PHYSICAL REVIEW B **69**, 100408(R) (2004)

Two-dimensional quantum *XY* model with ring exchange and external field

R. G. Melko,[1] A. W. Sandvik,[2] and D. J. Scalapino[1]
[1]*Department of Physics, University of California, Santa Barbara, California 93106, USA*
[2]*Department of Physics, Åbo Akademi University, Porthansgatan 3, FIN-20500 Turku, Finland*
(Received 6 November 2003; published 19 March 2004)

We present the zero-temperature phase diagram of a square lattice quantum spin-1/2 XY model with four-site ring exchange in a uniform external magnetic field. Using quantum Monte Carlo techniques, we identify various quantum phase transitions between the XY order, striped or valence bond solid, staggered Néel antiferromagnet and fully polarized ground states of the model. We find no evidence for a quantum spin liquid phase.

DOI: 10.1103/PhysRevB.69.100408 PACS number(s): 75.10.Jm, 05.30.−d, 75.40.Mg

Studies of two-dimensional spin-1/2 quantum magnet and boson models have provided insight into novel quantum phases and quantum critical points.[1] Recently, interest has focused on models which have multisite ring exchange.[2–4] The ring exchange interaction, either alone or in competition with the usual spin or boson near-neighbor exchange, has been shown to promote a variety of exotic quantum ground states,[3] including in some cases a spin-liquid state.[4] Of particular importance is the class of two-dimensional model Hamiltonians that contain quantum spin-1/2 or boson operators interacting with ring exchange that can be simulated using quantum Monte Carlo (QMC) techniques without a negative sign problem. With modern algorithms, such models can be studied numerically on large lattices without approximation, providing a laboratory for surveying the critical behavior that separates various quantum phases.

One important model in this respect is the easy-plane J-K model[5] that has quantum $S=1/2$ spins on a square lattice with a near-neighbor exchange J and a four-site ring exchange K. This Hamiltonian is partially motivated by the undoped cuprate materials,[6] where ring-exchange processes are believed to contribute to experimental signatures beyond those explained by the near-neighbor Heisenberg model. The two-parameter J-K model, despite its simplicity, displays a surprisingly rich and complex phase diagram,[5,7] with three distinct zero-temperature phases. These are an XY ordered or superfluid phase for large J, a staggered Néel or boson charge-density wave (CDW) phase for large K, and a striped or valence bond solid (VBS) phase for intermediate K/J. The zero-temperature phase transition between the VBS and Néel phases is first order, however previous numerical results[5,7] indicate the existence of a continuous quantum critical point (QCP) at the zero-temperature superfluid-VBS boundary.

The question naturally arises as to the behavior of the easy-plane J-K model under the influence of a magnetic field. This is interesting both as a study of the evolution of the QCP, as well as the behavior of the ground-state phases away from half filling. Using stochastic series expansion (SSE) QMC, we present here the basic features of the zero-temperature phase diagram of the easy-plane model described by the Hamiltonian

$$H=-J\sum_{\langle ij\rangle}B_{ij}-K\sum_{\langle ijkl\rangle}P_{ijkl}-h\sum_{i}S_i^z, \tag{1}$$

where S_i^z is the z component of a quantum spin 1/2, $B_{ij}=S_i^+S_j^-+S_i^-S_j^+$ is a near-neighbor exchange, and $P_{ijkl}=S_i^+S_j^-S_k^+S_l^-+S_i^-S_j^+S_k^-S_l^+$ generates a four-site ring exchange. Here, $\langle ij\rangle$ denotes a pair of nearest-neighbor sites and $\langle ijkl\rangle$ are sites on the corners of a square plaquette on the $L\times L$ lattice. For $K=0$, this is the standard XY model in a uniform magnetic field, or alternatively hard-core bosons with a chemical potential. For $h=0$, this model is in an XY ordered or superfluid phase for temperatures less than the Kosterlitz-Thouless transition temperature of $T_{KT}/J\approx 0.68$.[8] With the application of a uniform magnetic field the average magnetization $m=\langle S^z\rangle$ of the XY superfluid increases from zero ($m=0$) until it saturates into a fully spin polarized ($m=1/2$) state at $h/J\simeq 4$.[9] For $J=0$ and $h=0$, the ground state of the system has Néel antiferromagnetic order.[3,5] For $h=0$, it was found[5,7] that an intermediate VBS phase exists for $7.9\lesssim K/J\lesssim 14.5$, in which the expectation value $\langle P_{ijkl}\rangle$ alternates in strength with a period of two lattice spacings in one of the lattice directions, suggesting the term "striped" order.

