PHYSICAL REVIEW B VOLUME 38, NUMBER 13 1 NOVEMBER 1988

Rapid Communications

The Rapid Communications section is intended for the accelerated publication of important new results. Since manuscripts submitted to this section are given priority treatment both in the editorial office and in production, authors should explain in their submittal letter why the work justifies this special handling. A Rapid Communication should be no longer than 3½ printed pages and must be accompanied by an abstract. Page proofs are sent to authors, but, because of the accelerated schedule, publication is not delayed for receipt of corrections unless requested by the author or noted by the editor.

Monte Carlo simulation of the $1/n^2$ plane rotator chain

R. Brown and E. Šimánek
University of California, Riverside, Riverside, California 92521
(Received 22 June 1988)

We report Monte Carlo simulation results for the susceptibility and specific heat of the one-dimensional plane rotator system with $1/n^2$ interaction. The data confirm the previously conjectured transition to a phase with infinite susceptibility. For the equivalent model of a tunnel junction, the Monte Carlo transition temperature implies that a transition from activated to metallic behavior takes place when the normal conductance of the junction exceeds $\hbar/2\pi e^2 = 0.65$ kΩ.

It is well known that long-range attractive interactions can induce critical behavior in low-dimensional spin systems.[1–5] For example, it has been proven rigorously[1] that the one-dimensional Ising chain with a power-law interaction $(1/n)^{1+\sigma}$ exhibits a phase transition for $0<\sigma<1$. The borderline case of $\sigma=1$ has received a particular attention because of its relation to the Kondo problem.[6] The Monte Carlo study[4] of the $1/n^2$ Ising-spin chain confirms the existence of a transition with a finite discontinuity of the magnetization predicted in previous theoretical works.[2,6] Relatively little attention has been given to Heisenberg or planar-rotator systems with long-range interactions in one dimensions. Using the classical version of the Bogoliubov inequality, derived by Mermin and Wagner,[7] Joyce[8] has proven rigorously that the one-dimensional isotropic Heisenberg model cannot be ferromagnetic for $\sigma \geq 1$. The one-dimensional planar-rotator model with $1/n^2$ interaction has recently received attention through its relation to the problem of mesoscopic tunnel junctions.[9] Using the functional-integral formulation of Ben-Jacob, Mottola, and Schön[10] we have pointed out[9] that the effective action of the junction is, at $T=0$, equivalent to the Hamiltonian of the one-dimensional planar-rotor model with $1/n^2$ interaction. Treating the action in Ref. 10 in the self-consistent harmonic approximation we have calculated the effective conductance of the tunnel junction as a function of nominal tunnel conductance.[9] When $T\rightarrow 0$, the effective dc conductance shows a precipitous transition from the activated to the ohmic regime when the nominal tunnel conductance exceeds a critical value of order $e^2/\hbar$. Since the effective dc conductance is proportional to an integral of the phase correlator (over imaginary time) and since the nominal tunnel conductance corresponds to the temperature of the $1/n^2$ model, the numerical results of Ref. 9 indicate a possibility of some kind of a phase transition in the $1/n^2$ planar rotator chain. Subsequently, one of us[11] has applied the Mermin inequality[12] to establish rigorously the absence of ferromagnetic order in this model. Consequently, the nature of the phase transition in the planar-rotator model is quite different from the $1/n^2$ Ising spin chain. Employing the low-temperature (harmonic) approximation, it has been shown that the spin correlation function shows a power-law decay and the susceptibility diverges below a critical temperature $T_0 = \pi^2 J_0/k_B$, where J_0 is the coupling constant.[11]

Both of these properties are reminiscent of the behavior of the two-dimensional planar-rotator model with short-range interactions.[13] According to Kosterlitz and Thouless[14] the low-temperature phase of the latter model is characterized by a power-law decay of the correlation function modified by the presence of pairs of tightly bound pairs of topological defects (vortices) of opposite sign. At the transition temperature the vortices unbind and create a new phase in which the correlations decay exponentially. It has been conjectured[11] that an analogous crossover in the decay law takes place in the spin correlation of the $1/n^2$ planar-rotator chain. The transition to ohmic conduction shown in our recent self-consistent harmonic calculations on tunnel junction[9] and the divergence of the susceptibility derived in the low-temperature approximation[11] provided initial support of this conjecture. Theoretical progress in this model is somewhat hampered by the fact that it does not possess a topologically stable defect. In fact, if the argument of Toulouse and Kléman[15] is applied to the ($d=1$, $n=2$) case, n being the order-parameter dimensionality, we find that the defect in the planar-rotator chain has an anomalous dimensionality $d-n=-1$. This is in contrast to the $1/n^2$ Ising-spin chain ($d=1$, $n=1$) and the two-dimensional Kosterlitz-

