Phase transition and spin dynamics in the two-dimensional easy-plane ferromagnet

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With the use of self-consistent spin-wave theory, the spin stiffness for the two-dimensional classical easy-plane ferromagnet is calculated. The Kosterlitz-Thouless transition temperature for the classical XY model is obtaind. The contribution of vortex-antivortex bound pairs to the central peak at low temperatures is discussed.

I. INTRODUCTION

It is now well known[1] that neither the spin-one-half XY model nor the infinite-spin or classical XY model in two dimensions (2D) can have a conventional second-order phase transition to a state with uniform transverse magnetization. The phase transition and the nature of the ordered phase in the infinite-spin or classical XY model are now very well understood due to the work of Kosterlitz and Thouless[2,3] (KT) and others. Advances in material science, experimental techniques, and numerical simulations have contributed to assess, in a variety of systems, the validity of the various theoretical ideas underlying the physics of phase transitions in two dimensions, and the KT theory has been applied to many physical systems including magnetic compounds,[4] superconducting and superfluid films,[5] and 2D arrays of coupled Josephson junctions.[6]

In the Kosterlitz-Thouless theory,[2] the two-dimensional classical XY model undergoes a vortex-unbinding transition in a narrow temperature region in which vortexes bound together in *neutral* pairs unbind. For temperatures low enough, all vortices are bound together in pairs and the unbinding transition starts at a critical temperature T_{KT} at which the model undergoes a thermodynamic phase transition, the Kosterlitz-Thouless transition. Above T_{KT}, not all vortices are bound in pairs: We have free vortices and bound pairs of vortices (in fact, a vortex and an antivortex). In this temperature region, the order-parameter correlation function has an exponential decay, while in the low-temperature phase we have a *quasi*-long-range order where the correlation function has a power-law decay.

The two-dimensional classical easy-plane Heisenberg model, which is described by the Hamiltonian

$$H=-\frac{J}{2}\sum_{\mathbf{r},\mathbf{a}}(S_{\mathbf{r}}^{x}S_{\mathbf{r}+\mathbf{a}}^{x}+S_{\mathbf{r}}^{y}S_{\mathbf{r}+\mathbf{a}}^{y}+\lambda S_{\mathbf{r}}^{z}S_{\mathbf{r}+\mathbf{a}}^{z}) , \qquad (1.1)$$

where $\mathbf{r}+\mathbf{a}$ labels the four nearest-neighbor sites of $\mathbf{r}$ and $0\le\lambda<1$ describes an exchange easy-plane anisotropy, is very similar to the classical XY model concerning static properties. It also undertakes a topological phase transition at some critical temperature $T_c(\lambda)$, above which vortex pairs dissociate.[7] The classical XY model is given by Eq. (1.1) with $\lambda=0$, but considering $\mathbf{S}_{\mathbf{r}}=(S_{\mathbf{r}}^{x},S_{\mathbf{r}}^{y},S_{\mathbf{r}}^{z})$. This model has a true dynamics. The planar rotator model has a Hamiltonian of the same form, but the spins have only two components, $\mathbf{S}_{\mathbf{r}}=(S_{\mathbf{r}}^{x},S_{\mathbf{r}}^{y})$, and an equation of motion cannot be defined in the same way as for the XY model.

In this paper we report a calculation of the spin stiffness for the two-dimensional classical easy-plane Heisenberg model. We obtain a formula for $T_c(\lambda)$ valid for general λ $(0\le\lambda<1)$. We also discuss briefly the dynamics of this model in the long-wavelength and low-temperature limit.

II. CALCULATION OF THE SPIN STIFFNESS

The Hamiltonian for the planar rotator model can be written as

$$H_p=-\frac{J}{2}\sum_{\mathbf{r},\mathbf{a}}\cos(\phi_{\mathbf{r}+\mathbf{a}}-\phi_{\mathbf{r}}) , \qquad (2.1)$$

where $\phi_{\mathbf{r}}$ is an angle associated with each lattice site. In any system $\langle\phi_{\mathbf{r}}^2\rangle$ diverges if $\phi_{\mathbf{r}}$ is measured relative to a fixed axis since a uniform rotation costs no energy. Thus we define $\phi_{\mathbf{r}}$ as the angle relative to the direction of the instantaneous total spin. At low temperatures the configurations with small angular differences between neighboring sites, i.e., $|\phi_{\mathbf{r}+\mathbf{a}}-\phi_{\mathbf{r}}|\ll 1$, are easily excited. One may hence expect that these are the important configurations for determining the thermodynamic properties. Provided all other configurations are neglected, H_p can be approximated by expanding the cosine in Eq. (2.1):

$$H_p\approx-\frac{J}{2}\sum_{\mathbf{r},\mathbf{a}}\left[1-\frac{(\phi_{\mathbf{r}+\mathbf{a}}-\phi_{\mathbf{r}})^2}{2}\right] . \qquad (2.2)$$

