Phase transition in the spatially anisotropic classical XY model

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The self-consistent harmonic approximation is applied to the classical three-dimensional spatially anisotropic $O(2)$ model on the cubical lattice. The spin stiffness and the magnetization are calculated.

By now it is well known that in two-dimensional systems having a XY-like continuous symmetry, a topological long-range order is developed at low temperatures and the order is destroyed by the unbinding of vortices at a critical temperature T_{KT}, the Kosterlitz-Thouless temperature. Experimentally, a great variety of critical phenomena has been associated with the universality class of the XY model.[1,2] However, despite their layered structure, there is no ideal two-dimensional material which shows the planar behavior, as there is always some coupling between adjacent planes.[3–12] An arbitrarily small coupling between adjacent planes will have a dramatic effect on the ordering in the three-dimensional (3D) case. This system, of course, will show the conventional long-range order and exhibit an usual second-order phase transition.

In this paper we consider the renormalization effects of the interlayer and intralayer coupling using the self-consistent harmonic approximation (SCHA). This technique, for the isotropic model, has been used extensively in the literature,[13–20] mainly in the context of high-T_c superconductors, since the XY model can be viewed as a model of superconductors for which the magnitude variations of the order parameter have been suppressed. Here we will generalize the SCHA to treat the spatially anisotropic XY model.

The spatially anisotropic classical XY model in three dimensions is defined by the Hamiltonian

$$H=-\sum_r\left[J_x\sum_x\cos(\phi_r-\phi_{r+x})+J_y\sum_y\cos(\phi_r-\phi_{r+y})+J_z\sum_z\cos(\phi_r-\phi_{r+z})\right], \tag{1}$$

where J_x,J_y,J_z are the coupling constants in the x,y, and z directions, respectively, and the sums are extended over all nearest-neighbor pairs on a cubic lattice.

The SCHA procedure consists in replacing the cosine potential in the Hamiltonian (1) by a variational harmonic potential of the form

$$H_0=\tfrac{1}{2}\sum_r\left[K_x\sum_x(\phi_r-\phi_{r+x})^2+K_y\sum_y(\phi_r-\phi_{r+y})^2+K_z\sum_z(\phi_r-\phi_{r+z})^2\right], \tag{2}$$

where K_i $(i=x,y,z)$ are effective coupling constants that take into account the nonlinearities of the interactions and that have to be adjusted in order to minimize the variational free energy given by

$$F=F_0+\langle H-H_0\rangle_0 , \tag{3}$$

where both, F_0 and the average $\langle\ .\ \rangle_0$ are evaluated with respect to H_0. Our calculations will be a generalization of those of Ariosa *et al.*,[14] wherein the SCHA was used to investigate the phase transition in the fully frustrated 2D XY model. Using Eqs. (1) and (2) the variational free energy becomes

$$F=-\frac{1}{\beta}\ln Z_0-\sum_r[J_xe^{-X/2}+J_ye^{-Y/2}+J_ze^{-Z/2}]-\frac{1}{2}\sum_r[K_xX+K_yY+K_zZ] , \tag{4}$$

where $Z_0=\mathrm{Tr}\{\exp(-\beta H_0)\}$, and

$$X=\langle(\phi_0-\phi_x)^2\rangle_0,\quad Y=\langle(\phi_0-\phi_y)^2\rangle_0,\quad X=\langle(\phi_0-\phi_z)^2\rangle_0 \tag{5}$$

is the nonsingular part of the lattice Green function.

In order to obtain the quantities X, Y, and Z, we shall first diagonalize the quadratic form H_0. An eight site basis is introduced on the array, in the following way

$$\mathbf{r}=\boldsymbol{\rho}+(a/2)(s\hat{x}+t\hat{y}+1\hat{z}) , \tag{6}$$

with

$$\boldsymbol{\rho}=2a(n_x\hat{x}+n_y\hat{y}+n_z\hat{z}),\quad s,t,l=\pm1 , \tag{7}$$

where a is the lattice constant and $\hat{x},\hat{y},\hat{z}$ the unit vectors on the x,y,z axes.