 © 1988 The American Physical Society

Thouless model ($d=2$, $n=2$) both of which involve zero-dimensional defects. The phase transition in the latter models can be regarded as a condensation of such stable topological defects for which a renormalization-group analysis is available.[6,16]

In the absence of a similar type of analysis for the $1/n^2$ planar-rotator chain, it seems natural to investigate the phase transition in this model by the Monte Carlo simulation method. In this paper, we report calculations of the susceptibility and the specific heat for this model using a Monte Carlo technique. The calculation involves a finite number N of rotators with the periodic boundary conditions described by a Hamiltonian H with periodic interaction $J(n-n')$:

$$\beta H = -\sum_{n,n'} J(n-n')\cos(\theta_n - \theta_{n'}) , \tag{1}$$

where

$$J(n) = \frac{J_0}{k_B T}\left(\frac{\pi/N}{\sin[(\pi/N)n]}\right)^2 . \tag{2}$$

We deviated from the traditional Metropolis Monte Carlo procedure[17] in that the angles θ_n were calculated directly from the probability distribution. It is easy to show that the probability distribution for angle θ_n of rotator n is *proportional* to

$$p(\theta_n) = \exp\{a[\cos(\theta_n - \phi) - 1]\} , \tag{3}$$

where

$$a = (E_{\sin}^2 + E_{\cos}^2)^{1/2} , \qquad \phi = \tan^{-1}\left(\frac{E_{\sin}}{E_{\cos}}\right) , \tag{4}$$

and

$$E_{\sin} = \sum_{n'} J(n-n')\sin(\theta_{n'}) , \qquad E_{\cos} = \sum_{n'} J(n-n')\cos(\theta_{n'}) . \tag{5}$$

The subtraction of one in Eq. (3) was needed to keep the exponent small for calculation purposes. Random deviates θ_n of the distribution (3) were calculated directly by the *rejection method*,[18] where the comparison function is given by

$$f(\theta_n) = \begin{cases} 1 & \text{for } a<1 , \\ 1/[1+0.5a(\theta_n-\phi)^2] & \text{for } a \geq 1 . \end{cases} \tag{6}$$

The "bell-shaped" nature of the Lorentzian distribution in Eq. (6) makes it an excellent comparison function for Eq. (3) when $a \geq 1$. It gives a rejection ratio (ratio of number of rejected points to the total) of about 10–42% for $a = 1-\infty$. Reference 18 also gives a very fast algorithm for calculating random deviates of the Lorentzian distribution. The comparison function for $a<1$ gives a rejection ratio of 0% to 53% for $a=0$ to 1.

Monte Carlo runs were made for $N=10$, 100, and 1000 rotators. The initial configuration was set to $\theta_n=0$ for all n. The system was then heated from $k_BT/J_0=0.1$ to 1.5 in steps of 0.1. Each point was made with 3000 passes; the first 1000 passes were used for equilibration followed by 2000 passes for calculating averages. A test run for 10 and 100 rotators indicated that 10000 passes for averaging gave no significant change to the curves, other than the expected smoothing. Cooling runs for 10 and 100 rotators with random initial configurations agreed with the heating runs. The 1000 passes for equilibration were found to be more than sufficient.

In Fig. 1 we plot the reduced susceptibility χ defined as

$$\chi = \frac{\langle M^2\rangle}{N^2} , \tag{7}$$

where M is the magnetization of the chain. The data confirm the crossover from the finite susceptibility to a diverging one as the temperature decreases through the transition temperature. In fact the temperature dependence of χ for N large is qualitatively similar to that for the Kosterlitz-Thouless transition.[19–21] According to the theory of this transition[16] the susceptibility diverges as T approaches T_c from above as $\exp[1.5/(T-T_c)^{1/2}]$. In this case the transition temperature can be determined by fitting this function to the Monte Carlo data.[19] At present there is no theory of the $1/n^2$ planar-rotator chain for $T<T_c$ and thus we estimate T_c qualitatively from the position of the precipitous onset of χ with decreasing temperature. For $N=1000$ this yields $T_c \sim (0.8\pm 0.1)J_0/k_B$. The true transition to infinite susceptibility for $N=\infty$ is probably close to this value as suggested by the specific-heat data discussed below.

