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Vortex contribution to the specific heat in the two-dimensional *XY* model

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We study the properties of topological excitations in the two-dimensional *XY* model by performing a loop expansion on the duality-transformed version of the model. The results for internal energy and heat capacity are in good agreement with recent Monte Carlo data.

I. INTRODUCTION

The *XY* model in two dimensions is a prototype model for systems which exhibit continuous symmetry and topological excitations. An understanding of this model can give valuable insights into a large number of related physical systems.

Topological excitations, unlike usual long-wavelength excitations, have a threshold energy and are localized in space. They play an essential role in phase transitions. Because of this, they have recently attracted increasing attention in many branches of physics such as low-temperature physics (superfluidity),[1] solid-state physics (melting),[2] and quantum field theory (quark confinement).[3] Topological excitations appear as points, lines, surfaces, etc., depending on the models and dimensionality. In the two-dimensional (2D) *XY* model they are points which can be interpreted as vortices in a two-dimensional superfluid film. In the 3D *XY* model the points become lines (vortex lines). In a 4D *XY* model, they would be surfaces. In all cases, they interact with each other with long-range Coulomb forces.

Such excitations acquire a special importance if a system has a symmetry which cannot be broken globally. Then it is *only* the topological excitations which can cause phase transitions. The case of two-dimensional U(1) symmetry is the best-known example. Hohenberg[4] and Mermin and Wagner[5] have proven that the macroscopic order parameter is zero at all temperatures, and in this sense the system should be always in a disordered state. This is due to the fact, that in two dimensions, fluctuations diverge as

$$(2\pi)^{-2}\int d^2k\, k^{-2}e^{i\mathbf{k}\cdot\mathbf{x}}$$

and are therefore so large that the system cannot sustain a finite order parameter on a macroscopic scale. Since the work of Kosterlitz and Thouless,[6] however, we know that this does not imply that there cannot be a phase transition. Vortex excitations can give a signal for an ordered state by binding themselves in pairs in low temperature. The phase transition takes place when tightly bound vortex pairs dissociate at high temperature.

For gauge models, it is an entirely different mechanism which forbids the global symmetry breakdown, as proved by Elitzur.[7] Here again, the topological excitations can induce phase transitions. In all these cases the localized excitations overcome the finite creation energy associated with them by carrying large configurational entropy.

Important as it is, there is no accurate method for taking vortex contributions into account. This is due to the fact that they are of an essentially nonperturbative nature. They contribute terms of the type $e^{-E/T}$ which cannot be expanded in powers of temperature (in gauge models, T is the coupling constant).

In the 2D *XY* model there exists an approximate way out of this dilemma. It is based on approximate replacement of the original model by a periodic Gaussian model in the partition function, as proposed first by Villain.[8] Then the vortices and long-wavelength excitations decouple and it is possible to exhibit the effect of the vortices with reasonable quality. Quantitatively, however, this replacement is a rather poor approximation, at least above the phase transition.[9]

Our approach is based upon a duality transformation[8,10] of the *XY* model which gives a precise definition of the topological excitations even in the high-temperature phase when their density is rather large. We split the partition function into two factors, one arising from the long-wavelength excitations, to be called spin waves, and another from the vortices. For the spin waves we find well-known perturbative methods to be useful.[11] For vortices we expand the fields around the classical values and take into account fluctuations up to two-loop corrections. Our results indicate that a perturbative approach proposed earlier by Savit[10] cannot be pursued in practice, due to the absence of a small parameter. The temperature ($T\to 0$) is not really his organizing parameter as he claims. In fact, we shall see that the reason lies in the fact that vortices modify the spin-wave spectrum beyond perturbative corrections.

As a test of our approach we have calculated the energy and heat capacity and compared them with existing Monte Carlo data.[12,13] We find good agreement.

II. MEAN-FIELD THEORY

One way of dealing with spin-wave excitations is to perform a mean-field approximation and calculate small fluctuations around it. The partition function of the 2D

XY model reads ($\beta=T^{-1}$)

$$Z=\prod_{\mathbf{x}}\int_{-\pi}^{\pi}d\theta(\mathbf{x})\frac{1}{2\pi}\exp\beta\sum_{\mathbf{x}i}\cos\nabla_i\theta(\mathbf{x}) , \qquad (2.1)$$

where $\theta(\mathbf{x})$ is the angle of the unit spin, ∇_i is defined by

$$\nabla_i\theta(\mathbf{x})=\theta(\mathbf{x}+\mathbf{i})-\theta(\mathbf{x}) ,$$

which measures relative orientation of nearest-neighbor spins, and $\mathbf{i}$ is the unit vector along each of the two coordinate axes.

The model is transformed to a more convenient form by inserting[14]

$$\int_{-i\infty}^{i\infty}\frac{d\alpha^1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{d\alpha^2}{2\pi i}\int_{-\infty}^{\infty}du^1\int_{-\infty}^{\infty}du^2\exp\sum_{a=1}^{2}\alpha^a(u^a-U^a)=\prod_{a=1}^{2}\int_{-\infty}^{\infty}du^a\delta(u^a-U^a)=1 \qquad (2.2)$$

for each component $U(\mathbf{x})=e^{i\theta(\mathbf{x})}$ in (2.1). In this way the partition function (2.1) is expressed as a path integral over two pairs of nonconstrained, real and pure imaginary variables,

$$Z=\prod_{\mathbf{x}}\int_{-i\infty}^{i\infty}\frac{d\alpha^1(\mathbf{x})}{2\pi i}\int_{-i\infty}^{i\infty}\frac{d\alpha^2(\mathbf{x})}{2\pi i}\int_{-\infty}^{\infty}du^1(\mathbf{x})\int_{-\infty}^{\infty}du^2(\mathbf{x})\exp\left[\sum_{\mathbf{x}}\{W(\alpha(\mathbf{x})\alpha^\dagger(\mathbf{x}))-\tfrac{1}{2}[\alpha^\dagger(\mathbf{x})u(\mathbf{x})+\alpha(\mathbf{x})u^\dagger(\mathbf{x})]\}\right.$$
$$\left.+\frac{\beta}{2}\sum_{\mathbf{x},\mathbf{i}}[u(\mathbf{x}+\mathbf{i})u^\dagger(\mathbf{x})+u^\dagger(\mathbf{x}+\mathbf{i})u(\mathbf{x})]\right] , \qquad (2.3)$$

where $I_0(z)$ is the modified Bessel function,[15]

$$I_0(z)=\int_{-\pi}^{\pi}d\theta\frac{1}{2\pi}e^{\beta\cos\theta} ,$$

α,u are complex fields, $\alpha=\alpha^1+i\alpha^2$, $\alpha^\dagger=\alpha^1-i\alpha^2$ and $u=u^1+iu^2$, $u^\dagger=u^1-iu^2$, and

$$W(\alpha,\alpha^\dagger)=\ln I_0\{[(\alpha^1)^2+(\alpha^2)^2]^{1/2}\} .$$

The exponent is minimal for the constant real mean fields $u(\mathbf{x})=u$ and $\alpha(\mathbf{x})=\alpha$,

$$u=I_1(\alpha)/I_0(\alpha) ,$$
$$\alpha=2bu , \qquad (2.4)$$

with $b=D\beta$ (D: dimensionality) and $I_1(\alpha)$, the modified Bessel function of order one. The free energy per lattice site is given by

$$-\beta f^{\mathrm{MF}}=bu^2-\alpha u+\ln I_0(\alpha) . \qquad (2.5)$$

For the one-loop correction we expand the exponent in (2.3) up to quadratic terms and find

$$-\beta Nf^{\mathrm{MF}}+\frac{1}{2!}\sum_{\mathbf{x}}(W_{\alpha\alpha}\{[\delta\alpha(\mathbf{x})]^2+[\delta\alpha^\dagger(\mathbf{x})]^2\}+2W_{\alpha\alpha^\dagger}\delta\alpha(\mathbf{x})\delta\alpha^\dagger(\mathbf{x})-\delta\alpha^\dagger(\mathbf{x})\delta u(\mathbf{x})-\delta\alpha(\mathbf{x})\delta u^\dagger(\mathbf{x}))$$
$$+\beta D\sum_{\mathbf{x}}\delta u^\dagger(\mathbf{x})\left[1+\sum_i\frac{\nabla_i\overline{\nabla}_i}{2D}\right]\delta u(\mathbf{x}) , \qquad (2.6)$$

where

$$\overline{\nabla}_i f(\mathbf{x})=f(\mathbf{x})-f(\mathbf{x}-\mathbf{i}) ,$$
$$W_{\alpha\alpha}=-\tfrac{1}{4}[I_1(\alpha)/I_0(\alpha)]^2+\tfrac{1}{2}I_0''(\alpha)/I_0(\alpha)-\tfrac{1}{4} ,$$
$$W_{\alpha\alpha^\dagger}=-\tfrac{1}{4}[I_1(\alpha)/I_0(\alpha)]^2+\tfrac{1}{4} .$$

Performing the Gaussian integrals, we obtain the one-loop correction,

$$-\beta f^{1\,\mathrm{loop}}=-\tfrac{1}{2}\int_{-\pi}^{\pi}d^Dk\frac{1}{(2\pi)^D}\times\ln\left[\frac{m^2}{2D}+\left[1-\frac{m^2}{2D}\right]\frac{\mathbf{K}\cdot\overline{\mathbf{K}}}{2D}\right]-\tfrac{1}{2}l , \qquad (2.7)$$

where m is a mass parameter for the size fluctuations of the field and is given by

$$\frac{m^2}{2D}=2-2b(1-u^2) ,$$
$$l=\int_{-\pi}^{\pi}d^Dk\frac{1}{(2\pi)^D}\ln(\mathbf{K}\cdot\overline{\mathbf{K}}) ,$$
$$\mathbf{K}\cdot\overline{\mathbf{K}}=2\sum_{i=1}^{D}(1-\cos k_i) .$$

For $D=2$, $l=1.16$.

