Some properties of a one-dimensional Ising chain with an inverse-square interaction

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We report some new results obtained for the thermodynamic properties and correlation functions of the one-dimensional Ising model with an inverse-square interaction between the spins. Using the Anderson and Yuval renormalization-group equations, we evaluate the correlation function and magnetic susceptibility for $T < T_c$. Monte Carlo data for the magnetization, specific heat, and spin-spin correlation function have also been obtained.

The one-dimensional Ising chain with a ferromagnetic inverse-square interaction has been the subject of a wide variety of analysis.[1-3] Here we report some results of an analytic evaluation of correlation functions and the susceptibility for $T < T_c$, based on the renormalization-group equations of Anderson and Yuval[2] and Kosterlitz,[3] and some results obtained from a Monte Carlo investigation of the system. The Monte Carlo calculations which are reliable at low temperatures complement the renormalization-group results which are correct just below T_c giving a full description of the ordered phase. We find from our analytic work that for $T < T_c$, the order-parameter correlation function $G(r) = \langle s(r)s(0)\rangle - \langle s\rangle^2$ decays as the power law $4(|t|)^{1/2}r^{-4(|t|)^{1/2}}$ where $t = (T - T_c)/T_c$. As $T \to T_c$ from below this goes over to $(\ln r)^{-1}$ giving rise to an unusual behavior in the susceptibility. It is infinite in the range $-\frac{1}{16} < t < 0$ and becomes finite again for $t < -\frac{1}{16}$. Above T_c the correlation length ξ has the form $e^{\pi/2\sqrt{t}}$ for t close to zero and crosses over to a Gaussian behavior for $t \gg 1$. The susceptibility scales as the correlation length.

The Monte Carlo study shows, in agreement with the work of Anderson and Yuval,[2] that a transition with a finite discontinuity in the magnetization takes place very close to the transition temperature $T_c \cong 0.79$ (see Fig. 1). At this point the susceptibility of an infinite system does indeed diverge. The accuracy of our Monte Carlo work is not sufficient to verify that the susceptibility remains infinite over the range $-\frac{1}{16} \leq t \leq 0$. However, it definitely shows that the susceptibility is finite for $t \lesssim -0.16$ and for $t \gtrsim 0.05$, where T_c has been taken to be 0.79. The Monte Carlo correlation functions (Fig. 2) fall off very slowly for $T \leq T_c$ and are in qualitative agreement with a r^{-2} decay for $T > T_c$. The analysis of the specific heat shows a peak at a temperature above T_c. It is not possible, based on our present Monte Carlo data, to make an unequivocal statement about whether the peak height becomes infinite in the thermodynamic limit. However, it should be noted that the scaling analysis does not predict any divergence in the specific heat. Consideration of the crossover between the essential singularity in the free energy near T_c and the molecular-field behavior for $T > 2T_c$ leads to the prediction of a finite peak in the specific heat at a temperature above T_c.

The Hamiltonian for the Ising chain with an r^{-2} interaction is

$$\beta H = -\frac{1}{2T}\sum_{i>j}\frac{s_i s_j - 1}{(r_i - r_j)^2} - h\sum s_i \ . \tag{1}$$

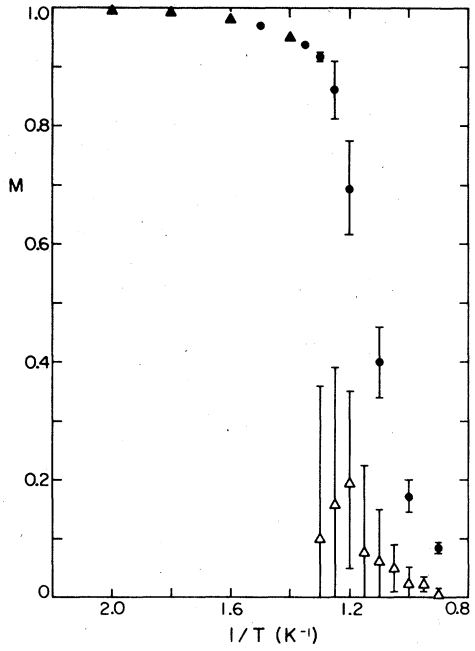

FIG. 1. Magnetization as a function of inverse temperature for a system of 256 spins. The solid dots are the magnetization in the presence of a local magnetic field perturbation described in the text and the open triangles are the magnitude of the magnetization in the absence of this field. The error bars give the rms fluctuation of block averages.

