

Classical phase diagram of $S \geq \frac{1}{2}$ Ising chains with long-range interactions: Finite-range scaling

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The classical phase diagram of an Ising chain for $S \geq \frac{1}{2}$ with long-range interaction in the form of $1/r^{1+\sigma}$ is determined. The calculation is performed by using the exact value of the critical exponent of the correlation length, $\nu = 1/\sigma$, given by the renormalization-group technique in the classical region, and applying a searching program based on the finite-range-scaling method. The results for the critical temperature in this approach are in excellent agreement with those calculated by the extensive Monte Carlo technique. This is strong support for the range-scaling method in the classical region.

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One of the methods used for the study of the critical properties of spin chains with long-range interaction is the finite-range-scaling (FRS) technique. This method, which was established by Glumac and Uzelac in 1988, is constructed in analogy with finite-size-scaling (FSS),¹ where the range of interaction, instead of the size, is scaled.² In this technique a spin chain with a finite range of interaction is exactly solved by using the transfer-matrix method, and then by the use of scaling properties and a proper extrapolating technique, the critical properties of the actual system are determined. The FRS method has been employed to study the critical properties of the one-dimensional $S = \frac{1}{2}$ Ising model,³ q -state Potts model,⁴ and recently for the $S > \frac{1}{2}$ Ising model⁵ with long-range interaction. This method can provide acceptable results for the critical temperature and critical exponent of the correlation length for Ising systems with long-range interaction in the form of $1/r^{1+\sigma}$ in the classical ($0 < \sigma \leq 0.5$) and the nonclassical ($0.5 < \sigma \leq 1$) regions.

In this report, the FRS method is exploited differently and the phase diagram of the $S \geq \frac{1}{2}$ Ising chain in the classical region is determined with higher precision than in our last report.⁵ In this approach, the exact critical exponent of the correlation length in the classical region given by the renormalization-group (RG) method ($\nu = 1/\sigma$) is adopted,⁶ and a search through the FRS method for a proper value of the critical temperature, which leads to the precise value for the critical exponent, is performed.

The Hamiltonian of the system under consideration can be written as

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

TABLE I. The critical coupling K_c ($\equiv 1/T_c$) for different values of σ in the classical region for the $S = \frac{1}{2}$ Ising chain by the traditional FRS methods $K_c^{(1)}$ (Ref. 2 for $N=9$), $K_c^{(2)}$ (Ref. 5 for $N=20$), the more recent FRS method $K_c^{(3)}$, and by the Monte Carlo simulations method $K_c^{(MC)}$.

σ	$K_c^{(1)}$	$K_c^{(2)}$	$K_c^{(3)}$	$K_c^{(MC)}$
0.1	0.053307	0.0463	0.047570	0.0476168 (6)
0.2	0.094768	0.091583	0.092316	0.0922314 (15)
0.3	0.1375	0.1359	0.13664	0.136110 (2)
0.4	0.1823	0.18127	0.18248	0.181150 (3)
0.5	0.2305	0.22947	0.2314	0.229155 (6)

where $s_i = -S, \dots, S$ 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 one. Based on the FRS method, the critical exponent of the correlation length, ν_N , for the chain with a finite range of interaction N , can be determined through the transfer matrix \mathbf{T} ,

$$\langle \mathbf{s} | \mathbf{T} | \mathbf{s}' \rangle = \delta(s_2, s'_1) \delta(s_3, s'_2) \cdots \delta(s_N, s'_{N-1}) \times \exp \left\{ \sum_{m=1}^N K_{N+1-m} s_m s'_m \right\} \quad (2)$$

and is given as

$$\nu_N^{-1} = \ln[\xi'_N(t)/\xi'_M(t)] / \ln(N/M) - 1, \quad (3)$$

where M is chosen as $N-1$, $K_i = (S^{-2} \beta J / i^{1+\sigma})$ and ξ' is the derivative of the correlation length ξ with respect to $t = (T - T_c) / T_c$, in the vicinity of the critical temperature of the system. For the correlation length ξ_N we have