To study the effect of the uniform magnetic field h on the ground-state properties of the easy-plane J-K model, we use the SSE quantum Monte Carlo simulation method[10] that was previously applied to the $h=0$, J-K model.[5,7] In order to implement the SSE method, the operators in the Hamiltonian (1) are represented as four-spin *plaquette* operators. Diagonal operators involving h terms are added to or removed from the SSE basis-state expansion using a simple Metropolis probability algorithm. Off-diagonal (J or K term) operators are sampled using the *directed-loop* algorithm,[7,10] which becomes increasingly important for simulation efficiency with increasing magnetic-field strength. The directed-loop equations[10] for the J-K-h model are only slightly more complicated than for the pure J-K model,[7] and are presented elsewhere.[11] The QMC algorithms were tested on $L=4$ lattice sizes against exact diagonalization results and previous QMC simulations on the pure XY and J-K models. In this paper, simulations were carried out on square lattices of linear dimension L (number of spins $N=L^2$) at temperatures $T=1/\beta$ low enough to ensure convergence into the ground state.

A variety of physical observables of direct relevance to the ground states of the model are accessible through the SSE method. It is straightforward to calculate the internal

RAPID COMMUNICATIONS

energy[10] since its statistical estimator is just the number n of plaquette operators in the SSE basis-expansion operator sequence multiplied by T: $E=-\langle n\rangle/\beta$. The spin stiffness (or superfluid density in the boson representation) is defined in terms of the energy response to a twist ϕ in the periodic boundary of the lattice by

$$\rho_s=\frac{\partial^2 E}{\partial\phi^2}, \tag{2}$$

and is directly estimated using the winding number fluctuations in the SSE simulation.[12] In addition we calculate the plaquette structure factor

$$S_p(q_x,q_y)=\frac{1}{L^2}\sum_{a,b} e^{i(\mathbf{r}_a-\mathbf{r}_b)\cdot\mathbf{q}}\langle P_{a_1a_2a_3a_4}P_{b_1b_2b_3b_4}\rangle. \tag{3}$$

Here, $a_1,\ldots,a_4$ are the sites belonging to plaquette a, located at $\mathbf{r}_a$. In the VBS phase, the square of the magnitude of the order parameter per site is $\langle M_P\rangle^2=[S_p(\pi,0)+S_p(0,\pi)]/2L^2$. Similarly, the square of the order parameter $\langle M_S\rangle$ of the Néel ordered phase is obtained from the S^z structure factor

$$S_s(q_x,q_y)=\frac{1}{L^2}\sum_{j,k} e^{i(\mathbf{r}_j-\mathbf{r}_k)\cdot\mathbf{q}}\langle S^z_j S^z_k\rangle, \tag{4}$$

with $\langle M_S\rangle^2=S_s(\pi,\pi)/L^2$. Here, j and k are lattice sites located at lattice coordinate $\mathbf{r}_j$. The quantities $\langle M_P\rangle^2$ and $\langle M_S\rangle^2$ are expected to decrease as $1/L^2$ (signifying short-range correlations) in phases without the respective order, but tend to a finite value for large L in phases where long-range order occurs.

