Critical properties of $S>\frac{1}{2}$ Ising chains with long-range interactions

M. Barati* and A. Ramazani
Department of Physics, Shiraz University, Shiraz 71454, Iran
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The phase diagram and critical exponent of the correlation length for an Ising chain with a long-range interaction in the form of $1/r^{1+\sigma}$ for $S=1/2,1,3/2,2$ is calculated by the finite-range scaling technique. The spin dependence of the critical temperature and critical exponent ν in the classical and nonclassical regions is also studied. It is observed that, with a good approximation, the critical exponent of the correlation length is independent of the magnitude of spin in both the classical and nonclassical regions.

I. INTRODUCTION

It is well known that the one-dimensional spin models with a long-range interaction exhibit an ordered state at low temperatures when the interaction falls off sufficiently slowly. The spin-$\frac{1}{2}$ Ising ferromagnet with a long-range interaction proportional to $1/r_{ij}^{1+\sigma}$ (r_{ij} is the distance between spins at sites i and j) has been studied extensively. For this system, the existence of a phase transition at a nonzero critical temperature is proved for $0<\sigma\leqslant 1$.[1,2] In addition, the critical phenomena in the system exhibit a more complicated behavior than in the system with a short-range interaction. The manifestation of such a complication can be observed clearly in the behavior of the critical exponents in the nonclassical region especially at the border of $\sigma=1$. Therefore the study of different properties of these systems requires a more profound understanding of the critical phenomena.

The critical properties of spin-$\frac{1}{2}$ systems with a long-range interaction have been investigated by the series expansion method,[3] the renormalization group (RG) method in reciprocal space in the form of an ε expansion around $\sigma=0.5$ (Ref. 4) and $\sigma=1$ (Ref. 5), the real-space RG method,[6] the finite-range scaling (FRS) method,[7,8] the coherent anomaly method (CAM),[9] and advanced Monte Carlo simulations.[10]

There are different interests in the study of the systems with a long-range interaction. From the fundamental theoretical point of view, the investigation of such systems lets one understand the effect of the range of the interaction on the critical properties of these systems. From another point of view, there are several applications for such systems. It has been shown that critical fluctuations may give rise to long-range Casimir forces between uncharged particles immersed in a critical fluid.[11] It has also been observed that the random exchange (Levy-flight) processes can generate effective interactions which decay algebraically at long distances.[12] Other related problems deal with spin systems with a long-range RKKY-like interaction $[\cos(ar)/r^{\alpha}]$ which is present in spin glasses[13] and critical phenomena in highly ionic systems.[14] A problem that is of particular interest is the $\sigma=1$ case. Under this form of interaction $(1/r^2)$, the $S=1/2$ can be mapped onto the spin-$\frac{1}{2}$ Kondo problem[15] and generally $S>1/2$ may be related to the higher-spin generalization of the Kondo problem.[16]

In the present work, the FRS method employed by Glumac and Uzelac[7,8] is followed and extended to study the magnetic phase diagram and the correlation length critical exponent ν of a one-dimensional Ising chain with a long-range interaction in the form of $1/r^{1+\sigma}$ for $S=1/2,1,3/2,2$. In this investigation, the critical temperature and the critical exponent ν in the classical ($0<\sigma\leqslant 0.5$) and nonclassical ($0.5<\sigma\leqslant 1$) regions are determined for different values of S and their behavior with respect to the parameters σ and S is obtained. In addition, the results for the critical exponent of the correlation length in the classical region are compared with the value of $1/\sigma$ predicted by the RG method[4] and confirmed by advanced Monte Carlo results.[10]

The Hamiltonian of the system under consideration can be written as

$$H=-S^{-2}\sum_{i,j} J_{ij}s_i s_j, \tag{1}$$

where $s_i=-S,\ldots,S$ and $J_{ij}=J/|i-j|^{1+\sigma}$ in which the lattice spacing is one unit. The S^{-2} factor in the Hamiltonian is entered as a normalization factor such that the magnitude of the large value of each spin is normalized to 1. The main idea of this approach is that the true infinite range of the interaction is truncated to the Nth first neighbors and the problem in this finite range is solved exactly with the Hamiltonian of Eq. (1). Then the $N\to\infty$ behavior of the system is deduced by using the range scaling relation and an appropriate extrapolating technique.

