Critical point in a two-dimensional planar model

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Transfer matrix formalism has been used to study the phase transition in a two-dimensional isotropic planar model where one dimension is taken to be spatial and the second dimension is temporal. Character expansion has been used to calculate the eigenvalues of the transfer matrix operator. This has ensured very rapid convergence around the critical point. Fluxes have been generated at each lattice site of the spatial dimension by Monte Carlo simulation. Mass gap and free energy have been found in both theoretical calculation and computer simulation separately for different values of temperature. From the results I infer an algebraic divergence of correlation length rather than a Kosterlitz-Thouless type. The value of critical temperature is found to be $k_B T_c/J=0.899$. [S1063-651X(97)01904-1]

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INTRODUCTION

In usual two-dimensional (2D) systems, at above absolute zero temperature, long-range order is said to be absent. Peierls [1] showed that the localization of particles on their lattice sites is destroyed by long wavelength lattice waves. Similarly, using the spin-wave theory of Bloch [2], one finds that the spontaneous magnetization is destroyed by long wavelength spin waves. Again, more general proofs using Bogoliubov inequalities have shown that under very general conditions, long-range order is destroyed for 2D crystals, magnets, superconductors, and superfluids [3]. However, high-temperature series expansions for 2D spin systems and certain other computer simulations suggest that there exists a phase transition even in the absence of long-range order.

Kosterlitz and Thouless [4] (KT) studied these 2D systems within a unified theoretical model and investigated the possibility of a phase transition with short-range order. First, they showed that it is possible to get long-range order, called topological order, and that there is a phase transition characterized by a sudden change in the response of the system to an external perturbation. Later, they established the presence of vortices in 2D systems [5]. They contend that the 2D low-temperature phase is characterized by a power-law decay in pair correlation function (as predicted by harmonic theory) modified by the presence of pairs of tightly bound topological defects of ''opposite sign.'' At the transition temperature, the pairs unbind to create a new phase where the correlations decay exponentially. In crystals, the topological defects are dislocations, in magnets they are spin vortices, and in superfluid helium they are quantum vortices. The three component spin model (Heisenberg model) will not sustain vortices because the singularity at the core of the vortex can be avoided by the core spins pointing outside the plane. Thus in this case KT predict that there is no phase transition.

However, the two component spin model, called the planar (or XY) spin model, can support vortices and should therefore exhibit the KT transition. In a planar model, the low-temperature phase of the system contains massless spin waves whereas the high-temperature phase is completely disordered. The vortices condense for $T>T_c$ and disorder spin-spin correlation function. Since this work of Kosterlitz and Thouless, this problem area has been explored by many research workers in a variety of means and ways. Out of these, I mention the results of relevant papers in Sec. IV of the present paper. In this section, I merely mention these papers to show the vast amount of work that has already been done on this problem. Analytical work has been done by Mattis [6], Migdal [7], and Stump [8]. Series expansion methods were tried by Hamer *et al.* [9], Luck [10], Hornby and Barber [11], Alton and Hamer [12], etc. Many computational methods have been used by Heys and Stump [13], Tobochnik and Chester [14], Fox *et al.* [15], Janke and Nather [16], Gupta, Delapp, and Batrouni [17], Biferale and Petronzio [18], etc. Although some of the papers on this problem have questioned KT-type transition, most of them have agreed firmly upon a KT transition.

The present paper is another independent attempt to verify KT transition on the basis of the lattice model. If I use a lattice model, probably it is not driven by vortex condensation. I expect a different approach to calculate the critical temperature and exponents and thus compare them with previously existing results. In this paper we have constructed the Hamiltonian in Euclidian formulation as explained later. This was previously done in only one paper (e.g., by Hamer *et al.* [9]), but there the methodology was much different. Here, I have used two very unique and useful methods: while calculating mass gap, I have used the character expansion [19] method and in computing the same, I have used the Neumann-Ulam stochastic method [20]. The usefulness of these methods has been discussed in appropriate sections.

Usually, as temperature T approaches its critical value T_c from above, the correlation length $\xi(T)$ diverges as [21]

$$\xi(T)\sim|T-T_c|^{-\nu}.$$

This is called algebraic divergence. But, renormalization group calculations by Kosterlitz [5] show

$$\xi(T)\sim\exp\left[b\left(\frac{T_c}{T-T_c}\right)^{1/2}\right],\quad T>T_c+$$

which is called exponential divergence. Our aim in this paper is to establish which of these two expressions is valid for $T>T_c$.

This paper is divided into two parts. In the first part, I have used character expansion, a perturbative method to calculate free energy and mass gap of the planar model in 2D, based on transfer matrix formalism. This is described in Sec. II. In the second part, a mainframe computer (IBM 360) has been used to create Monte Carlo simulation of the 2D lattice spin model and both free energy and mass gap have been computed. This has been described in Sec. III. Results of the computed values have been fitted by least squares method in Sec. IV to verify the nature of the divergence of correlation length $\xi(T)$ (which is inverse of mass gap). In Sec. V I compare my results with those of other relevant papers. In Sec. VI a conclusion is given.

