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Two-dimensional XY model with multiple symmetry-breaking fields

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A generalization of the José, Kadanoff, Kirkpatrick, and Nelson (JKKN) model to multiple symmetry-breaking fields in the classical two-dimensional (2D) XY model is achieved by applying symmetry arguments to the renormalization-group equations. The generalized model is analyzed with the use of a renormalized spin-wave—vortex-gas technique, with finite-size effects included. Numerical examples of the generalized model are given for the case of a classical 2D XY model with a onefold symmetry-breaking field and a sixfold symmetry-breaking field. Applications of the generalized JKKN model are discussed in connection with the susceptibility measurements on $CoCl_2$ intercalated graphite.

I. INTRODUCTION

In recent years, theoretical research on the two-dimensional XY model (2D XY) has attracted much interest. The studies of vortex-unbinding transitions by Kosterlitz and Thouless,[1,2] Berezinskiĭ,[3] and Villain[4] have shown that the low-temperature vortex-bound phase has a correlation function which decays algebraically with distance, yielding a phase with infinite susceptibility. On the other hand, the effect of a symmetry-breaking field in the 2D XY model has been investigated by Pokrovskii and Uimin[5] using the self-consistent harmonic approximation and scaling theory. Their work on symmetry-breaking fields and the vortex-unbinding transition are neatly unified in the work of José, Kadanoff, Kirkpatrick, and Nelson (JKKN)[6] applying the Villain approximation to the XY action. The JKKN model reveals an interesting phase diagram for $p \geq 4$ (p is the index of the symmetry-breaking field) as well as the duality symmetry of spin-wave excitations and vortices. Their phase diagram indicates that when $p>4$, there is a band of temperatures $T_{c1}<T<T_{c2}$, where the system is governed by Gaussian fluctuations and the susceptibility diverges. The correlation function critical exponents η at T_{c1} and T_{c2} are related by duality with $\eta(T_{c2})=T_{c2}/2\pi J$ and $\eta(T_{c1})=1/[p^2\eta(T_{c2})]$, where J is the ferromagnetic exchange coupling. The band of temperatures collapses into a multicritical line when $p=4$; a theoretical analysis of this line has been made by Kadanoff.[7]

The important work on the critical properties of the 2D XY model with or without one symmetry-breaking field is handicapped in two important aspects with regard to experimental comparisons. The first problem with the testing of these theories is the presence of finite-size effects, and the second is the presence of more than one symmetry-breaking field. It is the purpose of this paper to approximately incorporate these two effects into the JKKN model so that the gap between theory and experiment [e.g., magnetic susceptibility measurements on $CoCl_2$ graphite intercalation compounds (GIC's)] is bridged.

The finite-size effect necessarily reveals itself in any experimental testing of the JKKN theory because the divergent susceptibility must be bounded in any experimental setup by the size of the system for $T<T_{KT}$ (the Kosterlitz-Thouless transition temperature) in the absence of symmetry-breaking fields and at temperatures in the range $T_{c1}<T<T_{c2}$ in the presence of a p-fold symmetry-breaking field with $p>4$. The presence of finite-size effects makes the quantitative study of critical exponents in the critical region extremely difficult. Therefore, it seems more sensible to study the correction to scaling over an extended region of temperatures. Since correction to scaling involves nonuniversal properties of the system, a close interaction between experiment and theory is needed. In this paper, we illustrate the method of the renormalized spin-wave vortex gas in the study of finite-size modifications to the JKKN description. We leave the details of comparison with experimental systems to a separate paper.[8,9] The finite-size analysis follows a paper[9,10] on the finite-size Kosterlitz-Thouless transition, where more details about the matching scheme can be found.

The second problem in comparing the JKKN analysis with experimental data concerns the presence of an external field. This external field (the finite probing field in susceptibility measurements) is usually present in the experimental setup. But according to JKKN, no matter how small this onefold symmetry-breaking field, it will renormalize to a large value so that phase transitions are eliminated. Therefore, the theoretical analysis of JKKN, if applied consistently, can never be tested in its original form by the experimental measurement of the susceptibility. Rather, it is necessary to generalize the JKKN model to include multiple symmetry-breaking fields. This is the second subject discussed in this paper.

With both finite-size effects and multiple symmetry-breaking field effects incorporated, we discover that a wealth of complicated phenomena are possible. First of all, the presence of finite-size effects implies that the symmetry-breaking field cannot be renormalized without limit. Secondly, the presence of two symmetry-breaking fields opens the interesting possibility of competing symmetry-breaking fields of different indices. A low-temperature analysis of competing symmetry-breaking fields with an angular dependence of one of the fields, with a planar "spin-flip" transition, has been reported by Szeto *et al.*[9] In the present paper, we focus our attention on the temperature dependence of the susceptibility illustrated through the numerical computation of this quantity.

In Sec. II we construct the action of the generalized JKKN model. In Sec. III two symmetry principles are used to write down the renormalization-group equations for the generalized JKKN model. A qualitative discussion of the renormalization-group equations is the subject of Sec. III. In Sec. IV we develop the renormalized spin-wave—vortex-gas theory of the correlation function, incorporating the finite-size effect. In Sec. V the correlation function is integrated to obtain the susceptibility, and several figures illustrating the numerical solution of the generalized JKKN model are presented. Finally, Sec. VI is devoted to the application of this analysis to experiment.

