Superfluid phases of lattice bosons with ring-exchange interaction

Robert Schaffer, Anton A. Burkov, and Roger G. Melko
Department of Physics and Astronomy, University of Waterloo, Ontario, Canada N2L 3G1
(Received 9 November 2008; revised manuscript received 10 June 2009; published 7 July 2009)

We examine the superfluid phase of a hard-core boson model with nearest-neighbor exchange J and four-particle ring-exchange K at half filling on the square lattice. At zero temperature we find that the uniform superfluid in the pure-J model is quickly destroyed by the inclusion of negative-K ring-exchange interactions, favoring a state with a (π,π) ordering wave vector. Minimization of the mean-field energy suggests that another type of superfluid state, characterized by nonzero bond chirality, is formed. We also study the behavior of the finite-T Kosterlitz-Thouless phase transition in the uniform superfluid phase, by forcing the Nelson-Kosterlitz universal jump condition on the finite-T spin-wave superfluid density. Away from the pure J point, T_{KT} decreases rapidly for negative K, while for positive K, T_{KT} reaches a maximum at some $K\neq 0$ in agreement with recent quantum Monte Carlo simulations.

DOI: 10.1103/PhysRevB.80.014503 PACS number(s): 67.25.dj, 67.80.kb, 05.30.Jp, 67.85.Bc

I. INTRODUCTION

The road to discovering new quantum phenomena such as exotic phases or unconventional quantum-phase transitions is paved by the understanding of quantum Hamiltonians with competing microscopic interactions. Recent work has shown that competing kinetic energy terms, particularly four-particle "ring-exchange," is a fertile venue for the study of valence-bond solids and unconventional quantum-phase transitions.[1–4]

Long relegated to toy models of easy-plane spin systems or simple boson theories, the understanding of U(1) Hamiltonians has resurfaced as critical for the engineering of exotic quantum phases of ultracold atoms in optical lattices. Buchler *et al.*[5] presented the design of a ring-exchange interaction for bosonic cold atoms in two-dimensional (2D) square optical lattices. There, a conventional nearest-neighbor hopping term competes with a four-particle ring-exchange, which arises out of the hopping of boson pairs on the corners of square lattice plaquettes to an intermediate molecular state and back to the (opposite) plaquette corners. The Hamiltonian proposed in Ref. 5 can be written,

$$H=-J\sum_{\langle ij\rangle}(b_i^{\dagger}b_j+b_ib_j^{\dagger})-K\sum_{\langle ijkl\rangle}(b_i^{\dagger}b_jb_k^{\dagger}b_l+b_ib_j^{\dagger}b_kb_l^{\dagger}), \tag{1}$$

where the first term is the usual boson hopping, and the second is the ring-exchange interaction. Here, i and j are neighboring sites, lying opposite to sites l and k (respectively), which together form the basic square plaquette of the 2D lattice. This model has drawn significant attention recently from proposals that it may harbor an exotic quantum liquid phase that possesses d-wave correlations—a so-called d-wave Bose liquid (DBL) phase[6]—including extensive numerical investigation using exact diagonalization and the density matrix renormalization group.[7]

The main difficulty with the Hamiltonian (1) that prevents an exact solution in 2D for large systems (or the thermodynamic limit) is the presence of the prohibitive "sign-problem" in quantum Monte Carlo (QMC) simulations for the parameter regime $K<0$. In fact, the same model in the parameter regime without the sign problem, $K>0$, has been solved by QMC previously both at half filling[2] and in the presence of a symmetry-breaking chemical potential.[8] In this model, it was demonstrated[2] that the uniform superfluid phase that dominates for large J is destroyed by increasing the magnitude of the ring-exchange interaction, which realizes first a $(\pi,0)$ valence-bond solid (VBS) for $8<K/J<14$, and a (π,π) charge-density-wave (CDW) for $K>14$. The intermediate superfluid to VBS quantum-phase transition was studied intensely[9] as one of the first candidates for a *deconfined* quantum critical point.[10] However, other interesting behavior occurs in the model, in particular in the experimentally relevant regime of finite temperatures, where relatively little attention has been paid.[9]

In order to elucidate the mechanism by which the superfluid phase, which occurs for dominant J in Eq. (1), is destroyed by the four-site K interaction, we explore in this paper the behavior of the model using linear spin-wave (SW) theory. First, we calculate the dispersion and superfluid density ρ_s at $T=0$, where its behavior as a function of K indicates the realization of a phase with (π,π) symmetry for $K/J<-2$. Exploring the ordering nature of this phase in mean-field theory reveals a (π,π) modulated in-plane order parameter, which can be interpreted as a type of superfluid with bond-phase chirality. In the uniform superfluid phase, we also calculate the superfluid density at finite-temperature, and estimate the position of the Kosterlitz-Thouless (KT) transition using the universal jump condition. Interestingly, for $K>0$ the linear spin-wave theory reproduces the QMC result[9] that the maximum temperature of the KT transition does *not* occur when $K=0$, rather it happens at some intermediate value of K/J.