I. THE MODEL

Of the two dimensions, I take one to be spatial and the other to be temporal. The Hamiltonian of the system is $O(n)$ invariant (in our case $n=2$). We also consider nearest neighbor interaction with interaction coupling constant J to be unity. The Hamiltonian can then be given by

$$H=-\sum_{i,k}^{N}(\hat{S}_{i,k}S_{i-1,k}+\hat{S}_{i,k}\hat{S}_{i,k-1})$$
$$=\sum_{i,k}^{N}[\cos(\theta_{i,k}-\theta_{i-1,k})+\cos(\theta_{i,k}-\theta_{i,k-1})],\quad(1.1)$$

where I considered a finite lattice of N^2 sites satisfying periodic boundary condition. i is the index along the spatial axis and k is that for the temporal axis. Also, the system is devoid of any external field.

The partition function can be written as

$$Z=\int_0^{2\pi}\prod_{i,k}^{N}d\theta_{i,k}e^{-\beta H}.\quad(1.2)$$

But Z can be written in terms of transfer matrix T as

$$Z\sim\lim_{N\gg1}\mathrm{Tr}(\hat{T}^N)\quad(1.3)$$

(provided the largest eigenvalue state of $\hat{T}$ is unique).

This can be verified by considering the relation

$$\hat{H}=\lim_{\epsilon\to0}\left(-\frac{\hbar}{\epsilon}\right)\ln\hat{T},\quad(1.4)$$

where $\epsilon=\tau_k-\tau_{k-1}$ and $\tau=-it$, t being the time coordinate [10].

We have thus analytically continued time to imaginary region, thus the Minkowsky space has shifted to Euclidian space. But, no Wick's rotation is visible apparently in the formalism, because $t\to i\tau$ has been done by hand and implicitly in constructing the Hamiltonian H as given by Eq. (1.1).

II. CALCULATIONS FOR FREE ENERGY AND MASS GAP

The partition function appropriate for the planar model is obtained from Eqs. (1.1) and (1.2) as

$$Z(\beta)=\prod_{i,k}^{N}\int_0^{2\pi}d\theta_{i,k}\exp\{\beta\cos(\theta_{i,k}-\theta_{i-1,k})$$
$$+\beta\cos(\theta_{i,k}-\theta_{i,k-1})\}.\quad(2.1)$$

This has a global invariance, i.e.,

$$\theta_{i,k}\to\theta_{i,k}+\phi\quad\text{for all } i \text{ and } k.$$

Taking matrix elements in the $|\theta\rangle$ representation where $|\theta_i\rangle$'s are mutually orthogonal, one gets

$$\langle\theta_{k'}|\int d\zeta\ e^{\beta\cos\zeta}e^{\zeta\partial/\partial\theta_i}|\theta_k\rangle$$
$$=\int d\zeta\ e^{\beta\cos\zeta}\langle\theta_{k'}|(\theta_k+\zeta)\rangle$$
$$=\int d\zeta\ e^{\beta\cos\zeta}\delta(\theta_{k'}-\overline{\theta_k+\zeta})$$
$$=e^{\beta\cos(\theta_{k'}-\theta_k)}.$$

Let $\theta_{i,k}-\theta_{i,k-1}=\theta_{k'}-\theta_k$, which represents a translation along the time axis. Then I write the structure of the transfer matrix from Eq. (1.3) as

$$\hat{T}=\prod_{i}^{N}\int d\theta_i\left[\exp\{\beta\cos(\theta_i-\theta_{i-1})\}\int d\zeta\ e^{\beta\cos\zeta}e^{\zeta\partial/\partial\theta_i}\right].\quad(2.2)$$

This is diagonal in $|\theta\rangle$ representation. To work in flux representation,

$$|n_1,n_2,\ldots n_{M-1}\rangle=\int d\theta_1 d\theta_2\cdots d\theta_{M-1}$$
$$\times\exp\left(-i\sum_j n_j\theta_j\right)|\theta_1,\theta_2,\ldots,\theta_{M-1}\rangle,$$

and using the relations

$$\int dx'\int dx\ e^{a\partial/\partial x'}f(x)=\int dx'\int dx\ f(x+a)\,\delta(x'-x),$$

$$In(\beta)=\frac{1}{\pi}\int_0^{\pi}e^{\beta\cos\zeta}\cos(n\zeta)d\zeta.$$

(In being the modified Bessel function of order n), I get from Eq. (2.2)

$$T=\prod_i \int_0^{2\pi} d\theta_i \exp\left(\frac{\beta}{2}(e^{i(\theta_i-\theta_{i-1})} + e^{-i(\theta_i-\theta_{i-1})})\right)\int d\zeta\ e^{\beta\cos\zeta} e^{\zeta\partial/\partial\theta_i}|\theta\rangle$$

$$=\prod_i \int_0^{2\pi} d\theta_i \int d\zeta\ e^{\beta\cos\zeta} e^{\zeta\partial/\partial\theta_i} \times \exp\left(\frac{\beta}{2}(L_+^i L_-^{i+1}+L_-^i L_+^{i+1})\right)|\theta\rangle.$$

Now $|n\rangle=\int d\theta\ e^{-in\theta}|\theta\rangle$.