The specific heat was obtained by differentiation of the energy $\langle E\rangle$ with respect to the temperature. Another method, in which the specific heat was obtained from the energy fluctuations $\langle E^2\rangle - \langle E\rangle^2$, gave the same results, but with slightly larger error. The plots of the specific heat for the three different values of N are shown in Fig. 2. The peak of the specific heat exhibits an interesting behavior as a function of N. The temperature $T_p(N)$ of the maximum *decreases* with N and tends to level off to a constant value for $N>100$. It should be pointed out that a

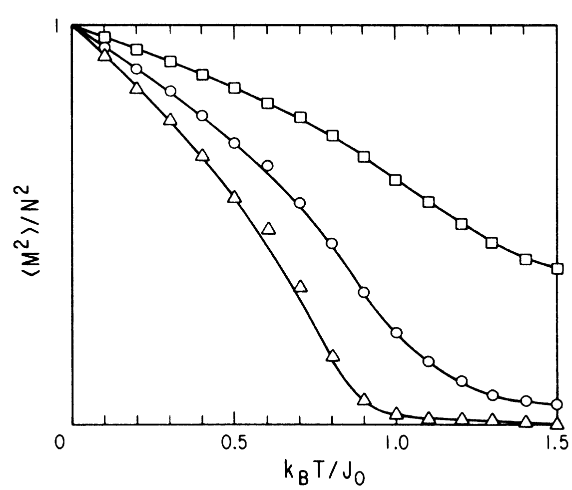

FIG. 1. The reduced susceptibility $\chi = \langle M^2\rangle/N^2$ vs temperature for different lattice sizes. □, ○, and △ denote the susceptibility for $N=10$, 100, and 1000, respectively. The solid lines are a guide to the eye.

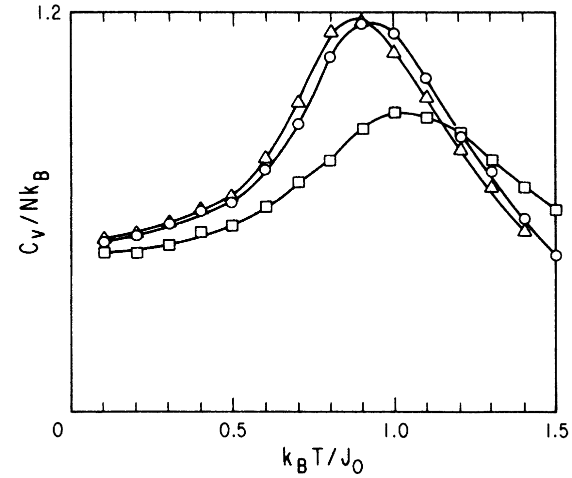

FIG. 2. The temperature and size dependence of specific heat. □, ○, and △ denote the specific heat for $N=10$, 100, and 1000, respectively. The solid lines are a guide to the eye.

decrease of $T_p(N)$ with N is also exhibited in the data of Ref. 4 for the $1/n^2$ Ising-spin chain, although less pronounced. Similar to the latter work, the maximum of the specific heat $C_v^{\max}(N)$ also increases with N but, as seen in Fig. 2, a saturation of the specific-heat peak takes place for $N>100$. Once saturation is reached $C_v^{\max}(N)$ becomes independent of N. It should be noted that the simulations of the Kosterlitz-Thouless model exhibit such an independence for all values of N considered. The N dependence of the specific-heat data obtained in the present work and also in the $1/n^2$ Ising-spin model is presumably due to the long-range interactions.

It should also be noted that even for the size $N=1000$ the specific heat is rounded. This is similar to the nondivergent specific heat of the Kosterlitz-Thouless transition. The rounding of the specific heat is not inconsistent with the divergence of the susceptibility since the energy, involving local correlations, is given by integration of fluctuations over all length scales which tends to wash out the diverging contribution at the infinite scale.

The transition temperature $T_p(N)$ for $N=1000$ is $(0.9\pm0.1)J_0/k_B$ and is presumably close to the transition temperature in the $N=\infty$ chain. In the Monte Carlo simulation of the Kosterlitz-Thouless transition,[19] the specific-heat peak is about 15% above the susceptibility transition. In view of this, the present estimate of susceptibility transition at $T_c\sim(0.8\pm0.1)J_0/k_B$ seems consistent with this trend.

