Vortex excitations and specific heat of the planar model in two dimensions

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The density of vortex excitations and their contribution to the specific heat are discussed for the Villain planar model. Exact results are derived for the low- and high-temperature limits, and a renormalization-group interpolation scheme is developed for intermediate temperatures.

I. INTRODUCTION

The planar model is relevant to experiment in that it describes superfluid behavior in systems of ^{4}He.[1,2] Furthermore, the planar model in two dimensions is the prototype of a model exhibiting topological long-range order and a novel type of phase transition. For details the reader is referred to the pioneering work of Kosterlitz and Thouless[2] and recent reviews.[3–5] There are two types of elementary excitations in the planar model: spin waves and vortices. In the low-temperature phase, spin waves coexist with bound vortex-antivortex pairs and the system exhibits topological long-range order. The phase transition is associated with the unbinding of vortex pairs and, in the high-temperature phase, free vortices are present. The purpose of this paper is to study the statistical thermodynamics of the vortex excitations and, in particular, to calculate as a function of temperature their average density, n, and contribution to the specific heat, c.

The calculation is performed for the Villain planar model,[6,7] in which the spin-wave and vortex excitations decouple. The thermodynamic properties of the model can be investigated exactly in the low- and high-temperature limits. This is discussed in Secs. II A and II B. Approximate results over the full temperature range are then obtained by a renormalization-group (RG) procedure, which is described in Sec. II C. The temperature dependence of the thermodynamic quantities discussed here is of experimental interest. However, we note that the detailed features of the curves are model dependent and, therefore, the calculation predicts only the general behavior of the quantities. A discussion of the results and further comments are presented in Sec. III.

For the purpose of establishing notation, some basic results for the Villain planar model on a square lattice are reviewed. The partition function for the model is[6,7]

$$Z_V=\left[\prod_j \int_0^{2\pi} \frac{d\theta_j}{2\pi}\right] \exp\left[\sum_{\langle i,j\rangle} V(\theta_i-\theta_j)\right] \quad , \tag{1.1a}$$

$$e^{V(\theta)}=\sum_{m=-\infty}^{+\infty} e^{-K(\theta-2\pi m)^2/2} \quad . \tag{1.1b}$$

Here K^{-1} is the dimensionless temperature parameter. The partition function (1.1) decomposes exactly into spin-wave and vortex-gas contributions, $Z=Z_{\rm SW}Z_{\rm VG}$,[7]

$$Z_{\rm SW}=\left[\prod_j \int_{-\infty}^{+\infty} \frac{d\phi_j}{2\pi}\right] \exp\left[-\tfrac{1}{2}K\sum_{i,j}\phi_i G_{ij}^{-1}\phi_j\right] \quad , \tag{1.2a}$$

$$Z_{\rm VG}=\left[\prod_j \sum_{m_j=-\infty}^{+\infty}\right] \exp\left[-\tfrac{1}{2}(2\pi)^2K\sum_{i,j} m_i G_{ij} m_j\right] \quad , \tag{1.2b}$$

where the Green's function is defined by

$$\sum_{\langle i,j\rangle}(\phi_i-\phi_j)^2\equiv\sum_{i,j}\phi_i G_{ij}^{-1}\phi_j \quad . \tag{1.3}$$

The continuous field, ϕ_i, describes the spin-wave excitations and the set of integers, m_i, the vorticity of the vortex excitations. For large lattices the diagonal elements of the Green's function, G_{ii}, diverge. This imposes the restriction that only configurations with $\sum_j m_j=0$ contribute to Eq. (1.2b). The reduced lattice Green's function $G_{ij}'=2\pi(G_{ii}-G_{ij})$ behaves for large r like[7]

$$G_{ij}'=\ln(r_{ij}/a_0)+C \tag{1.4}$$

and assumes the value $C=\pi/2$ for $r_{ij}=a_0$, where a_0 is the lattice spacing. With this approximation the vortex-gas contribution (1.2b) becomes[7]