II. GENERALIZED JKKN ACTION

The classical 2D XY model with a p-fold symmetry-breaking field is defined by the action

$$\mathscr{A}_p(\theta)=-K\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\{1-\cos[\theta(\mathbf{r})-\theta(\mathbf{r}')]\}+h_p\sum_{\mathbf{r}}\cos[p\theta(\mathbf{r})] \tag{1}$$

with $\langle \mathbf{r},\mathbf{r}'\rangle$ summed over first-nearest neighbors on a 2D lattice, K is the effective ferromagnetic coupling, and h_p is the phenomenological p-fold symmetry-breaking field strength (JKKN).[6] This action can be rewritten into the Coulomb-gas excitation representation via the Villain approximation,[4]

$$\mathscr{A}_{\mathrm{JKKN}}=\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}-\frac{K}{2}[\theta_r-\theta_{r'}-2\pi m(\mathbf{r},\mathbf{r}')]^2+(\ln y_0)\sum_{\mathbf{R}}S_{\mathbf{R}}^2(m)+(\ln y_p)\sum_{\mathbf{r}}n^2(\mathbf{r})+ip\sum_{\mathbf{r}}n(\mathbf{r})\theta(\mathbf{r})\ . \tag{2}$$

Here $m(\mathbf{r},\mathbf{r}')$ is an integer field defined on link $(\mathbf{r},\mathbf{r}')$, and $S_{\mathbf{R}}(m)$ is the plaquette sum of $m(\mathbf{r},\mathbf{r}')$ around the dual lattice vector $\mathbf{R}$, $n(\mathbf{r})$ is a site integer field, and y_p is the symmetry-breaking field activity, given for small h_p by $\frac{1}{2}h_p$ and y_0 is the vortex activity parameter introduced by JKKN to control fluctuations of the vortex variable.

JKKN have shown[6] that the critical properties of the partition function

$$Z_p(K,h_p)=\prod_{\mathbf{r}}\int_0^{2\pi}\frac{d\theta(\mathbf{r})}{2\pi}e^{\mathscr{A}_p(\theta)} \tag{3}$$

can be approximated by that of

$$Z_{\mathrm{JKKN}}(2\pi K,y_0,y_p)=\sum_{[m(\mathbf{r},\mathbf{r}')]}\sum_{[n(\mathbf{r})]}\prod_{\mathbf{r}}\int_0^{2\pi}\frac{d\theta(\mathbf{r})}{2\pi}e^{\mathscr{A}_{\mathrm{JKKN}}(\theta,m,n)}\ , \tag{4}$$

which satisfies the duality relation

$$Z_{\mathrm{JKKN}}(2\pi K,y_0,y_p)=Z_{\mathrm{JKKN}}\left[\frac{p^2}{2\pi K},y_p,y_0\right]\left[\frac{p}{2\pi K}\right]^N\ , \tag{5}$$

where N is the total number of sites in the system.

We will construct the generalization of the $\mathscr{A}_p$ action in Eq. (1) for the multiple symmetry-breaking field action $\mathscr{A}_{p_1,p_2,\ldots,p_l}$ with the JKKN approximation (2). The key observation that JKKN made in generalizing Villain's model to include a p-fold symmetry-breaking field is that for small h_p we have $h_p=2y_p$, and

$$e^{2y_p\cos(p\theta)}\approx 1+2y_p\cos(p\theta)\approx\sum_{n_p=0,\pm1}e^{(\ln y_p)n_p^2+2\pi i n_p p\theta}\ , \tag{6}$$

the Villain model being a special case of the JKKN model with $y_0=1$ and $y_p=0$.

By repetitively applying Eq. (6) we can write the action $\mathscr{A}_{p_1,\ldots,p_l}$ for l symmetry-breaking fields of indices $p_1,\ldots,p_l$ as

$$\mathscr{A}_{p_1,\ldots,p_l}=\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}-\frac{K}{2}[\theta_r-\theta_{r'}-2\pi m(r,r')]^2+(\ln y_0)\sum_{R}S_R^2(m)+\sum_{j=1}^{l}(\ln y_{p_j})\sum_{r}n_{p_j}^2(r)+i\sum_{j=1}^{l}p_j\sum_{r}n_{p_j}(r)\theta(r)\ , \tag{7}$$

where n_{p_j} is a site integer field defined by symmetry p_j and the partition function is given by

$$Z(2\pi K,y_0,y_{p_1},\ldots,y_{p_l})=\sum_{[m(r,r')]}\sum_{[n_{p_1}(r)]}\cdots\sum_{[n_{p_l}(\mathbf{r})]}\left[\prod_{\mathbf{r}}\int_0^{2\pi}\frac{d\theta(r)}{2\pi}\right]e^{\mathscr{A}_{p_1,\ldots,p_l}}\ , \tag{8}$$

which is an approximation to the 2D XY model with l symmetry-breaking fields, with the action defined by

$$\mathscr{A}(\theta,h_{p_1},\ldots,h_{p_l})=-K\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\{1-\cos[\theta(\mathbf{r})-\theta(\mathbf{r}')]\}^2+\sum_{j=1}^{l}h_{p_j}\sum_{\mathbf{r}}\cos[p_j\theta(\mathbf{r})] . \tag{9}$$