II. LINEAR SPIN-WAVE THEORY AT $T=0$

In order to study the destruction of the uniform superfluid phase by the competing ring-exchange interaction parameterized by K, we begin by examining the behavior of the system at $T=0$ in a linear spin-wave analysis. To begin, it is helpful to write our hard-core boson Hamiltonian as the analogous 2D spin-1/2 XY model using the standard mapping: $b_i^{\dagger}\rightarrow S_i^{+}$

and $b_i \rightarrow S_i^-$. This transforms the Hamiltonian Eq. (1) into

$$H = -J\sum_{\langle ij\rangle}(S_i^+S_j^- + S_i^-S_j^+) - K\sum_{\langle ijkl\rangle}(S_i^+S_j^-S_k^+S_l^- + S_i^-S_j^+S_k^-S_l^+), \tag{2}$$

which can be written with S^x and S^y operators as

$$H = -2J\sum_{\langle ij\rangle}(S_i^xS_j^x + S_i^yS_j^y) - 2K\sum_{\langle ijkl\rangle}(S_i^xS_j^xS_k^xS_l^x + S_i^xS_j^xS_k^yS_l^y - S_i^xS_j^yS_k^xS_l^y + S_i^xS_j^yS_k^yS_l^x + S_i^yS_j^xS_k^xS_l^y - S_i^yS_j^xS_k^yS_l^x + S_i^yS_j^yS_k^xS_l^x + S_i^yS_j^yS_k^yS_l^y). \tag{3}$$

As mentioned above, the ground state of the pure-J Hamiltonian is a bosonic superfluid, or an in-plane ferromagnet in the spin language, with an order parameter $\langle S^x\rangle \neq 0$ at zero temperature. We therefore perform our spin-wave expansion around this ordered state, treating the K term of the Hamiltonian as a perturbation. As first demonstrated by Gomez-Santos and Joannopoulos,[11] the proper Holstein-Primakoff representation in the case of the XY model is

$$S_i^x \approx \frac{1}{2} - a_i^\dagger a_i,$$

$$S_i^y \approx \frac{1}{2i}(a_i^\dagger - a_i), \tag{4}$$

giving us a leading order approximation to the Hamiltonian in terms of bosonic spin-wave operators a_i and $a_i^\dagger$. Writing the Hamiltonian in Fourier space gives the linear spin-wave Hamiltonian

$$H = H_{\text{MF}} + \sum_{\mathbf{k}}[A_{\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}}) + B_{\mathbf{k}}(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}}a_{-\mathbf{k}})]. \tag{5}$$

Here, the mean-field energy is

$$H_{\text{MF}} = -JN - \frac{KN}{8}, \tag{6}$$

while the coefficients $A_{\mathbf{k}}$ and $B_{\mathbf{k}}$

$$A_{\mathbf{k}} = JU_{\mathbf{k}} + KV_{\mathbf{k}}, \tag{7}$$

$$B_{\mathbf{k}} = JW_{\mathbf{k}} + KX_{\mathbf{k}} \tag{8}$$

are defined in terms of

$$U_{\mathbf{k}} = 2 - \frac{1}{2}\gamma_{\mathbf{k}}, \tag{9}$$

$$V_{\mathbf{k}} = \frac{1}{2} - \frac{1}{4}\gamma_{\mathbf{k}} + \frac{1}{4}\cos k_x \cos k_y, \tag{10}$$

$$W_{\mathbf{k}} = \frac{1}{2}\gamma_{\mathbf{k}}, \tag{11}$$

$$X_{\mathbf{k}} = \frac{1}{4}\gamma_{\mathbf{k}} - \frac{1}{4}\cos k_x \cos k_y, \tag{12}$$

where

$$\gamma_{\mathbf{k}} = \cos k_x + \cos k_y. \tag{13}$$

This form for the SW Hamiltonian reduces to that obtained by Bernardet *et al.*[12] in the limit of the simple XY model ($K=0$) and the absence of an external magnetic field. Following Ref. 12, we diagonalize Eq. (5) using a Bogoliubov transformation,

$$a_{\mathbf{k}} = u_{\mathbf{k}}\alpha_{\mathbf{k}} - v_{\mathbf{k}}\alpha_{-\mathbf{k}}^\dagger, \quad a_{\mathbf{k}}^\dagger = u_{\mathbf{k}}\alpha_{\mathbf{k}}^\dagger - v_{\mathbf{k}}\alpha_{-\mathbf{k}}, \tag{14}$$