Expanding all functions of $\boldsymbol{\rho}$ in Fourier series, H_0 can be written as

$$H_0=\sum_q\sum_{s,t,l=\pm1}\sum_{s',t',l'=\pm1}\psi^*_{s,t,l}(\mathbf{q})M_{stls't'l'}(\mathbf{q})\psi_{s',t',l'}(\mathbf{q}) \tag{8}$$

with the matrix M given by

$$M=\begin{bmatrix} m_1 & m_2 & m_3 & m_4 & 0 & 0 & 0 & 0\\ m_2 & m_1 & 0 & 0 & m_3 & m_4 & 0 & 0\\ m_3 & 0 & m_1 & 0 & m_2 & 0 & m_4 & 0\\ m_4 & 0 & 0 & m_1 & 0 & m_2 & m_3 & 0\\ 0 & m_3 & m_2 & 0 & m_1 & 0 & 0 & m_4\\ 0 & m_4 & 0 & m_2 & 0 & m_1 & 0 & m_3\\ 0 & 0 & m_4 & m_3 & 0 & 0 & m_1 & m_2\\ 0 & 0 & 0 & 0 & m_4 & m_3 & m_2 & m_1 \end{bmatrix} , \tag{9}$$

where $m_1=K_x+K_y+K_z$, $m_2=-K_z\cos q_z$, $m_3=-K_y\cos q_y$, $m_4=-K_x\cos q_x$, and $\psi_{x,t,l}(\mathbf{q})$ are the normal coordinates. The eigenvalues of M are given by

$$\begin{aligned}
\omega_1&=K_x(1-\cos q_x)+K_y(1-\cos q_y)+K_z(1-\cos q_z)\ ,\\
\omega_2&=K_x(1+\cos q_x)+K_y(1-\cos q_y)+K_z(1-\cos q_z)\ ,\\
\omega_3&=K_x(1-\cos q_x)+K_y(1+\cos q_y)+K_z(1-\cos q_z)\ ,\\
\omega_4&=K_x(1-\cos q_x)+K_y(1-\cos q_y)+K_z(1+\cos q_z)\ ,\\
\omega_5&=K_x(1+\cos q_x)+K_y(1+\cos q_y)+K_z(1-\cos q_z)\ ,\\
\omega_6&=K_x(1+\cos q_x)+K_y(1-\cos q_y)+K_z(1+\cos q_z)\ ,\\
\omega_7&=K_x(1-\cos q_x)+K_y(1+\cos q_y)+K_z(1+\cos q_z)\ ,\\
\omega_8&=K_x(1+\cos q_x)+K_y(1+\cos q_y)+K_z(1+\cos q_z)
\end{aligned}\tag{10}$$

and the eigenvectors by

$$\begin{aligned}
\Delta_1&=A(1;1;1;1;1;1;1;1)\ ,\\
\Delta_2&=A(1;1;1;-1;1;-1;-1;-1)\ ,\\
\Delta_3&=A(1;1;-1;1;-1;1;-1;-1)\ ,\\
\Delta_4&=A(1;-1;1;1;-1;-1;1;-1)\ ,\\
\Delta_5&=A(1;1;-1;-1;-1;-1;1;1)\ ,\\
\Delta_6&=A(1;-1;1;-1-1;1;-1;1)\ ,\\
\Delta_7&=A(1;-1;-1;1;1;-1;-1;1)\ ,\\
\Delta_8&=A(1;-1;-1;-1;1;1;1;-1)\ ,
\end{aligned}\tag{11}$$

with $A=(2\sqrt{2})^{-1}$. Thus, for each site (ρ,s,t,l) we have

$$\psi_{stl}(\rho)=\frac{1}{\sqrt{N}}\sum_q \exp\left[i\mathbf{q}\cdot\rho+i\frac{s}{2}q_x+i\frac{t}{2}q_y+i\frac{1}{2}q_z\right]\times\sum_m a_m(\mathbf{q},s,t,l)\psi_m(\mathbf{q})\ ,\tag{12}$$

where $a_m(\mathbf{q},s,t,l)$ is the (s,t,l) component of the eigenvectors Δ_m in (12). Then we can write