III. RENORMALIZATION-GROUP EQUATIONS

After the generalized JKKN action is defined, we proceed to derive the renormalization group equations. The two important symmetry principles used to determine the renormalization-group equations uniquely in lowest order of $y_0,y_{p_1},\ldots,y_{p_l}$ are the duality symmetry limits, when all but one of the symmetry-breaking fields vanish, and the global rotational symmetry of the free energy with respect to rotation of the coordinate axis. Duality symmetry refers to the invariance of the partition function when $2\pi K\to p^2/2\pi K$, $y_p\to y_0$, and $y_0\to y_p$, as indicated by Eq. (5). Duality symmetry is broken when more than one symmetry-breaking field are present, but it is a required symmetry when all but one of the h_p's vanish. The rotational symmetry refers to the freedom of choosing the two-dimensional coordinate system in defining the action, with the resulting partition function unchanged, since we integrate over all angles θ. This symmetry allows us to choose a coordinate system such that certain mixed terms of the form h_ph_q, $p\neq q$, will not appear in the renormalization-group equations since the renormalization group must respect the symmetry of the free energy.

To make use of these symmetry restrictions, we first write the most general form of the renormalization-group equations for the 2D XY model with two symmetry-breaking fields and we then eliminate those mixed terms using symmetry arguments. The generalization to more than two symmetry-breaking fields can be made similarly. In differential form with the scaling parameter $l\equiv\ln(|\mathbf{r}|/a_0)$, we have

$$\begin{aligned}\frac{dK^{-1}(l)}{dl}&=B_T(K^{-1}(l),h_p(l),h_q(l),y_0(l)) ,\\ \frac{dy_p(l)}{dl}&=B_p(K^{-1}(l),h_p(l),h_q(l),y_0(l)) ,\\ \frac{dy_q(l)}{dl}&=B_q(K^{-1}(l),h_p(l),h_q(l),y_0(l)) ,\\ \frac{dy_0(l)}{dl}&=B_0(K^{-1}(l),h_p(l),h_q(l),y_0(l)) .\end{aligned} \tag{10}$$

We then perform a Taylor expansion up to second order of the B's in their arguments. First, we consider the restriction imposed by duality. According to the analysis of JKKN, when h_q vanishes, all the linear terms in B_T vanish and B_T is given to second order in its arguments by

$$\begin{aligned}B_T&=a_0y_0^2-a_py_p^2+\cdots ,\\ B_p&=y_p\left[2-\frac{p^2}{2\pi K}\right]+\cdots ,\\ B_0&=(2-\pi K)y_0+\cdots ,\end{aligned} \tag{11}$$

with

$$\begin{aligned}a_0&=4\pi^3e^{-\pi^2K} ,\\ a_p&=\pi p^2K^{-2}e^{-p^2/4K} ,\end{aligned} \tag{12}$$

where the $\cdots$ refer to high-order terms in the Taylor expansion. The exponential form of the K dependence in a_p and a_0 is characteristic of 2D XY systems.

Thus, the most general form of the B's consistent with JKKN's analysis for two symmetry-breaking fields is given by

$$\begin{aligned}B_T&=a_0y_0^2-a_py_p^2-a_qy_q^2+b_{pq}y_py_q+\cdots ,\\ B_q&=y_q\left[2-\frac{q^2}{2\pi K}\right]+\cdots ,\end{aligned} \tag{13}$$

with B_p and B_0 unchanged from Eq. (11).

The second symmetry property of the 2D XY action with h_p and h_q perturbations will now be used to show that $b_{pq}=0$. First consider just one symmetry-breaking-field h_p term in the A_p action. By rotating our coordinate axis so that $\theta\to\theta'=\theta+\pi/p$, the resulting h_p term in the A_p action will change from $h_p\cos(p\theta)$ to $-h_p\cos(p\theta)$, but the partition function is unchanged since we integrate over all θ when the canonical ensemble average is performed. This implies

$$Z_p(K,h_p)=Z_p(K,-h_p) , \tag{14}$$

and the renormalization-group equation must have this reflection symmetry. Consequently, $B_T(K^{-1},y_p,y_0)$ cannot contain a term of the form y_py_0 as this violates the reflection symmetry. Similarly, when we have two symmetry-breaking fields of indices p and q, we can perform a global rotation of our coordinate axis by ϕ (independent of x), so that

$$h_p\cos(p\theta)+h_q\cos(q\theta)\to h_p\cos(p\theta)\cos(p\phi)+h_q\cos(q\theta)\cos(q\phi)-h_p\sin(p\theta)\sin(p\phi)-h_q\sin(q\theta)\sin(q\phi) . \tag{15}$$

By choosing $\phi=m\pi/p=n\pi/q$ for some integers m and n, we can make the sine terms disappear and we have

$$h_p\cos(p\theta)+h_q\cos(q\theta)\to(-1)^mh_p\cos(p\theta)+(-1)^nh_q\cos(q\theta) , \tag{16}$$

so that terms of form h_ph_q will change to $(-1)^{m+n}h_ph_q$. As long as $(m+n)$ is odd, odd power terms of (h_ph_q) will violate the symmetry of the partition function Z_{pq},

$$Z_{pq}(K,(h_ph_q),\ldots)=Z_{pq}(K,-(h_ph_q),\ldots) , \tag{17}$$

and cannot appear in the expansion of B_T. In solid-state experiments, the interesting case involves the combination of a onefold field (corresponding to Zeeman coupling to an external field) with a q-fold field where $q=2,4,6$. Whereas a twofold symmetry-breaking field can be a model for antiferromagnetic coupling, a fourfold and sixfold symmetry-breaking field corresponds to the crystalline anisotropy of a square and triangular lattice, respectively. Thus, for these combinations of p and q, we have $b_{pq}=0$.

