

Striped Phase in a Quantum XY Model with Ring Exchange

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We present quantum Monte Carlo results for a square-lattice $S = 1/2$ XY model with a standard nearest-neighbor coupling J and a four-spin ring exchange term K . Increasing K/J , we find that the ground state spin stiffness vanishes at a critical point at which a spin gap opens and a striped bond-plaquette order emerges. At still higher K/J , this phase becomes unstable and the system develops a staggered magnetization. We discuss the quantum phase transitions between these phases.

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Ring exchange interactions have for a long time been known to be present in a variety of quantum many-body systems [1] and have been investigated rather thoroughly in solid ^3He [2]. They are also important for electrons in the Wigner crystal phase [3,4]. In strongly correlated electron systems, such as the high- T_c cuprates and related antiferromagnets, ring exchange processes are typically much weaker than the pair exchange J [5] and are often neglected. Four-spin ring exchange has, however, been argued to be responsible for distinct features in the magnetic Raman [6] and optical absorption spectra [7]. Neutron measurements of the magnon dispersion have also become sufficiently accurate to detect deviations from the standard pair exchange Hamiltonian (the Heisenberg model) and such discrepancies have been attributed to ring exchange [8,9]. Recently, ring exchange has attracted interest as a potentially important interaction that could lead to novel quantum states of matter, in particular, 2D electronic spin liquids with fractionalized excitations [10–15]. Furthermore, for bosons on a square lattice ring exchange has been shown to give rise to an “exciton Bose liquid” phase [16].

Here we study the effects of ring exchange in one of the most basic quantum many-body Hamiltonians—the spin-1/2 XY model on a 2D square lattice. We use a quantum Monte Carlo method (stochastic series expansion, hereafter SSE [17–19]) to study the low-temperature behavior of this system including a four-spin ring term. Defining bond and plaquette exchange operators

$$B_{ij} = S_i^+ S_j^- + S_i^- S_j^+ = 2(S_i^x S_j^x + S_i^y S_j^y), \quad (1)$$

$$P_{ijkl} = S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+, \quad (2)$$

the Hamiltonian is

$$H = -J \sum_{\langle ij \rangle} B_{ij} - K \sum_{\langle ijkl \rangle} P_{ijkl}, \quad (3)$$

where $\langle ij \rangle$ denotes a pair of nearest-neighbor sites and $\langle ijkl \rangle$ are sites on the corners of a plaquette. For $K = 0$

this is the standard quantum XY model, or, equivalently, hard-core bosons at half-filling with no interactions apart from the single-occupancy constraint. This system undergoes a Kosterlitz-Thouless transition at $T/J \approx 0.68$ [20,21] and has a $T = 0$ ferromagnetic moment $M_x = \langle S_i^x \rangle \approx 0.44$ [22,23]. The K term corresponds to retaining only the purely x and y terms of the full cyclic exchange.

In a soft-core version of the pure ring model ($J = 0$), Paramekanti *et al.* recently found a compressible but non-superfluid phase (exciton Bose liquid) for weak on-site repulsion U [16]. As the hard-core limit is approached they found a transition to a staggered charge-density-wave phase. Hence, the ground state of the spin Hamiltonian (3) can be expected to change from an easy-plane ferromagnet with a finite spin stiffness ρ_s and a magnetization $\langle M_x \rangle$ at low K/J to an Isinglike antiferromagnet with vanishing ρ_s and a staggered magnetization $\langle M_S \rangle = (-1)^{x_i+y_i} \langle S_i^z \rangle$ at large K/J . The central result of our simulations is that the competing J and K interactions give rise to yet a third phase at $K/J \sim 10$; a striped bond-plaquette phase where the expectation values $\langle B_{ij} \rangle$ and $\langle P_{ijkl} \rangle$ alternate in strength with a period of two lattice spacings in one of the lattice directions. An example of this order is illustrated in Fig. 1. A similar columnar “bond charge” phase was recently predicted based on a lattice field theory including a plaquette term [13]. The field theory also has fractionalized phases, of which we have found no evidence. Hence, the microscopic mechanisms leading to fractionalized spin liquids remain to be clarified.

