Magnetic phase diagram of an alternating Ising chain with long-range interactions

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The phase diagram of a two-sited magnetic Ising chain, with a long-range interaction in the form of $1/r^{1+\sigma}$, is studied. In this investigation, the finite-range scaling technique is employed and a proper transfer matrix is developed. The critical temperature of the chain, as a function of each type of interaction, i.e., the interaction between the similar sites and different sites, in both the classical and nonclassical regions is calculated. The results indicate that the critical temperature is strongly affected by the interaction range parameter σ for both types of interaction, but its behavior is quite different for each of the interactions. The behavior of the system is explained by calculating the strength of each interaction using the mean-field approximation. The study of the critical exponent of the correlation length indicates that the exponent is, within a good approximation, independent of the interaction constants.

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I. INTRODUCTION

The study of the critical behavior of the systems with a long-range interaction has attracted much attention for their application and their theoretical interest in the last three decades. The investigation of such systems is more complicated than those performed on the system with a short-range of interaction. One of the models that has been extensively investigated is the spin-$\frac{1}{2}$ Ising chain with a long-range of interaction proportional to $1/r_{ij}^{1+\sigma}$ (r_{ij} is the distance between spins at sites i and j). The model exhibits a phase transition in the whole region of $0<\sigma\leqslant 1$ (Refs. 1 and 2). However, for the region of $0<\sigma\leqslant 0.5$ the critical exponents are mean-field type (and thus it is known as the classical region), whereas for $0.5<\sigma\leqslant 1$, the so-called nonclassical region, are nontrivial and known only approximately.[3]

Along with the attempt on the critical exponent determination, there has been a special interest in the study of the phase diagram and the critical temperature for such models. In this regard, techniques such as the series expansion method,[4] the cluster approach,[5] the Bethe lattice approximation,[6] the finite-range scaling method (FRS),[7] the renormalization group method in direct space,[8] the coherent anomaly method,[9] the cycle expansion method,[10] the Onsager field reaction theory,[11] the Monte Carlo simulations,[12,13] and a cluster mean-field approach combined with the finite-size scaling[14] have been developed.

A method that has the ability of providing good result for the critical temperature of such systems in both the classical and nonclassical regions is the finite-range scaling technique. The results evaluated by this technique are in good agreement with those calculated by the Monte Carlo simulations in the classical region and with the conjectured value of $\pi^2/6$ at the borderline value $\sigma=1$ in the nonclassical region.[15] The FRS method was introduced by Glumac and Uzelac in 1988,[7] and has been applied for the study of the critical properties and the phase diagram of the one-dimensional $S=1/2$ Ising model,[16] q-state Potts model,[17] and recently for $S>1/2$ Ising model[18] with a long-range interaction.

In this paper, the FRS method is employed and a proper transfer matrix is developed to study the phase diagram and the critical exponent of the correlation length of a spin-$\frac{1}{2}$ Ising chain with two alternating magnetic sites with a long-range interaction in the form of $1/r_{ij}^{1+\sigma}$ in both the classical and nonclassical regions. For this model with an alternating magnetic sites A and B, the Hamiltonian is written as

$$H=-\sum_{i,j} J_{ij}s_is_j\,. \tag{1}$$

Here $s_i=\pm 1$ is a classical Ising spin at site i, and J_{ij} is defined as

$$J_{ij}=\begin{cases} J_{AA}/|i-j|^{1+\sigma} & \text{if sites } i \text{ and } j \text{ occupied by } A \text{ and } A\\ J_{BB}/|i-j|^{1+\sigma} & \text{if sites } i \text{ and } j \text{ occupied by } B \text{ and } B,\\ J_{AB}/|i-j|^{1+\sigma} & \text{if sites } i \text{ and } j \text{ occupied by } A \text{ and } B \end{cases} \tag{2}$$

where the distance between alternating sites is considered to be one unit and J_{AA}, J_{BB}, and J_{AB} are defined as the interaction constants when the corresponding magnetic sites are one unit apart.

As is seen, the interactions within the system be considered as the interaction between two different magnetic sites A and B with distances proportional to the nearest neighbor by an odd number, and the interaction between similar sites A and A or B and B with the corresponding distances by an even number of the nearest-neighbor distances. The A-B interaction can be considered as coupling between the two independent chains A and B. The main idea is to investigate the role of each interaction, for different values of σ, in the phase diagram as well as the critical exponent of the correlation length in both the classical and nonclassical regions.