The constant term in (2.2) may be absorbed into the definition of the ground-state energy.

We note, however, that in writing (2.2) all anharmonic terms present in (2.1) have been neglected. One way to take into account these terms is to write (2.2) as

$$H_0=\frac{1}{2}\rho_s J\sum_{\mathbf{r},\mathbf{a}}(\phi_{\mathbf{r}+\mathbf{a}}-\phi_{\mathbf{r}})^2 , \qquad (2.3)$$

where ρ_s is the spin stiffness (or helicity modulus). Pokrovsky and Uimin[8] have calculated ρ_s using a self-consistent spin-wave theory, and in spite of the fact that their theory does not incorporate the vortex pair mechanism, it provides good estimates for ρ_s and the critical temperature for the planar rotator model. The stiffness ρ_s has also been calculated using a self-consistent harmonic approximation variational method.[6,9]

Here we will perform a calculation of the spin stiffness for Hamiltonian (1.1), the planar rotator model described above being a particular case of our more general theory.

We start by writing Hamiltonian (1.1) in terms of the polar representation for the spin at site $\mathbf{r}$:

$$\mathbf{S}_\mathbf{r}=\left[S\left[1-\left[\frac{S^z_\mathbf{r}}{S}\right]^2\right]^{1/2}\cos\phi_\mathbf{r},S\left[1-\left[\frac{S^z_\mathbf{r}}{S}\right]^2\right]^{1/2}\sin\phi_\mathbf{r},S^z_\mathbf{r}\right] . \tag{2.4}$$

We find

$$H=-\frac{J}{2}\sum_{\mathbf{r},\mathbf{a}}\left\{S^2\left[1-\left[\frac{S^z_\mathbf{r}}{S}\right]^2\right]^{1/2}\left[1-\left[\frac{S^z_{\mathbf{r}+\mathbf{a}}}{S}\right]^2\right]^{1/2}\cos(\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r})+\lambda S^z_\mathbf{r}S^z_{\mathbf{r}+\mathbf{a}}\right\} . \tag{2.5}$$

In order to obtain the long-wavelength limit of Hamiltonian (2.5), analogous to Hamiltonian (2.3), we argue as follows: If we calculate the time derivative of $\phi_\mathbf{r}$ through Hamiltonian (2.5), using the equation of motion $\dot{\Phi}_\mathbf{r}=\{\Phi_r,H\}$, where $\{\ ,\ \}$ denotes the Poisson bracket and $\{S^z_n,\Phi_n\}=\delta_{nm}$ is the fundamental Poisson bracket for the polar representation of a spin vector, we find (setting $\lambda=0$ for simplicity)

$$\dot{\phi}_\mathbf{r}=-4J[1+\mathcal{O}(\nabla\phi_\mathbf{r})^2]S^z_\mathbf{r}\approx-4JS^z_\mathbf{r} . \tag{2.6}$$

This is exactly the same result that we find considering the quadratic Hamiltonian obtained by expanding Hamiltonian (2.5) into powers of $(S^z/S)^2$ and $(\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r})^2$ with no need to introduce any renormalizing factor. Otherwise, the time derivative of $S^z_\mathbf{r}$ is related to the angle difference $\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r}$ and its analytic expression depends on which Hamiltonian is used, whether it is the one given by (2.5) or its quadratic expression. This means that in obtaining the correct long-wavelength limit of (2.5), we must be aware of the coefficient to be put on the $(\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r})^2$ term. The behavior of $\dot{S}^z_\mathbf{r}$ with both Hamiltonians of interest leads to the conclusion that the renormalization factor can be determined by the calculus of $\dot{S}^z_\mathbf{r}$ with Hamiltonian (2.5). We find, in the reciprocal space,