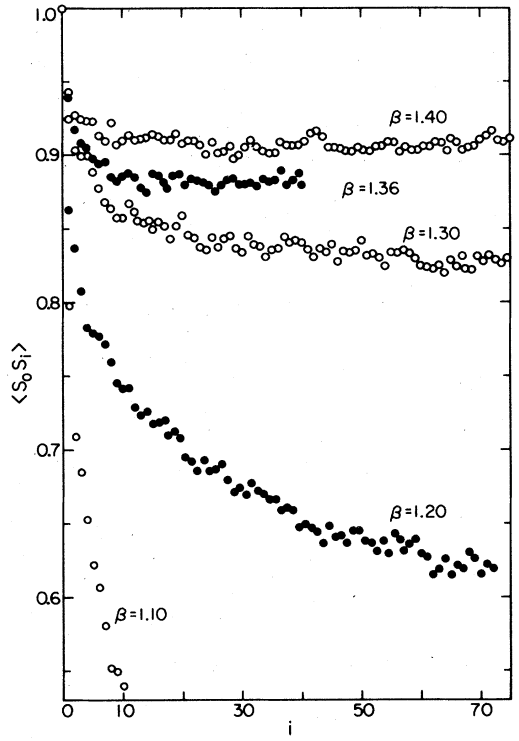

FIG. 2. Monte Carlo correlation function $\langle s_i s_j \rangle$ vs $|i-j|$ at different values of the temperature.

Here T is measured in units of the exchange energy J, $|r_i - r_j|$ is the distance between the ith and jth spins, $s_i = \pm 1$ and a is the lattice spacing. With the magnetic field $h = 0$, mean-field theory gives a transition temperature

$$T_M = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \simeq 1.645 \ldots . \tag{2}$$

Now, as expected, the fluctuations prevent the system from ordering at T_M. However, as the temperature drops below T_M, the spins tend to line up and the dominant excitations are kinks at which a spin reversal occurs. The leading terms in the action for a chain with n kinks can be written as

$$\beta H = -\frac{1}{T} \sum_{j \neq k} (-1)^{j-k} \ln \left| \frac{r_j - r_k}{a} \right| + n\mu \ . \tag{3}$$

Here the kinks are labeled sequentially by j and k. The logarithmic terms represent the interaction between kinks at sites j and k and the chemical potential μ is associated with the local energy to form a kink in the absence of h.

In the temperature range where Eq. (3) is appropriate, Anderson and Yuval[2] scaled the lattice spacing $a \rightarrow a(1+dl)$ and obtained the following renormalization-group equations for the temperature field $\phi = (1/T) - 1$, the chemical potential field, $y = e^{-\mu/t}$, and the magnetic field h,

$$\frac{d\phi}{dl} = -4y^2 \ , \tag{4}$$

$$\frac{dy}{dl} = -y\phi \ , \tag{5}$$

$$\frac{dh}{dl} = h(1-2y^2) \ . \tag{6}$$

It should be noted that to the lowest order in y^2 the exact form of Eq. (4) would have a factor $(1+\phi)$ multiplying the right-hand side. For the present purposes $\phi << 1$ and hence we feel justified in replacing this factor by unity. Equations (4) to (6) are a correct description of the system for small y. It is obvious from Eq. (5) that for $\phi > 0$ ($T < 1$) the y iterates to zero, and hence in the regime $1 >> \phi > 0$ these equations describe the system adequately. On the other hand, if we are above the transition $T > 1$, y grows under iteration and reliable conclusions cannot be drawn. In this work we will not use these equations in this range.

A first integral of Eqs. (4) and (5) is easily seen to be

$$y^2 - \tfrac{1}{4}\phi^2 = C \ , \tag{7}$$

where C is a constant. This constant has been evaluated by Anderson and Yuval[2] and shown to be approximately equal to t. For $T < T_c$, where the number of kinks is small, the flow always terminate on the $y = 0$ axis and one obtains a line of critical points ending at $T = T_c$. For $T > T_c$, y iterates to larger and larger values and the local RG equations based on a dilute "kink gas" must be mapped onto an appropriate high-temperature description.

We illustrate the use of Eqs. (4)–(6) in computing various thermodynamic quantities by calculating the correlation function $G(r)$ at $T = T_c$. The prescription for expressing the required correlation function with increased lattice spacing is

$$\langle s(r)s(0) \rangle = e^{-2l} \exp\left[2 \int_0^l y_h(l')\,dl'\right] \langle s(r/e^l)s(0) \rangle \ . \tag{8}$$