where $\alpha_{\mathbf{k}}$ and $\alpha_{\mathbf{k}}^\dagger$ are destruction and creation operators for quasiparticles of momentum $\mathbf{k}$. The bosonic commutation relations are satisfied if

$$u_{\mathbf{k}} = \cosh(\varphi_{\mathbf{k}}), \quad v_{\mathbf{k}} = \sinh(\varphi_{\mathbf{k}}), \tag{15}$$

where φ_k is determined by the requirement that it diagonalizes our Hamiltonian. This yields

$$u_{\mathbf{k}}^2 = \frac{1}{2}\left(\frac{A_{\mathbf{k}}}{\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}} + 1\right), \tag{16}$$

$$v_{\mathbf{k}}^2 = \frac{1}{2}\left(\frac{A_{\mathbf{k}}}{\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}} - 1\right), \tag{17}$$

and thus the diagonalized spin-wave Hamiltonian[12]

$$H = H_{\text{MF}} + \sum_{\mathbf{k}}(\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2} - A_{\mathbf{k}}) + \sum_{\mathbf{k}}\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}(\alpha_{\mathbf{k}}^\dagger\alpha_{\mathbf{k}} + \alpha_{-\mathbf{k}}^\dagger\alpha_{-\mathbf{k}}). \tag{18}$$

It is the diagonal SW Hamiltonian, in this generalized form, that we now proceed to use to analyze the behavior of our superfluid phase at zero temperature.

A. Dispersion

We begin by studying the dispersion, which is obtained immediately from Eq. (18)

$$\omega_{\mathbf{k}} = 2\sqrt{A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2}. \tag{19}$$

This can be examined as a function of K/J for the Hamiltonian Eq. (2). For $K=0$ and $\mathbf{k}\rightarrow 0$, one reproduces the expected linear dispersion,[12] a feature which survives for moderate $K>0$ (at least to first order in the SW theory)—see Fig. 1. No soft modes develop in the $K>0$ dispersion until very large values of $K/J \approx 10^3$, which is well above the critical value of $K/J=7.91$ where a phase transition to a $(\pi,0)$ VBS is known from QMC.[2] In contrast is the behavior of the dispersion in the $K<0$ regime, which is intractable to QMC methods due to the negative sign problem. In this case, the dispersion reveals the development of soft modes at $\mathbf{k}=(\pi,\pi)$. The value of $\omega_{(\pi,\pi)}$ tends toward 0 as K/J approaches -2, as illustrated in Fig. 1. This indicates that an ordered phase with (π,π) symmetry is realized for suffi-

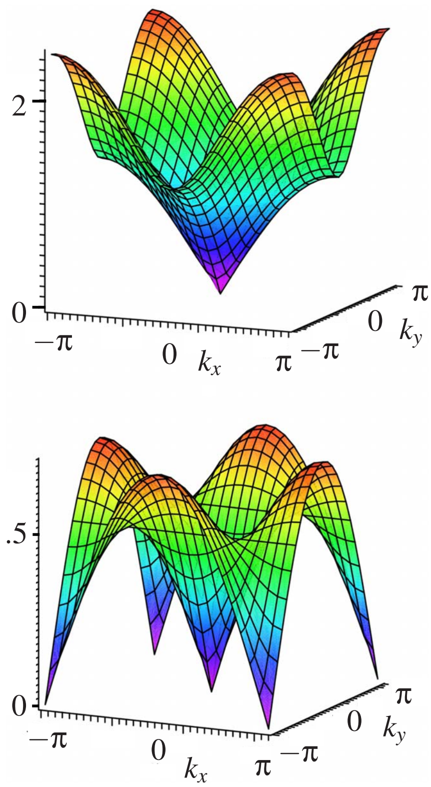

FIG. 1. (Color online) The dispersion $\omega_{\mathbf{k}}$, as a function of $\mathbf{k}=(k_x,k_y)$, for $K/J=2$ (top) and $K/J=-2$ (bottom).

ciently large $|K|$. The nature of this ordering is discussed in Sec. III.