$$Z_{\rm VG}={\rm Tr}'_{\{m\}}\exp\left[\tfrac{1}{2}(2\pi K)\sum_{i\neq j} m_i m_j \ln\left(\frac{r_{ij}}{a_0}\right) + \ln y \sum_j m_j^2\right] \quad , \tag{1.5a}$$

$$y=\exp(-\tfrac{1}{2}\pi^2 K) \quad . \tag{1.5b}$$

This partition function is equivalent to that of a two-dimensional Coulomb gas of positive and negative charges, m_j, with $\sum_j m_j=0$, and a temperature-controlled fugacity y. It is often useful to consider K and y in Eq. (1.5a) as independent parameters. The planar model is then recovered by imposing Eq. (1.5b).

The partition function (1.2) determines the reduced free-energy density

$$f=\lim_{N\to\infty}\frac{1}{N}\ln Z \ , \tag{1.6}$$

from which the thermodynamic quantities of interest are obtained by means of derivatives,

$$n=\frac{\partial f}{\partial \ln y}=\lim_{N\to\infty}\frac{1}{N}\sum_j \langle m_j^2\rangle \ , \tag{1.7a}$$

$$\frac{c}{k_B}=K^2\frac{\partial^2 f}{\partial K^2} \ . \tag{1.7b}$$

The derivative in Eq. (1.7a) is taken at constant K, while the derivatives with respect to K in Eq. (1.7b) are taken along the locus (1.5b). The spin-wave contribution to the specific heat is $c/k_B=\frac{1}{2}$. The vortex contributions are discussed below.

II. STATISTICAL THERMODYNAMICS OF VORTEX EXCITATIONS

A. Limit of low temperatures

In this section, a low-temperature approximation to the partition function (1.5) is developed. In this limit the fugacity, y, is small and the corrections to the ground state with $m_j=0$ are due to pairs of vortices of equal and opposite vorticity, $m_j=\pm 1$. Since these excitations form a dilute gas of neutral pairs, their interaction is neglected[8] and the grand canonical partition function in independent pair approximation ob-

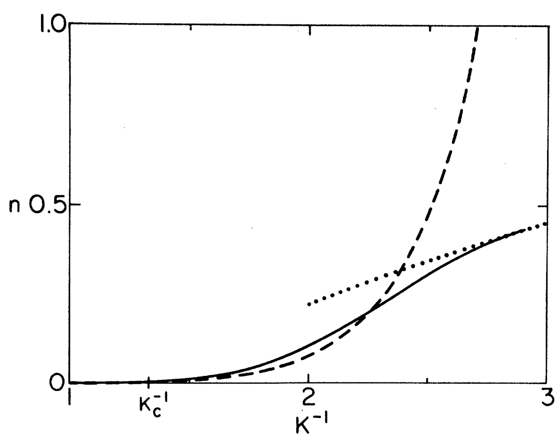

FIG. 1. Average density of vortex excitations for the Villain planar model in two dimensions from an approximate renormalization-group approach (full curve) and comparison with exact low- and high-temperature results (dashed and dotted curves, respectively). The transition occurs at $K_c^{-1}\simeq 1.33$.

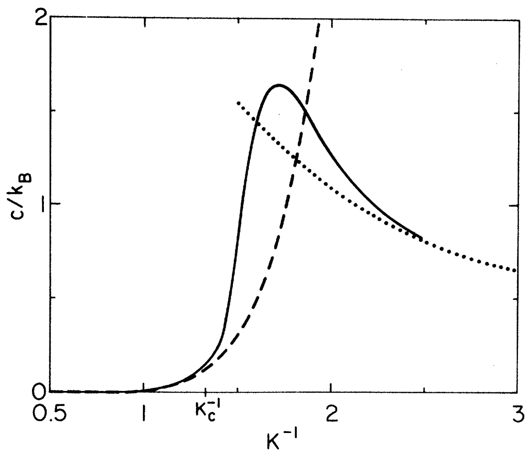

FIG. 2. Specific heat of the vortex excitations for the Villain planar model in two dimensions from an approximate renormalization-group approach (full curve) and comparison with exact low- and high-temperature results (dashed and dotted curves, respectively). The transition occurs at $K_c^{-1}\simeq 1.33$. The asymptotic behavior at high temperatures is $c/k_B=\frac{1}{2}$.