The SSE simulation method [17–19] that we use here has previously been applied to a variety of spin and boson models with two-particle interactions, including the Hamiltonian (3) with $K = 0$ (the XY model) [23]. The generalization to include the four-spin K term is relatively straightforward, although nontrivial new procedures had to be developed for large- K/J simulations [24]. Bond and plaquette strengths such as those shown in Fig. 1 were obtained using open-boundary rectangular $L_x \times L_y$ lattices with $L_y = 2L_x$. The translational and rotational

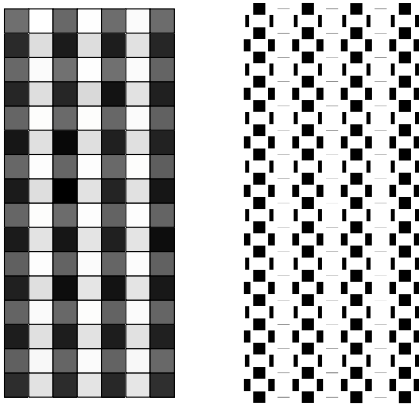


FIG. 1. Plaquette (left) and bond (right) strengths at the center of a 64×128 open-boundary lattice at $K/J = 10$ and $T = J/8$. The plaquette strengths are represented by shades of gray with the weakest $\langle P_{ijkl} \rangle = 0.222$ (white squares) and strongest 0.468 (black squares). The bond strengths are indicated by the width of the line segments, with the weakest $\langle B_{ij} \rangle = 0.181$ and the strongest 0.505.

symmetries are then broken and a unique static bond-plaquette strength pattern can be observed when $K/J \sim 10$ at $T/J \lesssim 0.5$. For $K/J \lesssim 8$ no order is visible at the centers of large lattices at any temperature. The modulations seen within the stripes in Fig. 1 are strongest at the four corners of the lattice and decrease as the center is approached. They also decrease as the lattice size is increased and in the thermodynamic the striped state should therefore be analogous to the fourfold degenerate columnar spin-Peierls state of Ref. [13].

Our conclusion that the stripes are stable is based on finite-size scaling of correlation functions on periodic $L \times L$ lattices. The striped phase can be detected using the bond or plaquette correlations. Here we consider the plaquette structure factor

$$P(q_x, q_y) = \frac{1}{L^2} \sum_{a,b} e^{i(\mathbf{r}_a - \mathbf{r}_b) \cdot \mathbf{q}} \langle P_{a_1 a_2 a_3 a_4} P_{b_1 b_2 b_3 b_4} \rangle, \quad (4)$$

where a_1, \dots, a_4 are the sites belonging to plaquette a . We have studied the full \mathbf{q} dependence and only found peaks at $(0, \pi)$ and $(\pi, 0)$. Hence, the modulations within the stripes seen in Fig. 1 are indeed induced by open boundaries. The spin structure factor is defined as

$$S(q_x, q_y) = \frac{1}{L^2} \sum_{j,k} e^{i(\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{q}} \langle S_j^z S_k^z \rangle, \quad (5)$$

where $r_i = (x_i, y_i)$ is the lattice coordinate. We will analyze the staggered and striped order parameters per site, defined as

$$\langle M_S^2 \rangle = S(\pi, \pi)/L^2, \quad (6)$$

$$\langle M_P^2 \rangle = P(\pi, 0)/L^2. \quad (7)$$

The spin stiffness (the superfluid density in the boson representation) is defined by

$$\rho_s = \frac{\partial^2 E(\phi)}{\partial \phi^2}, \quad (8)$$

where $E(\phi) = \langle H(\phi) \rangle / L^2$ and the twist ϕ is imposed in the x or y direction so that the corresponding bond operators (1) become $B_{ij}(\phi) = \cos(\phi)(S_i^x S_j^x + S_i^y S_j^y) + \sin(\phi)(S_i^x S_j^y - S_i^y S_j^x)$. The derivative at $\phi = 0$ in Eq. (8) can be directly estimated using the winding number fluctuations in the SSE simulations [25].

Figure 2 shows the spin stiffness and the stripe order parameter on an $L = 64$ lattice at $T = J/8$ (where the results are almost converged to their ground state values). The stiffness becomes very small at $K/J \approx 8$, where the stripe order increases significantly. Finite-size scaling shows that the stripe order survives in the thermodynamic limit. Results for $K/J = 8.5$ and temperatures sufficiently low to give the ground state are shown in Fig. 3. For $L \geq 32$ the data graphed versus $1/L$ fall on a straight line, which extrapolates to a nonzero value as $L \rightarrow \infty$. Based on results [16] for the soft-core version of the $J = 0$ model (or $K \rightarrow \infty$) the staggered magnetization can be expected to be nonzero for large K . However, as also shown in Fig. 3, at $K/J = 8.5$ $\langle M_S^2 \rangle$ decreases as $1/L^2$ for large lattices, implying that the spin-spin correlations are short ranged [$S(\pi, \pi)$ is finite]. Figure 3 also shows results for $K/J = 64$, where the scaling behaviors of the two quantities is reversed— $\langle M_P^2 \rangle$ decays as $1/L^2$ whereas $\langle M_S^2 \rangle$ extrapolates to a nonzero value. Note that the size dependence of M_S^2 is nonmonotonic, with a minimum around $L \approx 10$. Such nonmonotonicity has previously been observed for a spatially anisotropic spin model [26] where it was attributed to the presence of two different low-energy scales in the system. The nonmonotonicity seen at $K/J = 64$ in Fig. 3 indicates that the stripe correlations remain strong with a correlation length ~ 10 lattice spacings. The location of the minimum in $\langle M_S^2 \rangle$ moves to lower $1/L$ as K/J is decreased, indicating growing stripe correlations. The strong stripe correlations