B. Zero-temperature superfluid density

The most important quantity characterizing the superfluid phase is the superfluid density (or spin stiffness), defined as the second derivative of the free energy with respect to a uniform twist ϕ of the in-plane spin components across the system. At zero temperature, one replaces the free energy by the ground-state energy, hence we use the definition

$$\rho_s = \frac{\partial^2 E(\phi)}{\partial^2 \phi}, \tag{20}$$

which is valid for $\phi \to 0$. This is equivalent to finding the incremental energy per spin resulting from the twist,

$$\frac{\Delta E}{N} = \frac{\langle H(\phi)\rangle}{N} - \frac{\langle H(0)\rangle}{N} = \frac{1}{2}\rho_s \phi^2. \tag{21}$$

Thus, we are faced with the task of finding $H(\phi)$. To do this, we consider the spins in a site-dependent rotated reference frame, defined via the standard rotation operator about the z axis.[13] The relevant transformations become

$$S_j^x \to S_j^x \cos \phi_j - S_j^y \sin \phi_j,$$

$$S_j^y \to S_j^x \sin \phi_j + S_j^y \cos \phi_j, \tag{22}$$

which can also be written in terms of the spin raising and lowering operators,

$$S_j^+ \to S_j^+ e^{i\phi_j},$$

$$S_j^- \to S_j^- e^{-i\phi_j}. \tag{23}$$

We assume a uniform twist across the spins in the system, so that the twist $\phi_i - \phi_j \equiv \phi$, where i and j are nearest neighbors in the x or y direction. We find that, using the labeling of Eq. (1), $\phi_j = \phi_k$, $\phi_i = \phi_l$, and thus the ϕ dependence of the ring-exchange term cancels. This gives for our twisted Hamiltonian

$$H(\phi) = -2J\sum_{\langle ij\rangle}[(S_i^x S_j^x + S_i^y S_j^y)\cos \phi + (S_i^x S_j^y - S_i^y S_j^x)\sin \phi]$$
$$- K\sum_{\langle ijkl\rangle}(S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+). \tag{24}$$

The linear components of the term proportional to sin ϕ cancel, so in linear spin-wave theory the twist effectively scales the nearest-neighbor exchange value $J \to J\cos \phi$. Thus, $H(\phi)$ is obtained directly from the Hamiltonian Eq. (5), with the redefinition of

$$H_{\mathrm{MF}}(\phi) = -JN\cos \phi - \frac{KN}{8}, \tag{25}$$

$$A_{\mathbf{k}}(\phi) = JU_{\mathbf{k}} \cos \phi + KV_{\mathbf{k}}, \tag{26}$$

$$B_{\mathbf{k}}(\phi) = JW_{\mathbf{k}} \cos \phi + KX_{\mathbf{k}}, \tag{27}$$

but with the coefficients $U_{\mathbf{k}}$, $V_{\mathbf{k}}$, $W_{\mathbf{k}}$, and $X_{\mathbf{k}}$ unchanged from Eqs. (9)–(12). Expanding cos ϕ as $1-\phi^2/2$, and noting that at zero temperature, the thermal expectation value is

$$n_{\mathbf{k}} = \langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}\rangle = \langle \alpha_{-\mathbf{k}}^\dagger \alpha_{-\mathbf{k}}\rangle = 0, \tag{28}$$

we find that

$$\rho_s = \frac{J}{2} + \frac{1}{2N}\sum_{\mathbf{k}}\{JU_{\mathbf{k}} - (A_{\mathbf{k}}^2 - B_{\mathbf{k}}^2)^{-1/2}\cdot[J^2(U_{\mathbf{k}}^2 - W_{\mathbf{k}}^2)$$
$$+ JK(U_{\mathbf{k}}V_{\mathbf{k}} - W_{\mathbf{k}}X_{\mathbf{k}})]\}. \tag{29}$$

Note that we have divided by a factor of two to account for the fact that Eq. (18) is defined with respect to a twist in a single lattice bond, while Eq. (22) considers a twist in each bond in the lattice, a total of 2N bonds.

The $T=0$ superfluid density calculated in this linear SW theory, Eq. (29), is plotted in Fig. 2 for a range of K/J. Note that, as in the above section, we have set $J=1/2$ to correspond to the usual definition of the XY spin model (when $K=0$). The superfluid density curve has its maximum at $K/J=0$, with a value of $\rho_s=0.2709$, which can be compared to the best numerical estimate for the ground state spin stiffness in the XY model using finite-size scaling quantum Monte Carlo techniques, $\rho_s=0.2696(2)$.[14] Away from this maximum at $K=0$, the superfluid density declines monotonically with increasing $|K|$. On the positive K side, ρ_s decreases relatively gradually, only becoming zero for an extremely large value of $K \approx 10^3$. This is consistent with the above results for the dispersion, which indicate that no soft modes develop for moderate values of positive K. Again, exact QMC results have revealed a $T=0$ quantum phase transition

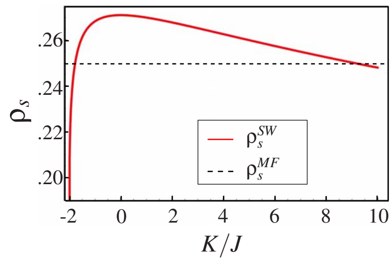

FIG. 2. (Color online) The superfluid density as a function of K/J. The dashed line is the mean-field result, $\rho_s=0.25$. The linear SW result for $K/J=0$ is $\rho_s=0.2709$, which can be compared to the best known exact results $\rho_s=0.2696(2)$ (Ref. 14).

to a valence-bond solid phase at $K/J\approx 7.91$,[2] reiterating the limitations of the linear SW theory calculation in this regime.