IV. QUALITATIVE FEATURES OF THE RENORMALIZATION-GROUP EQUATIONS

From our discussion in Sec. III, the renormalization-group equations for the generalized JKKN model with two symmetry-breaking fields of indices p and q in lowest order are

$$\begin{aligned}\frac{dK^{-1}}{dl}&=a_0y_0^2-a_py_p^2-a_qy_q^2\,,\\ \frac{dy_p}{dl}&=y_p\left[2-\frac{p^2}{2\pi K}\right],\\ \frac{dy_q}{dl}&=y_q\left[2-\frac{q^2}{2\pi K}\right],\\ \frac{dy_0}{dl}&=y_0(2-\pi K)\,.\end{aligned}\tag{18}$$

The case $y_p=y_q=0$ corresponds to the Kosterlitz recursive relation, with y_0 and K^{-1} renormalized to large values when $2-\pi K>0$. For $2-\pi K<0$, then $y_0(l)\rightarrow 0$ as $l\rightarrow\infty$, so that $K^{-1}(l)\rightarrow K^{-1}(\infty)$ and we have a continuous line of fixed points. When only $y_q(0)=0$, then y_p will renormalize to a large value when $2-p^2/2\pi K>0$; otherwise it will renormalize to small values. Thus, the JKKN phase diagram can be obtained by observing that for $p>4$, there will be K_{c1}^{-1} and K_{c2}^{-1} ($K_{c1}^{-1}<K_{c2}^{-1}$), such that for $K^{-1}>K_{c2}^{-1}\approx\pi/2$, we have $(y_0,K^{-1})\rightarrow(\infty,\infty)$ as $l\rightarrow\infty$ and the system is in the Kosterlitz-Thouless vortex-gas state; for $K^{-1}<K_{c1}^{-1}$, $y_p\rightarrow\infty$, $K^{-1}\rightarrow 0$ as $l\rightarrow\infty$, so that we have the low-temperature p-fold clock-model phase; for $K_{c1}^{-1}<K^{-1}<K_{c2}^{-1}$, the system is in a phase governed by large Gaussian fluctuations with both the symmetry-breaking field spin-wave excitation and free-vortex excitation small since both y_p and $y_0\rightarrow 0$ when $l\rightarrow\infty$. For $p=4$, the region of this Gaussian fluctuation phase (disordered XY vortex bound phase) will be squeezed into a line; the analysis of this multicritical line has been performed by Kadanoff.[7]

When a p-fold and a q-fold symmetry-breaking field are both present, the situation is fairly complicated. For example, in the usual case of a susceptibility measurement, a onefold probing field is also present. Since $2-1/2\pi K>2-p^2/2\pi K$ for all $p>1$, the onefold field will always dominate over the other symmetry-breaking fields of higher index in its rate of renormalization. In general, in a mixture of a p-fold and a q-fold field, with $p>q$, the q-fold field will dominate. The interesting investigation from the point of view of an experimental test of the JKKN model is to see the various crossovers from a q-fold-dominated regime to a p-fold-dominated regime when the initial values of y_p and y_q are different. Consider $p<q$ but $y_p(0)<y_q(0)$, then y_p will renormalize with a faster rate so that it will at some scale l_{pq}^* be equal to $y_q(l_{pq}^*)$. For scale $l<l_{pq}^*$, the q-fold symmetry-breaking field dominates over the p-fold field and for $l>l_{pq}^*$, the reverse is true. A similar analysis can be performed in the comparison of a p-fold field activity y_p with the vortex activity y_0. In general, there will be various length scales where the crossover from one phase to another takes place. The exact behavior of these crossovers will be governed by the following:

(i) The size of the system since it implies an upper bound l_m to the scaling parameter l.

(ii) The initial values of the activities in question. [For example, if $p<q$ and $y_p(0)>y_q(0)$, then the system will never exhibit a q-fold clock-model phase.]

These investigations necessarily invoke finite-size studies, which are relevant in experimental situations. The next section will thus address the finite-size effect for the generalized JKKN model.