The outline of the paper is as follows: the FRS method is briefly explained in Sec. II A, the transfer matrix method for this case is developed in Sec. II B, and the extrapolating method is introduced in Sec. II C. In Sec. III, the behavior of the critical temperature and the correlation length critical exponent ν and their dependence on the magnitude of the spin S is investigated. The concluding remarks are given in Sec. IV.

II. THEORY AND METHODS

A. Finite-range scaling

The FRS method has been constructed in analogy with finite-size scaling (FSS),[17] with a scaled range of interaction.[7] The basic idea is to truncate the range of the interaction in the system to a certain range and obtain precise information about the critical behavior of the true infinite system by using scaling properties.

Let $A_\infty(t)$ be some physical quantity which algebraically diverges in the vicinity of the critical point $t=0$ for an infinite long-range system, i.e.,

$$A_\infty(t)\simeq A_0 t^{-\rho} \tag{2}$$

where $t=(T-T_c)/T_c$, T_c is the critical temperature, ρ is the related critical exponent, and A_0 is a constant. Analogous to the FSS hypothesis, it is assumed that for a large finite range N and small t, $A_N(t)$ can be written as

$$A_N(t)=A_\infty(t)f(N/\xi_\infty), \tag{3}$$

where f is a homogeneous function with the following properties:

$$\lim_{x\to\infty} f(x)=1, \quad \lim_{x\to 0} f(x)=\text{const}\times x^{\rho/\nu}. \tag{4}$$

By applying Eq. (3) to the correlation length $\xi_\infty(t)=\xi_0 t^{-\nu}$, the standard procedure gives the condition for the critical temperature through the fixed point equation

$$\xi_N(t^*)=(N/M)\xi_M(t^*) \tag{5}$$

and the expression for the correlation length critical exponent ν,

$$\nu_N^{-1}=\ln[\xi_N'(t^*)/\xi_M'(t^*)]/\ln(N/M)-1, \tag{6}$$

where ξ' is the derivative of the correlation length ξ with respect to t. According to the FSS method, M and N must be two close integers for better convergency.

It is interesting to note that the critical behavior in this scaling approach (unlike the FSS approach[18]) depends essentially on the range of the interaction. Therefore, applicability of the method in both the mean-field ($0<\sigma\leqslant 0.5$) and nonclassical regions ($0.5<\sigma\leqslant 1$) is expected.

B. Transfer matrix

Applicability of the FRS method depends on the possibility of the exact determination of the results for a finite range of interaction. For Ising chains with the interaction truncated at the Nth neighbors, the exact calculation can be obtained by applying a proper transfer matrix. The Hamiltonian of the chain can be written as

$$-\beta H=\sum_{i=1}^{L}\sum_{j=1}^{N} K_j s_i s_{i+j}, \tag{7}$$

where $K_j=S^{-2}\beta J/j^{1+\sigma}$ and L and N are the number of magnetic sites and the range of interaction, respectively.

In order to set up a proper transfer matrix, the chain is considered as a strip with columns of height N where each column, regarding the $2S+1$ possible states of the spins, can be imagined as a system with $(2S+1)^N$ possible states which interact only with their nearest neighbors. The transfer matrix for the chain can be written as

$$\langle \mathbf{s}|\mathbf{T}|\mathbf{s}'\rangle=\exp\left\{\sum_{k=1}^{N} K_k\left[\sum_{n=1}^{N-k} s_n s_{n+k}+\sum_{n=1}^{k} s_{N+n-k}s_n'\right]\right\}, \tag{8}$$

where $s_n=-S,\ldots,S$ is a member of the state vector $|\mathbf{s}\rangle$ with N components, i.e.,

$$|\mathbf{s}\rangle=|s_1,s_2,\ldots,s_N\rangle. \tag{9}$$

Equation (8) can also be written as a product of N matrices T_n, where each matrix would add one more site to the column,[19]

$$\mathbf{T}=\mathbf{T}_1\mathbf{T}_2\cdots\mathbf{T}_{N-1}\mathbf{T}_N. \tag{10}$$