By directly observing the behavior of the spin stiffness (superfluid density) and the VBS and Néel order parameters, we are able to map out the phase boundaries of the J-K-h model as illustrated in Fig. 1. In general, we find no persistent regions of quantum disorder (i.e., a spin liquid state) in the vicinity of the $h=0$ quantum critical point. Rather, the QCP appears to evolve smoothly into a quantum phase transition between the superfluid and VBS regions for $0\leqslant h\lesssim 6$. The J-K-h model also exhibits a direct superfluid to Néel order transition for $6\lesssim h\lesssim 11$, a feature not contained in the $h=0$ phase diagram. Finally, for large h, the model finds a fully polarized spin state with $m=1/2$. This latter phase transition is strongly first order for $K/J\gtrsim 5$, displaying pronounced metastability and hysteresis effects in the simulation (see Fig. 2). Renormalization group treatments of two-dimensional bosons,[13] as well as spin-wave corrected mean-field theory and simulations of a hard-core boson Hamiltonian[9] indicate that at $K=0$, the pure XY model exhibits a continuous transition to the fully polarized state at $h=4J$. This suggests that a tricritical point (TCP in Fig. 1) exists on the phase boundary somewhere between $0<K/J\lesssim 5$, above which the transition to the fully polarized state becomes first order.

The energy crossover and magnetization hysteresis of Fig. 2 provide one indicator of a first-order transition. Alternatively, one may look for an abrupt discontinuity in the order parameter (for large system sizes) or for double-peaked probability histograms for data in the transition region. To illustrate this we turn now to a detailed set of simulation results for the superfluid-Néel phase boundary along cut B in Fig. 1. As illustrated in Fig. 3, the boson and superfluid densities develop significant discontinuities for larger systems as the phase boundary is traversed. This abrupt discontinuity does not appear for $L<20$, illustrating that the transition is caused by an avoiding level crossing and that large lattices sizes are necessary to quantify the behavior of this model. The first-order nature is apparent in double-peaked magnetization histograms, which were observed for data in the "discontinuity" regions for $L=16$, indicating a phase coexistence. For

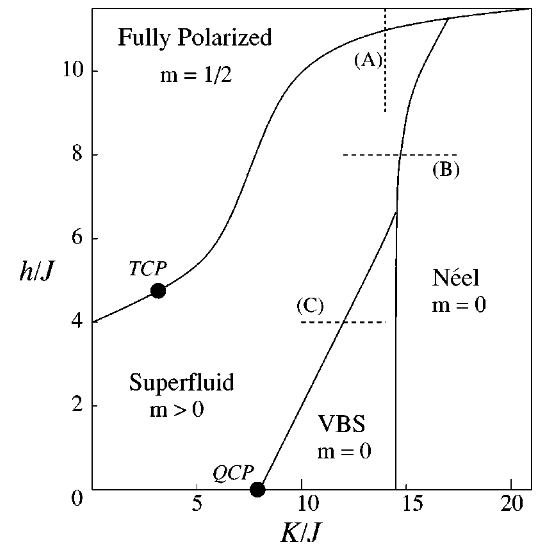

FIG. 1. The schematic zero-temperature phase diagram of the easy-plane J-K-h model. Phase boundaries are drawn as solid lines. Dashed lines indicate cuts along which we have examined the transitions between the various phases, as discussed in the text.

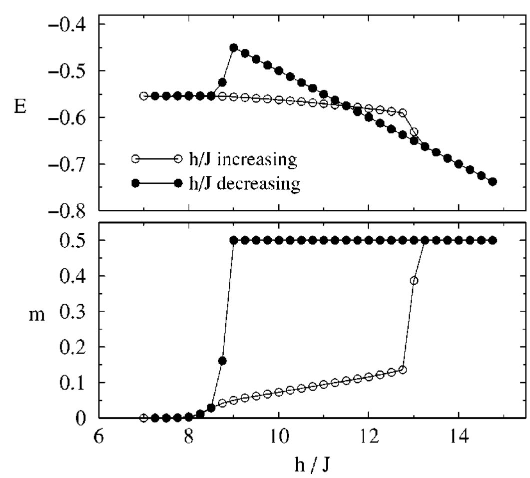

FIG. 2. The ground-state energy (E) and magnetization (m) of an $L=8$ system along cut A in the phase diagram Fig. 1. This set of simulations was performed with parameters $K/J=14$ and $\beta J=3.2$. The hysteresis effects were obtained by systematically increasing and then decreasing K/J in steps, with system configurations stored at the end of one K/J step and used to begin the next.