$$H_0=\sum_q\sum_{m=1}^{8}\omega_m(\mathbf{q})|\psi_m(\mathbf{q})|^2\tag{13}$$

which leads to the following expression (equipartition principle):

$$\omega_m(\mathbf{q})\langle|\psi_m(\mathbf{q})|^2\rangle_0=T/2\ ,\tag{14}$$

where we have taken the Boltzmann constant equal to the unity. We can now compute the averages X, Y, Z, obtaining

$$X=\frac{1}{N}\sum_q\sum_m[a_m^2(-1,1,1)+a_m^2(1,1,1)-2a_m(-1,1,1)a_m(1,1,1)\cos q_x]T/2\omega_m(\mathbf{q})\ ,\tag{15}$$

$$Y=\frac{1}{N}\sum_q\sum_m[a_m^2(1,1,1)+a_m^2(1,-1,1)-2a_m(1,1,1)a_m(1,-1,1)\cos q_y]T/2\omega_m(\mathbf{q})\ ,\tag{16}$$

$$Z=\frac{1}{N}\sum_q\sum_m[a_m^2(1,1,1)+a_m^2(1,1,-1)-2a_m(1,1,1)a_m(1,1,-1)\cos q_z]T/2\omega_m(\mathbf{q})\ .\tag{17}$$

In the following we will take $J_x=J_y=J$, since this is the case of more physical interest. Replacing the sum in q in (15), (16), and (17) by an intergral, the effective coupling constant can be calculated analytically. However since we have to solve a self-consistent equation to obtain K and K_z this would lead to a lengthy calculation. Thus to obtain a simple expression we will make the usual Debye approximation by using the small q limit of the mode frequencies. Strictly speaking this is not necessary and the full momentum dependence can be maintained. We will use the Debye approximation just as a matter of simplicity. We should note that more precise results (perhaps closer to Monte Carlo) could be obtained by keeping the full q dependence in Eqs. (15)–(17). Comparing the calculations, for a few values of K and K_z, using the two procedures, we have found a difference which ranged from 3% to 5%.

In the two limits $J_z\ll J$ and $J_z\approx J$ we have obtained

(a) $J_z\ll J$

$$K\approx J\exp\left\{-\frac{T}{16K}\left[\frac{5}{2}+\frac{1}{1+K_z/K}+\frac{1}{2+K_z/K}+\left[\frac{2\pi^2+24}{48\pi}\right]\left[\frac{K_z}{K}\right]\ln\left[\frac{K_z}{K}\right]\right]\right\}\ ,\tag{18}$$

$$K_z\approx J_z\left[\frac{K_z}{K}\right]^{Td/16K}\exp\left[-\frac{T}{16K}\left[\frac{2}{1+K_z/K}+\frac{1}{2+K_z/K}+c\right]\right]\ ,\tag{19}$$

where

$$d=(\pi^2+12)/12\pi;c=(\pi/12)\ln(4/\pi)+(1/\pi)\ln\pi\ .\tag{20}$$

(b) $J_z\approx J$

$$K\approx J\exp\left\{\frac{-T}{16}\left[\frac{3K+K_z}{2K^2+KK_z}+\frac{3K+K_z}{2K^2+2KK_z}+\frac{1}{2K}\left[\frac{1}{1-g}-\frac{g\tanh^{-1}(1-g)^{1/2}}{(1-g)^{3/2}}\right]\right]\right\}\ ,\tag{21}$$

$$K_z\approx J_z\exp\left\{-\frac{T}{16}\left[\frac{2K+2K_z}{K_z^2+2K_zK}+\frac{2K+2K_z}{(K+K_z)^2}+\frac{1}{K}\left[\frac{\tanh^{-1}(1-g)^{1/2}}{(1-g)^{3/2}}-\frac{1}{(1-g)}\right]\right]\right\}\tag{22}$$

with $g=K_z/K$.