tained,

$$Z_{\mathrm{IP}}=\sum_{n=0}^{\infty} y^{2n}n!(\hat{Z})^n(n!)^{-2}=\exp(y^2\hat{Z}) \ , \tag{2.1}$$

in terms of the canonical partition function for one pair,

$$\hat{Z}=N\sum_{\vec{r}\neq 0}\exp\left(-2\pi K\ln\left|\frac{\vec{r}}{a_0}\right|\right) \ . \tag{2.2}$$

This yields for the free energy in the limit $K^{-1}<<\pi$,

$$f_{\mathrm{IP}}=y^2(K-\pi^{-1})^{-1} \ . \tag{2.3}$$

The results for the density of vortex excitations, n, and specific heat, c, obtained according to Eq. (1.7) are shown as dashed curves in Figs. 1 and 2.

B. Limit of high temperatures

In this section, the partition function for the vortex gas is calculated for high temperatures. It is convenient to rewrite Z_{VG} as

$$Z_{\mathrm{VG}}=\left(\prod_j\sum_{m_j=-\infty}^{+\infty}\right)\exp\left(-\tfrac{1}{2}(2\pi)^2K \times\sum_{i,j}m_im_j(G_{ij}+\kappa\delta_{ij})\right) \ , \tag{2.4a}$$

with

$$\kappa=-\tfrac{1}{4}(1+2K^{-1}\ln y\,\pi^{-2}) \ . \tag{2.4b}$$

κ is zero on the locus (1.5b) and increases slowly with decreasing y at constant K.

In the limit of very high temperatures all vortex pairs are dissociated and the Debye-Hückel approximation applies.[9] The corresponding partition function can be evaluated exactly. It is obtained from Eq. (2.4a) by replacing the sums over integer m's by integrals, thus neglecting the "quantization" of vorticity. The free energy in this approximation is

$$f_{\rm DH}=\tfrac{1}{2}\ln(2\pi)-\tfrac{1}{2}\int\frac{d^2q}{(2\pi)^2}\ln[(2\pi)^2K(G_{\vec q}+\kappa)] \tag{2.5a}$$

$$=\tfrac{1}{2}\{\ln(2K^{-1})-[(1+4\pi\kappa)/4\pi\kappa]\ln(1+4\pi\kappa)\}\ , \tag{2.5b}$$

where Eq. (2.5b) follows by integrating over a circular Brillouin zone of radius $a=2\sqrt{\pi}$ and using the small-q approximation for the Fourier components of the Green's function, $G_{\vec q}=(4-2\cos q_x-2\cos q_y)^{-1}\simeq q^{-2}$. The Debye-Hückel specific heat is constant, $c/k_B=\frac{1}{2}$.

Corrections to the Debye-Hückel approximation can be obtained via a high-temperature series expansion. Applying to Eq. (2.4) the Poisson summation formula and the mathematical steps that led to the factorization of the original partition function into Eq. (1.2), one finds $Z_{\rm VG}=Z_{\rm DH}\tilde Z$ with

$$\tilde Z=\left[\prod_j\sum_{p_j=-\infty}^{+\infty}\right]\times\exp\left[-\frac{1}{2K}\sum_{i,j}p_ip_j(G_{ij}+\kappa\delta_{ij})^{-1}\right]\ , \tag{2.6}$$

where p extends over all integers and G_{ij}^{-1} is defined by Eq. (1.3).

When $\kappa=0$, Eq. (2.6) is the partition function of the solid-on-solid or discrete Gaussian model with coupling constant $1/K$.[10] Therefore, the strong-coupling expansion for that model[11,12] can be used to generate high-temperature corrections to the Debye-Hückel behavior. The expansion parameter is $\chi=\exp(-K^{-1})$.