Here r is measured in units of the lattice spacing and $y_h(l) = 1 - 2y^2(l)$ is the l-dependent magnetic eigenvalue. Scaling, so that $l = \ln r$, we have

$$\langle s(r/e^l)s(0) \rangle = \langle s(1)s(0) \rangle \simeq 1$$

and

$$\langle s(r)s(0) \rangle = \exp\left[-4 \int_0^{\ln} r y^2(l')\,dl'\right] = \exp\left[4 \int_{y(0)}^{y(l)} \frac{y\,dy}{\phi}\right] , \tag{9}$$

where Eq. (5) has been used in the last step. Using

Eq. (7), the last equation can be easily integrated. To complete the calculation we need the function $y(l)$. For $T=T_c$, Eq. (7) yields $\phi=2y$ and hence Eq. (5) can be integrated to give $y(l)=(2l)^{-1}$. Consequently

$$\langle s(r)s(0)\rangle=\bar{s}^2 e^{(1/\ln r)} \tag{10}$$

and

$$G(r)=\bar{s}^2(e^{(\ln r)^{-1}}-1)\simeq \bar{s}^2/\ln r \ , \tag{11}$$

where $\bar{s}\sim e^{-y(0)}$. This is an interesting limiting result in that the importance of the logarithmic term, which signifies marginality, is paramount. Without it, we would not obtain a physically meaningful correlation function. This is distinct from the Kosterlitz-Thouless transition[4] in the 2D (two-dimensional) XY model where the logarithmic correction at $T=T_c$ merely modifies the $r^{-1/4}$ falloff.

For $T<T_c$, but close to it similar considerations yield

$$G(r)=\bar{s}^2\frac{4\sqrt{|t|}}{r^{4(|t|)^{1/2}}} \ , \tag{12}$$

which correctly reduces to Eq. (11) as $t\to 0$. Equation (12) implies the temperature-dependent exponent

$$\eta=1+4\sqrt{|t|} \ . \tag{13}$$

At $T=T_c$, this yields $\eta=1$, a result which has been conjectured to be exact by Fisher, Ma, and Nickel.[5] It follows from Eq. (12) that the correlation drops off increasingly rapidly as T decreases below T_c in contrast to the 2D XY model. This is consistent with the existence of long-range order for the present problem and the interpretation of $G(r)$ as the healing of a disturbance in this order. An interesting consequence shows up in the susceptibility χ, which can be expressed as

$$\chi\simeq\int_1^\infty G(r)\,dr\simeq\int_1^\infty\frac{dr}{r^{4(|t|)^{1/2}}} \ . \tag{14}$$

For $-\frac{1}{16}<t<0$ this clearly diverges. It is finite for $t<-\frac{1}{16}$ and proportional to $1/(4\sqrt{|t|}-1)$. As $t\to-\frac{1}{16}$ form below the behavior is $(t+\frac{1}{16})^{-1}$.

Turning now to $T>T_c$, we note that Eqs. (4)–(6) are no longer valid except perhaps in the immediate vicinity of T_c. To extract more information one has to resort to the Gaussian approximation which will be valid at high temperature. In the Gaussian approximation the specific heat is strongly divergent.[6] In the vicinity of T_c, on the other hand, we know from Anderson and Yuval, [2] that the specific heat is severely suppressed by the fluctuations. Consequently, we have a picture in which for $T\gg T_c$ that the specific heat is rising rapidly as T decreases and close to T_c is becoming very small again. This suggests the existence of a peak in the crossover function for the specific heat with the crossover occurring from the Anderson-Yuval behavior to a Gaussian behavior. The susceptibility is finite for $T>T_c$ and scales as the correlation length.

The Metropolis Monte-Carlo procedure[7] was used to simulate the system. Here 3000 passes were used to equilibrate the system and another 12 000 passes were used to calculate the averages. The averaging has been performed over both heating and cooling runs. At least six independent runs were taken with different initial conditions and no systematic errors attributable to hysteresis were found. Since the Monte-Carlo calculation involves a finite number N of spins with periodic boundary conditions, the action of Eq. (1) becomes (within an additive constant)

$$\beta H=-\frac{1}{2T}\sum_{i>j}\frac{(\pi^2/N^2)(s_is_j-1)}{\sin^2[(\pi/N)(i-j)]}-h\sum s_i \ . \tag{15}$$

Calculations were performed for $N=16$, 32, 64, 128, and 256.

The magnetization for 256 spins is shown in Fig. 1. The error bars represent the rms fluctuations. These errors are negligible for $\beta>1.4$. For $N=256$ and zero magnetic field at $\beta=1.6$, $m(0)=0.9819$ with a rms fluctuation of ± 0.0003. It is also worth noting that the heating and cooling runs agree to within a tenth of a percent. The picture of Anderson and Yuval is borne out very well. Close to $\beta=1.30$ there is a sharp drop in the magnetization. According to Anderson and Yuval the magnetization would have a finite jump at $\beta=1.27$ corresponding to $T_c=0.79$.