So the above becomes

$$\hat{T}=\prod_j \hat{I}_{n_j}(\beta)\prod_i \exp\left(\frac{\beta}{2}(\hat{L}_+^i\hat{L}_-^{i+1}+\hat{L}_-^i\hat{L}_+^{i+1})\right)|n\rangle. \tag{2.3}$$

Here $\beta^{-1}=k_BT/J$, k_B being the Boltzmann constant, J is the nearest neighbor coupling constant, and T is the physical temperature. Actually, n_i is the number of fluxes at the ith spatial site.

$$\hat{L}_-^j=e^{-i\theta_j},\quad \hat{L}_+^j=e^{i\theta_j},\quad \text{and}\quad \hat{L}_+^j\hat{L}_-^j=1.$$

$\hat{L}_+$ and $\hat{L}_-$ can be identified as the flux generating and flux annihilating operators, respectively.

Using binomial expansion, one gets

$$\prod_i e^{(\beta/2)(L_+^iL_-^{i+1}+L_-^iL_+^{i+1})} = \prod_i \sum_{n=0}^{\alpha}\sum_{k=0}^{n}\left(\frac{\beta}{2}\right)^n \frac{1}{(n-k)!k!}(L_+^iL_-^{i+1})^{n-2k}$$

$$=\prod_i \sum_{\zeta=-\alpha}^{\alpha}\sum_{k=0}^{\alpha}\frac{(\beta/2)^{\zeta+2k}}{k!(\zeta+k)!}(L_+^iL_-^{i+1})^{\zeta}$$

$$=\prod_i \sum_{\zeta=-\alpha}^{\alpha} I_\zeta(\beta)(L_+^iL_-^{i+1})^{\zeta}.$$

So the transfer matrix in Eq. (2.3) can be written as

$$\hat{T}=\hat{T}_0\hat{T}_1, \tag{2.4a}$$

where

$$\hat{T}_0=\prod_i \hat{I}_{n_i}(\beta)[I_0(\beta)]^M \tag{2.4b}$$

(M being the number of links in the one-dimensional chain) and

$$\hat{T}_1=\prod_i\left[1+\frac{I_1}{I_0}(\hat{L}_+^i\hat{L}_-^{i+1}+\hat{L}_-^i\hat{L}_+^{i+1}) + \frac{I_2}{I_0}[(\hat{L}_+^i\hat{L}_-^{i+1})^2+(\hat{L}_-^i\hat{L}_+^{i+1})^2]+\vartheta\left(\frac{I_1}{I_0}\right)^3\right]. \tag{2.4c}$$

The sort of expansion in Eq. (2.4c) is called character expansion [19]. This is more advantageous than the strong-coupling expansion because I_0 is the largest eigenvalue (i.e., larger than I_1, I_2, I_3, etc.) for all values of the argument and therefore the expansion works well even near the phase transition point.

I take x as the perturbative expansion parameter (whose value will be set equal to 1 at the end) for the T_1 operator which may be taken as the perturbation operator with T_0 as the unperturbed one with eigenvalues and eigenkets as follows:

$$\hat{T}_0|\phi_i\rangle=e^{\lambda_i}|\phi_i\rangle \tag{2.5}$$

(λ_i must be calculated).

Let

$$\hat{T}|\psi_i\rangle=e^{k_i}|\psi_i\rangle \tag{2.6}$$

since $\vartheta(I_1/I_0)^2\sim\vartheta(I_2/I_0)$, therefore they compile as the second order term. Now, expansion of $\hat{T}_1$ yields

$$\hat{T}_1=1+x\hat{H}_1+x^2\hat{H}_2+\vartheta(x^3),$$

where

$$\hat{H}_1=\left(\frac{I_1}{I_0}\right)\left(\sum_i (L_+^iL_-^{i+1}+L_-^iL_+^{i+1})\right)$$

and

$$H_2=\left(\frac{I_2}{I_0}\right)\left(\sum[(L_+^iL_-^{i+1})^2+(L_-^iL_+^{i+1})^2]\right) + \frac{1}{2}\left(\frac{I_1}{I_0}\right)^2\left(\sum_i\sum_j (L_+^iL_+^jL_-^{i+1}L_-^{j+1}+L_+^iL_+^{j+1}L_-^jL_-^{i+1}+L_+^{j+1}L_-^jL_+^iL_-^{j+1}+L_+^{i+1}L_+^jL_-^iL_-^{j+1}+L_+^{i+1}L_+^{j+1}L_-^iL_-^j)\right).$$

I also define

$$|\psi_i\rangle=|\phi_i\rangle+x|\psi_i^{(1)}\rangle+x^2|\psi_i^{(2)}\rangle+\vartheta(x^3), \tag{2.7}$$

$$k_i=\lambda_1+xk_i^{(1)}+x^2k_i^{(2)}+\vartheta(x^3). \tag{2.8}$$

Using Rayleigh-Schrödinger perturbation theory, I obtain the perturbed energy states as follows.