$$\langle\dot{S}^z_\mathbf{q}\dot{S}^z_{-\mathbf{q}}\rangle=4JS^2T(1-\gamma_\mathbf{q})\left\langle\left[1-\left[\frac{S^z_\mathbf{r}}{S}\right]^2\right]^{1/2}\times\left[1-\left[\frac{S^z_{\mathbf{r}+\mathbf{a}}}{S}\right]^2\right]^{1/2}\times\cos(\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r})\right\rangle , \tag{2.7}$$

where the brackets mean a thermal average and $\gamma_\mathbf{q}=[\cos q_x+\cos q_y]/2$. Following this reasoning, the quadratic form of Hamiltonian (2.5) is found to be

$$H_0=\frac{J}{2}\sum_{\mathbf{r},\mathbf{a}}\left[\frac{S^2}{2}\rho_s(\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r})^2+(S^z_\mathbf{r})^2-\lambda S^z_\mathbf{r}S^z_{\mathbf{r}+\mathbf{a}}\right] , \tag{2.8}$$

where the stiffness ρ_s is given by

$$\rho_s=\left\langle\left[1-\left[\frac{S^z_\mathbf{r}}{S}\right]^2\right]^{1/2}\left[1-\left[\frac{S^z_{\mathbf{r}+\mathbf{a}}}{S}\right]^2\right]^{1/2}\times\cos(\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r})\right\rangle . \tag{2.9}$$

This equation includes terms describing out-of-plane fluctuations which were obtained here in a self-consistent way.

Hamiltonian (2.8) can be written, using Eq. (2.6) and taking for the moment $\lambda=0$,

$$H_0=\frac{JS^2\rho_s}{2}\sum_{\mathbf{r},\mathbf{a}}\frac{1}{2}(\phi_{\mathbf{r}+\mathbf{a}}-\phi_\mathbf{r})^2+\frac{\alpha}{2}\sum_\mathbf{r}\dot{\phi}^2_\mathbf{r} , \tag{2.10}$$

with $\alpha=J/16$. This Hamiltonian is similar to that found by Côté and Griffin.[10] However, in their result, the factor α is left undetermined. Equation (2.10) has also been used to describe periodic artificially layered high-T_c superconductors[6] where J is the Josephson coupling constant and α an effective self-capacitance.

Hamiltonian (2.8) can be diagonalized using standard methods.[11] Although we are interested in the classical model, it is more convenient to use the quantum formalism and, then, take the classical limit. Introducing the canonical transformation

$$\phi_\mathbf{q}=\frac{1}{\sqrt{2S}}\left[\frac{1+\lambda\gamma_\mathbf{q}}{\rho_s(1-\gamma_\mathbf{q})}\right]^{1/4}(a^\dagger_\mathbf{q}+a_{-\mathbf{q}}) , \tag{2.11}$$

$$S^z_\mathbf{q}=i\left[\frac{S}{2}\right]^{1/2}\left[\frac{\rho_s(1-\gamma_\mathbf{q})}{1+\lambda\gamma_\mathbf{q}}\right]^{1/4}(a^\dagger_\mathbf{q}-a_{-\mathbf{q}}) , \tag{2.12}$$

where $a^\dagger_\mathbf{q}$ and $a_{-\mathbf{q}}$ are the boson creation and annihilation operators, respectively, we obtain

$$H_0=\sum_\mathbf{q}\omega_\mathbf{q}\left[a^\dagger_\mathbf{q}a_\mathbf{q}+\frac{1}{2}\right] , \tag{2.13}$$

where

$$\omega_\mathbf{q}=4JS[\rho_s(1-\gamma_\mathbf{q})(1+\lambda\gamma_\mathbf{q})]^{1/2} . \tag{2.14}$$

The normalized spin-wave frequency is thus given by

$$\frac{\omega_q(T)}{\omega_q(T=0)}=\sqrt{\rho_s} . \tag{2.15}$$

Before proceeding with our calculation, let us remark that the second moment $\langle \omega_q^2 \rangle^z$ for the relaxation function $S^{zz}(q,\omega)$ is given exactly by[12]

$$\langle \omega_q^2 \rangle^z=\frac{4JT(1-\gamma_q)}{\langle S_q^z S_q^z \rangle}\langle S_{\mathbf{r}}^{\perp} S_{\mathbf{r+a}}^{\perp} \rangle , \tag{2.16}$$

where

$$\langle S_{\mathbf{r}}^{\perp} S_{\mathbf{r+a}}^{\perp} \rangle = \langle S_{\mathbf{r}}^{x} S_{\mathbf{r+a}}^{x} \rangle + \langle S_{\mathbf{r}}^{y} S_{\mathbf{r+a}}^{y} \rangle .$$