The internal energy is calculated from (2.7) and (2.5),

$$\frac{U}{D}=-u^2-\frac{1}{2}\left[1-\frac{m^2}{2D}\right]^{-1}\times\left\{1-\int_{-\pi}^{\pi}\frac{d^Dk}{(2\pi)^D}\left[\frac{m^2}{2D}+\left[1-\frac{m^2}{2D}\right]\frac{\mathbf{K}\cdot\overline{\mathbf{K}}}{2D}\right]^{-1}\times\frac{\partial}{\partial b}\left[\frac{m^2}{2D}\right]\right\} . \qquad (2.8)$$

The integral can be expressed by means of the number of closed random walks of length n,[16,17] C_n, i.e., $C_0=1$, $C_2=2D$, $C_4=6D(2D-1)$,

$$\frac{U}{D}=-u^2+\tfrac{1}{2}\sum_{n=2,4,6,\ldots}\frac{1}{D^n}\left[1-\frac{m^2}{2D}\right]^{n-1}C_n\frac{\partial}{\partial b}\left[\frac{m^2}{2D}\right]. \tag{2.9}$$

Expanding u in powers of α, we have

$$u=1-\frac{1}{2\alpha}-\frac{1}{8\alpha^2}-\frac{1}{8\alpha^3}-\cdots,$$

$$\alpha=2bu=2b\left[1-\frac{1}{4b}-\frac{3}{32b^2}-\frac{9}{128b^3}-\cdots\right],$$

so that

$$\frac{1}{\alpha}=\frac{1}{2b}\left[1+\frac{1}{4b}+\frac{5}{32b^2}+\frac{17}{128b^3}+\cdots\right],$$

$$1-\frac{m^2}{2D}=\frac{1}{4b}+\frac{3}{16b^2}+\cdots,$$

and

$$\frac{\partial}{\partial b}\frac{m^2}{2D}=\frac{1}{4b^2}+\frac{3}{8b^3}+\cdots.$$

The internal energy is now given by

$$\frac{U}{D}\cong-1+\frac{t}{2}+\frac{t^2}{8}+\frac{3t^3}{32}+\frac{1}{2D}\frac{t^3}{8}+O(t^4). \tag{2.10}$$

In Figs. 1 and 2 we have plotted the internal energy and the heat capacity for the full result based on Eqs. (2.7) and (2.5), and compared them with Monte Carlo data.[12,13] While the internal energy shows satisfactory agreement with the data, the specific heat displays a rather large discrepancy. This is due to the neglect of vortex excitations. If we want to calculate their effects, mean-field methods are not very useful. In terms of the fields u,α a vortex is a complicated solution of the nonlinear field equations, which is practically impossible to solve. Thus we have to develop a better procedure which exhibits vortices in a more direct fashion.

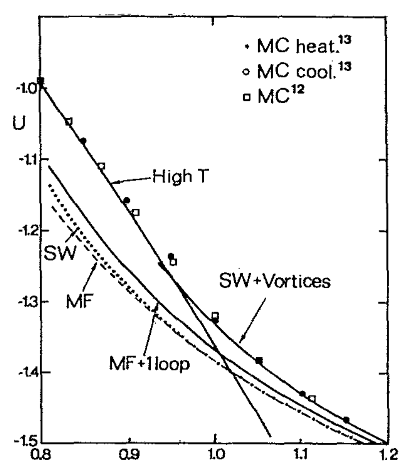


FIG. 1. Internal energy $U=-\partial(-\beta f)/\partial\beta$ for 2D XY model within various approximations are shown: MF, the mean field approximation from Eq. (2.5); MF + 1 loop from Eq. (2.8), SW the Hartree-Fock approximation to the spin-wave contribution, Eq. (4.23), and SW + vortices from Eqs. (4.32) and (5.22). MC, the Monte Carlo data have been taken from Refs. 12 and 13 and high T, the high-temperature expansion up to β^{12} from Ref. 19.

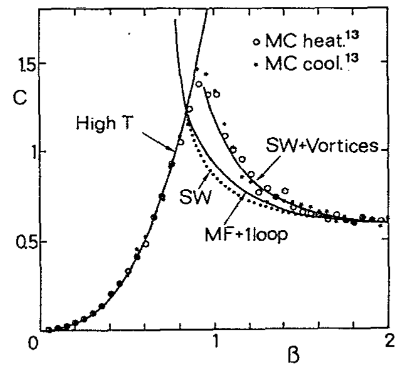


FIG. 2. Specific heat $C=-\beta^2\partial U/\partial\beta$ obtained in a way similar to that in Fig. 1.

III. DUALITY TRANSFORMATION

In order to separate the spin contribution clearly from the vortex contribution, we apply the duality transformation.[8,10] It amounts to rewriting the partition function in terms of variables conjugate to each pair of adjacent spins. In the superfluid film interpretation of the model, these variables correspond to the superfluid current density. Substituting the Fourier expansion

$$e^{\beta\cos\theta}=\sum_{b=-\infty}^{\infty}e^{ib\theta}I_b(\beta)$$

in (2.1), we find

$$Z=\prod_{\mathbf{x}}\int_{-\pi}^{\pi}d\theta(\mathbf{x})\frac{1}{2\pi}\sum_{b_i(\mathbf{x})=-\infty}^{\infty}I_{b_i(\mathbf{x})}(\beta)$$

$$\times\exp i\sum_{\mathbf{x}i}b_i(\mathbf{x})\nabla_i\theta(\mathbf{x})$$

$$=\prod_{\mathbf{x},i}\sum_{b_i(\mathbf{x})=-\infty}^{\infty}\delta_{\sum_j\nabla_j b_j(\mathbf{x}),0}I_{b_i(\mathbf{x})}(\beta), \tag{3.1}$$

where the Fourier coefficient $I_b(\beta)$,

$$I_b(\beta)=\int_{-\pi}^{\pi}d\theta\frac{1}{2\pi}e^{\beta\cos\theta+ib\theta}, \tag{3.2}$$

is the modified Bessel function of order b (Ref. 15) for an integer b. The divergence free condition in (3.1) can be satisfied by an integer field $a(\mathbf{x})$ via $b_i(\mathbf{x})=\epsilon_{ij}\overline{\nabla}_j a(\mathbf{x})$, where ϵ_{ij} is an antisymmetric tensor in two dimensions, $\epsilon_{12}=-\epsilon_{21}=1$, $\epsilon_{11}=\epsilon_{22}=0$. Using Poisson's formula

$$\sum_{a=-\infty}^{\infty}g(a)=\sum_{l=-\infty}^{\infty}\int_{-\infty}^{\infty}dA\,g(A)e^{2\pi ilA},$$

we transform the integer field $a(\mathbf{x})$ into a continuous one $A(\mathbf{x})$ in (3.1):

$$Z=\prod_{\mathbf{x}}\int_{-\infty}^{\infty}dA(\mathbf{x})\sum_{l(\mathbf{x})=-\infty}^{\infty}\exp\left[\sum_{\mathbf{x},i}\ln I_{b_i(\mathbf{x})}(\beta)+2\pi i\sum_{\mathbf{x}}l(\mathbf{x})A(\mathbf{x})\right]$$
$$=I_0(\beta)^{DN}\prod_{\mathbf{x}}\int_{-\infty}^{\infty}dA(\mathbf{x})\sum_{l(\mathbf{x})=-\infty}^{\infty}\exp\left[\sum_{\mathbf{x},i}W(b_i(\mathbf{x}))+2\pi i\sum_{\mathbf{x}}l(\mathbf{x})A(\mathbf{x})\right], \tag{3.3}$$

with

$$b_i(\mathbf{x})=\epsilon_{ij}\bar{\nabla}_jA(\mathbf{x}), \quad W(b)=\ln(I_b(\beta)/I_0(\beta)). \tag{3.4}$$

From the structure of Eq. (3.4) we may interpret $b_i(\mathbf{x})$ as magnetic fields and $A(\mathbf{x})$ as "vector potential" (which is a scalar in two dimensions, in spite of its name). It is well known that the superfluid current in ^{4}He has such a vector-potential representation with a local coupling $A\cdot l$ to vortices. In the absence of vortices the system is described only by spin waves. Their partition function is given by

$$Z_{\rm SW}=\prod_{\mathbf{x}}\int_{-\infty}^{\infty}dA(\mathbf{x})\exp\sum_{\mathbf{x},i}\ln I_{b_i(\mathbf{x})}(\beta)$$
$$=I_0(\beta)^{DN}\prod_{\mathbf{x}}\int_{-\infty}^{\infty}dA(\mathbf{x})\exp\sum_{\mathbf{x},i}W(b_i(\mathbf{x})). \tag{3.5}$$

The vortex part then may be defined by

$$Z_{\rm vort}=Z/Z_{\rm SW}, \tag{3.6}$$

so that

$$Z=Z_{\rm vort}Z_{\rm SW}.$$

IV. SPIN WAVES

The spin-wave (SW) contribution may be evaluated via an expansion of the Bessel Function[15] in a power series in $1/\beta$,

$$I_b(\beta)\simeq\frac{e^\beta}{\sqrt{2\pi\beta}}\left[1-\frac{(2b)^2-1}{8\beta}+\frac{[(2b)^2-1][(2b)^2-9]}{2!(8\beta)^2}+\cdots\right]. \tag{4.1}$$

In this way one arrives at a field energy

$$S[A]=-\sum_{\mathbf{x},i}W(b_i(\mathbf{x}))\simeq-\sum_{\mathbf{x},i}\left[\frac{W^{(2)}(0)}{2!}b_i^2(\mathbf{x})+\frac{W^{(4)}(0)}{4!}b_i^4(\mathbf{x})+\cdots\right], \tag{4.2}$$

where $W^{(2)}(0)$ and $W^{(4)}(0)$ are given by

$$W^{(2)}(0)\simeq-\frac{1}{\beta}\left[1+\frac{1}{2\beta}+\frac{13}{24\beta^2}+\frac{7}{8\beta^3}+\cdots\right],$$
$$W^{(4)}(0)\simeq\frac{1}{\beta^3}\left[1+\frac{3}{\beta}\cdots\right], \tag{4.3}$$

and a partition function

$$Z_{\rm SW}=I_0^{DN}(\beta)\prod_{\mathbf{x}}\int_{-\infty}^{\infty}dA(\mathbf{x})e^{-S[A]}.$$

This expression allows for a simple low-temperature limit. For $\beta\gg1$, only the first term in the field energy survives and the integral over A can immediately be performed giving

$$Z_{\rm SW}=I_0(\beta)^{DN}\left[\frac{2\pi}{-W^{(2)}(0)}\right]^{1/2}\det{}^{-1/2}(-\nabla\cdot\bar{\nabla}). \tag{4.4}$$

The higher-order terms can in principle be calculated order by order in perturbation theory.