V. FINITE-SIZE ANALYSIS OF THE SUSCEPTIBILITY

The renormalization-group equations for the generalized JKKN model indicate that crossover from one phase to another occurs at different length scales for different initial values of activities and temperature. Furthermore, the existence of a disordered XY phase governed by Gaussian fluctuations for a single p-fold symmetry-breaking field with $p>4$ implies that the divergent susceptibility in this phase is bounded by finite size. Therefore, the incorporation of finite size into the JKKN model or its generalized version is necessary for the comparison with experiment. In this section, we will employ the renormalized spin-wave—vortex-gas techniques to discuss the finite-size effect. The analysis on the simpler case of the 2D XY model without symmetry-breaking fields has been reported elsewhere.[10]

The renormalized spin-wave—vortex-gas technique makes use of the spin-wave description for the correlation function by replacing the bare coupling $(K^{-1}(0),y_p(0),y_q(0),y_0(0))$ with the corresponding terms renormalized $(K^{-1}(l),y_p(l),y_q(l),y_0(l))$ at the length scale l. When the renormalized couplings are within the validity limit of the renormalization-group equation, the correlation function can be written as

$$\begin{aligned}g(r)&=\langle[\mathbf{S}(r)-\langle\mathbf{S}\rangle]\cdot[\mathbf{S}(0)-\langle\mathbf{S}\rangle]\rangle\\ &=\langle\cos[\theta(\mathbf{r})-\theta(0)]\rangle-\langle\cos\theta\rangle^2\\ &=e^{-\langle[\theta(\mathbf{r})-\theta(0)]^2\rangle_{\rm SW}/2}-e^{-\langle\theta^2\rangle_{\rm SW}}\,,\end{aligned}\tag{19}$$

where $\langle\ \rangle_{\rm SW}$ denotes the harmonic spin-wave average. These spin-wave averages with bare coupling give

$$\tfrac{1}{2}\langle[\theta(\mathbf{r})-\theta(\mathbf{0})]^2\rangle_{\rm SW}=\int_{\rm BZ}\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{1-e^{i\mathbf{k}\cdot\mathbf{r}}}{\gamma(0)-\gamma(\mathbf{k})+p^2h_p(0)+q^2h_q(0)}\tag{20}$$

and

$$\langle\theta^2\rangle_{\rm sw}=\int_{\rm BZ}\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{1}{\gamma(0)-\gamma(\mathbf{k})+p^2h_p(0)+q^2h_q(0)}\ , \tag{21}$$

where

$$\gamma(\mathbf{k})=\sum_{\mathbf{r}}e^{i\mathbf{k}\cdot\mathbf{r}}\frac{J_{\rm eff}(\mathbf{r})}{T}\ , \tag{22}$$

and the integration is performed over a circular Brillouin zone of area equal to the original two-dimensional Brillouin zone of the system.

The discussion of finite-size effects enters in many ways. The first one is that the position vector $\mathbf{r}$ must be inside the finite system so that the maximum limit of $|\mathbf{r}|$ is L, the linear size of the system. The second one concerns the boundary conditions. The spin-wave spectrum is usually obtained by imposing periodic boundary conditions with $\mathbf{k}$ space being divided into Brillouin zones. We can also solve the spin-wave problem for other boundary conditions and the correlation function will accordingly be modified. The third way finite-size effects enter is through the existence of an infrared cutoff of the allowed values of $\mathbf{k}$, the lowest possible value of k being π/L. This is important since the Gaussian propagator will never diverge when the range of k excludes zero. Finally, the critical region is smeared out for finite systems.

The integration over the Brillouin zone can be written as

$$\int_{\rm BZ}\frac{d^2\mathbf{k}}{(2\pi)^2}=\frac{a_0^{-2}}{(2\pi)^2}\int_{\Lambda a_0/L}^{\Lambda}k\,dk\int_0^{2\pi}d\theta \tag{23}$$

with the cutoff parameter Λ given by

$$a_0^{-2}\frac{\Lambda^2}{4\pi}\left[1-\frac{a_0^2}{L^2}\right]=A_{\rm BZ}\ , \tag{24}$$

where $A_{\rm BZ}$ is the area of the Brillouin zone. We also perform a standard small-k expansion of $\gamma(\mathbf{k})$ so that

$$\gamma(\mathbf{0})-\gamma(\mathbf{k})=\frac{J_{\rm eff}(\mathbf{0})}{T}k^2=K(\mathbf{0})k^2\ . \tag{25}$$

These standard approximations for the Brillouin-zone integral yield

$$\begin{aligned}-\tfrac{1}{2}\langle[\theta(r)-\theta(0)]^2\rangle_{\rm sw}&=\frac{-T}{2\pi J_{\rm eff}(0)}\times\int_{\Lambda a_0/L}^{\Lambda}\left[\frac{1-J_0(kr)}{k^2+u^2(0)}\right]k\,dk\\&=\ln M^2(u(0))+C(u(0)r)\ ,\end{aligned} \tag{26}$$

where

$$\begin{aligned}\ln M^2(u(0))&=\frac{-T}{2\pi J_{\rm eff}(0)}\int_{\Lambda a_0/L}^{\Lambda}\frac{k\,dk}{k^2+u^2(0)}\ ,\\C(u(0)r)&=\frac{T}{2\pi J_{\rm eff}(0)}\int_{\Lambda a_0/L}^{\Lambda}\frac{J_0(kr)k\,dk}{k^2+u^2(0)}\ ,\end{aligned} \tag{27}$$

and

$$\begin{aligned}u^2(0)&=\frac{[p^2h_p(0)+q^2h_q(0)]}{J_{\rm eff}(0)}T\\&=K^{-1}(0)[p^2h_p(0)+q^2h_q(0)]\ .\end{aligned} \tag{28}$$

Thus, the correlation function in the spin-wave approximation with bare coupling is given by

$$g(r)=M^2(u(0))(e^{C(u(0)r)}-1)\ . \tag{29}$$

In this equation, $h_p(0)$, $h_q(0)$, and $T/J_{\rm eff}(0)$ $[=K^{-1}(0)]$ are the initial values (bare coupling). We replace them by the renormalized values $h_p(l)$, $h_q(l)$, and $K^{-1}(l)$ with $l=\ln(r/a_0)$. The renormalized coupling at length scale l is obtained by integration of the renormalization group equation from 0 to l.