$$\xi_N = \frac{1}{\ln(\lambda_1 / \lambda_2)}, \quad (4)$$

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

The critical exponent ν for the chain with an infinite range of interaction can be obtained by the least-squares fitting of the ν_N s to the convergence relation

$$\nu_N^{-1} = \nu^{-1} + A/N^x, \quad (5)$$

TABLE II. The calculated value of the critical temperature for the $S=1, \frac{3}{2}$, and 2 Ising chains by the more recent FRS method $T_c^{(N)}$ and by the traditional FRS technique $T_c^{(T)}$ in the classical region.

$S \setminus \sigma$	0.1		0.2		0.3		0.4		0.5	
	$T_c^{(T)}$	$T_c^{(N)}$								
1	14.0	14.06	7.32	7.2801	4.99	4.9561	3.78	3.748	3.026	2.991
$\frac{3}{2}$	11	11.730	6.03	6.0823	4.16	4.146	3.17	3.143	2.55	2.515
2	9.6	10.5604	5.4	5.47950	3.73	3.737	2.86	2.834	2.30	2.271

used in the FSS method, where A is a constant and x_ν is the convergence exponent of ν . It is obvious that as the temperature in Eq. (3) approaches the actual transition temperature of the system, the critical exponent obtained by Eq. (5) through the fitting procedure approaches its real value. This way, one can design a searching computer program to obtain the transition temperature corresponding to the exact value of the critical exponent of the correlation length ν , predicted by RG technique in the classical region. Thus, the eigenvalues λ_1 and λ_2 of the transfer matrix for the $S=\frac{1}{2}$ Ising chain with an accuracy of 10^{-17} are calculated and then ξ_N for five different values of the range of interaction up to $N=20$ is obtained. The inverse transition temperatures (critical coupling), for different values of σ in the classical region, calculated by our method and those given by the extensive Monte Carlo simulations technique,⁷ are presented in Table I. As is seen from the table, the results obtained by our method are in good agreement (with an uncertainty of less than 1%) with the best available results by the Monte Carlo technique in the entire classical region, and they are in an excellent agreement (uncertainty is even less than 0.1%) for the lower half of this region. Although the results for the upper half of this region given by the traditional FRS method are more accurate than those of our approach, they are not however reliable in the other half of this region. This can be seen from Table I where the transition temperature increases in a non-predictable way as σ decreases, such that at $\sigma=0.1$ it has a value even larger than the upper limit value predicted by the mean-field theory. It is interesting to note that the results given by this method, in contrast with those calculated by the traditional FRS method, are almost insensitive to the range of interaction N for the lower half of the classical region. Here the value of the critical temperature for $\sigma=0.1$ increases only less than 0.01% (from 21.06 to 21.021) and approaches the Monte Carlo value as the range of interaction is increased from 9 to 20, whereas this increase, under the same condition, is about 15% as is seen in Table I, where the traditional FRS method is employed.

As was discussed before, the FRS method was constructed in analogy with the finite-size-scaling technique. However, the FSS method is not applicable in the classical region where the size is an irrelevant scaling parameter,⁸ whereas the range of interaction is still a good scaling parameter.³ Therefore, the similarity between the two techniques disappears in the classical region. As a result, the applicability of the convergence relation (5) which has been proven in the process of establishing the FSS method,⁹ is not clearly verified by the FRS technique in the classical region.

In the early investigation of the Ising systems using the FRS technique by Glumac and Uzelac, the convergence relation (5) was employed, but the low precision of the results, particularly for small values of σ , persuaded them to use another convergence relation in the form $\nu^{-1}=B+A[(N-1)/N]^x$, where a better result was deduced.³ Our results as presented in Table I, which are calculated by employing the FRS technique together with the convergence relation (5), clearly show that calculating ν_N through Eq. (3) at the exact transition temperature (the temperature given by Monte Carlo simulations) leads to the exact value of $1/\sigma$ for the critical exponent of the correlation length ν (the value predicted by RG technique). This excellent agreement strongly supports the applicability of the FRS technique together with

TABLE III. The calculated values of the critical temperature for small values of σ by the more recent FRS method, together with the corresponding values predicted by the real-space renormalization group method for (a) $S=\frac{1}{2}$, (b) $S=1$, (c) $S=\frac{3}{2}$, and (d) $S=2$.