The outline of the paper is as follows: in the Sec. II A, the FRS and the extrapolation method is briefly explained. In Sec. II B the transfer matrix method for this case (a chain with alternating magnetic sites) is developed. In Sec. III, the behavior of the critical temperature and the critical exponent of the correlation length as a function of J_{AA} and J_{AB} is analyzed. The concluding remarks are given in Sec. IV.

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II. THEORY AND METHODS

A. Finite-range scaling and extrapolation method

The FRS has been constructed in analogy with the finite-size scaling (FSS),[19] where in the first method the range of interaction is scaled.[7] The basic idea is to truncate the range of interaction in the system to a certain range, and then by using scaling properties obtain a precise information about the critical behavior of the true infinite system.

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

$$A_\infty(t)\simeq A_0 t^{-\rho}, \tag{3}$$

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. Then, analogous to the FSS hypothesis, it is assumed that for large finite range N and small t, $A_N(t)$ can be written as

$$A_N(t)=A_\infty(t)f(N/\xi_\infty), \tag{4}$$

where f is a homogeneous function with the following properties:

$$\lim_{x\to\infty} f(x)=1, \qquad \lim_{x\to 0} f(x)=\text{const}\times x^{\rho/\nu}. \tag{5}$$

By applying equation (4) 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

$$\xi_N(t^*)=(N/M)\xi_M(t^*). \tag{6}$$

The critical exponent of the correlation length can be obtained by expanding and linearizing Eq. (6) around t^*. Thus for the chain with a finite range of interaction N, the corresponding critical exponent ν_N can be written as

$$\nu_N^{-1}=\ln[\xi_N'(t^*)/\xi_M'(t^*)]/\ln(N/M)-1, \tag{7}$$

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 closed integer for better convergence.

The critical temperature and the critical exponent of the correlation length given by Eqs. (6) and (7) depend on the selected range of interaction N. In order to obtain the correct answer for the true Ising system, a proper method of extrapolation should be employed. On the basis of FSS analysis,[20] a power-law convergence for T_c and ν in the large limit of N is expected. Thus, in order to obtain the true critical temperature and the critical exponent of the correlation length, the results for $K_{c,N}(\equiv 1/T_{c,N})$ and ν_N^{-1} are fitted to the form

$$Y_N=Y_e+A/N^x \tag{8}$$

in the least-squares approximation (LSA). Y_e and x denote the extrapolated quantity and the exponent of the fitting, respectively. The calculations are performed by considering three largest values of N (=14, 16, 18), and the extrapolation of K_c is done for the whole range of $0<\sigma<1$. Since the behavior of the data for $\sigma=1$ is nonmonotonic, the simple convergence expression is not applicable anymore. However, the variation of data for the selected value of N is not very significant and therefore the extrapolation value can be obtained by fitting the data to a linear relation with $1/N$ [i.e., $x=1$ in Eq. (8)].

B. Transfer matrix

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

$$-\beta H=\sum_{i=1,3,\ldots}^{L-1}\left[\sum_{j=1,3,\ldots}^{N-1} K_j^{AB}(s_i s_{i+j}+s_{i+1}s_{i+j+1}) + \sum_{j=2,4,\ldots}^{N-2}(K_j^{AA}s_i s_{i+j}+K_j^{BB}s_{i+1}s_{i+j+1})\right], \tag{9}$$

where $K_j^{xy}=\beta J_{xy}/j^{1+\sigma}$ 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 two possible states of the spins, can be imagined as a system with 2^N possible states that interact only with their nearest neighbors.[7] The transfer matrix for the chain can be written as