The above expressions are self-consistent equations giving the effective coupling constants K and K_z for each temperature. The critical temperature T_c is reached when the self-consistent equations for the coupling constants admit no solutions but the trivial one $K=0$, $K_z=0$. Figure 1 shows a plot of the critical temperature

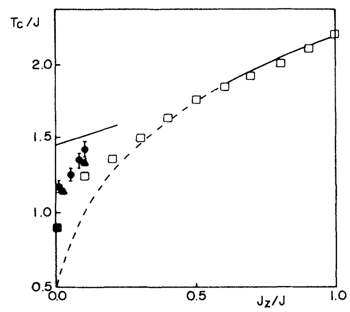

FIG. 1. Critical temperature as a function of anisotropy ratio J_z/J. Open squares, solid circles, and triangles are Monte Carlo data from Refs. 11, 26, and 29. Solid and dashed lines as in text.

(in the two limits discussed above) versus J_z/J (solid line) compared with Monte Carlo data from Refs. 11, 21, and 26. The dashed line represents the critical temperature calculated using the following expression $T_c/J=(J_z/J)^{1/3}2.2$, obtained by the mapping of the anisotropic continuum model onto the isotropic one [see discussion after Eq. (27)]. For $J=J_z$ we have $T_c/J=6/e=2.20$ which is consistent with Monte Carlo results[9,22,23] and the high temperature series of Ferer *et al.*[24] for the 3D isotropic planar model. For $J_z=0$ we recover the previous result for the 2D planar rotator (Ref. 2), $T_c/J=4/e=1.47$. This value is above the Monte Carlo result $T_c/J=0.90$. This happens because the SCHA does not incorporate the effect of polarization by bound vortex pairs. As was shown by Pires and Gouvea,[25] if we include vortex effects we obtain a good agreement with the Monte Carlo estimate. However if we apply the procedure of Ref. 25 for a small value of J_z, for instance $J_z/J=0.02$, we obtain the renormalized value for the critical temperature $T^*/J=1.07$, quite below the Monte Carlo estimate $T_c/J=1.14$, whereas the bare SCHA gives $T_c/J=1.50$. This discrepancy for the renormalized value T^* (considering that the inclusion of vortex effects worked well for $J_z=0$ in Ref. 25) may be associated with the fact that for $J_z\neq 0$ the transition does not have a Kosterlitz-Thouless character; the phase transition of the anisotropic XY model is of second order. For larger values of J_z/J we cannot, of course, apply the formalism developed in Ref. 25.

For $J_z/J \ll 1$ we have obtained the following expression for the transition temperature

$$T_c=T_0[1-\Delta(5/16-p\ln\Delta)]^{-1} , \tag{23}$$

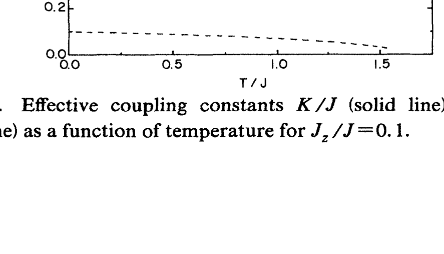

FIG. 2. Effective coupling constants K/J (solid line) and K_z/J (dashed line) as a function of temperature for $J_z/J=0.1$.

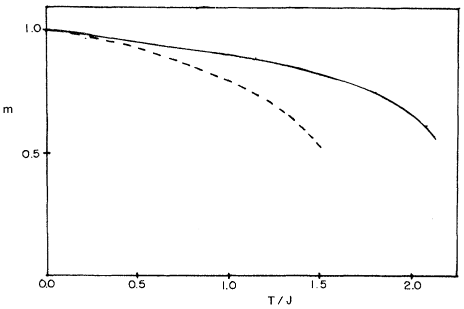

FIG. 3. Magnetization as a function of temperature for $J_z/J=1$ (solid line) and $J_z/J=0.1$ (dashed line).

where $\Delta=J_z/J, p=(2\pi^2+24)/48\pi$ and $T_0=4J/e$ is the transition temperature for the planar rotator.