There exists also a simple relation between these one-site matrices, i.e.,

$$\mathbf{U}^T\mathbf{T}_{n+1}\mathbf{U}=\mathbf{T}_n, \tag{11}$$

where $\mathbf{T}_{N+1}=\mathbf{T}_1$ and $\mathbf{U}$ is the translation operator in a direction perpendicular to the strip as given by

$$\langle \mathbf{s}|\mathbf{U}|\mathbf{s}'\rangle=\delta(s_1,s_N')\,\delta(s_2,s_1')\,\delta(s_3,s_2')\cdots\delta(s_{N-1},s_{N-2}')\times\delta(s_N,s_{N-1}'), \tag{12}$$

where $\mathbf{U}^N=\mathbf{1}$ and $\mathbf{U}^{N-1}=\mathbf{U}^T=\mathbf{U}^{-1}$. Therefore $\mathbf{T}$ can be written as

$$\mathbf{T}=(\mathbf{U}\mathbf{T}_N)^N=\tilde{\mathbf{T}}^N, \tag{13}$$

where

$$\langle \mathbf{s}|\tilde{\mathbf{T}}|\mathbf{s}'\rangle=\delta(s_2,s_1')\,\delta(s_3,s_2')\cdots\delta(s_N,s_{N-1}')\times\exp\left\{\sum_{m=1}^{N} K_{N+1-m}s_m s_N'\right\}. \tag{14}$$

It is interesting to note that the $\tilde{\mathbf{T}}$ matrix has only $2S+1$ nonzero elements in each row which reduces the required computer memory tremendously. Applying the standard derivation, the correlation length is obtained as

$$\xi_N=\frac{N}{\ln(\lambda_1/\lambda_2)}=\frac{1}{\ln(\mu_1/\mu_2)}, \tag{15}$$

where λ_1 and λ_2 are the largest and second-largest eigenvalues of $\mathbf{T}$, and μ_1 and μ_2 are the largest and second-largest eigenvalues of $\tilde{\mathbf{T}}$, respectively.

A power method can be used for calculating μ_1. Then, by factorizing μ_1, a similar technique is employed to calculate μ_2. Details of the methods have been discussed extensively in the numerical literature.[20]

C. Extrapolation procedure

The critical temperature and exponent ν, given by Eqs. (5) and (6), depend on the selected range of the interaction N. In order to obtain the correct answer for the true Ising system, a proper method of extrapolation should be employed.

From the scaling hypotheses one expects to observe a power-law convergency for a critical behavior of the same type. Based on this theory, the FRS is similar to the FSS

TABLE I. (a) The extrapolated values of the critical temperature as a function of S and σ. (b) The critical temperature convergence exponent x_T as a function of S and σ.

(a)

S/σ	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
$\frac{1}{2}$	21.6	10.919	7.359	5.5167	4.3579	3.5436	2.9269	2.4299	2.0054	1.640
1	14.0	7.32	4.99	3.78	3.026	2.499	2.103	1.789	1.530	1.317
$\frac{3}{2}$	11	6.03	4.16	3.17	2.55	2.11	1.79	1.535	1.326	1.154
2	9.6	5.4	3.73	2.86	2.30	1.92	1.63	1.40	1.21	1.06

(b)

S/σ	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
$\frac{1}{2}$	0.857	1.021	1.132	1.193	1.218	1.217	1.20	1.22	1.90	1
1	0.88	1.01	1.12	1.19	1.24	1.27	1.32	1.46	2.60	1
$\frac{3}{2}$	0.9	1.0	1.1	1.2	1.26	1.31	1.38	1.55	2.3	1
2	1.0	1.1	1.2	1.2	1.3	1.3	1.4	1.6	2.2	1

technique[21] and convergency is mainly affected by the leading irrelevant field and the related critical exponent $y_3<0$. Therefore a power-law convergency for T_c and ν is used for large values of N:

$$T_{c,N}=T_c+aN^{y_3-1/\nu} \tag{16}$$

and

$$\nu_N^{-1}=\nu^{-1}+b(T_{c,N}-T_c)N^{1/\nu}+cN^{y_3}=\nu^{-1}+b'N^{y_3}, \tag{17}$$

where a, b, b', and c are constants. Thus, in order to obtain the true critical temperature and the correlation length critical exponent ν, the results for $K_{c,N}(=1/T_{c,N})$ and ν_N^{-1} are fitted to the form

$$\rho_N=\rho_e+A/N^{x_\rho} \tag{18}$$

in the least-squares approximation (LSA). Here ρ_e and x_ρ denote the extrapolated quantity and the convergence exponent, respectively.

It should be noted that the FSS technique is not applicable in the mean-field (MF) region.[21] Therefore a fitting based on Eq. (18) in this region is quite optional. Here, in the MF region the fitting in the form

$$\rho_N=B+A\left(\frac{N-1}{N}\right)^{x_\rho} \tag{19}$$

for ν evaluation, as suggested by Glumac and Uzelac,[7] is accepted. The results which have been evaluated through Eq. (19) for $S=1/2$ are in better agreement with the values predicted by the RG method.