The renormalized spin-wave expression for the correlation function

$$g(r)\equiv G_L(r)=M^2(u(l))(e^{C(u(l)r)}-1) \tag{30}$$

has an exponential decay form for both the high-temperature and low-temperature limits. At low temperature $[K^{-1}<\max(4\pi/p^2,\ 4\pi/q^2)]$, the renormalized value of the symmetry-breaking field is large, so that M^2 does not vanish and has the value

$$\begin{aligned}M^2&=M^2(u[l_m=\ln(L/a_0)])\\&=\left[\frac{\Lambda^2+u^2(l_m)}{(\Lambda a_0)^2/L^2+u^2(l_m)}\right]^{-1/4\pi K(l_m)}\ ,\end{aligned} \tag{31}$$

where M is the magnetization. On the other hand, the value for $C(u(l)r)$ is given by

$$\begin{aligned}C(u(l)r)&=\frac{1}{2\pi K(l)}\left[\int_0^{\infty}-\int_0^{\Lambda a_0/L}-\int_{\Lambda}^{\infty}\right]\frac{J_0(kr)k\,dk}{k^2+u^2(l)}\\&\simeq\frac{1}{2\pi K(l)}\left[\mathscr{K}_0(u(r)r)-\int_0^{\Lambda a_0/L}\frac{J_0(kr)k\,dk}{k^2+u^2(l)}\right]\ .\end{aligned} \tag{32}$$

Here $\mathscr{K}_0$ is the zero-order Bessel function of the second kind, J_0 is the zero-order Bessel function of the first kind, and the last term in the k integral of the first equality is dropped because of the oscillatory nature of $J_0(x)$ for large x. At large r, we make use of the asymptotic expansion of the Bessel function to obtain

$$C(u(l)r)\approx\frac{1}{2\pi K(l)}\left[\left[\frac{\pi}{2u(l)r}\right]^{1/2}e^{-ru(l)}\right]\ll 1\ , \tag{33}$$

so that

$$e^{C(u(l)r)}-1\approx 1+C(u(l)r)-1=C(u(l)r) \tag{34}$$

has an exponential tail with decay parameter $u^{-1}(l)$. The other exponential form of the correlation function is given at high temperature where the symmetry-breaking fields renormalize to small values while the vortex activity y_0 renormalizes to large values. The magnetization is small, and vanishes in the limit of infinite size ($L \to \infty$). In this case, short-range order sets in by the Kosterlitz-Thouless vortex-unbinding mechanism, with the Ornstein-Zernike form of the correlation function at high temperature given by

$$g_H(r) = f(r/\xi)e^{-r/\xi} , \tag{35}$$

where $f(r/\xi)$ is the correction function to scaling and ξ is the correlation length.

In the extreme case where $L \to \infty$ and $h_1 \to 0$, the renormalized spin-wave expression for the correlation function can be matched to this high-temperature form $g_H(r)$. In actual computations, the high-temperature region can be defined by the criterion that the renormalized temperature $K^{-1}(l^*)$ at some length scale l^*, determined by the initial condition $(K^{-1}(0), y_p(0), y_q(0), y_0(0))$, is twice the critical temperature K_c^{-1} for the Kosterlitz-Thouless transition. The exact choice of the matching point l^* and the value $K^{-1}(l^*)$ can be fixed by experiment or by a high-temperature-series expansion, since these matching schemes produce qualitatively similar results. Numerically, the quantitative difference is small between different matching schemes [such as different values of the ratio $K^{-1}(l^*)/K_c^{-1}$ in the neighborhood of 2]. The procedure used in matching the correlation function is identical to the analysis we made for the computation of the susceptibility for the finite-size Kosterlitz-Thouless transition.[10] We first integrate the renormalization-group equation until $K^{-1}(l^*) \approx 2K_c^{-1}$ and then match the correlation function to the high-temperature form $g_H(r)$ by requiring the continuity of the functions, as well as their first and second derivatives at $r^* = a_0 e^{l^*}$. The correction function $f(r/\xi)$ used for $g_H(r)$ has the form

$$f(r/\xi) = A(r/\xi)^{-\alpha} \tag{36}$$

with A, α, and ξ fixed by the continuity requirements.

In the next section we present the numerical calculations of the differential magnetic susceptibility for the finite-size 2D *XY* model with two symmetry-breaking fields using the renormalized spin-wave—vortex-gas expression for the correlation function discussed in this section.