In Fig. 2 we show our calculation for K and K_z as a function of temperature for $J_z/J=0.1$. As we can see at low temperatures the behavior is linear in T. For the 2D XY model there is no spontaneous magnetization and both the correlation length ξ and the magnetic susceptibility χ are infinite for temperatures below the Kosterlitz-Thouless temperature. For our model the magnetization is given by

$$\begin{aligned} m &= \langle \cos\psi_{s,t,l}(\rho)\rangle \\ &= \exp\{-(T/8\pi)(4/\sqrt{\pi K K_z})\tan^{-1}(\tfrac{1}{2}\sqrt{\pi K_z/K}) \\ &\quad +(1/K)\ln[(\pi K_z+4K)/\pi K_z]\} . \end{aligned} \tag{24}$$

In the limit $J_z \ll J$ Eq. (24) leads to

$$m \approx (K_z/K)^{T/8\pi K} \tag{25}$$

which would be compared with the result predicted by spin-wave calculations:

$$m=(J_z/J)^{T/8\pi J} . \tag{26}$$

In Fig. 3 we show the magnetization m as a function of temperature for $J_z/J=1$ and $J_z/J=0.1$. We see that the magnetization decreases drastically near T_c, where the three-dimensional critical fluctuations grow up and the spectrum $\omega_2, \ldots, \omega_8$ becomes relevant. As in the isotropic case the SCHA gives a first-order phase transition (with infinite slope of the order parameter) at T_c. This feature is an artifact of the approximation. Nonetheless the reasonable agreement for the critical temperature with Monte Carlo data suggests that the approximation is semiquantitatively reliable except insofar as the order of the transition is concerned. Of course for T close to the transition point, the behavior of the layered system is three dimensional, and the magnetization m should scale as $(T_c-T)^{\beta}$ with $\beta\approx\frac{1}{3}$.

The utility of the SCHA is not restricted to the calculation of the transition temperature (this could be performed using other techniques[26]) but also to give renormalized temperature-dependent coupling constants K and K_z that appear in the expressions of several thermodynamical variables, for instance, spin wave and topological excitations energy.

We should however remark that the stiffness, given by

$\rho=K/J$, is not an order parameter. For instance, in 2D the system can be described by a function $\rho(q^2)$ that plays the role of a dielectric susceptibility in the vortex gas.[27] In the low temperature phase we have $\rho=\rho(0)\neq 0$. Above the transition point, $\rho(q^2)\approx q^2(q^2+\xi^{-2})^{-1}$, where ξ is the correlation length. Thus is this region only for large distances r (short wavelength q) we have $\rho=0$.

The spin wave energy is given by

$$\omega(\mathbf{q})=4K\left[\sin^2\frac{q_x}{2}+\sin^2\frac{q_y}{2}\right]+4K_z\sin^2\frac{q_z}{2}\ , \tag{27}$$

while up to now no expression has been obtained for the energy of topological excitations occurring in the continuum limit of Hamiltonian (1), i.e.,

$$H=\frac{J}{2}\int\left[\left[\frac{\partial\phi}{\partial x}\right]^2+\left[\frac{\partial\phi}{\partial y}\right]^2+\frac{J_z}{J}\left[\frac{\partial\phi}{\partial z}\right]^2\right]dx\,dy\,dz\ . \tag{28}$$

The transformation $(x,y,z)=(\sqrt{\alpha}x',\sqrt{\alpha}y',z'/\alpha)$ with $\alpha=(J/J_z)^{1/3}$ yields an isotropic 3D model. Using the value of the critical temperature of the isotropic 3D planar rotator $T_c/J=2.2$ we obtain $T_c/J=(J_z/J)^{1/3}2.2$. This relation should hold as far as the continuum limit is valid. Of course the continuum approximation in the z direction breaks down for $J_z/J\ll 1$.

Comparing the critical temperature calculated using the above expression with our theoretical calculation (and Monte Carlo data) in Fig. 1, we see that this breaking down should happen for J_z/J below 0.3. In this region, instead of $(\partial\phi/\partial z)^2$ it would be better to approximate $\mathbf{S}_i\cdot\mathbf{S}_j$ by $\mathbf{S}_i\cdot\langle\mathbf{S}_j\rangle=m\cos\phi$, where m is the magnetization and i and j are in different layers. We have then

$$H=\frac{1}{2}\int\{J[(\partial\phi/\partial x)^2+(\partial\phi/\partial y)^2]+J_z m\cos\phi\}dx\,dy,\quad J_z\ll J\ . \tag{29}$$

Using now the lowest energy solution for Hamiltonian (29), calculated by Hudak,[28] we have for the energy of a bound pair a distance r apart

$$E(r)=16\pi J\ln(r/a_0)+2^{11/2}\pi\sqrt{JJ_z m}\,(r/a_0)\ , \tag{30}$$

where a_0 is a cutoff constant of the order of the lattice parameter. For large pair separation $(r/a_0\gg 1)$ the second term on the right-hand side of (29) dominates. For temperatures greater than zero we have then

$$E(r)=C(T)r, r\gg a_0\ , \tag{31}$$

where $C(T)=2^{11/2}\pi\sqrt{K(T)K_z(T)m(T)}$.