At low temperatures and in the classical limit, we have, from (2.12),

$$\langle S_q^z S_q^z \rangle = S\left[\frac{1-\gamma_q}{1+\lambda\gamma_q}\right]^{1/2}\frac{1}{\beta\omega_q} . \tag{2.17}$$

Thus, using Eqs. (2.14) and (2.16), we obtain

$$\langle \omega_q^2 \rangle^z=\omega_q^2\left[\frac{\langle S_{\mathbf{r}}^{\perp} S_{\mathbf{r+a}}^{\perp} \rangle}{S^2}\right] . \tag{2.18}$$

So the stiffness as defined by Eq. (2.9) gives correctly the second moment.

For calculating ρ_s we approximate $\langle \cdots \rangle$ in Eq. (2.9) by $\langle \cdots \rangle_0$. In this approximation $\phi_{\mathbf{r}}$ and $S_{\mathbf{r}}^z$ are uncoupled variables and we find

$$\rho_s=\left\langle\left[1-\left[\frac{S_{\mathbf{r}}^z}{S}\right]^2\right]^{1/2}\left[1-\left[\frac{S_{\mathbf{r+a}}^z}{S}\right]^2\right]^{1/2}\right\rangle_0 \times\exp\left[-\frac{1}{2}\langle(\phi_{\mathbf{r+a}}-\phi_{\mathbf{r}})^2\rangle_0\right] . \tag{2.19}$$

Using Eq. (2.11), we obtain, for the exponential factor,

$$\begin{aligned} F&=\frac{1}{2}\langle(\phi_{\mathbf{r+a}}-\phi_{\mathbf{r}})^2\rangle_0 \\ &=\frac{1}{S}\frac{1}{N}\sum_{\mathbf{k}}\left[\frac{1}{2}+\frac{1}{e^{\beta\omega_{\mathbf{k}}}-1}\right](1-\cos\mathbf{k}) \\ &\quad\times\left[\frac{1+\lambda\gamma_{\mathbf{k}}}{\rho_s(1-\gamma_{\mathbf{k}})}\right]^{1/2} . \end{aligned} \tag{2.20}$$

Using a long-wavelength approximation, we get

$$F=\frac{1}{2S\sqrt{2}\rho_s^{1/2}}\frac{1}{(2\pi)^2}\int\int \kappa\, d^2\kappa \coth(b\kappa/2) , \tag{2.21}$$

where $b=\sqrt{8}JS\rho_s^{1/2}/T$. In the quasiclassical case $b \ll 1$, we find

$$F=\frac{t}{4S^2\rho_s}+\frac{\pi^2}{9t} , \tag{2.22}$$

where $t=T/J$. The first term is the classical result; the second is a first quantum correction.

For the out-of-plane fluctuations, we have, in the classical limit,

$$\left\langle\left[1-\left[\frac{S_{\mathbf{r}}^z}{S}\right]^2\right]\left[1-\left[\frac{S_{\mathbf{r+a}}^z}{S}\right]^2\right]\right\rangle_0 \approx 1-\left\langle\left[\frac{S_{\mathbf{r}}^z}{S}\right]^2\right\rangle_0 =1-\frac{T}{4JS^2}I(\lambda) , \tag{2.23}$$

where

$$I(\lambda)=\frac{1}{(2\pi)^2}\int d^2k\frac{1}{1+\lambda\gamma_{\mathbf{k}}} . \tag{2.24}$$

Substituting the above equations into (2.19), we obtain, in the classical limit,

$$\rho_s=[1-\Theta I(\lambda)]e^{-\Theta/\rho_s} , \tag{2.25}$$

where $\Theta=T/4JS^2$. This is a self-consistent equation giving the stiffness ρ_s for each temperature.