VI. NUMERICAL RESULTS FOR THE SUSCEPTIBILITY

The magnetic susceptibility χ is given by the fluctuation-dissipation theorem as the integral of the correlation function over the volume of the system. For finite systems, χ can be written as

$$\chi = \frac{1}{VT} \int_V d^2\mathbf{r}' \int_V d^2\mathbf{r} [\langle \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r}') \rangle - \langle \mathbf{S} \rangle^2] . \tag{37}$$

We can extract the finite-size effect by approximating this double integral by

$$\chi = \frac{1}{T} \int_V d^2\mathbf{r} [\langle \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(0) \rangle - \langle \mathbf{S} \rangle^2] \tag{38}$$

with the correlation function given by

$$\begin{aligned} g(r) &\equiv \langle \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(0) \rangle - \langle \mathbf{S} \rangle^2 \\ &= g_L(r) \quad \text{for } r \le r^* \\ &= g_H(r) \quad \text{for } r > r^* , \end{aligned} \tag{39}$$

where r^* is the matching point of $g_L(r)$ and $g_H(r)$.

The numerical procedure that was used consists of solving the set of differential equations [Eq. (18)], thereby obtaining the renormalized coupling; then, the correlation function with renormalized coupling is integrated to obtain the susceptibility. In practice, we augment the renormalization-group equations (18) with the fluctuation-dissipation theorem in differential form,

$$\frac{d(T\chi)}{dl} = e^{2l + \ln g(e^l)} , \tag{40}$$

where $g(e^l) = g_L(r)$, and integrate the augmented system of differential equations. At each step of integration we check the conditions for the validity of the renormalization-group equation. When $y_0(l)$ is large, so that the system is in the high-temperature region, we perform a matching of g_L to g_H and stop the integration of the system of differential equations.

The numerical results provide us with a map of $\chi(T, H_p, H_q)$. The interesting case from the experimentalist's point of view is a map of $\chi(T, H_p, H_1 = H_{\text{ext}})$. Here H_{ext} is the externally applied field and H_p is the intrinsic anisotropy field of the specific two-dimensional magnetic system. In experimental situations, the intrinsic anisotropy field is fixed, but the external field can be varied.

In Fig. 1 we show the correlation function versus distance for different temperatures normalized to J_{eff}. The two symmetry-breaking fields are the onefold external field and the sixfold symmetry-breaking field corresponding to the $CoCl_2$ intercalated-graphite system.[9] The size of the system[11] is 30×30. The values of the fields h_1 and h_6 are related to the physical applied field $H_1 = H_{\text{ext}}$ (in Oe) and the p-fold anisotropy by the relations

$$Th_1 = \frac{H_1 s}{J_{\text{eff}}} \tag{41}$$

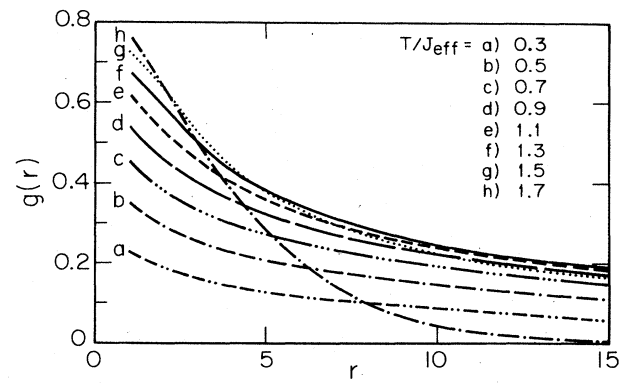

FIG. 1. The calculated correlation function $g(r)$ vs r of a 30×30 system with a onefold field of 1 Oe and a sixfold field of 10 Oe is plotted vs distance r for different temperatures, T/J_{eff}. The value of J_{eff} is 7.125 K, corresponding to the experimental value for $CoCl_2$ GIC.

and

$$Th_6 = \frac{H_6 s^6}{J_{\rm eff}} , \tag{42}$$

where s is the spin magnitude. The sixfold field arises from the sixfold anisotropy of the free energy

$$F_{\rm anisotropy} \propto M_+^6 + M_-^6$$
$$= 2M^6 \cos(6\theta) \tag{43}$$

for $M_\pm = \langle S_\pm \rangle$.

The initial value of the vortex activity parameter y_0 is set to 1, corresponding to the original Kosterlitz-Thouless theory. In Fig. 1 we see the sharp decay of the $T/J_{\rm eff} = 1.7$ correlation function with distance. This is due to the vortex unbinding at high temperature. The susceptibility is the area under the correlation-function curves. In Fig. 2 we show the temperature dependence of the magnetic susceptibility for systems of different sizes. In the limit of infinite size,[6] we have the JKKN description of the susceptibility when h_1 approaches 0. The calculated field dependence of the susceptibility for a 30×30 system is shown in Fig. 3 for $H_{\rm ext} = 0$, 2, 4, 6, 8, and 10 Oe and $H_6 = 10$ Oe. The value of the effective exchange coupling $J_{\rm eff}$ used in these figures is 7.125 K, corresponding to the experimental value for $CoCl_2$ GIC's.[8,12,13] From Fig. 3 we can see the important effect of the onefold symmetry-breaking field on suppressing the susceptibility. These results show that in the comparison of experimental data with theories of two-dimensional magnetism, caution must be exercised in taking into account the effects of the probing field in the actual measurements, since the usual theoretical predictions are made for the limit of zero probing field. These results also illustrate the finite-size modifications of the theory of the critical properties of the two-dimensional XY model with symmetry-breaking fields. The application of these numerical results to experimental studies of two-dimensional magnetism are reported elsewhere.[8,9]