Thus $C(T)$ decreases with increasing temperature and in fact vanishes at T_c. This means that the interplane coupling effectively ceases to be felt by the vortices for $T>T_c$, the model effectively reducing to a two-dimensional planar model. The decoupling of the planes retrieves the 2D functional form of the vortex-antivortex interaction.[29,30]

Since our theory can be generalized to include dynamical terms in Hamiltonian (1) (an S^z component for the magnetic system, and a time derivative, $\partial\phi/\partial t$, for the superconductor) we hope it will play, for the layered system, the same role that the former SCHA have played for the isotropic model.

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[1] P. Minnhagen, Rev. Mod. Phys. **59**, 1001 (1987).

[2] D. G. Wiesler *et al.*, Z. Phys. B **93**, 277 (1994).

[3] V. L. Berezinskii, and A. Ya Blank, Sov. Phys. JETP **37**, 369 (1973).

[4] V. L. Pokrovsky and G. V. Uimin, Sov. Phys. JETP **38**, 847 (1978).

[5] C. Tsallis, Nuovo Cimento **34B**, 411 (1976).

[6] S. Hikami and T. Tsuneto, Prog. Theor. Phys. **63**, 387 (1980).

[7] N. Parza and J. E. van Himbergen, Ann. Phys. (NY) **134**, 286 (1981).

[8] S. T. Chui, Phys. Rev. B **12**, 2863 (1983).

[9] S. T. Chui and M. R. Giri, Phys. Lett. A **128**, 49 (1988).

[10] H. Weber and H. J. Jensen, Phys. Rev. B **44**, 454 (1991).

[11] D. Baeriswyl *et al.*, Braz. J. Phys. **22**, 140 (1992).

[12] A. S. T. Pires *et al.*, Phys. Rev. B **49**, 9663 (1994).

[13] D. Ariosa and H. Beck, Phys. Rev. B **43**, 344 (1991).

[14] D. Ariosa *et al.*, J. Phys. I (France) **51**, 1373 (1990).

[15] D. Spisak, Physica B **190**, 407 (1993).

[16] D. M. Wood and D. Stroud, Phys. Rev. B **25**, 1600 (1982).

[17] Y. E. Lozovik and S. G. Akopov, J. Phys. C **14**, L31 (1981).

[18] R. S. Fishman and D. Stroud, Phys. Rev. B **38**, 290 (1988).

[19] R. S. Fishman, Phys. Rev. B **38**, 11 996 (1988).

[20] D. Ariosa and H. Beck, Helv. Phys. Acta **65**, 499 (1992).

[21] P. Minnhagen and P. Olsson, Phys. Rev. Lett. **67**, 1039 (1991).

[22] C. Kawabata and K. Binder, Ann. Israel Phys. Soc. **2**, 988 (1978).

[23] G. Kohring *et al.*, Phys. Rev. Lett. **57**, 1358 (1986).

[24] M. Ferer *et al.*, Phys. Rev. B **8**, 5205 (1973).

[25] A. S. T. Pires and M. E. Gouvea, Phys. Rev. B **48**, 12 689 (1993).

[26] B. Chattopadhyay and S. R. Shenoy, Phys. Rev. Lett. **72**, 400 (1994).

[27] M. V. Feigelman, Sov. Phys. JETP **49**, 395 (1979).

[28] O. Hudak, Phys. Lett. **89A**, 245 (1982).

[29] P. Minnhagen and P. Olsson, Phys. Rev. B **44**, 4503 (1991).

[30] S. W. Pierson, Phys. Rev. Lett. **73**, 2496 (1994).