Plugging the series values (2.7) and (2.8) into the eigenvalue Eq. (2.6) and taking matrix elements, I get

$$\langle\phi_j|\hat{T}|\psi_i\rangle=\langle\phi_j|e^{k_i}|\psi_i\rangle$$

or

$$\langle\phi_j|\hat{T}_0\hat{T}_1|\psi_i\rangle=\langle\phi_j|e^{(\lambda_i+xk_i^{(1)}+x^2k_i^{(2)}+\cdots)}|\psi_i\rangle,$$

$$\langle\phi_j|\hat{T}_0\hat{T}_1|\psi_i\rangle=e^{\lambda_j}\langle\phi_j|[1+x\hat{H}_1+x^2H_2+\vartheta(x^3)] \times[|\phi_i\rangle+x|\psi_i^{(1)}\rangle+x^2|\psi_i^{(2)}\rangle+\vartheta(x^3)],$$

$$\langle\phi_j|e^{\lambda_i}+xk_i^{(1)}+x^2k_i^{(2)}+\cdots|\psi_i\rangle$$
$$=e^{\lambda_i}\left(1+xk_i^{(1)}+x^2k_i^{(2)}+\frac{x^2}{2}(k_i^{(1)})^2+\vartheta(x^3)\right)$$
$$\times[\delta_{ij}+x\langle\phi_j|\psi_i^{(1)}\rangle+x^2\langle\phi_j|\psi_i^{(2)}\rangle+\vartheta(x^3)].$$

Of course, I can take the normalizing conditions,

$$\langle\phi_i|\psi_i^{(k)}\rangle=0 \quad \text{for all } k.$$

Then, for $i=j$, I have

$$e^{\lambda_i}\left[1+x\langle\phi_i|\hat{H}_1|\phi_i\rangle+x^2\langle\phi_i|\hat{H}_2|\phi_i\rangle+x^2\langle\phi_i|H_1|\psi_i^{(1)}\rangle+\vartheta(x^3)=e^{\lambda_i}\left(1+xk_i^{(1)}+x^2k_i^{(2)}+\frac{x^2}{2}(k_i^{(1)})^2+\vartheta(x^3)\right)\right.$$

where

$$k_i=\langle\phi_1|\hat{H}_1|\phi_i\rangle, \tag{2.9}$$

and

$$k_i^{(2)}=\langle\phi_i|\hat{H}_1|\psi_i^{(1)}\rangle+\langle\phi_i|\hat{H}_2|\phi_i\rangle-\tfrac{1}{2}[\langle\phi_i|\hat{H}_1|\phi_i\rangle]^2. \tag{2.10}$$

And for $i\neq j$, I have

$$e^{\lambda_i}[x\langle\phi_j|\psi_i^{(1)}\rangle+x^2\langle\phi_j|\psi_i^{(2)}\rangle+x\langle\phi_j|\hat{H}_1|\phi_i\rangle+x^2\langle\phi_j|\hat{H}_1|\psi_i^{(1)}\rangle+x^2\langle\phi_j|\hat{H}_2|\phi_i\rangle+\vartheta(x^3)]$$
$$=e^{\lambda_i}[x\langle\phi_j|\psi_i^{(1)}\rangle+x^2\langle\phi_j|\psi_i^{(2)}\rangle+x^2k_i^{(1)}\langle\phi_j|\psi_i^{(1)}\rangle+\vartheta(x^3)]\Rightarrow e^{\lambda_j}[\langle\phi_j|\hat{H}_1|\phi_i\rangle+\langle\phi_j|\psi_i^{(1)}\rangle]=e^{\lambda_i}\langle\phi_j|\psi_i^{(1)}\rangle.$$

So I get

$$|\psi_i^{(1)}\rangle=\sum_{j=1}|\phi_j\rangle\langle\phi_j|\hat{H}_1|\phi_i\rangle\frac{1}{e^{\lambda_i-\lambda_j}-1} \tag{2.11a}$$

and

$$k_i^{(2)}=\langle\phi_i|\hat{H}_2|\phi_i\rangle-\frac{1}{2}[\langle\phi_i|\hat{H}_1|\phi_i\rangle|]^2+\sum_{j=i}\frac{|\langle\phi_i|\hat{H}_1|\phi_j\rangle|^2}{e^{\lambda_i-\lambda_j}-1}. \tag{2.11b}$$

Below I calculate the eigenvalues of different order.

The unperturbed values follow.

(i) Ground state. The ground-state eigenket of $\hat{T}_0$ is

$$|\phi_0\rangle=|0,0,\ldots\rangle$$

$$\therefore\hat{T}_0|\phi_0\rangle=[I_0(\beta)]^{2M}|\phi_0\rangle=e^{\lambda_0}|\phi_0\rangle\rightarrow\lambda_0=2M\ \ln[I_0(\beta)]. \tag{2.12a}$$

(ii) First excited state. The eigenket is

$$\phi_k'=\frac{1}{\sqrt{M}}\sum_{r=1}^{M}e^{i\vec{k}\cdot\vec{r}}|0,0,\ldots,1_r,0,\ldots\rangle,$$

where k is the momentum of the ket in momentum space, $\vec{r}$ is the position vector of the links,

$$T_0|\phi_k^{(1)}\rangle=[I_0(\beta)]^{2M-1}I_1(\beta)|\phi_k^{(1)}\rangle=e^{\lambda_1}|\phi_k^{(1)}\rangle$$
$$\Rightarrow\lambda_1=\ln[\{I_0(\beta)\}^{2M-1}I_1(\beta)]. \tag{2.12b}$$

Now the perturbed values follow.