On the negative-K side, where no QMC results are available, the value of ρ_s drops rapidly as it approaches -2. In SW theory, there is a divergent negative contribution to ρ_s at this value of $K/J=-2$. This is of course an artifact of linear SW theory. As explained in the next section, one actually expects ρ_s to remain finite on the other side of the transition, where an ordered phase with (π,π) symmetry is realized.

III. BOND-CHIRAL SUPERFLUID PHASE FOR $K<0$

Examining our linear SW theory results of the previous section, for $K/J<-2$ we expect the development of a phase with (π,π) as the ordering wave vector. We can further elucidate the nature of the ordering in this phase by minimizing the mean-field energy of the ring-exchange Hamiltonian, Eq. (1), under the constraint of order with (π,π) symmetry. By representing the quantum spins as classical spin vectors,

$$S_i^x=\frac{1}{2}\sin\,\theta_i\,\cos\,\phi_i, \tag{30}$$

$$S_i^y=\frac{1}{2}\sin\,\theta_i\,\sin\,\phi_i, \tag{31}$$

$$S_i^z=\frac{1}{2}\cos\,\theta_i, \tag{32}$$

we rewrite Eq. (3), which simplifies to the following Hamiltonian:

$$H=-\frac{J}{2}\sum_{\langle ij\rangle}\sin\,\theta_i\,\sin\,\theta_j\,\cos(\phi_i-\phi_j) - \frac{K}{8}\sum_{\langle ijkl\rangle}\sin\,\theta_i\,\sin\,\theta_j\,\sin\,\theta_k\,\sin\,\theta_l\,\cos(\phi_i-\phi_j+\phi_k-\phi_l). \tag{33}$$

Note that the angle of the classical vector from the x axis, ϕ_i, should not be confused with the phase twist variable defined in the previous section. Restricting ourselves to half filling, we look for solutions to the angles θ_i and ϕ_i in the form

$$\theta_i=\theta_0+\theta_1 e^{i\boldsymbol{\pi}\cdot\mathbf{r}_i}, \tag{34}$$

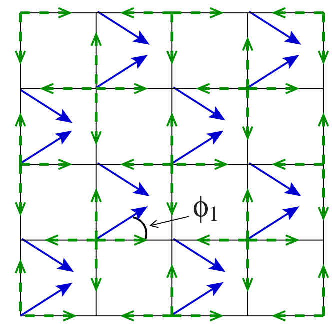

FIG. 3. (Color online) The (π,π) superfluid phase as obtained from mean-field theory, for $K/J<-2$. Solid (blue) arrows show the angles of deviation of the classical spin vectors from the x direction (the out-of plane deviation is zero). The direction of the dashed (green) arrows correspond to the sign of the bond chirality $\mathcal{J}$, Eq. (39).

$$\phi_i=\phi_0+\phi_1 e^{i\boldsymbol{\pi}\cdot\mathbf{r}_i} \tag{35}$$

[where $\boldsymbol{\pi}=(\pi,\pi)$] by minimizing the classical energy Eq. (33). The solution is

$$\theta_0=\pi/2, \tag{36}$$

$$\theta_1=\phi_0=0, \tag{37}$$

$$\phi_1=\frac{1}{2}\arccos\left(\frac{2J}{K}\right). \tag{38}$$

This solution corresponds to a staggered canting of spins away from the x axis, as illustrated in Fig. 3. To describe this state, it is convenient to define a chirality $\mathcal{J}_{ij}$ associated with every bond,

$$\mathcal{J}_{ij}=(\mathbf{S}_i\times\mathbf{S}_j)_z=\sin(\phi_i-\phi_j). \tag{39}$$

In the bosonic language one can think of this state as a superfluid phase with a coexisting (π,π) bond-chirality wave. In spite of the fact that this superfluid breaks translational symmetry, this phase does not correspond to a density wave in the bosonic language. This is because the bond chirality does not have identical transformation properties to the S^z component of the (π,π) staggered magnetization, which would correspond to a (π,π) density wave. Specifically, $\mathcal{J}_{ij}$ does not change sign under (spin) time-reversal transformation, whereas the staggered magnetization does. We note however that, strictly speaking, this argument for the absence of density wave order only holds in the case of hard-core bosons at half filling. The possibility of coexisting superfluidity and charge-density order should be investigated separately for the cases of soft-core bosons away from half filling.