There is, however, a more convenient procedure based on the original formulation of the partition function in terms of the angular variables $\theta(\mathbf{x})$. For this we remember that the asymptotic expansion of $I_b(\beta)$, Eq. (4.1), can be obtained, in principle, directly from an evaluation of the integral

$$I_b(\beta)=\int_{-\infty}^{\infty}\frac{dh}{2\pi}e^{\beta\cos h+ihb} \tag{4.5}$$

via a saddle-point approximation around the *maximum at the origin* $h=0$. Equivalently, we may write

$$e^{\beta\cos h}=e^\beta\exp\left[-\frac{\beta}{2}h^2+\beta\left[\frac{h^4}{4!}-\frac{h^6}{6!}+\cdots\right]\right], \tag{4.6}$$

with a truncated series for $\cos h$, and evaluate this integral order by order in perturbation theory, with $\beta h^2/2$ being the free part and the bracket the interaction. In order to shorten the notation, let us denote the truncated (subscript t) expression (4.6) by $\exp(\beta\cos_t h)$. Then we rewrite $Z_{\rm SW}$ as

$$Z_{\rm SW}=\prod_{\mathbf{x}}\int_{-\infty}^{\infty}dA(\mathbf{x})\prod_{\mathbf{x},i}\int_{-\infty}^{\infty}\frac{dh_i(\mathbf{x})}{2\pi}\times\exp\left[\beta\sum_{\mathbf{x},i}\cos_t h_i(\mathbf{x})+i\sum_{\mathbf{x},i}b_i(\mathbf{x})h_i(\mathbf{x})\right]$$
$$=\prod_{\mathbf{x},i}\int_{-\infty}^{\infty}\frac{dh_i(\mathbf{x})}{2\pi}\prod_{\mathbf{x}}\left[2\pi\delta\left[\sum_{i,j}\epsilon_{ij}\nabla_jh_i(\mathbf{x})\right]\right]\times\exp\left[\beta\sum_{\mathbf{x},i}\cos_t h_i(\mathbf{x})\right]. \tag{4.7}$$

Introducing

$$h_i(\mathbf{x})=\nabla_i\theta(\mathbf{x})+\epsilon_{ij}\bar{\nabla}_j\gamma(\mathbf{x}), \tag{4.8}$$

we change the two variables h_1,h_2 into θ and γ. Then, (4.8) after γ integration becomes

$$Z_{SW}=\prod_{\mathbf{x}}\int_{-\infty}^{\infty}\frac{d\theta(\mathbf{x})}{2\pi}\exp\left[\beta\sum_{\mathbf{x},i}\cos_t\nabla_i\theta(\mathbf{x})\right]. \tag{4.9}$$

The difference with the original model is the tacit under standing that $\exp\beta\cos_t\cdots$ has to be treated perturbatively, as defined by (4.6), around the maximum $\nabla_i\theta(\mathbf{x})=0$ only. It is this restriction which makes Z_{SW} free of vortices.

For a partition function like this there exists an efficient way of summing the perturbative series via normal ordering.[11] The basis for this is Wick's rule for harmonically fluctuating fields

$$e^{i\lambda\phi}=e^{-(\lambda^2/2\langle\phi^2\rangle)}:e^{i\lambda\phi}:\,, \tag{4.10}$$

where $\langle\cdots\rangle$ denotes the harmonic average and the dots denote the normal ordering. Applying this to

$$\beta\sum_{\mathbf{x},i}\cos_t\nabla_i\theta(\mathbf{x})\,,$$

we obtain

$$\beta\sum_{\mathbf{x},i}e^{-(1/2)\langle(\nabla_i\theta)^2\rangle}\{-\tfrac{1}{2}(\nabla_i\theta)^2+:[\cos\nabla_i\theta-1+\tfrac{1}{2}(\nabla_i\theta)^2]:+1+\tfrac{1}{2}\langle(\nabla_i\theta)^2\rangle\}\,,$$

such that the partition function in (4.9) takes the form

$$Z_{SW}=e^{ND\beta^R(1+(1/2)\langle(\nabla_i\theta)^2\rangle)}\prod_{\mathbf{x}}\int_{-\infty}^{\infty}\frac{d\theta(\mathbf{x})}{2\pi}\exp\left[-\frac{\beta^R}{2}\sum_{\mathbf{x},i}(\nabla_i\theta)^2+\beta^R\sum_{\mathbf{x},i}\sum_{n=2}^{\infty}\frac{(-1)^n}{(2n)!}:(\nabla_i\theta)^{2n}:\right] \tag{4.11}$$

with the renormalized inverse temperature

$$\beta^R=\beta e^{-(1/2)\langle(\nabla_i\theta)^2\rangle}\quad(i=1,2)\,. \tag{4.12}$$

Since

$$\langle(\nabla_i\theta)^2\rangle=\frac{1}{D\beta^R}\quad(i=1,2)\,,$$

(4.12) becomes

$$\beta^R=\beta e^{-(1/2D\beta^R)}\,, \tag{4.13}$$

the Hartree-Fock self-consistent equation.

For small β^{-1}, (4.13) can be solved by iteration,

$$\begin{aligned}b^R&\cong b-\frac{1}{2}-\frac{1}{8b}-\frac{1}{12b^2}+\cdots\,,\\ t^R&=\frac{1}{b^R}\simeq t+\frac{t^2}{2}+\tfrac{3}{8}t^3+\tfrac{1}{3}t^4+\cdots\,,\end{aligned} \tag{4.14}$$

with $b=D\beta$, $b^R=D\beta^R$. The result is tabulated in Table I. There exists a solution only for $b\geq(e/2)\sim1.359$, which for $D=2$ and $D=3$ comprises the entire low-temperature phase [$D=2$: $b_c=(2/0.89)=2.247$, $t_c=(0.89/2)=0.445$; $D=3$: $b_c=(3/2.2)=1.36$, $t_c=0.733$]. For larger D, Hartree-Fock equations cannot be used up to the critical point which for $D\to\infty$ converges to the mean-field values $b_c\to2$, $t_c\to\frac{1}{2}$. Only the expansion (4.14) can, if they are truncated after the maximal reliable power in t. Neglecting the interactions, the θ integrals in (4.11) can be performed and we obtain from the lowest Hartree-Fock approximation

TABLE I. Self-consistent inverse temperature β^R in Eq. (4.13) as a function of inverse temperature β is tabulated ($D=2$).

β	β^R
0.7	0.3222
0.8	0.4700
0.9	0.5885
1.0	0.6995
1.1	0.8069
1.2	0.9124
1.3	1.0166
1.4	1.1199
1.5	1.2226
1.6	1.3249
1.7	1.4268
1.8	1.5284
1.9	1.6298
2.0	1.7310

$$Z_{SW}^{HF}=e^{Nb^R[1+(1/2b^R)]}\left[\frac{1}{(4\pi b^R)^{1/2}}\right]^N\det\left[-\frac{\nabla\cdot\bar{\nabla}}{2D}\right]^{-1/2}, \tag{4.15}$$

which amounts to the free-energy density

$$\begin{aligned}-\beta f_{SW}^{HF}&=b^R+\tfrac{1}{2}-\tfrac{1}{2}\ln(4\pi b^R)-\tfrac{1}{2}l\\ &=b+\frac{1}{8b}+\frac{1}{24b^2}+\cdots-\tfrac{1}{2}\ln(4\pi b)-\tfrac{1}{2}l\,,\end{aligned} \tag{4.16}$$

with

$$l=\int_{-\pi}^{\pi}d^Dk\frac{1}{(2\pi)^D}\ln\left[\frac{\mathbf{K}\cdot\bar{\mathbf{K}}}{2D}\right] \tag{4.17}$$

being equal to -0.22004 and -0.11837 for $D=2,3$, respectively. Using

$$\frac{\partial b^R}{\partial b}=\left[1-\frac{1}{2b^R}\right]^{-1}e^{-(1/2b^R)}=\frac{b^R}{b}\left[1-\frac{1}{2b^R}\right]^{-1}, \tag{4.18}$$

the internal energy per site and dimension

$$\frac{U}{D}=-\frac{1}{D}\frac{\partial}{\partial\beta}(-\beta f)=-\frac{\partial}{\partial b}(-\beta f) \tag{4.19}$$

is found to be simply

$$\frac{U_{\rm SW}^{\rm HF}}{D} = -e^{-(1/2b^R)} = -\frac{b^R}{b}$$
$$\simeq -1 + \frac{1}{2b} + \frac{1}{8b^2} + \frac{1}{12b^3} + \cdots$$
$$= -1 + \frac{t}{2} + \frac{t^2}{8} + \frac{t^3}{12} + \cdots \; . \qquad (4.20)$$

This energy is reliable only up to the power t^2. If we want to go beyond this power, the interaction energy has to be considered. The lowest Feynman diagram due to the second order in the quartic interaction which gives a free energy of order t^2

$$-\beta f^{(2)} = \frac{1}{2!}$$ 

$$= \frac{1}{2!}\left[\frac{\beta^R}{4!}\right]^2 4! \sum_{\mathbf{x},\mathbf{x}',i,j} \langle \nabla_i\theta(\mathbf{x})\nabla_j'\theta(\mathbf{x}')\rangle^4$$
$$= \frac{1}{2!}\left[\frac{\beta^R}{4!}\right]^2 4! \sum_{\mathbf{x},\mathbf{x}',i,j} \left[\nabla_i\nabla_j' \frac{1}{\beta^R} v(\mathbf{x}-\mathbf{x}')\right]^4 , \qquad (4.21)$$

where $v(\mathbf{x}-\mathbf{x}')$ is the Coulomb propagator (Appendix B),

$$v(\mathbf{x}-\mathbf{x}') = -\left[\frac{1}{\nabla_i\overline{\nabla}_i}\right]_{\mathbf{x},\mathbf{x}'} .$$

The dominant part of this comes from the D $\mathbf{x}=0$ diagonal pieces,

$$\sum_{\mathbf{x}=0,i=j} \langle \nabla_i\theta(\mathbf{x})\nabla_j\theta(\mathbf{x})\rangle^4 = \frac{D}{(b^R)^4} , \qquad (4.22)$$

and reads

$$-\beta f^{(2)} = \frac{1}{D}\,\frac{1}{2!4!}\,\frac{1}{(b^R)^2} . \qquad (4.23)$$

The $\mathbf{x}\neq 0$ and the off-diagonal $i\neq j$ contributions are extremely small. In order to calculate them let us now go to the special case of $D=2$ dimensions. Then the $i=j$, $\mathbf{x}=\pm 1, \pm 2$ terms are

$$\langle \nabla_1\theta(1)\nabla_1\theta(0)\rangle = \frac{2}{b^R}[v(2,0)-2v(1,0)+v(0,0)]$$
$$= \frac{2}{b^R}\left[-1+\frac{2}{\pi}-2(-\tfrac{1}{4})\right] = \frac{0.2732}{b^R} , \qquad (4.24)$$
$$\langle \nabla_1\theta(2)\nabla_1\theta(0)\rangle = -\frac{2}{b^R}[v(-1,1)-2v(0,1)+v(1,1)]$$
$$= -\frac{2}{b^R}\left[-\frac{1}{\pi}-2(-\tfrac{1}{4})+\left[-\frac{1}{\pi}\right]\right]$$
$$= \frac{0.2732}{b^R} ,$$

such that the sum in (4.21) is changed from $2/(b^R)^4$ to

$$\frac{2}{(b^R)^4} + \frac{8}{(b^R)^4}(0.2732)^4 = \frac{2}{(b^R)^4}(1+0.022) , \qquad (4.25)$$

i.e., by only 2%. For $x=\pm 21$, the contribution is entirely negligible since

$$\langle \nabla_1\theta(21)\nabla_1\theta(0)\rangle = -\frac{2}{b^R}[v(3,0)-2v(2,0)+v(1,0)]$$
$$= -\frac{2}{b^R}\left[-\frac{17}{4}+\frac{12}{\pi}-2\left[-1+\frac{2}{\pi}\right] + \left[-\frac{1}{4}\right]\right]$$
$$= -\frac{0.0930}{b^R} , \qquad (4.26)$$

such that the fourth power $2/(b^R)^4$ changes only by 1/100%.