σ	(a)	
	$T_c(\text{FRS})$	$2/\sigma$
0.02	100.95	100.00
0.04	51.127	50.00
0.06	34.432	33.333
0.08	26.059	25.000
	(b)	
		$((S+1)/3S)2/\sigma$
0.02	67.08	66.66
0.04	34.095	33.333
0.06	22.992	22.222
0.08	17.415	16.666
	(c)	
		$((S+1)/3S)2/\sigma$
0.02	55.78	55.55
0.04	28.39	27.77
0.06	19.166	18.5185
0.08	14.526	13.888
	(d)	
		$((S+1)/3S)2/\sigma$
0.02	50.28	50.00
0.04	25.53	25.00
0.06	17.245	16.666
0.08	13.075	12.500

the convergence relation (5) in the classical region. In other words, the FRS method in the classical region is quite similar to the FSS method in the nonclassical region. It should be mentioned that the large uncertainty in the results obtained by the use of relation (5) in the early investigation could have been caused by the use of small values of N in those investigation.

The results for $S > \frac{1}{2}$ using the FRS method and the traditional technique are presented in Table II. Because of the limitation of the computer memory [the required memory for the transfer matrix is in the order of $(2S+1)^N$ units], five values for N with the highest values of 13, 10, and 9 for $S = 1, \frac{3}{2},$ and 2 is considered, respectively. The uncertainty in this calculation depends in a complicated way on the values of S and σ and reduces by decreasing them. The significant digits of the data were determined by reducing the maximum value of the range of interaction from N to $N-1$. As is seen from Table II, the results for the small values of σ are noticeably different from those reported before using the traditional FRS technique.⁵

Before opening the discussion about the results for $S > \frac{1}{2}$, we should point out that, to the best of our knowledge, there is not any report on the phase diagram of $S > \frac{1}{2}$ Ising chains with long-range interaction, except the one reported by us using the traditional FRS technique.⁵ Considering the universality of ν (its independence on S), and the existence of the same convergence behavior in the extrapolation procedure for different values of S , one expects that the data in the

lower half of the classical region for $S > \frac{1}{2}$ by the more recent method to be more reliable than those reported by the traditional FRS technique as they were for $S = \frac{1}{2}$ system. Another advantage of the more recent method is with regard to the computational limit in the evaluation of the results. This limit depends on the value of S and the range of the interaction, N . As the value of S increases one has to reduce the maximum range of the interaction in order to circumvent the problem of approaching the limit. Since for small values of σ the FRS method is less sensitive to N , this method would be more applicable than the traditional FRS technique for systems with $S > \frac{1}{2}$ in the lower half of the classical region.

The high precision of this method for small values of σ encouraged us to check the predicted value of $T_c = 2/\sigma$ by a real-space renormalization-group method for the $S = \frac{1}{2}$ Ising chain.¹⁰ The results have been presented in Table III(a). As is seen, our results successfully support this prediction. Similar comparison was made for the system with other values of S . The results for $S = 1$ to $S = 2$ are shown in Tables III(b)–III(d), respectively. The results show that as σ approaches zero, the transition temperature approaches $((S+1)/3S)2/\sigma$, which is expected in the classical limit, $\sigma \rightarrow 0$, for different values of S , in analogy with the prediction of the real-space group method for $S = \frac{1}{2}$. In conclusion, in spite of the invalidity of the finite-size scaling in the classical region, our results with the finite-range-scaling technique strongly support the validity of the FRS method in the classical region as the FSS does in the nonclassical region.

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