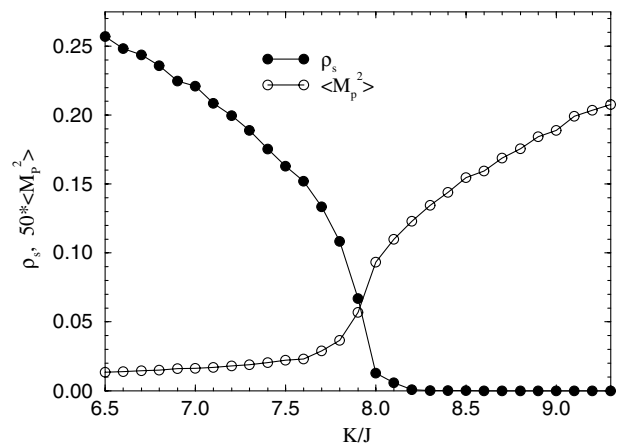


FIG. 2. Spin stiffness and plaquette-stripe order parameter vs ring-exchange coupling for a 64×64 system with periodic boundary conditions at $T = J/8$.

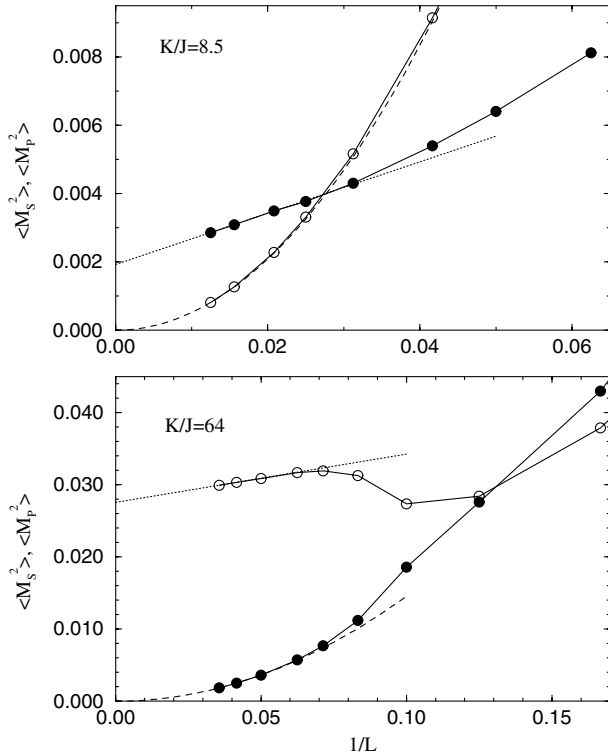


FIG. 3. Finite-size scaling of the ground state staggered magnetization (open circles) and the plaquette-stripe order parameter (solid circles) at $K/J = 8.5$ and 64 . The dotted straight lines show extrapolations of the infinite-size order parameters. The dashed curves show the form $\sim 1/L^2$ expected asymptotically when there is no long-range order.

in the staggered phase makes it difficult to determine the $\langle M_S \rangle$ versus K/J curve. Our simulations show that the stripe order persists at least for K/J up to 12, and also that the staggered correlations are short ranged up to this coupling. The stripe correlations are short ranged for $K/J \geq 16$. Between $K/J = 12$ and 16 the two phases could either coexist or be separated by a first-order transition. Simulations of larger lattices will be required in order to clarify the interesting transition region.