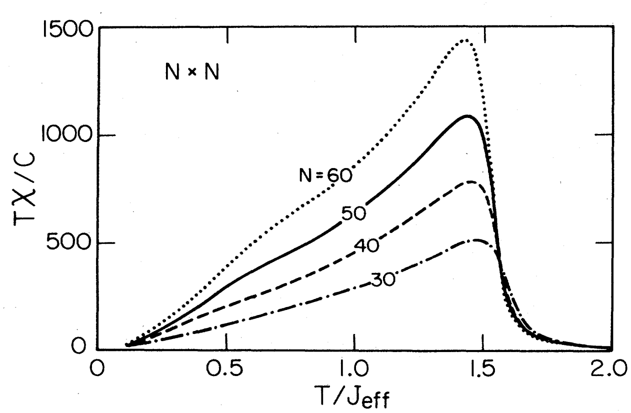

FIG. 2. Temperature dependence of the reduced susceptibility for systems of different sizes ($N \times N$ for $N = 30,40,50,60$) with a sixfold field $H_6 = 10$ Oe, but no onefold field. The value of $J_{\rm eff}$ is 7.125 K, corresponding to the experimental value for $CoCl_2$-GIC's, and C is the Curie constant.

VII. CONCLUSIONS

We have generalized the JKKN treatment of the two-dimensional classical XY model with one symmetry-breaking field to include multiple symmetry-breaking fields, so that the effects of an external field on the susceptibility could be considered. The action, the renormalization-group equations, and the effect of the competition between the two symmetry-breaking fields of different indices are discussed. We have also generalized the JKKN analysis to include finite-size effects using the renormalized spin-wave—vortex-gas theory for the spin-spin correlation function. Our results connect the theoretical work for the critical region in the JKKN model with experimental studies of two-dimensional magnetism, so that the experimental studies in the divergent susceptibility region and the effect of the external field can be compared with theoretical calculations.

The numerical calculations of the susceptibility allow the first systematic analysis to be made of the experimental data on $CoCl_2$ intercalated graphite, which have accumulated over almost a decade.[8,11,14–18] The magnetic

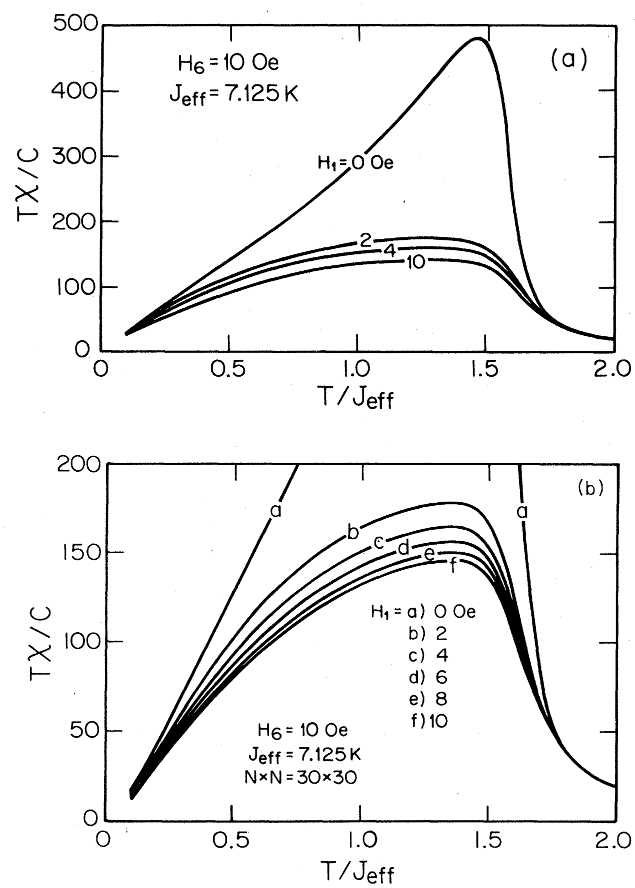

FIG. 3. Temperature dependence of the reduced susceptibility $\chi T/C$ for a 30×30 system with a sixfold field of 10 Oe and different values of the onefold field, $H_1 = 0$, 2, 4, 6, 8, and 10 Oe. The value of $J_{\rm eff}$ is 7.125 K, corresponding to the experimental values of $CoCl_2$-GIC's, and C is the Curie constant. (a) The scale is chosen to display the $H_1 = 0$ curve. (b) The results of (a) are replotted on a reduced scale to display the field dependence in the range $2 \leq H_1 \leq 10$ Oe.

properties of $CoCl_2$ GIC's exhibit a wealth of phenomena, ranging from the high-stage case of vanishing interplane coupling, to the possibility of studying Lifshitz points and two-dimensional spin-flop—transition phenomena in the low-stage case where the interplane coupling plays a crucial role on the magnetic properties. The generalized JKKN model is a unified attempt toward the explanation of experimental studies on samples with vanishing interplane coupling.

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