Unlike the uniform superfluid density discussed in this model in Sec. II B, the bond-chiral phase has a mean-field superfluid density,

$$\rho_s = \frac{J^2}{|K|},$$

that vanishes as $K \to -\infty$. No instabilities to other ordered phases are present in the theory at the mean-field level. It is therefore only possible to speculate on the remaining $T=0$ phase diagram for $K<-2$.

One point on the $K<0$ phase diagram where the ordered state is known is at $K/J=-\infty$, which is expected to harbor a phase equivalent to the (π,π) CDW found by QMC simulations for $K/J>14$. To see this, consider the limit $K/J\to\infty$, where the Hamiltonian Eq. (1) for $K<0$ maps exactly onto the Hamiltonian with $K>0$, via a rotation of spins on one of the sublattices by $\pi/2$ around the z axis. Therefore, for finite values of $-\infty<K/J<-2$, two possibilities exist for the evolution of the bond-chiral superfluid state to the CDW; there can be a direct transition between the superfluid and the CDW, or there may be an intermediate valence-bond solid phase like found by QMC for $K/J \gtrsim 8$.

IV. FINITE-TEMPERATURE KOSTERLITZ-THOULESS TRANSITION

We turn now to a discussion of the uniform superfluid phase in the J-K model at finite temperatures. The goal of this section will be to map out the finite-temperature phase boundaries of the superfluid phase in our linear SW theory, to compare (at least in part) to the results obtained in other studies. In the QMC work of Ref. 9, the phase boundary reported has a nontrivial shape, reaching a maximum for a positive value of $K\neq 0$. We are interested in whether this feature can be captured by our SW theory, therefore elucidating the physical mechanism by which this maximum at $K\neq 0$ occurs. To do this, we first develop an expression for the superfluid density for $T>0$ (Sec. IV A), then use it to estimate the SW Kosterlitz-Thouless transition through the universal jump condition (Sec. IV B).

A. Finite-temperature superfluid density

At finite temperatures, we may calculate the superfluid density by recalling its original definition as the response of the free energy with respect to a twist. Calculating the partition function from Eq. (18) we obtain the free energy

$$F = H_{\mathrm{MF}}(\phi) + \sum_{\mathbf{k}} \left(\sqrt{A_{\mathbf{k}}(\phi)^2 - B_{\mathbf{k}}(\phi)^2} - A_{\mathbf{k}}(\phi)\right) + T\sum_{\mathbf{k}} \ln(1 - e^{-\omega_{\mathbf{k}}(\phi)/T}), \tag{40}$$

with the dispersion redefined as

$$\omega_{\mathbf{k}}(\phi) = 2\sqrt{A_{\mathbf{k}}(\phi)^2 - B_{\mathbf{k}}(\phi)^2}. \tag{41}$$

As noted previously, the twist-dependent terms in $H(\phi)$ are proportional to $\cos\phi$, so we can write for $\phi\to 0$

$$F = F(\phi=0) + \frac{2N}{2}\rho_s\phi^2 + \ldots \tag{42}$$

which is properly normalized with $2N$ being the number of lattice bonds. Therefore, we obtain for the superfluid density

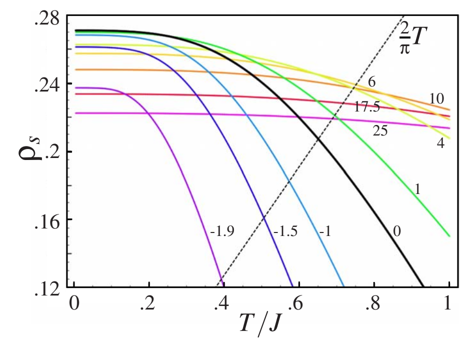

FIG. 4. (Color online) The superfluid density, calculated from Eq. (48), as a function of the temperature. Lines are labeled by the parameter value K/J. The universal jump [Eq. (49)] is illustrated as a dashed line. The exact value for the Kosterlitz-Thouless transition for $K/J=0$ is $T_{KT}=0.6860(2)$, from unbiased QMC calculations (Ref. 15).