III. RESULTS AND DISCUSSION

A. Critical temperature

In order to determine the critical temperature for an Ising chain with a long-range interaction by the FRS technique, we have to find the value of the fixed point through Eq. (5). In this calculation the limitation of the computer memory for saving the elements of the transfer matrix $\tilde{\mathbf{T}}$ causes a restriction on the range of interaction N. For $S=1/2,1,3/2,2$ the maximum range of interaction is limited to $N=20,13,10,9$, respectively. It must be noted that the $S=1/2$ Ising chain has already been investigated with the FRS technique.[8] However, in order to have a better comparison of the results, the $S=1/2$ system along with the other systems with higher values of S was studied with the same degree of accuracy. Our results for $S=1/2$ apart from a few percent discrepancy caused by the different accuracy in the calculation are compatible with the reported values.

The two largest eigenvalues of the transfer matrix were calculated with 17 digits and the values of the $T_{c,N}$ could be determined with an accuracy of $10^{-8}J/k$. In order to find the critical temperature for a given S and σ, an extrapolation for five fixed points with a larger interaction range based on Eq. (18) was performed. It should be noted that $T_{c,N}$ has nonmonotonic behavior for $\sigma=1$ (the limiting point for the presence of the phase transition). Therefore fitting through Eq. (18) in this case is not possible and the fitting is performed by imposing $x_T=1$ in the equation. This restriction does not have much effect on the final results because of a small variation of $T_{c,N}$s. The results for the critical temperature T_c and convergency exponent x_T are presented in Table I.

It must be remarked that the accuracy of the critical temperature determined by extrapolation depends on σ and S. The maximum possible value of the range of interaction N as well as the accuracy of the calculations decreases by increasing S. In addition, in the FRS method the convergency of the fixed points is reduced as σ decreases and the accuracy in the extrapolated critical temperature decreases. Thus, the accuracy of the results depends on S and σ. In this regard the significant digits of the data presented in this section were determined by the change of the maximum range of the interaction from $N-1$ to N.

TABLE II. The ratio of T_c/T_c^{MF} as a function of S and σ.

S/σ	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
$\frac{1}{2}$	0.96	0.929	0.885	0.832	0.773	0.711	0.644	0.574	0.499
1	0.97	0.948	0.911	0.868	0.819	0.767	0.713	0.656	0.601
$\frac{3}{2}$	0.97	0.953	0.919	0.879	0.833	0.785	0.734	0.682	0.631
2	0.98	0.955	0.922	0.883	0.839	0.792	0.743	0.694	0.644

TABLE III. (a) The extrapolated values of ν^{-1} for ν_N calculated in T_{ce} as a function of S and σ. For comparison, we cite the exact RG results. (b) The convergence exponent x_ν as a function of S and σ.

(a)

S/σ	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$\frac{1}{2}$	0.095	0.194	0.289	0.374	0.440	0.481	0.490	0.458
1	0.100	0.196	0.289	0.373	0.439	0.480	0.492	0.474
$\frac{3}{2}$	0.115	0.206	0.295	0.376	0.440	0.48	0.49	0.486
2	0.126	0.214	0.302	0.380	0.44	0.48	0.50	0.493
Exact RG	0.1	0.2	0.3	0.4	0.5			

(b)

S/σ	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$\frac{1}{2}$	0.94	0.91	0.81	0.70	0.62	0.57	0.56	0.65
1	0.96	0.91	0.83	0.75	0.70	0.68	0.74	1.23
$\frac{3}{2}$	0.94	0.89	0.83	0.77	0.74	0.76	0.9	1.4
2	0.92	0.88	0.82	0.77	0.76	0.8	0.9	1.5

In order to study the spin dependence of the critical temperature, the ratio T_c/T_c^{MF} for the range $0.2\leqslant\sigma\leqslant 1$ and for $S=1/2,1,3/2,2$ was calculated. T_c^{MF} is the mean-field critical temperature and is given by[10]

$$T_c^{MF}=\frac{2}{3}\frac{S+1}{S}\frac{J}{k}\sum_{n=1}^{\infty}\frac{1}{n^{1+\sigma}}=\frac{2}{3}\frac{S+1}{S}\frac{J}{k}\xi(1+\sigma), \quad (20)$$

where ξ is the Riemann zeta function. The results are shown in Table II. It should be mentioned that for a better comparison, the critical temperature calculation was carried out with $N=9$ for all values of S. It is seen from Table II that the ratio T_c/T_c^{MF}, as expected, increases with S increasing. However, the process of this approach strongly depends on the value of σ such that the rate of change of T_c/T_c^{MF} between $S=1/2$ and $S=2$ is only 2% for $\sigma=0.2$ and 29% for $\sigma=1$.