When $\kappa>0$ but small, the partition function (2.6) can be expanded in terms of κ. The coefficients are certain correlation functions of the solid-on-solid model that can also be evaluated by the strong-coupling expansion in χ. To fourth order in χ and first order in κ we obtain

$$\tilde f=(2\chi^2+4\chi^3+4\chi^4)+\tfrac{1}{2}K^{-1}\kappa(40\chi^2+96\chi^3+24\chi^4)\ . \tag{2.7}$$

For $\kappa=0$, Swendsen's[12] result is recovered when an error in his fourth-order coefficient is corrected.

In summary, for high temperatures the free energy of the vortex gas is given by

$$f_{\rm HT}=f_{\rm DH}+\tilde f\ , \tag{2.8}$$

with $\tilde f$ of Eq. (2.7) yielding the leading corrections to the asymptotic result $f_{\rm DH}$ of Eq. (2.5). Results for n and c up to the same order in χ along the locus $\kappa=0$ are shown as dotted curves in Figs. 1 and 2.

C. Interpolation for intermediate temperatures

In this section, an interpolation formula for the free energy at intermediate temperatures is developed, which improves an earlier calculation by Berker and Nelson.[9] The phase transition of the planar model being associated with the onset of dissociation of vortex pairs, the interaction among vortices is crucial in that temperature region. Kosterlitz[13] first proposed an RG method for treating these effects to order y^2 in a small-y expansion. The approach used the Coulomb-gas representation (1.5a) including approximation (1.4). Our interpolation procedure requires, at high temperatures, an expression for the free energy to which the RG result can be matched. For that purpose Eq. (2.8) is used, which results from Eq. (2.4) without approximation (1.4). Therefore, we employ recursion relations for the parameters K^{-1} and y,

$$\frac{dK^{-1}}{dl}=2\pi^4y^2K\ , \tag{2.9a}$$

$$\frac{dy^2}{dl}=2y^2(2-\pi K)\ , \tag{2.9b}$$

that follow from the sine-Gordon representation of the Villain model by means of a momentum-space RG procedure.[14-17] To order y^2 the Villain and sine-Gordon models are equivalent. Other treatments[13,16] lead to equations $dK^{-1}/dl=4\pi^3y^2h(K^{-1})$ with different functions $h(K^{-1})$, all of which assume $h(\pi/2)=1$ at the Kosterlitz-Thouless point. The recursion relation for the free energy to order y^2 is[18]

$$f(K,y)=e^{-2l^*}f(K(l^*),y(l^*))+\int_0^{l^*}dl\,e^{-2l}g_0(y(l))\ , \tag{2.10a}$$

$$g_0(y)=2\pi y^2\ . \tag{2.10b}$$

This expression describes in the standard line integral form[19] the scaling properties of the free energy between two points, (K,y) and (K^*,y^*), along an RG trajectory.

The flows generated by the recursion relations (2.9) are shown in Fig. 3. The relationship (1.5b) defines the initial locus. There exists a critical value K_c^{-1} such that flows originating in the physical sub-

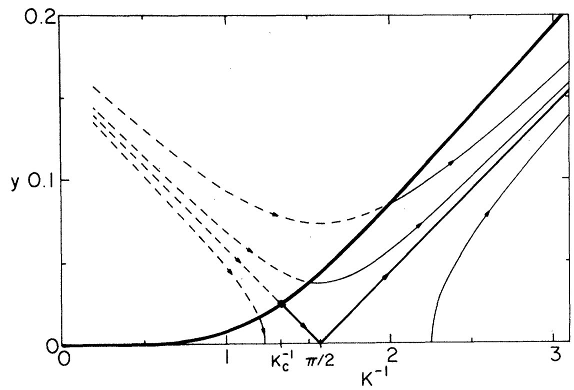

FIG. 3. Renormalization-group trajectories for the Villain planar model in two dimensions from Eqs. (2.9). The medium heavy lines separate regions with different flow properties and the heavy line is the locus of initial conditions, Eq. (1.5b). The critical point is indicated by a dot. The flows are terminated and the thermodynamic quantities matched to their high-temperature values when y reaches $y^* = 0.15$.