$$\rho_s(T) = \lim_{\phi\to 0}\frac{1}{N}\frac{\partial F}{\partial \phi^2} \tag{43}$$

$$= \lim_{\phi\to 0}\frac{J}{2} + \frac{1}{N}\sum_{\mathbf{k}}\left(\frac{1}{2}\frac{\partial \omega_{\mathbf{k}}(\phi)}{\partial\phi^2} - \frac{\partial A_{\mathbf{k}}(\phi)}{\partial\phi^2}\right) + \frac{T}{N}\sum_{\mathbf{k}}\frac{e^{-\omega_{\mathbf{k}}/T}}{1-e^{-\omega_{\mathbf{k}}/T}}\frac{1}{T}\frac{\partial\omega_{\mathbf{k}}(\phi)}{\partial\phi^2}, \tag{44}$$

where the important limits are evaluated as follows:

$$\lim_{\phi\to 0}\frac{\partial A_{\mathbf{k}}(\phi)}{\partial\phi^2} = -J\frac{U_{\mathbf{k}}}{2}, \tag{45}$$

$$\lim_{\phi\to 0}\frac{\partial B_{\mathbf{k}}(\phi)}{\partial\phi^2} = -J\frac{W_{\mathbf{k}}}{2}, \tag{46}$$

$$\lim_{\phi\to 0}\frac{\partial\omega_{\mathbf{k}}(\phi)}{\partial\phi^2} = \lim_{\phi\to 0}\frac{4}{\omega_{\mathbf{k}}}\left(A_{\mathbf{k}}\frac{\partial A_{\mathbf{k}}(\phi)}{\partial\phi^2} - B_{\mathbf{k}}\frac{\partial B_{\mathbf{k}}(\phi)}{\partial\phi^2}\right) = -2J\frac{A_{\mathbf{k}}}{\omega_{\mathbf{k}}}U_{\mathbf{k}} + 2J\frac{B_{\mathbf{k}}}{\omega_{\mathbf{k}}}W_{\mathbf{k}}. \tag{47}$$

Thus, this calculation yields the following expression for the superfluid density at finite-T:

$$\rho_s(T) = \frac{J}{2} + \frac{J}{2N}\sum_{\mathbf{k}} U_{\mathbf{k}} - \frac{J}{N}\sum_{\mathbf{k}}\left(1 + 2\frac{1}{e^{-\omega_{\mathbf{k}}/T}-1}\right)\times\left(\frac{A_{\mathbf{k}}}{\omega_{\mathbf{k}}}U_{\mathbf{k}} - \frac{B_{\mathbf{k}}}{\omega_{\mathbf{k}}}W_{\mathbf{k}}\right). \tag{48}$$

This SW expression for ρ_s as a function of temperature is plotted for several parameters K/J in Fig. 4.

B. Estimation of the Kosterlitz-Thouless transition

The superfluid density of Eq. (48), plotted as a function of T, decays slowly (see Fig. 4), crossing zero for relatively large temperatures. However, as is well known, the XY

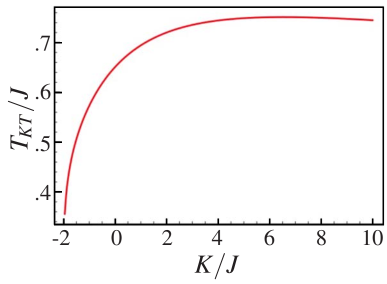

FIG. 5. (Color online) The KT transition phase boundary as calculated in linear SW theory. A maximum of $T_{KT}/J=0.751$ occurs at approximately $K/J=6.5$.

model realizes a Kosterlitz-Thouless[16] (KT) transition in any 2D lattice, which is manifest as a discontinuity in ρ_s precisely at T_{KT}. This, of course, cannot be captured by a simple spin-wave theory. We can, however, take advantage of the fact that the expected discontinuity in ρ_s in 2D models such as this obeys the so-called *universal jump* condition,

$$T_{KT} = \frac{\pi}{2}\rho_s(T_{KT}), \tag{49}$$

first found by Nelson and Kosterlitz.[17] One can thus hypothesize a reasonable estimate of T_{KT} by solving $T=\pi\rho_s(T)/2$, using $\rho_s(T)$ from our spin-wave theory. An important test of this idea can be performed at $K=0$ and $J=1/2$, the parameter values for the XY model. This is illustrated in Fig. 4, where the crossing point of the dashed line and the curve for $K/J=0$ is our SW theory solution to Eq. (49). The value of T_{KT} obtained by this procedure is 0.6507, remarkably close to the exact result of $T_{KT}=0.6860(2)$, obtained from unbiased QMC calculations.[15]

We thus generalize this procedure of calculating T_{KT} in our linear SW theory to nonzero values of K/J. Results are plotted in Fig. 5. As is evident by studying Fig. 4 closely, the SW theory reproduces the remarkable trend that T_{KT} *increases* for small to moderate values of $K>0$. In Fig. 4, the maximum in T_{KT} occurs at $K/J\approx 6.5$, before beginning to drop slowly. The phase boundary for the KT transition drops to zero for the large value of $K/J\approx 10^3$, well outside of the expected range of validity for the SW calculation. Clearly, a simple spin-wave theory cannot capture the physics of the superfluid-VBS quantum-phase transition that is observed in QMC simulations.