In order to probe the transition region we ran the simulations with a local magnetic field perturbation in which one spin was always held in the "up" direction. We see from Fig. 1 that the magnetization $m(h)$ is identical to $m(0)$ for $\beta>1.30$, but for $\beta\sim 1.30$ the local magnetic field perturbation causes a large change in the magnetization and hence indicates the existence of a critical region. The additional prediction of an infinite slope in the magnetization curve at the transition temperature cannot be verified by these techniques.

The Monte Carlo correlation function $\langle s_is_j\rangle$ at various temperatures is shown in Fig. 2. For $\beta\geq 1.3$ the function approaches a constant at large distances due to the long-range order in the system. At $\beta=1.2$ and 1.1 the data are consistent with an r^{-2} falloff. The susceptibility data have not been shown due to the limited accuracy in the vicinity of the transition point. It was found that at $\beta=1.30$ the susceptibility scales with the system size and hence would be infinite in the thermodynamic limit. It was found to be finite for $\beta\geq 1.5$ and for $\beta\leq 1.2$. The $N\to\infty$ behavior in the remaining region was not particularly transparent. We have seen above that the recursion relations lead to a divergent susceptibility in a finite temperature range in this region. Although our

Monte Carlo cannot verify this exactly, the data are not inconsistent with this assertion.

We turn now to the most interesting feature of the Monte Carlo simulation, the specific heat. We have calculated it from the fluctuation in the internal energy $\langle u^2\rangle - \langle u\rangle^2$ and also from the temperature derivative of the computed internal energy $\langle u\rangle$. In our simulations we have made sure that the two methods yield practically the same answer, a fact that assures us of the reliability of our simulations. The plots for different values of N are shown in Fig. 3. The interesting point is that at $\beta \simeq 1.10$, which is a temperature slightly higher than the transition temperature, the specific heat increases with the size of the system. The height of the peak at $\beta = 1.10$ is shown as a function of the system size in the inset. The accuracy of the data is quite high at this temperature and the conservative error bars represent the difference between heating and cooling runs. The variation of the specific-heat peak with the sample size shown in the inset of Fig. 3 does not follow the finite-size scaling behavior associated with a second-order transition. However, we cannot reliably distinguish between a specific-heat peak saturation or divergence within the sample sizes we have studied. This Monte Carlo finding is in contrast to the 2D XY model studies[8] where the peak was found to saturate rapidly with the system size.

In conclusion, we have on the basis of the Anderson-Yuval recursion relations, predicted the temperature-dependent exponent $\eta = 1 + 4\sqrt{-t}$, for $T < T_c$, and shown that this leads to a finite susceptibility for $T < 15T_c/16$. Our Monte Carlo studies supporting the Anderson prediction for the magnetization and our assertion of a finite low-temperature susceptibility have been presented. The investigation

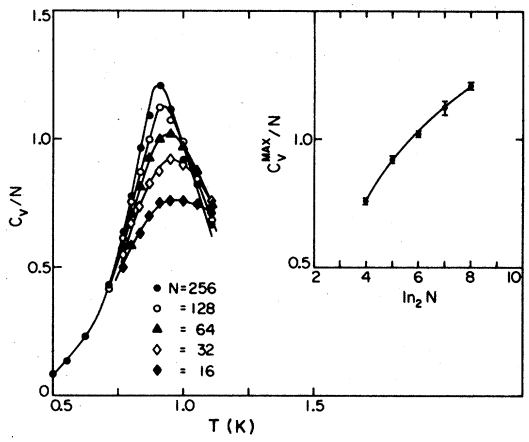

FIG. 3. Specific heat vs temperature for different lattice sizes N. The error bars represent the differences between heating and cooling runs. The insert shows the variation of the maximum of the specific heat with the system size.

of the specific heat by Monte Carlo techniques has shown the existence of a maximum at a temperature above T_c. Further study is required to establish whether the maximum is finite or an actual divergence. Arguments based on a crossover from Anderson-Yuval to Gaussian behavior have been given to predict a finite maximum at a temperature above T_c.

ACKNOWLEDGMENT

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[1]D. J. Thouless, Phys. Rev. 187, 732 (1969).
[2]P. W. Anderson and G. Yuval, J. Phys. C 4, 607 (1971).
[3]J. M. Kosterlitz, Phys. Rev. Lett. 37, 1577 (1976).
[4]J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973); see also J. M. Kosterlitz, *ibid.* 7, 1046 (1974).
[5]M. E. Fisher, S. Ma, and B. Nickel, Phys. Rev. Lett. 29, 917 (1972).
[6]See for example, P. Pfeuty and G. Toulouse, *Introduction to the Renormalization Group and to Critical Phenomena* (Wiley, New York, 1975), Chap. 2.
[7]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1089 (1953).
[8]J. E. Van Himbergen and S. Chakravarty (unpublished).