For the XY model, we have $I(0)=1$; however, for the planar rotator model, since no out-of plane fluctuations are allowed, we should take $I(0)=0$. In the latter case, we have $\rho_s=\exp(-\Theta/\rho_s)$, the result obtained by Pokrovsky and Uimin.[8]

At sufficiently low temperatures, we may expand Eq. (2.25), obtaining

$$\rho_s=1-[I(\lambda)+1]\frac{T}{4JS^2} . \tag{2.26}$$

The linear decrease of ρ_s at low temperature is characteristic of classical spin models. [A quantum calculation performed using Eq. (2.21) in the region $b \gg 1$ would lead to a cubic dependence with temperature.]

In Fig. 1 we show the normalized dispersion relation $\omega_q(T)/\omega_q(0)$ as a function of temperature, compared with simulation data from Ref. 13. The agreement could be improved, in principle, for high temperatures, including vortices effects (see next section).

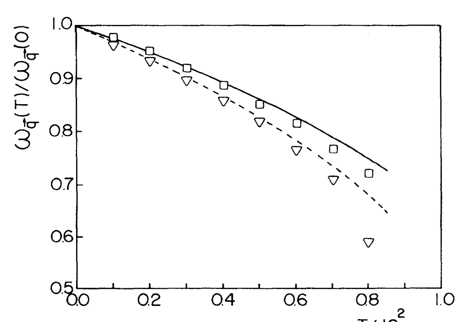

FIG. 1. Temperature dependence of the normalized spin-wave frequency. Here we compare our theoretical calculation with numerical simulation from Ref. 13: $\lambda=0$ (□ and solid curve); $\lambda=0.9$ (∇ and dashed curve). The solid and dashed curves apply to the present theory and the symbols to the Monte Carlo simulations.

III. RENORMALIZATION OF THE SPIN-WAVE FREQUENCY BY VORTEX PAIRS

At low temperatures $T \ll J$, only the long-wavelength fluctuations of ϕ, the scales of which are much greater than the distance between neighboring spins, are important. For these long-wavelength excitations, we can go over from the summation to an integration and replace the difference by a derivative in Eq. (2.10), obtaining

$$H=\frac{JS^2\rho_s}{2}\int[\nabla\phi(\mathbf{r})]^2d\mathbf{r}+\frac{\alpha}{2}\int\left[\frac{d\phi}{dt}\right]^2d\mathbf{r}\ , \tag{3.1}$$

where $\phi(\mathbf{r})$ is now a continuous field angle variable. This field splits into two parts:

$$\phi(\mathbf{r})=\varphi(\mathbf{r})+\psi(\mathbf{r})\ , \tag{3.2}$$

where $\varphi(\mathbf{r})$ is the spin-wave field and $\psi(\mathbf{r})$ the vortex field. If the vortex part $\psi(\mathbf{r})$ is ignored, the spin-wave frequency is given by Eq. (2.14). The effect of the bound vortex pairs is to renormalize the spin-wave excitations.

In a theory developed by Côté and Griffin,[10] the coupled equations of motion for the spin-wave and vortex fields are derived from a Lagrangian analogous to that used in classical electrodynamics of a continuous medium in analogy with the dielectric function in ordinary electrodynamics. This approach leads to an effective Hamiltonian

$$H_{s\omega}=\frac{1}{2}S^2J_T\int d\mathbf{r}(\nabla\varphi_0)^2+\frac{\alpha}{2}\int\left[\frac{d\phi}{dt}\right]^2d\mathbf{r}\ , \tag{3.3}$$

where $J_T=J\rho_s/\epsilon$ and ϵ is the dielectric function describing the effect of the bound pairs. Thus the equation of motion and the associated Hamiltonian look precisely as if we were dealing with a pure spin field, with no vortex configuration included. The effect of the bound vortices is completely buried in the renormalized exchange constant.

There is no explicity theoretical calculation for the dielectric function; however, for low temperatures, we can neglect the vortex contribution, since the vortices require a finite energy to be excited, and therefore Eq. (2.15) should give the correct spin-wave frequency. Near T_{KT}, vortex excitations become important and renormalization-group analysis shows that ϵ^{-1} exhibits a universal jump at $T=T_{\mathrm{KT}}$, in the short-wavelength limit, given by[14,15]

$$\lim_{T\to T_{\mathrm{KT}}^-}\frac{J_T(T)}{T}=\frac{2}{\pi}\ . \tag{3.4}$$

IV. PHASE TRANSITION

Equation (2.25) shows that there is a critical temperature T_c below which spin-wave-like excitations of ϕ are possible. This critical temperature is reached when Eq. (2.25) admits no solution but the trivial one ($\rho_s=0$). This situation corresponds to