space (1.5b) iterate towards $y = 0$ when $K^{-1} \leq K_c^{-1}$, and towards large values of y when $K^{-1} > K_c^{-1}$. The dissociation of vortex pairs begins at $K^{-1} = K_c^{-1}$. When $K^{-1} < K_c^{-1}$, Eqs. (2.9) and (2.10) determine the free energy completely since $y(l)$ tends to zero for large l. When $K^{-1} \gtrsim K_c^{-1}$, $y(l)$ eventually increases and begins to move outside the domain of validity of Eqs. (2.9). For sufficiently large (K^{-1}, y) the high-temperature series expansion of the previous section applies. Our interpolation consists in using the RG equations (2.9) and (2.10) up to such values and then matching the RG and high-temperature results. Roughly, the high-temperature approximation will be valid for temperatures above which the dissociation of vortex pairs is completed. A simple estimate of the mean separation between vortices in a pair indicates that the process of dissociation which begins at K_c^{-1} continues to about $2K_c^{-1}$.[20] We choose $y(l^*) = 0.15$ as matching locus, thus ensuring that $K^{-1}(l^*) > 2K_c^{-1}$. The actual matching is performed for the internal energy, $E = -\partial f/\partial K$, and vortex density, $n = \partial f/\partial \ln y$. Then one numerical differentiation is sufficient to obtain the specific heat. The results are shown as full curves in Figs. 1 and 2.

III. DISCUSSION OF RESULTS

The statistical thermodynamics of vortex excitations in the Villain planar model in two dimensions has been obtained. The partition function for this model factorizes exactly into spin-wave and vortex parts. The background spin-wave contributions have to be corrected at low temperatures for quantum effects neglected here.

The density of vortex excitations, shown in Fig. 1, increases smoothly as a function of temperature. At the transition temperature, $K_c^{-1} \simeq 1.33$, only 0.3% of the lattice sites are occupied by such excitations.

The specific heat, shown in Fig. 2, exhibits a pronounced maximum at a temperature larger than the transition temperature. The maximum is caused by the dissociation of more and more tightly bound vortex pairs with increasing temperature. At sufficiently high temperatures, when all vortices are unbound, the specific heat reaches the constant Debye-Hückel value, $c/k_B = \frac{1}{2}$. At low temperatures the specific heat rises exponentially and passes without an observable signature through the transition point at K_c^{-1}. The RG approach predicts an essential singularity at the transition.[13] The agreement between the specific heats in the independent pair approximation and the RG interpolation is very good almost up to the critical temperature, K_c^{-1}, where it is within 13%. About 10% below K_c^{-1} the specific heat begins to rise more steeply until it reaches a maximum value about 30% above K_c^{-1}. When most pairs are dissociated the interpolation follows the exact high-temperature behavior. The precise height, shape, and location of the specific-heat maximum are nonuniversal features that depend on the choice of model (i.e., the Villain interaction or a more general periodic interaction that allows for spin-wave vortex couplings) and details of the recursion relations (i.e., contributions of higher order in y^2, choice of cutoff function,[16] etc.). It is nevertheless safe to expect the peak to be located from 10 to 40% above the transition temperature.

Our RG interpolation scheme is in the spirit of an earlier calculation by Berker and Nelson.[9] The results for the specific heat agree below the critical temperature. However, the choice of a different matching locus and an improved high-temperature theory lead to a better description at higher temperatures.

Monte Carlo simulations[21,22] of the statistical thermodynamics of the planar model, $H = K \times \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$, yielded results for the specific heat with the same general features as Fig. 2, but sharper peak profiles and peak locations only 15% above the critical temperature. The two-dimensional Coulomb gas of unit charges has also been investigated by Monte Carlo techniques.[23] The results are most reliable for low temperatures, and we found them to be in excellent agreement with the independent pair approximation on a lattice, Eq. (2.2). Swendsen[12] pointed out that the discrete Gaussian or solid-on-solid model with quadratic interactions provides for a more efficient simulation. The exact equivalence between this model and the Villain planar model[7,10] would make possible a detailed comparison with the results of the RG calculation presented here over the full temperature range. So far, simulations have been performed only for a 10×10 lattice.[12]

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