Consider now the $i\neq j$ terms. The expression

$$\langle \nabla_1\theta(\mathbf{x})\nabla_2\theta(\mathbf{0})\rangle = \frac{2}{b^R}[v(\mathbf{x})-v(\mathbf{x}+1)+v(\mathbf{x}+1-2) - v(\mathbf{x}-2)] \qquad (4.27)$$

sums up the potentials around the plaquette (with alternating signs) lying to the lower right of the point $\mathbf{x}$. The largest contribution for the sum in (4.21) comes from the four plaquettes around the origin, each of which gives

$$\frac{2}{b^R}[v(0)-v(1,0)+v(1,-1)-v(0,-1)]$$
$$= \frac{2}{b^R}\left[-2\left[-\frac{1}{4}\right]+\left[-\frac{1}{\pi}\right]\right]$$
$$= \frac{1}{b^R}\left[1-\frac{2}{\pi}\right] = \frac{0.3633}{b^R} , \qquad (4.28)$$

such that (4.25) is modified to

$$\frac{2}{(b^R)^4}(1+0.032) + 4\frac{1}{(b^R)^4}\times 0.0574$$
$$= \frac{2}{(b^R)^4}(1+0.057) . \qquad (4.29)$$

If the plaquette lies farther away from the origin, it can be neglected. For example,

$$\langle \nabla_1\theta(1)\nabla_2\theta(0)\rangle = \frac{2}{b^R}[v(1,0)-v(2,0)+v(2,-1) - v(1,-1)]$$
$$= \frac{2}{b^R}\left[-\frac{1}{4}-\left[-1+\frac{2}{\pi}\right] + \left[\frac{1}{4}-\frac{2}{\pi}\right]-\left[-\frac{1}{\pi}\right]\right]$$
$$= \frac{0.0901}{b^R} , \qquad (4.30)$$

such that $2/(b^R)^4$ is modified by less than $\frac{3}{1000}$%. Hence, for $D=2$ we can make (4.23) more precise and have

$$-\beta f^{(2)} = \frac{1}{D}\,\frac{1}{2!4!}\,\frac{1}{(b^R)^2}1.057 . \qquad (4.31)$$

TABLE II. The internal energies and heat capacities obtained by various approximations and in a manner similar to that in Figs. 1 and 2, at chosen inverse temperatures, are tabulated.

		U			C	
β	SW	Vortices	SW + Vortices	SW	Vortices	SW + Vortices
0.95	−1.3355	6.88×10^{-2}	−1.27	0.925	0.38	1.31
1.0	−1.3824	5.06×10^{-2}	−1.33	0.861	0.32	1.18
1.1	−1.4566	2.71×10^{-2}	−1.43	0.777	0.21	0.98
1.2	−1.5135	1.43×10^{-2}	−1.55	0.726	0.13	0.85
1.5	−1.6272	2.02×10^{-3}	−1.63	0.645	0.03	0.67
2.0	−1.7300	6.34×10^{-5}	−1.73	0.592	0.001	0.59

Since the term $-\beta f^{(2)}$ is quite small compared to the leading powers in t up to the transition point $b^R \sim 2$, we may forget the 4.5% modifications due to the $\mathbf{x}\neq 0$ and $i\neq j$ parts of (4.21) and use (4.23) directly. A similar discussion holds for three dimensions.

Thus we arrive at a free energy, good to order t^3,

$$-\beta f_{\rm SW}^{\rm HF} = b^R + \frac{1}{2} + \frac{1}{48D(b^R)^2} - \tfrac{1}{2}\ln(4\pi b^R) - \tfrac{1}{2} l \ , \tag{4.32}$$

with an internal energy

$$\frac{U_{\rm SW}^{\rm HF}}{D} = \frac{b^R}{b}\left[-1 + \frac{1}{24D}\frac{1}{(b^R)^3}\left[1-\frac{1}{2b^R}\right]^{-1}\right] = -1 + \frac{t}{2} + \frac{t^2}{8} + \frac{t^3}{12} + \frac{1}{24D}t^3 + O(t^4) \ . \tag{4.33}$$

This expansion is to be compared with the mean-field result (2.10). They agree up to t^2. Even the terms of order t^3 would not differ greatly.

In Table II we have listed the results and Figs. 1 and 2 compared the internal energies and heat capacities with existing Monte Carlo data[12,13] in $D=2$ dimensions.

V. VORTICES

The vortex contribution is given by (3.6),

$$Z_{\rm vort} = \prod_{\mathbf{x}} \int_{-\infty}^{\infty} dA(\mathbf{x}) \sum_{l(\mathbf{x})=-\infty}^{\infty} \exp\left[\sum_{\mathbf{x},i} W(b_i(\mathbf{x})) + 2\pi i \sum_{\mathbf{x}} l(\mathbf{x})A(\mathbf{x})\right]\left[\prod_{\mathbf{x}} \int_{-\infty}^{\infty} dA(\mathbf{x}) \exp \sum_{\mathbf{x},i} W(b_i(\mathbf{x}))\right]^{-1} , \tag{5.1}$$

where

$$\begin{aligned} &W(b) = \ln[I_b(\beta)/I_0(\beta)] = W_0(b) + W_{\rm int}(b) \\ &W_0(b) = \tfrac{1}{2} W''(0) b^2 \ , \quad W_{\rm int}(b) = W(b) - W_0(b) \\ &W''(0) = -\int_{-\pi}^{\pi} d\theta \frac{1}{2\pi} e^{\beta\cos\theta}\theta^2 / I_0(\beta) \ . \end{aligned} \tag{5.2}$$

Although it is hard to evaluate this formula in general, it becomes quite simple at low temperatures since, there, only $l=0,\pm1$ contribute, corresponding to a dilute gas of oppositely charged pairs $(+-)$.[6] In this circumstance $l(x)$ may be regarded as an external field for $A(\mathbf{x})$. The strategy is then to imagine a certain configuration of $l(\mathbf{x})$ and later sum over all important patterns,

$$\begin{aligned} &Z_{\rm vort} = 1 + \prod_{\mathbf{x}} \sum_{l(\mathbf{x})\neq 0} Z[l(\mathbf{x})] \\ &Z[l(\mathbf{x})] = \prod_{\mathbf{x}} \int_{-\infty}^{\infty} dA(\mathbf{x}) \exp\left[\sum_{\mathbf{x},i} W(b_i(\mathbf{x})) + 2\pi i \sum_{\mathbf{x}} l(\mathbf{x})A(\mathbf{x})\right]\left[\prod_{\mathbf{x}} \int_{-\infty}^{\infty} dA(\mathbf{x}) \exp \sum_{\mathbf{x},i} W(b_i(\mathbf{x}))\right]^{-1} . \end{aligned} \tag{5.3}$$

The previous approaches[8,10] take advantage of the limiting form of $W(b_i)$ for large β (4.3),

$$W(b_i(\mathbf{x})) \simeq -\frac{1}{2\beta} b_i^2(\mathbf{x}) + \frac{1}{4!\beta^3} b_i^4(\mathbf{x}) - O(b_i^6/\beta^5) \ . \tag{5.4}$$

If only the first term is kept, it is easy to perform $A(\mathbf{x})$ integration. To the quadratic term this gives

$$\begin{aligned} Z_V[l(\mathbf{x})] &= \exp\left[-(4\pi^2/2)\beta \sum_{\mathbf{x},\mathbf{x}'} l(\mathbf{x}) v(\mathbf{x}-\mathbf{x}') l(\mathbf{x}')\right] = \exp\left[-(4\pi^2/2)\beta \sum_{\mathbf{x},\mathbf{x}'} l(\mathbf{x}) v'(\mathbf{x}-\mathbf{x}') l(\mathbf{x}')\right]\Bigg|_{\sum_{\mathbf{x}} l(\mathbf{x})=0} \\ &= e^{-\beta E_V[l(\mathbf{x})]}\Big|_{\sum_{\mathbf{x}} l(\mathbf{x})=0} \ , \end{aligned} \tag{5.5}$$

where $E_V[l(\mathbf{x})]$ is the energy for the configuration $[l(\mathbf{x})]$

$$E_V[l(\mathbf{x})]=\frac{(2\pi)^2}{2}\sum_{\mathbf{x},\mathbf{x}'} l(\mathbf{x})v'(\mathbf{x}-\mathbf{x}')l(\mathbf{x}') , \qquad (5.6)$$

and $v(\mathbf{x})$ and $v'(\mathbf{x})$ are Coulomb Green's functions in 2D, the latter being the divergence-subtracted Green's function. Some of the properties of the Coulomb propagator are summarized in Appendix A, for convenience. The condition in (5.5) originates from the divergence of $v(0)\sim\ln R$ (R: the system size) at the origin. The vortex configurations which do not satisfy the neutrality condition $\sum_{\mathbf{x}} l(\mathbf{x})=0$ give no contribution.