B. Critical exponent ν

The critical exponent of the correlation length ν_N was calculated by Eq. (6). In this calculation, the accuracy of the results is reduced to six or five digits because of the required differentiation procedure. The errors depend in a complicated way on the value of S and σ as in the case of the critical temperature, although the dependence is somewhat different from that in Sec. III A. The significant digits of data presented in this section have been determined by the method explained in the last section.

From Eq. (17), one expects to obtain better results for ν^{-1} in the nonclassical region if the expansion of Eq. (6) is performed around the extrapolated critical temperature T_{ce} instead of $T_{c,N}$. This was processed for $S=1/2$ by Glumac and Uzelac where a better convergency for ν_N was observed.[8] It is interesting to note that even in the MF region if the ν_N is calculated for the extrapolated critical temperature T_{ce} and the critical exponent ν is evaluated through Eq. (18), the results are in good agreement with the predicted values by the RG method.

The results for the inverse of the critical exponent of the correlation length, ν^{-1}, are presented in Table III(a) and the convergence exponent x_ν in Table III(b). As is seen from Table III(a), the results are in good agreement with the exact

TABLE IV. (a) The extrapolated values of ν^{-1} for ν_N calculated in $T_{c,N}$ as a function of S and σ. For comparison, we cite the exact RG results. (b) The convergence exponent x_ν for the nonclassical region as a function of S and σ.

(a)

S/σ	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
$\frac{1}{2}$	0.104	0.201	0.292	0.370	0.428	0.465	0.472	0.454	0.380	0.13
1	0.108	0.203	0.294	0.373	0.435	0.474	0.487	0.469	0.388	0.15
$\frac{3}{2}$	0.11	0.21	0.297	0.376	0.437	0.473	0.491	0.474	0.395	0.17
2	0.12	0.21	0.30	0.378	0.44	0.47	0.49	0.475	0.398	0.18
Exact RG	0.1	0.2	0.3	0.4	0.5					0

(b)

S/σ	0.6	0.7	0.8	0.9	1
$\frac{1}{2}$	2.4	2.6	1.6	0.49	0.19
1	0.97	0.9	0.72	0.41	0.21
$\frac{3}{2}$	0.8	0.8	0.66	0.42	0.23
2	0.8	0.8	0.63	0.41	0.23

RG prediction in the classical region. The small difference between the results in the border of the classical and nonclassical regions is mainly caused by a poor convergency originated from the logarithmic term. In the fitting procedure, ten points corresponding to the largest values of N for $S=1/2$ and five points for the other S's were used. For $\sigma=0.9$ the ν_N behave nonmonotonically which makes the fitting by Eq. (18) impossible and for $\sigma=1$ the fitting leads to a negative value for the convergence exponent x_ν.

As is seen in Table III, the critical exponent ν for a fixed σ is almost spin independent in both the MF and nonclassical regions. The small deviation for a small value of σ is caused mainly by the use of different values of N for different values of S. This observation indicates that the borderline between the MF and nonclassical regions is spin independent, and therefore the method of calculation through $T_{c,N}$ should be applicable for this determination. The critical exponent ν was also calculated through the fitting of ν_N in Eq. (18) and Eq. (19) for $0.5<\sigma\leqslant 1$ and $0<\sigma\leqslant 0.5$, respectively. The results of ν in both regions and x_ν in the nonclassical region are presented in Tables IV(a) and IV(b). The agreement between the two methods of calculation is good evidence of the spin-independent behavior of the critical exponent ν.

IV. CONCLUSIONS

The critical temperature and the correlation length critical exponent of an Ising chain with a long-range interaction in the form $1/r^{1+\sigma}$ were calculated for $S=1/2,1,3/2,2$ in the classical and nonclassical regions by the FRS technique.

The spin dependence of the critical temperature was investigated by the study of the ratio T_c/T_c^{MF}. It was observed that the spin dependence of the ratio is more pronounced for large values of σ. Likewise, it was observed that the critical exponent ν is almost independent of the magnitude of the spin in both the classical and nonclassical regions. This supports the prediction of universality for the critical exponent ν for Ising systems with a long-range interaction.

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*Electronic address: barati@physics.susc.ac.ir

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