Stripped phase in a quantum XY-model with ring exchange

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We present quantum Monte Carlo results for a square-lattice 2D 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 3 He 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 $J$ and are often neglected. Four-spin ring exchange has, however, been argued to be responsible for distinct features in the magnetic Raman 5 and optical absorption spectra 6. Neutron measurements of the magnon dispersion 7 have previously been applied to a variety of spin and lattice field-theory including a plaquette term 8. The SSE simulation method 9, 10, 11, 12, 13, 14, 15 that we use here has previously been applied to a variety of spin and boson models with two-particle interactions, including the Hamiltonian (4) with $K = 0$ (the XY-model) 16. The generalization to include the four-spin $K$-term is relatively straightforward, although non-trivial new procedures had to be developed for large-$K/J$ simulations 17. 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 symmetries are then broken and a unique static bond-plaquette strength pattern can be observed when $K/J \approx 10$ 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 limit. Results for $K/J=8$ and temperatures sufficiently low to give the ground state are shown in Fig. 3. For $L \gtrsim 32$ the data graphed versus $1/L$ fall on a straight line, which extrapolates to a non-zero value as $L \to \infty$. Based on results for the soft-core version of the $J=0$ model (or $K \to \infty$) the staggered magnetization can be expected to be non-zero for large $K$. However, as also shown in Fig. 3 at $K/J=8.5$ the $\langle M_2^z \rangle$ decreases as $1/L^2$ for large lattices, implying that the spin-spin correlations are short ranged in this case. Fig. 3 also shows results for $K/J=64$, where the scaling behaviors of the two quantities is reversed$-$(5) decays as $1/L^2$ whereas $\langle M_2^z \rangle$ extrapolates to a non-zero value. Note that the size-dependence of $M_2^z$ is non-monotonic, with a minimum around $L \approx 10$. Such non-monotonicity has been observed for a spatially anisotropic spin model where it was attributed to the presence of two different low-energy scales in the system. The non-monotonicity seen at $K/J=64$ in Fig. 3 indicates that
the uniform magnetic susceptibility, can be inferred also from the temperature dependence of
Fig. 2 indicates the opening of a spin gap. A spin gap
in Ref. 13). The vanishing of the spin stiffness seen in
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order, although we cannot exclude a very weakly
region.
First-order transition. Simulations of larger lattices will
the two phases could either co-exist or be separated by a
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 ∼ 1/L^2 expected asymptotically when there is no long-range order.

the stripe correlations remain strong with a correlation length ∼ 10 lattice spacings. The location of the minimum in ⟨M^2⟩ moves to lower 1/L as K/J is decreased, indicating growing stripe correlations. The strong stripe correlations in the staggered phase makes it difficult to
determine the ⟨M_S⟩ 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 ≥ 16. Between K/J = 12 and 16
the two phases could either co-exist 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-striped 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,

\[ \chi_u = \frac{1}{L^2 T} \left( \sum_i S_i^z \right)^2. \]  \hspace{1cm} (9)