It is well known[17] that $v'(\mathbf{x})$ is well approximated by the asymptotic value (A4) at all $\mathbf{x}$ ($\mathbf{x}\neq 0$)

$$v'(\mathbf{x})\sim -\frac{1}{2\pi}(\ln|\mathbf{x}|+1.617) .$$

Since this is the potential for which Kosterlitz and Thouless[6] have predicted the vortex unbinding transition, we expect the vortices to be bound in pairs and form a dilute gas at low temperatures. The contribution from the vortices is then simply given by

$$-\beta f_{\text{vort}}=\sum_m p(m)e^{-\beta E_V[m]} , \qquad (5.7)$$

where the sum is to be taken over various types of vortex pairs m and $p(m)$, the corresponding orientational factor.

The pair energies $E_V(m)$ can be explicitly obtained with help from Appendix B,

$$E_V=\begin{cases} \pi^2\simeq 9.87 , & p=4 , \text{ for } m=-+ \\[4pt] 4\pi\simeq 12.57 , & p=4 , \text{ for } m=\begin{smallmatrix} \cdot & + \\ - & \cdot \end{smallmatrix} \\[4pt] 4\pi^2\left[1-\dfrac{2}{\pi}\right]\simeq 14.35 , & p=4 , \text{ for } m=-\cdot+ \\[4pt] 4\pi^2\left[\dfrac{2}{\pi}-\dfrac{1}{4}\right]\simeq 15.26 , & p=8 , \text{ for } m=\begin{smallmatrix} \cdot & \cdot & + \\ - & \cdot & \cdot \end{smallmatrix} \\[4pt] \dfrac{16\pi}{3}\simeq 16.76 , & p=4 , \text{ for } m=\begin{smallmatrix} \cdot & \cdot & + \\ \cdot & \cdot & \cdot \\ - & \cdot & \cdot \end{smallmatrix} \end{cases} \qquad (5.8)$$

where dots among vortices indicate empty sites. Although this calculation is useful in understanding the model qualitatively, the results (5.8) and (5.7) do not account for the Monte Carlo data.[12,13] Indeed, the vortex pair energies (5.8) are so large that for $\beta\gtrsim 1$ their contribution is always negligible. The large error occurs when ignoring in (5.4) the higher-order terms in b_i. At first sight one may be tempted to improve the accuracy by taking the higher orders in b into account perturbatively. Unfortunately, this does not work. The reason is that all terms in the expansion (5.4) contribute to equal order in $1/\beta$. This is easy to see since $b_i\sim O(\beta)$ in (5.3), such that, indeed, every term in (5.4) becomes of the same order β. Therefore, the perturbative approach breaks down.

This may be contrasted with the spin-wave part. There, the typical value of b_i is $O(\sqrt{\beta})$, such that the higher terms decrease as β^{1-n} ($2n$ is the power of b_i) and assures the validity of the perturbative approach.

In the following we will avoid this difficulty by applying the *loop expansion*[16,18] to the *full* expression in (5.3). The loop expansion is the field-theoretic version of the saddle-point approximation for simple integrals and has been used successfully in many systems where fluctuations are weak. In general, we can write (5.3) as

$$Z[l(\mathbf{x})]=e^{-\beta E[l(\mathbf{x})]} , \qquad (5.9)$$

where $\beta E[l(\mathbf{x})]$ is the sum of connected graphs organized by a number of loops n,

$$\beta E[l(\mathbf{x})]=\beta\sum_{n=0}^{\infty} E_n[l(\mathbf{x})] . \qquad (5.10)$$

The lowest term, which is called the classical or tree term, is simply given by the field $A^{\text{cl}}(\mathbf{x})$ for which the exponential in the numerator of (5.3) is stationary,

$$-\beta E_0[l(\mathbf{x})]=\sum_{\mathbf{x},i} W(b_i^{\text{cl}}(\mathbf{x}))+2\pi i\sum_{\mathbf{x}} l(\mathbf{x})A^{\text{cl}}(\mathbf{x}) . \qquad (5.11)$$

The classical field is determined by the stationarity condition,

$$-\sum_{i,j}\epsilon_{ij}\nabla_j W'(b_i^{\text{cl}}(\mathbf{x}))+2\pi i l(\mathbf{x})=0 , \qquad (5.12)$$

which is the analog of the Maxwell equation, albeit nonlinear, for the magnetic field b_i, with an imaginary current il. For convenience we introduce the notation

$$\alpha_{\langle i\rangle}=\sum_j \epsilon_{ij}\alpha_j .$$

Then, $\alpha_{\langle 1\rangle}=\alpha_2$ and $\alpha_{\langle 2\rangle}=-\alpha_1$. If we use (5.2) and (3.4), we can solve (5.12) formally:

$$A^{\text{cl}}(\mathbf{x})=-2\pi i[W''(0)]^{-1}\sum_{\mathbf{x}'} v(\mathbf{x}-\mathbf{x}')[l(\mathbf{x}')-q(\mathbf{x}')] ,$$

$$b_i^{\text{cl}}(\mathbf{x})=-2\pi i[W''(0)]^{-1}\sum_{\mathbf{x}'}\overline{\nabla}_{\langle i\rangle}v'(\mathbf{x}-\mathbf{x}') \times[l(\mathbf{x}')-q(\mathbf{x}')] , \qquad (5.13)$$

with

$$q(\mathbf{x})=\frac{1}{2\pi i}\sum_i \nabla_{\langle i\rangle}W'_{\text{int}}(b_i^{\text{cl}}(\mathbf{x})) . \qquad (5.14)$$

The nonlinearity of Eq. (5.12) is entirely hidden in $q(\mathbf{x})$. The bare charge $l(\mathbf{x})$ is screened by this $q(\mathbf{x})$. Substituting (5.13) in (5.11), we have

$$\begin{aligned}-\beta E_0[l(\mathbf{x})]&=(2\pi)^2[W''(0)]^{-1}\tfrac{1}{2}\sum_{\mathbf{x},\mathbf{x}'}[l(\mathbf{x})v(\mathbf{x}-\mathbf{x}')l(\mathbf{x}')-q(\mathbf{x})v'(\mathbf{x}-\mathbf{x}')q(\mathbf{x}')]+\sum_{\mathbf{x},i}W_{\text{int}}(b_i^{\text{cl}}(\mathbf{x}))\\ &=(2\pi)^2[W''(0)]^{-1}\tfrac{1}{2}\sum_{\mathbf{x},\mathbf{x}'} l(\mathbf{x})v'(\mathbf{x}-\mathbf{x}')l(\mathbf{x}')-(2\pi)^2[W''(0)]^{-1}\tfrac{1}{2}\sum_{\mathbf{x},\mathbf{x}'}q(\mathbf{x})v'(\mathbf{x}-\mathbf{x}')q(\mathbf{x}')\\ &\quad+\sum_{\mathbf{x},i}W_{\text{int}}(b_i^{\text{cl}}(\mathbf{x}))\Big|_{\sum_{\mathbf{x}} l(\mathbf{x})=0} .\end{aligned} \qquad (5.15)$$

Making use of the large-β expansion

$$[W''(0)]^{-1}\simeq-\beta\left[1+\frac{1}{2\beta}+\frac{13}{24\beta^2}+\frac{7}{8\beta^3}+\cdots\right],$$

we see from (5.15), (5.10), (5.9), and (5.3) that the first term in (5.15) corresponds to the usual result (5.5) and could have been obtained by previous methods leading to Eq. (5.5) if a power expansion in b_i rather than in β^{-1} had been used for $W(b_i)$, i.e., $W(b_i)\simeq\frac{1}{2}W''(0)b_i^2+\cdots$. Because of induced vortex charge $q(\mathbf{x})$ and the full interactions we have found two extra terms in (5.15). Note that an arbitrary constant which could be added to $A^{\rm cl}(\mathbf{x})$ (5.13) does not contribute to E_0 because of the neutrality $\sum_{\mathbf{x}} l(\mathbf{x})=0$ in (5.15).

We can find higher-loop corrections by expanding the exponent in the numerator of (5.3) around $b_i=b_i^{\rm cl}(\mathbf{x})$ and the exponent in the denominator around $b_i=0$. Changing variables, we see

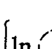
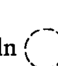
$$Z[l(\mathbf{x})]=e^{-\beta E_0[l(\mathbf{x})]}\left[\prod_{\mathbf{x}}\int d\,\delta A(\mathbf{x})\exp\left[-\tfrac{1}{2}\sum_{\mathbf{x},\mathbf{x}'}\delta A(\mathbf{x})g_{\mathbf{x}\mathbf{x}'}^{-1}\delta A(\mathbf{x}')+\sum_{\mathbf{x},i}\sum_{n=3}^{\infty}\frac{1}{n!}\lambda^{(n)}(\mathbf{x})\delta b_i^n(\mathbf{x})\right]\right]$$
$$\times\left[\prod_{\mathbf{x}}\int dA(\mathbf{x})\exp\left[-\tfrac{1}{2}\sum_{\mathbf{x},\mathbf{x}'}A(\mathbf{x})v_{\mathbf{x}\mathbf{x}'}^{-1}A(\mathbf{x}')+\sum_{\mathbf{x},i}\sum_{n=4,6,8,\ldots}\frac{1}{n!}\lambda^{o(n)}b_i^n(\mathbf{x})\right]\right]^{-1}, \tag{5.16}$$

where

$$g_{\mathbf{x}\mathbf{x}'}^{-1}=-\sum_i\nabla_{\langle i\rangle}\omega_i(\mathbf{x})\overline{\nabla}_{\langle i\rangle}\delta_{\mathbf{x},\mathbf{x}'},$$
$$v_{\mathbf{x}\mathbf{x}'}^{-1}=-\sum_i\nabla_i\overline{\nabla}_i\delta_{\mathbf{x},\mathbf{x}'},$$
$$\omega_i(\mathbf{x})=W''(b_i^{\rm cl}(\mathbf{x}))/W''(0),$$
$$\lambda_i^{(n)}(\mathbf{x})=W^{(n)}(b_i^{\rm cl}(\mathbf{x}))/[-W''(0)]^{n/2},$$
$$\lambda^{o(n)}=\lambda_i^{(n)}(\mathbf{x})\,|_{b_i^{\rm cl}(\mathbf{x})=0},$$
$$\delta b_i(\mathbf{x})=\overline{\nabla}_{\langle i\rangle}\delta A(\mathbf{x}),$$
$$b_i(\mathbf{x})=\overline{\nabla}_{\langle i\rangle}A(\mathbf{x}).$$

The higher corrections represent the difference of spin waves, expressed here by A fields, with and without vortices. The spin waves oscillate around a new minimum $A^{\rm cl}(\mathbf{x})$ when the vortices are present, while they are ordinary spin waves when the vortices are absent.