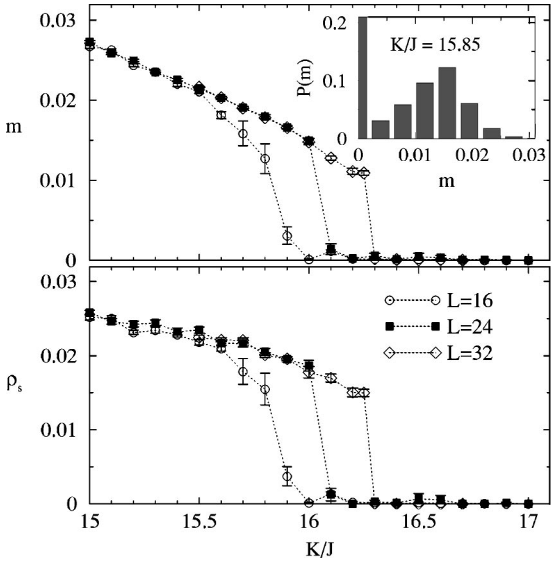

FIG. 3. Magnetization (m) and spin stiffness (ρ_s) of the superfluid-Néel transition, along cut B in the phase diagram Fig. 1. Model parameters are $h/J=8$, $\beta J=3.2$ for $L=16$ and $\beta J=4.0$ for the larger lattice sizes. The inset shows a double-peaked magnetization probability histogram $P(m)$ representing 5×10^5 Monte Carlo steps at a point on the $L=16$ data curve in the transition region. The lower peak is not Gaussian in shape, as the system is attracted to zero magnetization (the half-filled) state.

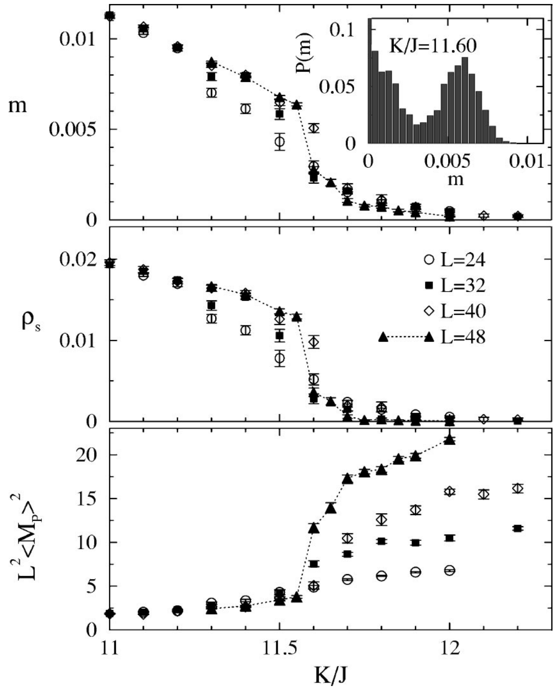

FIG. 4. Details of the magnetization, spin stiffness, and the VBS structure factor of the superfluid-VBS transition, along cut C in the phase diagram Fig. 1. Model parameters are $h/J=4$, $\beta J=3.2$ for $L=24$ and $\beta J=4.0$ for the larger lattice sizes. The inset shows a double-peaked magnetization probability histogram $P(m)$ representing 3.5×10^5 Monte Carlo steps at a point on the $L=48$ data curve in the transition region.