Fig. 4 shows the T-dependence for L = 80 (sufficiently
large to eliminate finite-size effects). The T → 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 being the behavior in the XY-model [18, 23, 27].
The behavior for K/J = 7.90 and 7.95 is consistent with
χ_u ∼ T at the critical coupling, which is indicative of
a T = 0 quantum critical point with dynamic exponent
z = 1 [23, 29]. At K/J ≈ 7.9 we have verified that the
stripe structure factor indeed exhibits non-trivial finite-
size scaling, P(π, 0) ∼ L^ε with ε < 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 co-existence 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-striped 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-striped transition could possibly, in an extended parameter space, connect to the
order-disorder transition in the two-dimensional Heisenberg antiferromagnet with frustrating interactions [31].
We also note that the staggered-striped-superfluid phase behavior versus J/K shows interesting similarities to the
high-T_c cuprates, where the pseudogap phase interven-
ing between the antiferromagnetic and superconducting
phases exhibits strong stripe correlations [30]. Although
the microscopic physics and symmetries are clearly differ-
ent, a detailed study of the staggered-striped 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 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 [31], 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 a exciton Bose liquid phase [6], 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 supersolid 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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[1] D. J. Thouless, Proc. Phys. Soc. 86, 893 (1965).
[2] M. Roger, J. H. Hetherington, and J. M. Delrieu, Rev. Mod. Phys. 55, 1 (1983); M. Roger et al., Phys. Rev. Lett. 80, 1308 (1998); G. Misguich et al., ibid. 81, 1098 (1998).
[3] K. Voelker and S. Chakravarty, Phys. Rev. B 64, 235125 (2001).
[4] B. Bernu, L. Candido, and D. M. Ceperley, Phys. Rev. Lett. 86, 870 (2001).
[5] B. S. Shastry and B. I. Shraiman, Phys. Rev. Lett. 65, 1668 (1990); Int. J. Mod. Phys. B 5, 365 (1991).
[6] M. Roger and J. M. Delrieu, Phys. Rev. B 39, 2299 (1989); Y. Honda, Y. Kuramoto, and T. Watanabe, Phys. Rev. B 47, 11320 (1993).
[7] J. Lorenzana, J. Eroles, and S. Sorella, Phys. Rev. Lett. 83, 5122 (1999).
[8] R. Coldea et al., Phys. Rev. Lett. 86, 5377 (2001).
[9] M. Matsuda et al., Phys. Rev. B 62, 8903 (2000).
[10] G. Misguich et al, Phys. Rev. B 60, 1064 (1999).
[11] T. Senthil and M. P. A. Fisher, Phys. Rev. B 63, 134521 (2001).
[12] L. Balents, M. P. A. Fisher, and S. M. Girvin, Phys. Rev. B 65, 224412 (2002).
[13] S. Sachdev and K. Park, Annals of Physics (N.Y.) 298, 58 (2002).
[14] R. D. Sedgewick, D. J. Scalapino, and R. L. Sugar Phys. Rev. B 65, 054508 (2002).
[15] E. Demler et al., Phys. Rev. B 65, 155103 (2002).
[16] A. Paramekanti, L. Balents, and M. P. A. Fisher, Phys. Rev. B 66, 054526 (2002).
[17] A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B 43, 5950 (1991); A. W. Sandvik, J. Phys. A 25, 3667 (1992).
[18] A. W. Sandvik, Phys. Rev. B 59, R14157 (1999).
[19] O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E 66, 046701 (2002).
[20] E. Loh, D. J. Scalapino, and P. M. Grant, Phys. Rev. B 31, 4712 (1985).
[21] K. Harada and N. Kawashima Phys. Rev. B 55, R11949 (1998).
[22] J. Oitmaa and D. B. Betts, Can. J. Phys. 56, 897 (1978); S. Zhang and K. J. Burne, Phys. Rev. B 45, 1052 (1992).
[23] A. W. Sandvik and C. J. Hamer, Phys. Rev. B 60, 6588 (1999).
[24] In order to implement the SSE “operator-loop” algorithm when the $K$-term is included, all operators in the Hamiltonian are expressed as plaquette operators, i.e., a bond-operator $B_{ij}$ is written as $B_{ij}I_{ik}$, where $I_{kl}$ is a unit operator. Constant operators $c_{ijkl}$ are introduced in order to carry out the SSE “diagonal update”. The operator-loops are one-dimensional closed operator paths along which substitutions of the types $c_{ijkl} \leftrightarrow B_{ij}I_{kl}$ and $B_{ij}I_{kl} \leftrightarrow P_{ijkl}$ are accomplished. The performance can be optimized using “directed loop” detailed balance equations of the type introduced in Ref. [9]. The above scheme does not work when $J = 0$ and is inefficient for large $K/J$. A new type of cluster update effecting substitutions of the type $P_{ijkl} \leftrightarrow c_{ijkl}$ has been developed in order to study large $K/J$. Further details of the simulation algorithm will be presented elsewhere.
[25] A. W. Sandvik, Phys. Rev. B 56, 11678 (1997).
[26] A. W. Sandvik, Phys. Rev. Lett. 83, 3069 (1999).
[27] P. Hasenfratz and F. Niedermayer, Z. Phys. B 92, 91 (1993).
[28] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. 60, 1057 (1988); Phys. Rev. B 39, 2344 (1989).
[29] A. V. Chubukov, S. Sachdev, and J. Ye, Phys. Rev. B 49, 11919 (1994).
[30] E. W. Carlson, V. J. Emery, S. A. Kivelson, and D. Orgad, cond-mat/0206217.
[31] N. Read and S. Sachdev, Phys. Rev. Lett. 62, 1694 (1989); L. Capriotti et al., ibid. 87, 097201 (2001); O. P. Sushkov, J. Oitmaa, and Z. Wei, Phys. Rev. B 63, 104420 (2001).
[32] F. Hébert et al., Phys. Rev. B 65, 014513 (2002).