Expanding the interaction terms and organizing the results according to the number of loops, we obtain for the one-loop correction in (5.10) and (5.9)

$-\beta E_1[l(\mathbf{x})]=-\frac{1}{2}\,{\rm tr}\left[\ln\right.$  $-\ln$  $\left.\Big|_{b^{\rm cl}=0}\right]$

$$=-\tfrac{1}{2}\,{\rm tr}\ln(g^{-1}\cdot v)\,, \tag{5.17}$$

where the broken line indicates the free propagator g or v in (5.16) and tr and the dot product are to be taken over $\mathbf{x}$ space. Separating out the interaction term from $\omega_i(\mathbf{x})$, we may rewrite (5.17),

$$-\beta E_1[l(\mathbf{x})]=-\tfrac{1}{2}\,{\rm tr}\ln\left[1-\sum_i\nabla_{\langle i\rangle}\cdot\omega^{\rm int}\cdot\overline{\nabla}_{\langle i\rangle}\cdot v\right]$$
$$\simeq-\tfrac{1}{2}\,{\rm Tr}(G^0\cdot\omega^{\rm int}-\tfrac{1}{2}G^0\cdot\omega^{\rm int}\cdot G^0\cdot\omega^{\rm int}$$
$$+\tfrac{1}{3}G^0\cdot\omega^{\rm int}\cdot G^0\cdot\omega^{\rm int}\cdot G^0\cdot\omega^{\rm int}+\cdots)$$
$$=-\tfrac{1}{2}\,{\rm Tr}\ln(1+G^0\cdot\omega^{\rm int})\,, \tag{5.18}$$

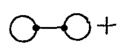
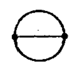
where we have introduced a free propagator G^0 for b_i, and the interaction

$$G_{ij}^0(\mathbf{x},\mathbf{x}')=-\overline{\nabla}_{\langle i\rangle}\nabla_{\langle j\rangle}v'(\mathbf{x}-\mathbf{x}'),$$
$$\omega_i^{\rm int}(\mathbf{x})=W_{\rm int}''(b_i^{\rm cl}(\mathbf{x}))/W''(0),$$

for which $\omega_i(\mathbf{x})=1+\omega_i^{\rm int}(\mathbf{x})$. Here, Tr and the dot product are to be taken in $(\mathbf{x},i)$ space, and should be interpreted as such from now on. To calculate the two-loop contribution, it is convenient to introduce a free propagator for δb_i,

$$G_{ij}(\mathbf{x},\mathbf{x}')=\overline{\nabla}_{\langle i\rangle}\overline{\nabla}'_{\langle j\rangle}g_{\mathbf{x},\mathbf{x}'}\,. \tag{5.19}$$

Denoting G by a solid line, we give the two-loop graphs to $-\beta E$

$-\beta E_2[l(\mathbf{x})]=\frac{1}{8}\Big[$  $-$  $\Big|_{b_i^{\rm cl}=0}\Big]+\frac{1}{8}$  $+\frac{1}{12}$ 

$$=\tfrac{1}{8}\sum_{\mathbf{x},i}[G_{ii}(\mathbf{x},\mathbf{x})\lambda_i^{(4)}(\mathbf{x})G_{ii}(\mathbf{x},\mathbf{x})-\tfrac{1}{4}\lambda^{o(4)}]$$
$$+\tfrac{1}{8}\sum_{\mathbf{x},\mathbf{x}',i,j}G_{ii}(\mathbf{x},\mathbf{x})\lambda_i^{(3)}(\mathbf{x})G_{ij}(\mathbf{x},\mathbf{x}')\lambda_j^{(3)}(\mathbf{x}')G_{jj}(\mathbf{x}',\mathbf{x}')+\tfrac{1}{12}\sum_{\mathbf{x},\mathbf{x}',i,j}\lambda_i^{(3)}(\mathbf{x})G_{ij}(\mathbf{x},\mathbf{x}')^3\lambda_j^{(3)}(\mathbf{x}')\,, \tag{5.20}$$

where we have made use of the fact that $G\,|_{b_i^{\rm cl}=0}=G^0$ and $G_{ii}^0(\mathbf{x},\mathbf{x}')=\frac{1}{2}$ for $i=1,2$.

Expanding g in powers of $\omega^{\rm int}$ in (5.19), we can show that

$$G=(1+G^0\cdot\omega^{\rm int})^{-1}\cdot G^0$$

and thus G obeys the Dyson equation,

$$G=G^0-G^0\cdot\omega^{\rm int}\cdot G\,. \tag{5.21}$$

So far, we have assumed an arbitrary configuration of $l(\mathbf{x})$, so that the loop expansions (5.20), (5.18), and (5.15) are completely general. We have seen in (5.8) that at low temperatures vortices are bound in pairs and characterized by its dipole moment. We expect this situation holds true even in our new results so that we can specialize the formula to the dilute gas of dipoles. The result is then the same as before [Eq. (5.8)] but with $\beta E[m]$ now given by (5.20), (5.18), (5.15), and (5.10).

Adding to the dipoles listed in (5.8) a quadrupole $\begin{matrix} + & - \\ - & + \end{matrix}$, we obtain

$$-\beta f^{\rm vort}=\sum_m p(m)e^{-\beta E[m]}+p(Q)e^{-\beta E[Q]} \tag{5.22}$$

with $Q=\begin{matrix} + & - \\ - & + \end{matrix}$ and $p(Q)=2$. Higher quadruples like

$$\begin{matrix} + & \cdot & - \\ - & + & \cdot \end{matrix} \quad \text{or} \quad \begin{matrix} + & \cdot & - \\ \cdot & \cdot & \cdot \\ - & + & \cdot \end{matrix}$$

are so strongly suppressed that we can ignore them, although the latter happens to appear in Fig. 7(b) of Ref. 12, due to fluctuations. Their naive pair energies E_V [to be compared with (5.8)] are

$$E_V\begin{bmatrix} + & \cdot & - \\ - & + & \cdot \end{bmatrix}=(2\pi)^2\left[\frac{7}{4}-\frac{4}{\pi}\right]\simeq 18.82 \quad (p=16)$$

and

$$E_V\begin{bmatrix} + & \cdot & - \\ \cdot & \cdot & \cdot \\ - & + & \cdot \end{bmatrix}=(2\pi)^2\left[\frac{9}{4}-\frac{16}{3\pi}\right]\simeq 21.81 \quad (p=16)\ .$$

The total free energy is then the sum of (5.22) and (4.32).

Because of the nonlinearity in the extremum condition (5.13), in general we cannot obtain explicitly the energy E in (5.22). Fortunately, there is a small parameter in this problem which we have found after a numerical calculation. It is the screening charge q defined in Eq. (5.14). Actually, the smallness of q permits also a more direct expansion in powers of q which we have not followed here. This procedure is explained in Appendix B. We shall make use of this smallness by following an iteration procedure which starts from $q(\mathbf{x})=0$ and converges rapidly. To solve (5.13) we first assume each configuration of m in (5.8) or Q in (5.22) and proceed by iterations, starting from $q(\mathbf{x})=0$. We find that 7×7 lattice points surrounding the assumed $l(\mathbf{x})\neq 0$ are sufficient to solve $\mathbf{b}^{\rm cl}(\mathbf{x})$. Beyond this area, $\mathbf{b}^{\rm cl}(\mathbf{x})=0$, practically. In Fig. 3 we have plotted $\mathbf{b}^{\rm cl},\mathbf{b}^{\rm cl}|_{q=0}$, and $q(\mathbf{x})$ on a lattice in the presence of $l(\mathbf{x})=\delta_{\mathbf{x},0}-\delta_{\mathbf{x},1}$ at $\beta=1$ and 1.5. Note that $b_i^{\rm cl}(\mathbf{x})$ is pure imaginary so that $\mathrm{Im}\mathbf{b}^{\rm cl}(\mathbf{x})$ is plotted. The magnetic fields $\mathbf{b}^{\rm cl}$ are largest at the sites occupied by $l(\mathbf{x})$ and decrease rapidly away from the occupied sites. Although, in the figure, $\mathbf{b}^{\rm cl}(\mathbf{x})$ does not appear to form the dipole fields, it does so in the remote regions. Comparing $\mathbf{b}^{\rm cl}(\mathbf{x})$ and $\mathbf{b}^{\rm cl}(\mathbf{x})|_{q(\mathbf{x})=0}$, we find that $q(\mathbf{x})$ gives rise to contributions to $\mathbf{b}^{\rm cl}(\mathbf{x})$: at $\beta=1$, $\sim 16\%$ at $\mathbf{x}=1$ and $\sim 10\%$ at $\mathbf{x}=0$; and at $\beta=1.5$, $\sim 8\%$ at $\mathbf{x}=0$ and 1. At $\beta=2$, the contribution is unimportant. The fields increase as the temperature rises. This is expected since the free fields $|\mathbf{b}^{\rm cl}(\mathbf{x})|_{q=0}$ grow linearly in β for large β [Eq. (5.13)]. The nonlinear charges $q(\mathbf{x})$ which are visible only at the occupied sites screen the bare charges $l(\mathbf{x})$: at $\beta=1$, $q(0)=-q(1)=0.227$ which amounts to $\sim 30\%$ of screening, and at $\beta=1.5$, $q(0)=-q(1)=-0.0928$ which

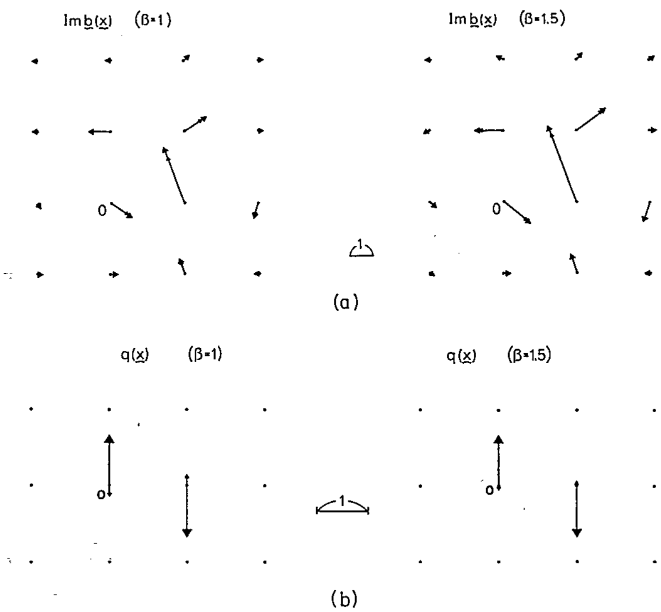


FIG. 3. (a) Classical values for the internal magnetic fields $\mathrm{Im}\mathbf{b}^{\rm cl}(\mathbf{x})$ (large arrows), $\mathrm{Im}b^{\rm cl}(\mathbf{x})|_{q(\mathbf{x})=0}$ (small arrows), and (b) nonlinear vortex charge $q(\mathbf{x})$ (small arrow) in Eq. (5.14), in the presence of the dipole pair $(+-)$: $l(\mathbf{x})=\delta_{\mathbf{x},0}-\delta_{\mathbf{x},1}$ (large arrow) at $\beta=1$ and 1.5 are displayed on a lattice. For $q(\mathbf{x})$ diagrams, up and down arrows denote positive and negative values, respectively. Note, $\mathbf{b}^{\rm cl}(\mathbf{x}),\mathbf{b}^{\rm cl}(\mathbf{x})|_{q(\mathbf{x})=0}$ are purely imaginary at these temperatures.