(i) First order. (a) Ground state,

$$k_0^{(1)}=\langle\phi_0|\hat{H}_1|\phi_0\rangle=0. \tag{2.13a}$$

(b) First excited state,

$$k_{k:1}^{(1)}=\frac{1}{\sqrt{M}}\langle\phi_k^{(1)}|\left(\frac{I_1}{I_0}\right)\sum_i(L_+^iL_-^{i+1}+L_-^iL_+^{i+1})$$
$$\times\sum e^{i\vec{k}\cdot\vec{r}}L_+^r|\phi_0\rangle$$
$$=2\cos k\left(\frac{I_1}{I_0}\right). \tag{2.13b}$$

(i) *Second order.* (a) Ground state,

$$\langle\phi_0|\hat{H}_2|\phi_0\rangle=0.$$

In $\langle\phi_0|\hat{H}_1|\phi_j\rangle$, the surviving matrix elements are of

$$|\phi_j\rangle=\frac{1}{\sqrt{M}}\sum_r e^{i\vec{k}\cdot(\vec{r}+\vec{r}+1)}|0,\ldots,1_r,-1_{r+1},0,\ldots\rangle$$

and

$$|\tilde{\phi}_j\rangle=\frac{1}{\sqrt{M}}\sum_r e^{i\vec{k}\cdot(\mathbf{r}+\mathbf{r}+1)}|0,\ldots,1_r,-1_{r+1},0,\ldots\rangle$$
$$=\frac{2MI_1^2}{I_0^2-I_1^2}\left(\frac{I_1}{I_0}\right)^2. \tag{2.14a}$$

(b) First excited state,

$$\langle \phi_k^{(1)}|H_1|\phi_k^{(1)}\rangle = 2\cos k\left(\frac{I_1}{I_0}\right),$$

$$H_1|\phi_{k=0}^{\langle 1\rangle}\rangle = \frac{1}{\sqrt{M}}\left(\frac{I_1}{I_0}\right)\left[\left(\sum_i (L_+^i L_-^{i+1} + L_-^i L_+^{i+1})\right) + \sum_r L_+^r\right]|\phi_0\rangle$$

$$= \frac{1}{\sqrt{M}}\left(\frac{I_1}{I_0}\right)\left(\sum_i [(L_+^i)^2 L_-^{i+1} + L_-^{i-1}(L_+^i)^2 + 2L_+^{i-1}L_-^i L_+^{i+1} + (M-3)(L_+^i L_-^{i+1} + L_-^i L_+^{i+1})]L_+^i\right)^* |\phi_0\rangle$$

$$\rightarrow \sum_{j\neq 1} \frac{|\langle \phi_{k=0}^{\langle 1\rangle}|\hat{H}_1|\phi_j\rangle|^2}{e^{\lambda_1-\lambda_j}-1}$$

$$= \left(\frac{I_1}{I_0}\right)^2\left(2\frac{I_2}{I_0-I_2} + 4\frac{I_1^2}{I_0^2-I_1^2} + 2(M-3)\frac{I_1^2}{I_0^2-I_1^2}\right). \tag{2.14b}$$

The $\langle \phi_k^{\langle 1\rangle}|\hat{H}_2|\phi_k^{\langle 1\rangle}\rangle$ term is calculated as

$$H_2|\phi_k^{(1)}\rangle = \frac{1}{\sqrt{M}}\left[\left(\frac{I_2}{I_0}\right)\sum_i [(L_+^i L_-^{i+1})^2 + (L_-^i L_+^{i+1})^2]\right.$$

$$+\frac{1}{2}\left(\frac{I_1}{I_0}\right)^2 \sum_i \sum_{j\atop i\neq j} (L_+^i L_+^j L_-^{i+1} L_-^{j+1}$$

$$+ L_+^i L_+^{j+1} L_-^j L_-^{i+1} + L_+^{i+1} L_+^j L_-^i L_-^{j+1}$$

$$\left. + L_+^{i+1} L_+^{j+1} L_-^i L_-^j)\right]\sum_r e^{i\vec{k}\cdot\vec{r}} L_+^r|\phi_0\rangle.$$

Some of the above matrix elements vanish. The surviving terms are

$$\frac{1}{\sqrt{M}}\left(\frac{I_1}{I_0}\right)^2 \sum L_+^{r-2} e^{i\vec{k}\cdot\vec{r}}|\phi_0\rangle$$

and

$$\frac{1}{\sqrt{M}}\left(\frac{I_1}{I_0}\right)^2 \sum_r^r I_+^{r+2} e^{i\vec{k}\cdot\vec{r}}|\phi_0\rangle.$$