$$T_c(\lambda)=\frac{4JS^2}{e+I(\lambda)}\ . \tag{4.1}$$

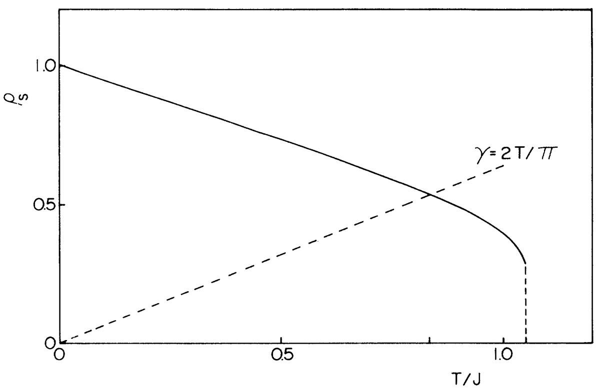

FIG. 2. Spin stiffness for the XY model. Dashed line is $\gamma=2T/\pi$. Crossing between the solid curve through the dashed line defines the Kosterlitz-Thouless temperature T_{KT}.

Thus we may conclude that the anharmonicity of the initial Hamiltonian (1.1) results in an abrupt disappearance of the stiffness ρ_s, which corresponds to the disappearance of the phase ordering. For the classical XY model, we find, from (4.1), $T_c(0)/JS^2=1.076$, while for the planar rotator model ($I=0$) we have $T_c/JS^2=1.47$; thus, $T_c(\lambda=0)=0.73T_c$ (planar rotator). The Kosterlitz-Thouless temperature for the XY model can be determined by the crossing between the $\rho_s(T)$ curve and the line $\gamma=J_T(T_{\mathrm{KT}})$ with $J_T(T)$ given by Eq. (3.4). In Fig. 2 we plot both curves, obtaining $T_{\mathrm{KT}}=0.83J$ (taking $S=1$), in good agreement with the value of the Monte Carlo simulation to the XY model.[16]

T_c given by Eq. (4.1) varies very slowly with λ except at the close vicinity of the isotropic limit ($\lambda\to 1$). For $\lambda\to 1$ we have

$$I(\lambda)\approx 0.66+\pi^{-1}\ln(1-\lambda)^{-1}\ ,$$

leading to

$$\frac{T_c}{JS^2}\overset{\lambda\to 1}{\approx}\frac{4\pi}{A+\ln(1-\lambda)^{-1}}\ , \tag{4.2}$$

with $A=10.6$. Taking vortices into account will change the value of A. Considering that for $\lambda\to 1$ the value of A is irrelevant and that, for $\lambda=0$, $4\pi/A=0.83$ is the KT temperature obtained above, we can take $A=15.14$ and write

$$\frac{T_c(\lambda)}{JS^2}=\frac{4\pi}{15.14+\ln(1-\lambda)^{-1}}\ . \tag{4.3}$$

This equation will give a good estimate for $T_c(\lambda)$ for all values of λ. In fact, Eq. (4.3) agrees quite well with Monte Carlo estimates of $T_c(\lambda)$ performed by Kawabata and Bishop.[17]

V. VORTEX DYNAMICS

In this section we will discuss the effect of the bound vortex pairs on the dynamics of the XY model below T_{KT}.

The vortex-antivortex bound pair static solution to Eq. (3.1) is given by[2]

$$\phi(\mathbf{r})=\tan^{-1}\left[\frac{y-y_1}{x-x_1}\right]-\tan^{-1}\left[\frac{y-y_2}{x-x_2}\right], \quad (5.1)$$

where the vortex is localized at point (x_1,y_1) and the antivortex at point (x_2,y_2). The vortex pairs are created as thermal excitation. The creation of such an excitation will, in addition to the interaction energy between members of the pair, involve a contribution E_0 which is determined by the energy needed to create a vortex pair with the two vortices on nearest-neighbor sites. We have, at low temperature,

$$E(r)=E_0+E_1\ln\left[\frac{r}{r_0}\right], \quad (5.2)$$

where r is the distance between the vortex and antivortex centers, r_0 is the lattice spacing, and

$$E_0=\pi^2 JS^2\left[1-\frac{T}{2JS^2}\right],$$
$$E_1=2\pi JS^2\left[1-\frac{T}{2JS^2}\right], \quad (5.3)$$

where we have used the low-T expansion for ρ_s in Eq. (5.3). Note that for the XY model, E_0 and E_1 are temperature dependent.