$K/J\gtrsim16.3$, the spin-spin structure factor [Eq. (4)] develops Bragg peaks at (π,π) (not illustrated), indicating Néel order. It is interesting to note that a similar phase transition between a superfluid and a (π,π) staggered solid is found in hard-core boson Hubbard models with nearest and next-nearest-neighbor repulsion.[14,15]

Finally we examine the *XY* superfluid-VBS transition along cut C. As illustrated in Fig. 4, simulation data for system size $L=24$ do not display an obvious sharp discontinuity as in Fig. 3. However, the presence of a small discontinuity in m and ρ_s for $L=32$–48 is suggested by the data. The inset of Fig. 4 displays a double-peaked magnetization probability histogram in the transition region, which indicates the presence of a first-order phase coexistence. This clearly precludes the existence of a continuous quantum phase transition, at least for the field value $h/J=4$ that was studied in cut C (see Fig. 1). The most immediate conclusion to draw is that the superfluid-VBS phase transition is weakly first order, either along its entirety (excluding the $h=0$ QCP), or up to a tricritical point at a field $0<h<4$. In this case, the difficulty in seeing a large discontinuity in the superfluid density or plaquette structure factor is due to the small h value and the closeness of the magnetization to zero. The persistence of a small region of superfluid density in apparent coexistence with a finite VBS order parameter (for example, the two data points for $L=48$, $K/J=11.60$, and 11.65 in Fig. 4) is due to the first-order metastability between the superfluid phase and the VBS phase that is obscured by statistical averaging. As a check, we observed the Monte Carlo time correlation between $S_p(\pi,0)$, $S_p(0,\pi)$, and the superfluid density ρ_s in the x and y directions at these points. In fact, we find that ρ_s show no preference for the x or y directions when stripe order is present. Rather, both ρ_s^y and ρ_s^x show very strong anticorrelations whenever $\langle M_P\rangle^2$ develops Bragg peaks.

In summary, using SSE QMC techniques, we have determined the ground-state phase diagram (Fig. 1) of the easy-plane *J-K-h* model. In addition to the *XY* superfluid, VBS, and Néel ordered phases observed for $h=0$,[5] we observe a large region of fully polarized order, which dominates the phase diagram for large h. The phase transition to the polarized state is continuous at small K/J and strongly first order for large K/J, suggesting the existence of a tricritical point somewhere on the phase boundary for intermediate K/J. Two other phase transitions were studied in detail, the superfluid-Néel and superfluid-VBS transitions. Both were first order for the parameter values investigated in detail here.

As indicated by our data, the *J-K-h* model does not appear to support a region of superfluid-VBS coexistence (i.e., a supersolid), which is observed near a similar transition between a superfluid and $(\pi,0)$ striped solid phase in a hard-core boson Hubbard model.[15,16] No additional ordered phases were observed in this model, in particular, incommensurate VBS stripes (or striped order away from half filling) which would have been indicated by Bragg peaks in the **q**-dependent structure factor $S_p(q_x,q_y)$ away from $(\pi,0)$.

In the context of the $h=0$ superfluid-VBS transition at $T=0$,[5,7] the existence of a continuous QCP does not require a continuous phase transition to develop smoothly as h is increased from zero. Conversely, the existence of a true continuous phase transition would provide additional supporting evidence for the existence of the $h=0$ QCP,[17] as well as a further region in which to explore the nature of the critical behavior associated with the transition from XY superfluid to VBS order. Ultimately, one would like to determine whether this QCP is an example of the ‘‘deconfined’’ quantum criticality recently discussed by Senthil *et al.*[18]

Finally, the inability of any significant region of a spin-liquid phase to develop in the vicinity of the QCP motivates further searches on related models. Of particular interest is the square lattice J-K ring model in a *staggered* magnetic field, which could conceivably destabilize the superfluid or VBS order near the QCP and promote the development of an extended region of disorder.[19] Work on this model is in progress.[11]

The authors would like to thank L. Balents and M. P. A. Fisher for insightful discussions and a critical reading of the manuscript. This work was supported by the National Science Foundation, Grant No. DMR02-11166 (D.J.S.), and by The Academy of Finland, Project No. 26175 (A.W.S.). Supercomputer time was provided by NCSA under Grant No. DMR020029N. A.W.S. would like to thank the Department of Physics at UCSB for hospitality and support during a visit.