Hence

$$\langle \phi_k^{\langle 1\rangle}|\hat{H}_2|\phi_k^{\langle 1\rangle}\rangle = 2\cos(2k)\left(\frac{I_1}{I_0}\right)^2 \tag{2.14c}$$

$$\therefore k_1^{(2)} = \left(2\cos(2k) - 2\cos^2 k + \frac{2I_2}{I_0-I_2} + \frac{2I_1^2}{I_0^2-I_1^2} + 2(M-3)\frac{I_1^2}{I_0^2-I_1^2}\right)\left(\frac{I_1}{I_0}\right)^2. \tag{2.14d}$$

Thus I get the difference between eigenvalues of the first excited state and the ground state as

$$\lambda_1 - \lambda_0 = \ln\left(\frac{I_1}{I_0}\right) \quad \text{(unperturbed)}, \tag{2.15a}$$

$$k_1^{(1)} - k_0^{(1)} = 2\cos k\left(\frac{I_1}{I_0}\right) \quad \text{(first order)}, \tag{2.15b}$$

$$k_1^{(2)} - k_0^{(2)} = \left(2\cos(2k) - 2\cos^2 k + \frac{2I_2}{I_0-I_2} - \frac{4I_1^2}{I_0^2-I_1^2}\right) \times \left(\frac{I_1}{I_0}\right)^2 \quad \text{(second order)}. \tag{2.15c}$$

Hence the mass gap at zero momentum value is given by

$$\Delta_{k=0}^{(\beta)} = k_1 - k_0 = \ln\left(\frac{I_1}{I_0}\right) + 2\left(\frac{I_1}{I_0}\right) + \left(\frac{I_1}{I_0}\right)^2\left(\frac{2I_2}{I_0-I_2} - \frac{4I_1^2}{I_0^2-I_1^2}\right). \tag{2.16}$$

Since free energy is the total energy of the ground state, it is given by

$$F = k_0 = M\left[\ln(I_0)^2 + \frac{2I_1^2}{I_0^2-I_1^2}\left(\frac{I_1}{I_0}\right)^2\right], \tag{2.17a}$$

and free energy per link is

$$f(\beta) = \frac{F}{M} = \ln[I_0(\beta)]^2 + \frac{2I_1^2}{I_0^2-I_1^2}\left(\frac{I_1}{I_0}\right)^2. \tag{2.17b}$$

The numerical values of $\Delta(\beta)$ and $f(\beta)$ have been listed using the above theoretical calculations in Table II in Sec. IV for β=0.10–1.00 and compared with independently computed values.

To show rapid convergence of the character expansion series given by Eq. (2.4c) and hence of the expression given by Eq. (2.16), I plot a graph for $\Delta(\beta)$ considering up to first order expansion and second order expansion separately in Fig. 1. The data for Fig. 1 have been calculated and listed in Table I.

III. METHOD OF COMPUTATION

A master program was written based on the Neumann-Ulam method [20]. This method is very efficient and devoid of various stochastic errors when applied on the transfer ma-

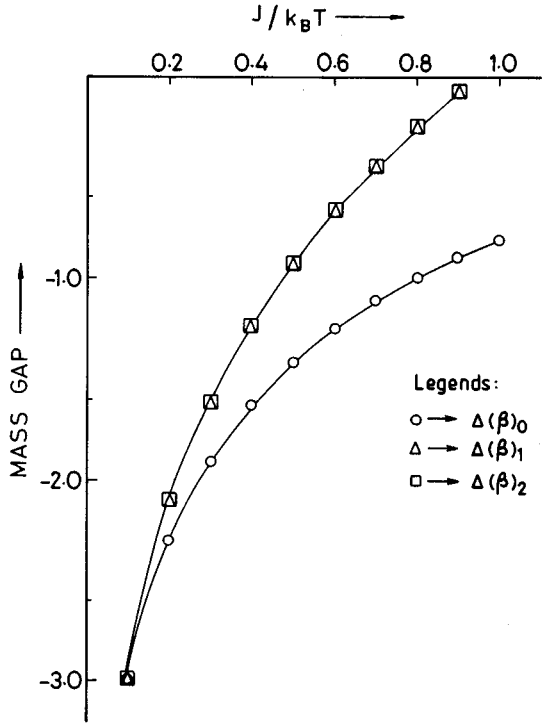

FIG. 1. Data from Table I have been plotted. We clearly see that curves for $\Delta(\beta)_1$ and $\Delta(\beta)_2$ are overlapping, convincing us of convergence even at second order of the character expansion.

trix formalism. The basic idea is like this: It involves a random walk in the space of basis states. At each step in the walk, one applies a projection operator to the current basis state in some stochastic fashion. Thus it makes transition to a new state or states. The number of times each basis state is visited during the walk is proportional to its amplitude in the ground-state wave function. This of course is multiplied by some weight function. In our problem, we apply this method as follows.

The transfer matrix operator $\hat{T}$ takes the linear link system from one time slice to another.