The superfluid-stripped transition appears to be of second order, although we cannot exclude a very weakly first-order transition (which was argued to be more likely in Ref. [13]). The vanishing of the spin stiffness seen in Fig. 2 indicates the opening of a spin gap. A spin gap can be inferred also from the temperature dependence of the uniform magnetic susceptibility,

$$\chi_u = \frac{1}{L^2 T} \left\langle \left(\sum_i S_i^z \right)^2 \right\rangle. \quad (9)$$

Figure 4 shows the T dependence for $L = 80$ (sufficiently large to eliminate finite-size effects). The $T \rightarrow 0$ susceptibility vanishes for K/J between 7.90 and 7.95, i.e., a spin gap is present above a critical coupling in this range. The temperature independence of χ_u at $K/J = 7.80$ at the two lowest temperatures is expected on account of this

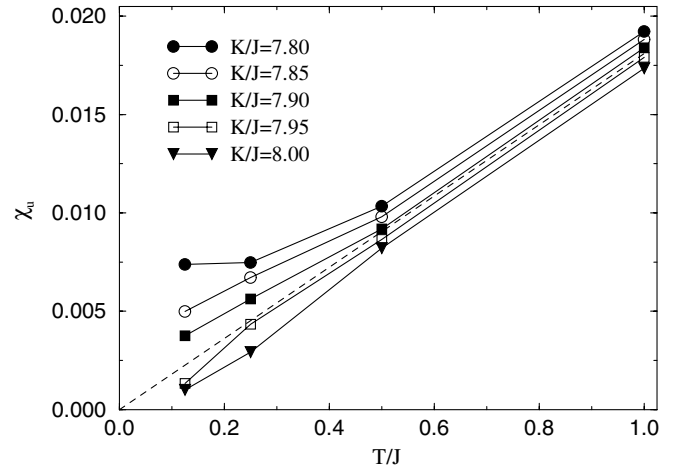


FIG. 4. Temperature dependence of the uniform magnetic susceptibility for $L = 80$ systems close to the superfluid-stripped transition. Statistical errors are of the order of the size of the symbols. The dashed line shows the linear behavior expected for a quantum phase transition with $z = 1$.

being the behavior in the XY model [18,23,27]. The behavior for $K/J = 7.90$ and 7.95 is consistent with $\chi_u \sim T$ at the critical coupling, which is indicative of a $T = 0$ quantum critical point with dynamic exponent $z = 1$ [28,29]. At $K/J \approx 7.9$ we have verified that the stripe structure factor indeed exhibits nontrivial finite-size scaling, $P(\pi, 0) \sim L^\epsilon$ with $\epsilon < 2$, but the statistical accuracy is not sufficient for determining the exponent to a meaningful precision. Nevertheless, power-law scaling for the same K/J at which the spin gap opens supports a continuous quantum phase transition with no intervening disordered phase or coexistence region.

In summary, the spin-1/2 XY model with ring exchange exhibits three different ground state orderings as a function of the strength of the ring term. The superfluid-stripped transition appears to be a continuous quantum phase transition, whereas the striped-staggered transition most likely is of first order. Since the sign of the J term in (3) is irrelevant (the sign of the K term is relevant) the superfluid-stripped transition could possibly, in an extended parameter space, connect to the order-disorder transition in the two-dimensional Heisenberg antiferromagnet with frustrating interactions [30]. We also note that the staggered-stripped-superfluid phase behavior versus J/K shows interesting similarities to the high- T_c cuprates, where the pseudogap phase intervening between the antiferromagnetic and superconducting phases exhibits strong stripe correlations [31]. Although the microscopic physics and symmetries are clearly different, a detailed study of the staggered-stripped transition may still be useful in this context.

In spite of the absence of a spin liquid phase, the presence of three distinct ordered ground states, and the phase transitions between them, puts the J - K model (3) in an important class among the basic quantum many-body Hamiltonians. Although the interesting large- K/J region

may not be of direct relevance to real systems, we expect this and the related model to be very useful as systems where complex quantum states and quantum phase transitions can be further explored on large lattices without approximations. Although other models, such as the frustrated J_1 - J_2 Heisenberg model [30], may show similar or potentially even more complex behavior, sign problems affecting quantum Monte Carlo makes it difficult to obtain conclusive results. It would clearly be interesting to study also the J - K model with a positive sign for the K term, in particular, to determine whether fractionalized spin liquid phases could arise, but unfortunately this also leads to sign problems.

The J - K model with the sign of K chosen here can be modified in several interesting ways and still be easily accessible to simulations using the SSE method. For example, when relaxing the hard-core constraint there should be a transition to an exciton Bose liquid [16], both as a function of on-site repulsion U for large K/J and as a function of K/J . It will also be interesting to include a magnetic field to “dope” the striped and staggered phases. Transitions between different charge-density phases and the question of the existence of doped super-solid phases have recently been studied numerically for boson models where charge-density phases are stabilized due to diagonal density-density interactions [32]. In contrast, the striped phase found here arises out of a competition between two kinetic terms and it may hence behave differently upon doping.

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