For dynamical solutions of the form $\phi(\mathbf{r}-\mathbf{v}t)$, where $\mathbf{r}$ is the bound pair velocity (one site apart), we find for the energy, using Eq. (3.1),

$$E(\mathbf{v})=E_0+av^2, \quad (5.4)$$

where $a=\alpha\pi^2$.

To calculate the density n of vortex pairs, it is usual to describe the thermally induced vortex excitations by a grand canonical ensemble of noninteracting vortex pairs. In this description we have[2,18]

$$n=\frac{2\pi}{r_0^4}\int_{r_0}^{L} r\,dr\,e^{-\beta E(r)}, \quad (5.5)$$

where L is an upper cutoff.

The Kosterlitz-Thouless theory predicts that well below T_{KT} all vortices will be tightly bound in pairs with the mean separation between members of a pair, d, being around one lattice spacing and very much smaller than R, the mean separation of one pair from another. As T_{KT} is approached, d increases while r decreases as more vortex pairs appear. At T_{KT}, the first pair unbinds; that is, there exist some pairs with d of the same order as R. However, for the discrete lattice, r does not vary continuously but in steps of the lattice parameter r_0. So, for a pair two sites apart, we have an interaction energy $E_2=2\pi JS^2[1-T/4JS^2]\ln 2$. Thus, for temperatures $T\ll E_2$, we expect all pairs to be just one site apart, and therefore for the discrete lattice the density should be given by

$$n=Ae^{-\beta E_0}, \quad (5.6)$$

the prefactor A being of order of the unity. This picture is confirmed by Monte Carlo simulations[19,20] which show that a pair with d greater than a lattice spacing appears at $T=0.95T_{KT}$.

The dynamic correlation function $S^{\alpha,\alpha}(\mathbf{q},\omega)$ $(\alpha=x,y)$ is given by

$$S^{\alpha\alpha}(\mathbf{q},\omega)=\frac{1}{(2\pi)^3}\int\int d\mathbf{r}\,dt\,e^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}\langle S_{\mathbf{r}}^{\alpha}(t)S_0^{\alpha}(0)\rangle . \quad (5.7)$$

In order to calculate $\langle S_{\mathbf{r}}^{\alpha}(t)S_0^{\alpha}(0)\rangle$, we use the picture of a gas of noninteracting bound pairs which are thermally activated and write

$$\langle S_{\mathbf{r}}^{x}(t)S_0^{x}(0)\rangle =S^2\int\int d\mathbf{R}\,d\mathbf{v}\,N(v)\cos\phi(\mathbf{r}-\mathbf{R}-\mathbf{v}t)\cos\phi(\mathbf{R}), \quad (5.8)$$

where $\mathbf{R}$ is the position of the pair and $N(v)=NP(v)$ is the number of pairs with velocity v. Within the Boltzmann statistics, the probability of finding a pair with velocity v is expressed as

$$P(v)=\frac{e^{-(v/v_\theta)^2}}{\pi v_\theta}, \quad (5.9)$$

where $v_\theta=\sqrt{T/a}$ is the thermal velocity. After performing all integrations, we find

$$S^{xx}(q,\omega)=\frac{n}{(2\pi)^3}\frac{|F_x(\mathbf{q})|^2}{q}v_\theta e^{-(\omega/qv_\theta)^2}, \quad (5.10)$$

where $|F_x(\mathbf{q})|^2$ is the form factor for the x component obtained using Eq. (5.1). A similar result holds for the y component. Because of the rotational symmetry in the XY plane, what is really important is the symmetrized correlation function

$$S^{1}(q,\omega)=\tfrac{1}{2}[S^{xx}(q,\omega)+S^{yy}(q,\omega)] . \quad (5.11)$$

This equation gives the vortex pair contribution to the central peak below T_{KT}. There is also indication that spin waves contribute to the central peak.[21] For spin-wave dynamics below T_{KT}, see Côté and Griffin,[10] and for vortex dynamics above T_{KT}, see Ref. 22.

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