneracy, respectively, and the isospins are quantum mechanical. Rigorous results are not available for the quantum model, but some qualitative and physical arguments can be made. In the quantum model, there are fluctuations about the classical ground state even at $T = 0$. Some aspects of these fluctuations manifest themselves in similar ways to thermal fluctuations, and serve to both stabilize and destabilize LRO. The $\theta = 0$, $\pi/2$, π, and $3\pi/2$ ordering directions are stabilized by renormalized spin-wave fluctuations that lift the O(2) degeneracy while also generating a gap. This conventional ordering is weakened by fast mode fluctuations. However, a simple-minded $2 + 1$ dimension argument implies that unlike thermal fluctuations, the disordering effects of fast mode physics destroy
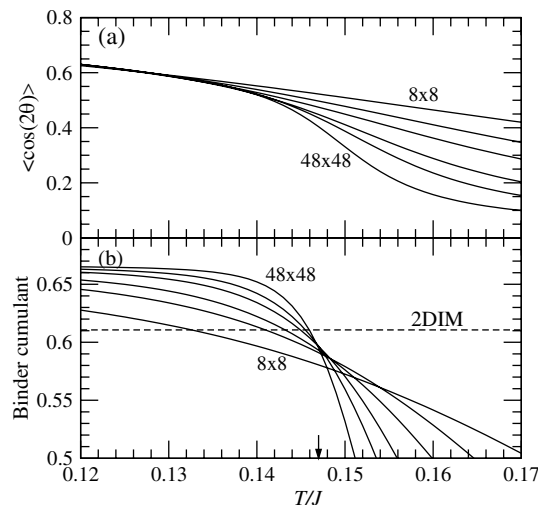

FIG. 1. (a) Directional order parameter against temperature T for the 2D compass model at various system sizes. (b) Binder cumulant against temperature. The critical temperature is estimated at $T_c/J = 0.147 \pm 0.001$. The dashed line shows the value of B for 2DIM at criticality.
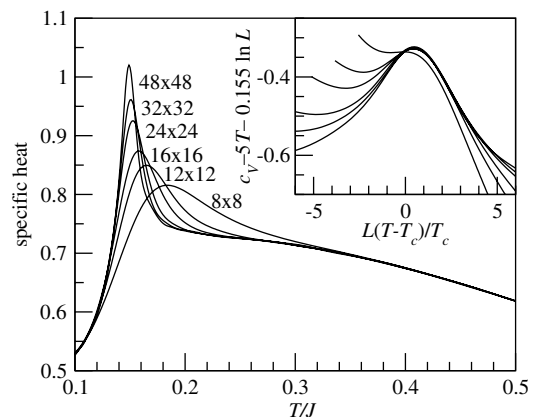

FIG. 2. Specific heat against temperature for the 2D compass model. Inset: Same data plotted using scaled variables.

the conventional ordering only if they are sufficiently strong. The same argument suggests that the disordering effect on directional ordering is even weaker. However, the true description of the fast mode physics involves understanding the physics of instanton tunneling of the quantum model, and is beyond the scope of this Letter. At any rate, we expect the directional ordering shown in the classical model to be stable against weak quantum fluctuations at low but finite T. Indeed, the $T = 0$ gap of the quantum model may actually stabilize the directional ordering at low T.

The directional ordering leaves the orbital degeneracy completely ($S = 1/2$) or partially ($S = 1$) unbroken. In the case of $S = 1$, the directional ordering reduces the triple orbital degeneracy to double degeneracy. In the case of $S = 1/2$, $S_{ix}^2 = S_{iy}^2 \equiv 1/4$, and the directional order parameter q is defined above $\equiv 0$. Instead, we define an alternative directional order parameter applicable for all S, namely, $r = \langle S_{ix}S_{i+x,x} - S_{iy}S_{i+y,y} \rangle$, which like q shows LRO in the direction of fluctuations in isospin space. An advantage of r over q is that it explicitly displays the energy difference between horizontal and vertical bonds and hence the broken lattice rotation symmetry. A consequence of this is that, when the couplings of the orbital isospin to lattice modes are included, the directional ordering is necessarily accompanied by a lattice distortion so that the bond lengths in horizontal and vertical directions become unequal.

Our results can be generalized to the compass model on the 3D cubic lattice, now with a three-component spin $\mathbf{S} = (S_x, S_y, S_z)$. Slow mode physics stabilize orderings along $\pm\hat{x}$, $\pm\hat{y}$, $\pm\hat{z}$. Restricting to the six special directions, we can then consider the corresponding six-state PCM [18]. The mapping we used to map the 2D four-state PCM into the 2D Ising model can be applied here too. However, in this case, the mapping does not result in an ordinary three-state Potts model, but in a three-state PCM, $H = -\sum_i n_{i\sigma}n_{i+x,\sigma} + n_{i\tau}n_{i+y,\tau} + n_{i\mu}n_{i+x,\mu}$, where $n_{i\sigma,\tau,\mu} = 0, 1$ and $n_{i\sigma} + n_{i\tau} + n_{i\mu} = 1$. There is no known solution to this model. Heuristic domain wall analysis suggests that directional ordering is stable at low T, but more rigorous calculation is necessary for this to be conclusive. Unlike the 2D case, the degeneracy of the directional ordered state, while less than the ground state degeneracy of $D = 3 \times (2 \times 2^L)^L$, is also macroscopic and found to be $3 \times 2 \times 2^L$. Notice that the fluctuation effects are stronger in 3D than 2D, and, in fact, in general, the higher the dimension, the stronger the fluctuations, a point previously pointed out by Khomskii and Mostovoy in Ref. [4].

In general, the real system may not correspond precisely to the compass model. As an example, we consider an additional isotropic XY coupling of strength J' which is identical for all the bonds. At low T ($T \lesssim J'$), this term suppresses the arbitrarily large 1D domains, and conven-

tional ordering given by $\langle \mathbf{S}_i \rangle \neq 0$ is stable. However, this ordering cannot persist beyond T of order J' since the correlation function for $\mathbf{S}_i$ is short ranged for all $T > 0$ when $J' = 0$. Furthermore, the J' term does not tend to disorder directional ordering, only to augment it to conventional ordering. Hence, for small J', we expect directional ordering to be stable at intermediate temperatures, and the directional ordered phase is robust and observable in systems with Hamiltonians close to the compass model.

In conclusion, we have established that the compass model has a low temperature phase characterized by $\langle \mathbf{S}_i \rangle = 0$, but with long-ranged correlations in the direction of fluctuations in both isospin and lattice spaces.

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