If $\hat{T}|\psi_i\rangle=\lambda_i|\psi_i\rangle$ then after L successive operations of the $\hat{T}$ operator on a general configuration state of ensemble, I get

$$\hat{T}^L|\phi\rangle=\sum_i C_i(\lambda_i)^L|\psi_i\rangle. \tag{3.1}$$

I can justly assume that $\max\lambda_i=\lambda_0$; then if $C_0\neq 0$ and the ground state is nondegenerate, I eventually get

$$\hat{T}^L|\phi\rangle \xrightarrow[L\gg 1]{} C_0(\lambda_0)^L|\psi_0\rangle. \tag{3.2}$$

This means that if $|\phi\rangle$ is such a wave function of the ensemble in which the total flux (summing over all the lattice sites) is zero, then after a large number of passes, I will arrive at the true ground state of the system.

But, if I start with an ensemble wave function $|\hat{\phi}\rangle$ which has altogether one unit of flux, thus making it orthogonal to the ground state, then eventually, after a large number of passes, I shall reach the first excited state, i.e.,

$$\hat{T}|\hat{\phi}\rangle \xrightarrow[L\gg 1]{} C_1(\lambda_1)^L|\psi_1\rangle. \tag{3.3}$$

The matrix elements of $\hat{T}$ can be written as

$$T_{n'n}\rightarrow\frac{T_{n'n}}{\Sigma_{n',n}T_{n'n}}R_n=P_{n'n}R_n, \tag{3.4}$$

where $P_{n'n}$ can be regarded as the probability of random walk from state n to n' and R_n is the residue or score (which has previously been regarded as some kind of weight function).

Of course, $\Sigma_{n,n'}P_{nn'}=1$.

Thus the general algorithm can be briefly stated below.

(1) Start out with an ensemble of states.
(2) Update them with probabilities $P_{n'n}$ by simulating random numbers and register the score R_n for each element in the ensemble.
(3) Regard R_n as the weight of the corresponding element of the ensemble.
(4) Making an integer out of $R_{n'}$ statistically branch out the corresponding state that many times.
(5) Since, due to branching out, the size of the ensemble changes, one has to ''renormalize'' the states after each pass.

TABLE I. Here β is the inverse temperature, $\Delta(\beta)_0$ is the zeroth order term in Eq. (2.16) given by expression (2.15a); $\Delta(\beta)_1$ is the zeroth plus first order term in Eq. (2.16) given by Eq. (2.15b) included with Eq. (2.15a) and $\Delta(\beta)_2$ is the zeroth plus first plus second order term in Eq. (2.16) given by Eq. (2.15c) included.

β	$\Delta(\beta)_0$	$\Delta(\beta)_1$	$\Delta(\beta)_2$
0.1	−2.996	−2.986	−2.897
0.2	−2.303	−2.103	−2.106
0.3	−1.909	−1.612	−1.605
0.4	−1.628	−1.236	−1.226
0.5	−1.417	−0.932	−0.917
0.6	−1.247	−0.672	−0.657
0.7	−1.108	−0.447	−0.435
0.8	−0.991	−0.249	−0.245
0.9	−0.892	−0.073	−0.083
1.0	−0.807	+0.086	−0.052

IV. RESULTS

In Table II I have furnished the theoretically calculated values of mass gap $[M(\beta)_{\text{th}}]$ and free energy per link $[f(\beta)]_{\text{th}}$. I have also given computed values of mass gap $[M(\beta)_c]$ and free energy per link $[f(\beta)_c]$. $M(\beta)_{\text{th}}$ is obtained from Eq. (2.16) and $f(\beta)_{\text{th}}$ is obtained from Eq. (2.17b).

One can see from Table II that both $M(\beta)_{\text{th}}$ and $M(\beta)_c$ tend to drop down to zero for $\beta\sim 1.0$. Also, the values are comparable to one another although those for free energy tally much better than the mass gap. This difference can be attributed to the calculation of free energy in the first excited state. There, some computational error might have crept in. The computed values also show that as the transition point is approached, the fluctuation in the values increases significantly. This is because near the transition point correlation

TABLE II. β is the inverse temperature. In the computation part, the statistics that have been used are number of spatial links equals 50, number of ensembles equals 1000, and number of time iterations (i.e., passes) equals 200.

	Calculated value		Computed value	
β	Mass gap $M(\beta)_{\text{th}}$	Free energy per link $f(\beta)_{\text{th}}$	Mass gap $M(\beta)_c$	Free energy per link $f(\beta)_c$
0.1	−2.897	0.005 01	2.888 (6)	0.004 89 (3)
0.2	−2.106	0.020 1	−2.090 (10)	0.020 1 (1)
0.3	−1.605	0.045 7	−1.592 (12)	0.045 1 (2)
0.4	−1.226	0.082 3	−1.222 (4)	0.081 9 (3)
0.5	−0.917	0.130	−0.926 (5)	0.128 (1)
0.6	−0.657	0.191	−0.635 (18)	0.186 (1)
0.7	−0.435	0.264	−0.361 (42)	0.256 (2)
0.8	−0.245	0.352	−0.165 (43)	0.336 (1)
0.9	−0.083	0.454	−0.192 (95)	0.444 (1)
1.0	−0.052	0.571	−0.096 (30)	0.573 (1)

between different lattice sites increases and more and more vortex-antivortex pairs form, thereby affecting the result.