On the negative-K side, the phase boundary drops rapidly to zero as K/J approaches -2, reflecting the $T=0$ SW theory result, that a transition to a (π,π) bond-chiral superfluid phase, discussed in the previous sections, happens at this point.

V. DISCUSSION

We have studied through linear spin wave theory the various mechanisms which destroy the uniform superfluid phase in the bosonic ring-exchange model Eq. (1) at half filling, motivated as a candidate to realize exotic phases in cold atomic gases in optical lattices.[5] As is known from previous QMC results,[2] sufficiently large ring-exchange $K>0$ promotes: first, a quantum-phase transition to a valence bond solid state; second, a quantum-phase transition to a (π,π) CDW state, at large K. In this paper, we have shown that a moderate value of $K/J<0$ is also sufficient to destroy the uniform superfluid phase, promoting an ordered state that is identified as a different superfluid phase with (π,π)-modulated bond chirality. In mean-field theory, this transition occurs at $K/J=-2$. Since this phase transition occurs in mean-field theory, it, and the corresponding (π,π)-modulated superfluid phase, is expected to be robust; however the actual critical value of $|K/J|$ would of course be larger than the mean-field value, if fluctuations were taken into account.

Further, we have studied the finite-temperature phase boundary of the uniform superfluid phase in linear SW theory, by calculating the superfluid density and estimating the Kosterlitz-Thouless transition temperature by forcing it to obey the universal jump condition. We find that this procedure yields good numerical agreement with exact QMC results for $K=0$. For $K<0$, the phase boundary monotonically decreases to $T=0$ at $K/J=-2$, indicating a transition to the (π,π) bond-chiral superfluid phase discussed above. Increasing $K>0$ from the XY point, the phase boundary initially increases, reaching a maximum for $K\neq 0$ before monotonically decreasing. This is in qualitative agreement with the trend identified with QMC simulations,[9] and allows us to attribute at least the initial increase in T_{KT} for small K/J to the physics of noninteracting spin waves. It is remarkable that such nontrivial information about this model, namely, the nonmonotonic behavior of T_{KT} as a function of K/J, and the existence of a bond-chiral superfluid phase, can be contained in such a simple analytical theory.

ACKNOWLEDGMENTS

We are indebted to P. Nikolic, A. Paramekanti, A. Sandvik, and D. Scalapino for enlightening discussions. Support for this work was provided by NSERC of Canada.

[1] A. Paramekanti, L. Balents, and M. P. A. Fisher, Phys. Rev. B **66**, 054526 (2002).
[2] A. W. Sandvik, S. Daul, R. R. P. Singh, and D. J. Scalapino, Phys. Rev. Lett. **89**, 247201 (2002).
[3] L. Balents and A. Paramekanti, Phys. Rev. B **67**, 134427 (2003).
[4] V. G. Rousseau, R. T. Scalettar, and G. G. Batrouni, Phys. Rev. B **72**, 054524 (2005).
[5] H. P. Büchler, M. Hermele, S. D. Huber, M. P. A. Fisher, and P. Zoller, Phys. Rev. Lett. **95**, 040402 (2005).
[6] O. I. Motrunich and M. P. A. Fisher, Phys. Rev. B **75**, 235116 (2007).
[7] D. N. Sheng, O. I. Motrunich, S. Trebst, E. Gull, and M. P. A.

Fisher, Phys. Rev. B **78**, 054520 (2008).
[8] R. G. Melko, A. W. Sandvik, and D. J. Scalapino, Phys. Rev. B **69**, 100408(R) (2004).
[9] A. W. Sandvik and R. G. Melko, Ann. Phys. **321**, 1651 (2006).
[10] T. Senthil, A. Vishwanath, L. Balents, S. Sachdev, and M. P. A. Fisher, Science **303**, 1490 (2004).
[11] G. Gomez-Santos and J. D. Joannopoulos, Phys. Rev. B **36**, 8707 (1987).
[12] K. Bernardet, G. G. Batrouni, J.-L. Meunier, G. Schmid, M. Troyer, and A. Dorneich, Phys. Rev. B **65**, 104519 (2002).
[13] A. W. Sandvik, Phys. Rev. B **56**, 11678 (1997).
[14] A. W. Sandvik and C. J. Hamer, Phys. Rev. B **60**, 6588 (1999).
[15] R. G. Melko, A. W. Sandvik, and D. J. Scalapino, Phys. Rev. B **69**, 014509 (2004).
[16] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[17] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).