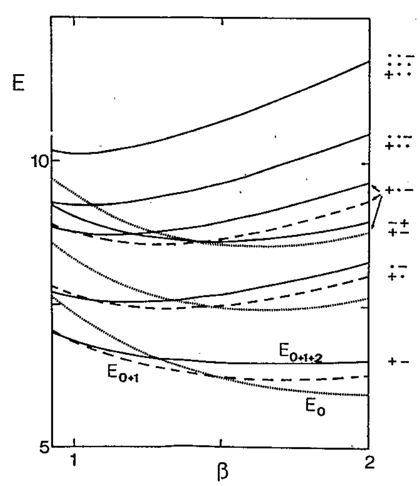


FIG. 4. Loop expansion of bound vortex energies, the zero-loop E_0 [Eq. (5.15)], up to one-loop E_{0+1} [Eq. (5.18)], and up to two-loop E_{0+1+2} [Eq. (5.20)] as a function of inverse temperature β are plotted.

amounts to $\sim 10\%$ of screening. At $\beta=2$, $q(\mathbf{x})$ is almost negligible.

Once $\mathbf{b}^{\text{cl}}(\mathbf{x})$ is determined, Eq. (5.15) gives the classical-level energies E_0 which are plotted in Fig. 4. The energies are 20–40 % less than the previous results of Eq. (5.8) and enhance the vortex contributions to heat capacity and internal energy. Of the three terms in Eq. (5.15), the second (q term) and the last term contribute $\sim 3\%$ and $\sim 8\%$ of E_0 for the $(+-)$ pair at $\beta=1.2$, respectively. The numbers at $\beta=1.0$ are $\sim 4\%$ and $\sim 12\%$, and at $\beta=1.6$, $\sim 1.5\%$ and $\sim 4\%$, respectively. For other pairs the numbers are roughly halved. The last two terms in Eq. (5.15) decrease for low temperatures and are most important for $(+-)$ pairs. The one-loop correction E_1 (5.18) to E_0 was evaluated in series up to $(\omega^{\text{int}})^3$ and was added to E_0 (Fig. 4). The correction is negative for $\beta<1.2\sim 1.5$ for our configurations. It gives E_0 a 7–9 % decrease at $\beta=1.0$ and a 2–4 % increase at $\beta=1.8$. To find the two-loop correction E_2 in (5.20), we needed the free propagator G in (5.19). This was obtained iteratively from the Dyson equation (5.21). The sum of the energies $E_{0+1+2}\equiv E_0+E_1+E_2$ is plotted in Fig. (4). The correction E_2 is of $\sim 0.5\%$ at $\beta=1.0$ and increases to a few percent at $\beta=1.8$. Our loop expansion is therefore a good approximation. It is important to evaluate higher-loop effects in a situation like ours when there exists no obvious expansion parameter, β being about unity in our case. It is known that the loop expansion works whenever a large overall constant factor appears in the exponent which suppresses the fluctuation. The present situation is different. Here the results are better for lower β. When β decreases, the spin waves tend to have shorter wave lengths and are naturally insensitive to a localized object like vortices. Consequently, the higher-loop effects should disappear as β decreases because they measure the difference between spin waves with and without vortices [Eq. (5.16)]. Table III shows our results for energies E_{0+1+2} against β. In the last row the previous results, Eq. (5.8), are inserted for comparison. For all configurations the energies are greatly reduced. For the $(+-)$ pair it is a $\sim 30\%$ reduction at $\beta=1.0$. This decrease is clearly reflected in the internal energy and heat capacity in Figs. 1 and 2 and in Table II. Here we have added the spin-wave contribution in (4.32) to the vortex part and used the standard thermodynamic formula, $U=-\partial(-\beta f)/\partial\beta$ and $C=-\beta^2\partial U/\partial\beta$. We have a good agreement with the Monte Carlo data.[12,13]

VI. DISCUSSIONS AND CONCLUSION

We have presented a new method to take into account topological excitations of nonlinear lattice models. As an example, we have calculated the heat capacity and the internal energy of the planar spin model in 2D and compared them with the recent Monte Carlo data (Figs. 1 and 2).[12,13] We have found good agreement. In particular, the peak of the heat capacity is well reproduced at the correct temperature. Our results indicate the importance of vortices in this model which are missed by the mean-field method described in Sec. II and the Hartree-Fock method in Sec. IV. The latter methods, relying on perturbation expansions in powers of T, focus attention only upon spin-wave fluctuations and ignore the nonperturbative effects arising from vortices which behave like $e^{-E/T}$ and cannot be expanded in powers of T.

In order to see the impact of the topological excitations, it is important to look at the specific heat since the internal energy is not sufficiently sensitive [for it, the two conventional methods suffice (Fig. 1 and Table II)]. In order to extract clearly the vortex content of the model, we have made use of the duality transformation.[8,10] Although this transformation has been used before, it has been applied mostly to the Villain model,[8] where it is trivial to perform. For the 2D XY model it has been analyzed, but improperly.[10] As discussed in Sec. V, the presence of vortices makes it impossible to expand the action for the dual variables in powers of $1/\beta$. In other words, β^{-1} is no longer a good expansion parameter. In fact, we have shown that the terms supposed to be of higher order are not really so but are all of the same order as the lowest one.

In the present approach we have, instead, resorted to the loop expansions,[16,18] regarding the vortices as external fields to the dual variables. This has given rise to nonlinear equations [Eq. (5.12)]. At the classical level they determine the internal magnetic fields in response to the

TABLE III. The bound vortex energies up to two-loop corrections $E_{0+1+2}\equiv E_0+E_1+E_2$ [Eqs. (5.20), (5.18), and (5.15)] for various types are tabulated for chosen temperatures and are compared with the previous temperature-independent results E_V [Eq. (5.8)] in the last row.

β	$+-$	$\cdot\,-$ / $+\,\cdot$	$+\cdot-$	$\cdot\,\cdot-$ / $+\cdot\,\cdot$	$\cdot\,\cdot-$ / $\cdot\,\cdot\,\cdot$ / $+\cdot\,\cdot$	$-+$ / $+-$
0.95	6.952	7.669	8.802	9.264	10.156	9.162
1.0	6.862	7.624	8.765	9.244	10.150	9.041
1.1	6.719	7.571	8.732	9.246	10.183	8.852
1.2	6.616	7.559	8.744	9.294	10.265	8.721
1.5	6.471	7.699	8.963	9.624	10.708	8.596
1.8	6.484	8.016	9.354	10.125	11.321	8.763
2.0	6.547	8.289	9.666	10.510	11.772	8.988
	9.87	12.57	14.35	15.26	16.76	14.35

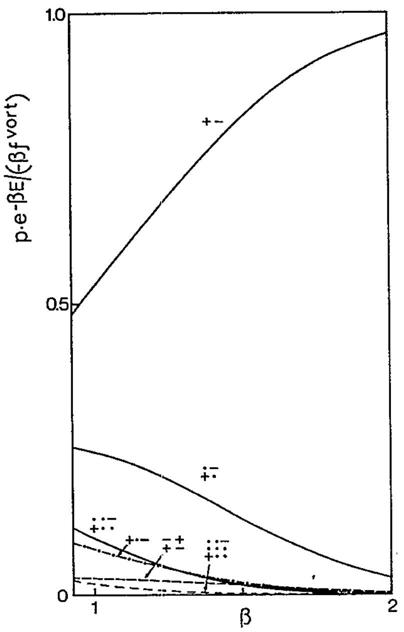


FIG. 5. Normalized importance of various bound vortices, $p(m)\exp(-\beta E[m])/(-\beta f^{\rm vort})$ and $p(Q)\exp(-\beta E(Q)]/(-\beta f^{\rm vort})$, as having appeared in Eq. (5.22), is plotted as a function of inverse temperature β.

vortex currents. The equations resemble the Maxwell equations, but with nonlinear field energy. They imply the renormalization of the bare charge $l(\mathbf{x})$ by the extra charge $q(\mathbf{x})$ which contains the nonlinearity screening effect (Fig. 3). For the vortex interactions (5.15), two new terms, one associated with the nonlinear charge $q(x)$ and the other with the nonlinear field energy, have been obtained in addition to a term which in the limit $\beta\to\infty$ reduces to the ordinary Biot-Savart-like term[8,10] $\sim lv'l$ [(5.6)]. Taking up to two-loop diagrams, we have determined the energies of various isolated neutral molecules of vortices, dipoles, and a quadruple within a few percent error (Table III and Fig. 4). [Notice that our energy of the $+-$ configuration (6.5) does not quite agree with the estimate of Tobochnik and Chester[12] extracted from the vortex density at $\beta=0.125$ (which is 9.4 ± 0.3). The reason is probably the slow equilibration of vortex configurations in Monte Carlo data.] This was achieved by solving first the nonlinear Maxwell equations numerically. In Fig. 5 the relative importance of various bound vortices is shown. A quadruple $\pm\mp$ detected by the Monte Carlo[12] simulation is seen to become as important as the dipoles as temperature increases.

The energies are now greatly reduced from the previous results (5.8) (Refs. 8 and 10) and are temperature dependent. Since these energies determine almost exclusively the free energy of the vortex part in the low-temperature phase (5.22), the reduction immediately enhanced the contributions from the vortices to the heat capacity and brought good agreement with the Monte Carlo data. The agreement extends even beyond the critical temperature (Fig. 2). Thus, our independent-molecule approximation interpolates even the low- and high-temperature phases smoothly, at least for macroscopic properties such as heat capacity. This is no surprise because the 2D XY model belongs to the Kosterlitz-Thouless[6] phase transition, so that it undergoes a smoother than second-order phase transition.