Taking the data of $M(\beta)_{\text{th}}$ and $M(\beta)_c$ from Table I, I have plotted them in a graph to see what is the critical value of β, i.e., for which value of β, they become zero. It is found that both can be extrapolated to the value of $\beta_c=1.112$. Taking this value of β_c as a constant parameter, I have fitted the following two functions by least squares method to find other parameters of the function.

(a) For Kosterlitz-Thouless expression,

$$M_1(\beta)=C\ \exp\left(-\frac{B}{\sqrt{|\beta_c-\beta|}}\right). \tag{4.1}$$

(b) For algebraic divergence expression,

$$M_2(\beta)=A|\beta_c-\beta|^{\nu}. \tag{4.2}$$

It is found that from Eq. (4.1)

$$\beta_c=1.112,$$

$$C=-10.496,$$

$$B=1.858,$$

and from Eq. (4.2)

$$\beta_c=1.112,$$

$$A=-2.102,$$

$$\nu=1.674.$$

A full graph has been plotted with $M(\beta)_{\text{th}}$, $M(\beta)_c$, $M_1(\beta)$, and $M_2(\beta)$ versus β for $0.1\leqslant\beta\leqslant1.0$ in Fig. 2. This graph clearly shows a much better fit of Eq. (4.2) in the algebraic divergence rather than the Kosterlitz-Thouless type.

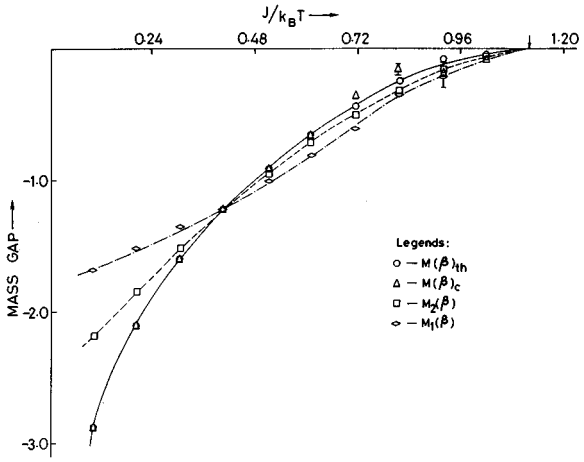

FIG. 2. Proximity of fitted curves to the computed curve $M(\beta)_c$. Here $M(\beta)_{\text{th}}$ is the calculated curve; $M_2(\beta)$ is the algebraic divergence fit and $M_1(\beta)$ is the KT type exponential fit to the observed data points. Obviously $M_2(\beta)$ is much better fit to $M(\beta)_c$ than $M_1(\beta)$.

V. DISCUSSION OF RESULTS

In my work, I find that towards the high-temperature side, the divergence of correlation follows an algebraic expression which contradicts the Kosterlitz-Thouless prediction. The value of ν has been obtained to be 1.674, which is far from the classical value of $\frac{1}{2}$. The value of critical temperature has been obtained to be $k_BT_c/J=0.899$.

Much work has been done in the computation of the planar model. Tobochnik and Chester [14] have used Metropolis Monte Carlo techniques to verify KT type transition. They have obtained the value of critical temperature $k_BT_c/J=0.89$. Shugard *et al.* [22], using a simulation of the roughening model which maps onto the planar model, find $k_BT_c/J=0.90$. McMillan [23] finds $k_BT_c/J=0.90\pm0.02$ in his simulation of a 1024 spin lattice.

Of the more recent results we have observed, Janke and Nather [16] have employed the 2D isotropic planar model to justify KT transition. They have used Villain's formulation of the Monte Carlo simulation to conclude an exponential divergence of KT transition with χ^2 estimate of $k_BT_c/J\simeq0.752\pm0.005$. A heavy computational load of work in this field has been due to Gupta, Delapp, and Batrouni [17] which again confirms a KT type transition and not a power-law divergence in the planar model. Their result is $k_BT_c/J\sim0.898\pm0.002$. In 1989, one paper by Biferale and Petronzio [18] used real space renormalization group computation to support again the KT type transition and the obtained value of $k_BT_c/J\sim0.899\pm0.002$.

Only one work so far by Seiler *et al.* [25] has challenged the KT type exponential divergence and has produced results in support of algebraic divergence of correlation length. They have used a high precision numerical study of the $Z(10)$ clock model which is a discrete version of the 2D planar spin model. Their value of $k_BT_c/J\sim0.990(10)$ for algebraic divergence and $k_BT_c/J\sim0.746$ for exponential divergence with a much higher χ^2 degree of freedom.

VI. CONCLUSION

I have used an independent approach in both theoretical calculation and the computation of the mass gap. In calcula-

tion, character expansion yielded more advantage over the usual strong-coupling expansion, as has been pointed out earlier. In computation, the Ulam-Neumann stochastic method has been employed which certainly is efficient as the close proximity between calculation and computed values show. But my results contradict most of the previous work in this area regarding the nature of divergence of the correlation length towards the high-temperature side of the critical point. Of course my results have obtained support from one standard paper, e.g., Seiler *et al.* [24]. The value of critical temperature though has been close to that of almost all these works. Whatever errors that have crept in in the value of critical temperature and the value of ν are because of insufficient computational accuracy.

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