[1] S. Sachdev and K. Park, Ann. Phys. (N.Y.) **298**, 58 (2002); R.D. Sedgewick, D.J. Scalapino, and R.L. Sugar, Phys. Rev. B **65**, 054508 (2002); T. Senthil and M.P.A. Fisher, *ibid.* **63**, 134521 (2001).

[2] L. Balents and A. Paramekanti, Phys. Rev. B **67**, 134427 (2003); A. Läuchli, G. Schmid, and M. Troyer, *ibid.* **67**, 100409 (2003).

[3] A. Paramekanti, L. Balents, and M.P.A. Fisher, Phys. Rev. B **66**, 054526 (2002).

[4] G. Misguich, C. Lhuillier, B. Bernu, and C. Waldtmann, Phys. Rev. B **60**, 1064 (1999); L. Balents, M.P.A. Fisher, and S.M. Girvin, *ibid.* **65**, 224412 (2002); M. Hermele, M.P.A. Fisher, and L. Balents, Phys. Rev. B **69**, 064404 (2004).

[5] A.W. Sandvik, S. Daul, R.R.P. Singh, and D.J. Scalapino, Phys. Rev. Lett. **89**, 247201 (2002).

[6] M. Roger and J.M. Delrieu, Phys. Rev. B **39**, 2299 (1989); Y. Honda, Y. Kuramoto, and T. Watanabe, *ibid.* **47**, 11 329 (1993); J. Lorenzana, J. Eroles, and S. Sorella, Phys. Rev. Lett. **83**, 5122 (1999); R. Coldea *et al.*, *ibid.* **86**, 5377 (2001).

[7] A. W. Sandvik and D. J. Scalapino (unpublished).

[8] K. Harada and N. Kawashima, J. Phys. Soc. Jpn. **67**, 2768 (1998); R.G. Melko, A.W. Sandvik, and D.J. Scalapino, Phys. Rev. B **69**, 014509 (2004).

[9] K. Bernardet, G.G. Batrouni, J.-L. Meunier, G. Schmid, M. Troyer, and A. Dorneich, Phys. Rev. B **65**, 104519 (2002).

[10] A.W. Sandvik, Phys. Rev. B **59**, 14 157 (1999); O.F. Syljuåsen and A.W. Sandvik, Phys. Rev. E **66**, 046701 (2002).

[11] R.G. Melko, A.W. Sandvik, and D.J. Scalapino (unpublished).

[12] E.L. Pollock and D.M. Ceperley, Phys. Rev. B **36**, 8343 (1987); A.W. Sandvik, *ibid.* **56**, 11 678 (1997).

[13] D.S. Fisher and P.C. Hohenberg, Phys. Rev. B **37**, 4936 (1987); S. Sachdev, T. Senthil, and R. Shankar, *ibid.* **50**, 258 (1994).

[14] G. Schmid, S. Todo, M. Troyer, and A. Dorneich, Phys. Rev. Lett. **88**, 167208 (2002).

[15] F. Hebert, G.G. Batrouni, R.T. Scalettar, G. Schmid, M. Troyer, and A. Dorneich, Phys. Rev. B **65**, 014513 (2001).

[16] E. Frey and L. Balents, Phys. Rev. B **55**, 1050 (1996); C. Pich and E. Frey, *ibid.* **57**, 13 712 (1997); G. Schmid and M. Troyer, cond-mat/0304657 (unpublished).

[17] However, differentiating numerically between a continuous or a weakly first-order superfluid-VBS phase transition for fields less than $h/J=4$ would be exceeding difficult using the techniques illustrated in this study, requiring lattice sizes of 10^4 sites or more.

[18] L. Balents and M.P.A. Fisher (private communication); T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M.P.A. Fisher, Science **303**, 1490 (2004); T. Senthil, L. Balents, S. Sachdev, A. Vishwanath, and M.P.A. Fisher, cond-mat/0312617 (unpublished).

[19] O.I. Motrunich and A. Vishwanath, cond-mat/0311222 (unpublished).