At this point we want to make a few critical comments on the results. The good agreement for $\beta\lesssim1$ is misleading in our opinion. This does not necessarily mean that our picture of noninteracting neutral molecules holds even for $\beta\lesssim1$ when the system is full of vortices of bound and free types. Rather, we speculate that the spin-wave contribution is overestimated by the Hartree-Fock method, to raise the specific heat and thus improve the better agreement. This overestimate may be illustrated by the one-dimensional (1D) XY model. It consists purely of spin waves and its partition function is exactly known. For it, the Hartree-Fock result is presented in Appendix C and is compared with the exact results in Fig. 6. Although the approximation is good for lower temperatures, the specific heat begins to override the true curve as $\beta\to0$. The exact result tells us that the heat capacity which is given by powers of $1/\beta$ for low temperatures is taken over by powers of β for high temperatures. The deviation occurs because the asymptotic series in $1/\beta$ is unable to take care of this transformation.

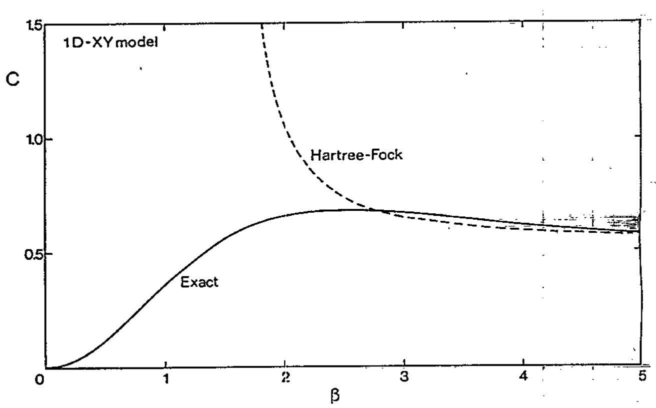


FIG. 6. Exact and Hartree-Fock results for the heat capacity for the 1D XY model in Eqs. (C5) and (C6) are plotted as a function of β.

Notice that the full expansion in $1/\beta$ is really the asymptotic expansion, i.e., it is formally divergent if it is considered up to the infinite order. The Hartree-Fock method, however, gives rise to a finite result owing to the partial resummation.

Actually, for $\beta>1$, the Hartree-Fock full series for the inverse temperature β^R in (4.13) is not really needed. For $\beta=1$, for example, β^R is already determined by a few lower-order terms in the power series expansion of $\exp-1/(2D\beta^R)$ which correspond to the lowest Feynman diagrams in the perturbative expansion.

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APPENDIX A: COULOMB GREEN'S FUNCTION $v(\mathbf{x})$ AND $v'(\mathbf{x})$

The Coulomb Green's function $v(\mathbf{x})$ and $v'(\mathbf{x})$ are given by

$$v(\mathbf{x})=-\left[\frac{1}{\nabla_i\overline{\nabla}_i}\right]_{\mathbf{x},0}=\int_{-\pi}^{\pi}d^2k\frac{1}{(2\pi)^2}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{2\sum_{i=1,2}(1-\cos k_i)},$$
$$v'(\mathbf{x})=v(\mathbf{x})-v(0)=\int_{-\pi}^{\pi}d^2k\frac{1}{(2\pi)^2}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}-1}{2\sum_{i=1,2}(1-\cos k_i)},\tag{A1}$$

respectively. In the latter propagator $v'(\mathbf{x})$, the logarithmic singularity of $v(\mathbf{x})$ at the origin has been subtracted. The values of $v'(\mathbf{x})$ are known.[17] We list some of them:

$$\begin{aligned}&\mathbf{x}:\ (0,0)\ ,\\ &v'(\mathbf{x}):\ 0\ ,\\ &\mathbf{x}:\ (1,0)\ ,\ (1,1)\ ,\\ &v'(\mathbf{x}):\ -\tfrac{1}{4}\ ,\ -1/\pi\ ,\\ &\mathbf{x}:\ (2,0)\ ,\ (2,1)\ ,\ (2,2)\ ,\\ &v'(\mathbf{x}):\ -1+\frac{2}{\pi}\ ,\ \frac{1}{4}-\frac{2}{\pi}\ ,\ -\frac{4}{3\pi}\ .\end{aligned}\tag{A2}$$

Note the properties of $v'(\mathbf{x})=v'(x_1,x_2)$,

$$v'(\mathbf{x})=v'(|x_1|,|x_2|)=v'(|x_2|,|x_1|)\ .\tag{A3}$$

For large $|\mathbf{x}|$, $v'(\mathbf{x})$ behaves as

$$v'(\mathbf{x})\sim\frac{1}{2\pi}[\ln|\mathbf{x}|+\ln(2\sqrt{2}e^{\gamma})]\ ,\tag{A4}$$

with $\gamma=0.577\,216\ldots$, Euler's, constant.

APPENDIX B: SMALL-q EXPANSION OF EQ. (5.13)

In the limit $q\to 0$, we can solve the nonlinear equation (5.13) by expanding the right-hand side of Eq. (5.14) in $q(\mathbf{x})$,

$$\begin{aligned}q(\mathbf{x})&=\frac{1}{2\pi i}\sum_i\nabla_{\langle i\rangle}W'_{\rm int}\left[b_i^{0\rm cl}(\mathbf{x})+\sum_{\mathbf{x}'}V_i(\mathbf{x}-\mathbf{x}')q(\mathbf{x}')\right]\\ &\simeq\frac{1}{2\pi i}\sum_i\nabla_{\langle i\rangle}W'_{\rm int}(b_i^{0\rm cl}(\mathbf{x}))\equiv q^0(\mathbf{x})\ ,\end{aligned}\tag{B1}$$

where

$$b_i^{0\rm cl}\equiv-\frac{2\pi i}{W''(0)}\sum_{\mathbf{x}'}\overline{\nabla}_{\langle i\rangle}v'(\mathbf{x}-\mathbf{x}')l(\mathbf{x}')\ ,$$
$$V_i(\mathbf{x})\equiv\frac{2\pi i}{W''(0)}\overline{\nabla}_{\langle i\rangle}v'(\mathbf{x})\ .$$

The magnetic fields $\mathbf{b}^{\rm cl}(\mathbf{x})$ are then given up to $O(q)$ by

$$b_i^{\rm cl}(\mathbf{x})\simeq b_i^{0\rm cl}(\mathbf{x})+\sum_{\mathbf{x}'}V_i(\mathbf{x}-\mathbf{x}')q^0(\mathbf{x}')\ .\tag{B2}$$

Similarly, the classical contribution $-\beta E_0$ in Eq. (5.15) is expanded up to $O(q)$,

$$-\beta E_0[l(\mathbf{x})]\simeq\frac{(2\pi)^2}{W''(0)}\frac{1}{2}\sum_{\mathbf{x},\mathbf{x}'}l(\mathbf{x})v'(\mathbf{x}-\mathbf{x}')l(\mathbf{x}')+\sum_{\mathbf{x},i}\left[W_{\rm int}(b_i^{0\rm cl}(\mathbf{x}))+W'_{\rm int}(b_i^{0\rm cl}(\mathbf{x}))\sum_{\mathbf{x}'}V_i(\mathbf{x}-\mathbf{x}')q^0(\mathbf{x}')\right]\ .\tag{B3}$$

For higher loops in Eqs. (5.20) and (5.18) one may simply assume $\mathbf{b}^{\rm cl}(\mathbf{x})=\mathbf{b}^{0\rm cl}(\mathbf{x})$, since they are already small corrections to $-\beta E_0$.

APPENDIX C: HARTREE-FOCK APPROXIMATION FOR 1D *XY* MODEL

The *XY* model in one dimension is given by

$$Z=\prod_x\int_{-\pi}^{\pi}d\theta(x)\frac{1}{2\pi}\exp\left[\beta\sum_x\cos\nabla\theta(x)\right]\ .\tag{C1}$$

Integrating the angles one by one and ignoring the boundary effects, which is unimportant in the thermodynamic limit, we find

$$Z=\left[\int_{-\pi}^{\pi}d\theta\frac{1}{2\pi}e^{\beta\cos\theta}\right]^N=I_0(\beta)^N\ .\tag{C2}$$

Therefore, the model has no topological excitation and is described entirely by angle fluctuations. Then, for low temperatures the Hartree-Fock approximation may be sufficient. Thus, we consider

$$Z_{\rm SW}=\int_{-\infty}^{\infty}d\theta\frac{1}{2\pi}e^{\beta\cos_t\theta}\ ,\tag{C3}$$

with $\cos_t\theta$ defined as in (4.6) and apply the normal ordering. This gives

$$Z_{\rm SW}=\exp\left[\beta^R\left[1+\frac{1}{2\beta^R}\right]\right]\int_{-\infty}^{\infty}\frac{d\theta}{2\pi}\times\exp\beta^R\left[-\tfrac{1}{2}\theta^2+:\left[\cos\theta-1+\frac{\theta^2}{2}\right]:\right]\ ,\tag{C4}$$

with $\beta^R=\beta\exp(-\frac{1}{2}/\beta^R)$. Taking up to three loops, we find

$$\begin{aligned}-\beta f_{\rm sw}^{\rm HF}&=\beta^R+\tfrac{1}{2}-\tfrac{1}{2}\ln(2\pi\beta^R)+\frac{1}{2\times4!}\frac{1}{(\beta^R)^4}\ ,\\ U_{\rm sw}^{\rm HF}&=-\frac{\beta^R}{\beta}+\frac{1}{3!}\frac{1}{\beta(\beta^R)^3(2\beta^R-1)}\ ,\\ C_{\rm sw}^{\rm HF}&=\frac{1}{2\beta^R-1}\left[\frac{1}{3!(\beta^R)^3}+\beta^R\right]+\frac{1}{(2\beta^R-1(\beta^R)^2}\\ &\quad+\frac{2}{3\beta^R(2\beta^R-1)^3}\ .\end{aligned}\tag{C5}$$

The exact results are

$$\begin{aligned}&-\beta f=\ln I_0(\beta)\ ,\\ &U=-I_1(\beta)/I_0(\beta)\ ,\\ &C=\beta^2\left[1-\frac{I_1(\beta)}{\beta I_0(\beta)}-\left[\frac{I_1(\beta)}{I_0(\beta)}\right]^2\right]\ .\end{aligned}\tag{C6}$$

The heat capacities in (A6) and (A5) are plotted in Fig. 6.

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