It should be noted that the Gaussian approximation of Ref. 11, yields a transition temperature $T_0=\pi^2J_0/k_B$ which is an order of magnitude larger than the present Monte Carlo value. This leads to interesting implications for the transition to ohmic conduction in tunnel junctions. Comparing the partition function for the model (1) with the path integral for the junction partition function, the transition temperature T_c is found to be related to the critical value of nominal junction conductance R_n^{-1} as follows:[11]

$$\frac{\hbar}{2\pi e^2R_n}=\frac{J_0}{k_BT_c}\,. \tag{8}$$

For $T_c=T_0=\pi^2J_0/k_B$, as given by Ref. 11, the critical resistance is, according to Eq. (8), equal to $R_N=\pi\hbar/2e^2$. This is close to the estimate by Imry and Strongin[22] predicting a metallic behavior in a single tunnel junction if its resistance falls below $\hbar/e^2\simeq4.1$ kΩ. On the other hand, from the present Monte Carlo work we deduce $T_c\simeq J_0/k_B$ which yields for the critical resistance a considerably lower value of $\hbar/2\pi e^2\simeq0.65$ kΩ. The latter value is not inconsistent with some data on the normal-sheet film resistance at which the normal-state activation energy vanishes.[23] In contrast with the onset of metallic behavior in normal junctions, the onset of phase coherence in a superconducting junction seems to take place at the universal resistance $R_N=\hbar/e^2$, the latter value being relatively firmly established both theoretically[24] and experimentally.[25] Hence the present work suggests that a superconducting coherence may take place in junctions and their arrays which would, in the absence of local superconductivity, be in an insulating state.

While the present work was in progress we were made aware of unpublished work by Romano[26] describing a Monte Carlo simulation of the $1/n^2$ chain of planar rotators. The latter work confines itself to temperatures above the transition temperature which is found to be $1.15J_0/k_B$. The saturation of the specific-heat data at $N\geq1000$ observed by Romano[26] is also in agreement with the present work.

We thank Harold Cooper and H. M. Jaeger for valuable discussions, S. Romano for sending us his results before publication, and D. Scharffenberg for computational assistance. The computations were done on a VAX 8700, computer time was generously allocated by the Academic Computing Center at the University of California, Riverside.

[1]F. Dyson, Commun. Math. Phys. **12**, 91 (1969).
[2]D. J. Thouless, Phys. Rev. **187**, 732 (1969).
[3]M. Fisher, S. Ma, and B. Nickel, Phys. Rev. Lett. **29**, 917 (1972).
[4]J. Battacharjee, S. Chakravarty, J. L. Richardson, and D. J. Scalapino, Phys. Rev. B **24**, 3862 (1980).
[5]H. Kunz and C. E. Pfister, Commun. Math. Phys. **46**, 245 (1976).
[6]P. W. Anderson and G. Yuval, J. Phys. C **4**, 607 (1971).
[7]N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).
[8]G. S. Joyce, J. Phys. C **2**, 1531 (1969).
[9]R. Brown and E. Šimánek, Phys. Rev. B **34**, 2957 (1986).
[10]E. Ben-Jacob, E. Mottola, and G. Schön, Phys. Rev. Lett. **51**, 2064 (1983).
[11]E. Šimánek, Phys. Lett. A **119**, 477 (1987).
[12]N. D. Mermin, J. Math. Phys. **8**, 1061 (1967).
[13]F. J. Wegner, Z. Phys. **206**, 465 (1967).

[14]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

[15]G. Toulous and M. Kléman, J. Phys. Lett. (Paris) **37**, L149 (1976).

[16]J. M. Kosterlitz, J. Phys. **7**, 1046 (1974).

[17]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).

[18]W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes: The Art of Scientific Computing* (Cambridge Univ. Press, Cambridge, 1986).

[19]Jan Tobochnik and G. V. Chester, Phys. Rev. B **20**, 3761 (1979).

[20]S. Miyashita, H. Nishimori, A. Kuroda, and M. Suzuki, Prog. Theor. Phys. (Kyoto) **29**, 341 (1963).

[21]The spread of the χ curves, seen in Fig. 1 on changing N, is largely removed if one plots $\langle M^2\rangle/N$ vs T as it is done in Ref. 20.

[22]Y. Imry and M. Strongin, Phys. Rev. B **24**, 6353 (1981).

[23]H. M. Jaeger (private communication).

[24]M. P. A. Fisher, Phys. Rev. Lett. **57**, 885 (1986).

[25]B. G. Orr, H. M. Jaeger, and A. M. Goldman, Phys. Rev. B **32**, 7586 (1985).

[26]S. Romano (unpublished).