$$\langle \mathbf{s}|\mathbf{T}|\mathbf{s}'\rangle=\exp\Bigg\{\sum_{k=1,3,\ldots}^{N-1} K_k^{AB}\left[\sum_{n=1}^{N-k} s_n s_{n+k}+\sum_{n=1}^{k} s_{N+n-k}s_n'\right] + \sum_{k=2,4,\ldots}^{N} K_k^{AA}\left[\sum_{n=1,3,\ldots}^{N-k-1} s_n s_{n+k} + \sum_{n=1,3,\ldots}^{k-1} s_{N+n-k}s_n'\right] + \sum_{k=2,4,\ldots}^{N} K_k^{BB}\left[\sum_{n=2,4,\ldots}^{N-k} s_n s_{n+k} + \sum_{n=2,4,\ldots}^{k} s_{N+n-k}s_n'\right]\Bigg\}, \tag{10}$$

where $s_n=1,-1$ is a member of the state vector $|\mathbf{s}\rangle$ with N components, i.e.,

$$|\mathbf{s}\rangle\equiv|s_1,s_2,\ldots,s_N\rangle. \tag{11}$$

Equation (10) can also be written as a product of N matrices T_n, where each matrix would add one more site to the column.[21] Considering the shape of the chain, we have

$$\mathbf{T}=\mathbf{T}_1^A\mathbf{T}_2^B\cdots\mathbf{T}_{N-1}^A\mathbf{T}_N^B, \tag{12}$$

where $\mathbf{T}_n^A$ and $\mathbf{T}_m^B$ would add nth site of A and mth site of B to the columns, respectively. There exists also a simple relation between these one-site matrices, i.e.,

$$(\mathbf{U}^T)^2\mathbf{T}_{n+2}^{A(B)}\mathbf{U}^2=\mathbf{T}_n^{A(B)}, \tag{13}$$

where $\mathbf{T}_{N+2}^B=\mathbf{T}_2^B$, $\mathbf{T}_{N+1}^A=\mathbf{T}_1^A$, and $\mathbf{U}$ is the translation operator in a direction perpendicular to the strip as given by

$$\langle \mathbf{s}|\mathbf{U}|\mathbf{s}'\rangle=\delta(s_1,s_N')\,\delta(s_2,s_1')\,\delta(s_3,s_2')\ \ldots\ \delta(s_{N-1},s_{N-2}')\times\delta(s_N,s_{N-1}'), \tag{14}$$

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

$$\mathbf{T}=[\mathbf{U}^2\mathbf{T}_{N-1}^A\mathbf{T}_N^B]^{N/2}=[\mathbf{U}(\mathbf{U}\mathbf{T}_{N-1}^A\mathbf{U}^T)\mathbf{U}\mathbf{T}_N^B]^{N/2}=[\tilde{\mathbf{T}}^A\tilde{\mathbf{T}}^B]^{N/2}=\tilde{\mathbf{T}}^{N/2}, \tag{15}$$

where

$$\langle \mathbf{s}|\tilde{\mathbf{T}}^B|\mathbf{s}'\rangle=\langle \mathbf{s}|\mathbf{U}\mathbf{T}_N^B|\mathbf{s}'\rangle=\delta(s_2,s_1')\,\delta(s_3,s_2')\cdots\delta(s_N,s_{N-1}')\times\exp\left[\sum_{m=1,3,\ldots}^{N-1}K_{N+1-m}^{BB}s_ms_N'+\sum_{m=2,4,\ldots}^{N}K_{N+1-m}^{AB}s_ms_N'\right], \tag{16}$$

$$\langle \mathbf{s}|\tilde{\mathbf{T}}^A|\mathbf{s}'\rangle=\langle \mathbf{s}|\mathbf{U}(\mathbf{U}\mathbf{T}_{N-1}^A\mathbf{U}^T)|\mathbf{s}'\rangle=\delta(s_2,s_1')\,\delta(s_3,s_2')\cdots\delta(s_N,s_{N-1}')\times\exp\left[\sum_{m=1,3,\ldots}^{N-1}K_{N+1-m}^{AA}s_ms_N'+\sum_{m=2,4,\ldots}^{N}K_{N+1-m}^{AB}s_ms_N'\right]. \tag{17}$$

It is interesting to note that the $\tilde{\mathbf{T}}^A$ and $\tilde{\mathbf{T}}^B$ matrices have only two nonzero elements in each row that reduces the required computer memory tremendously. Applying the standard derivation, the correlation length is obtained as

$$\xi_N=\frac{N}{\ln(\lambda_1/\lambda_2)}=\frac{2}{\ln(\mu_1/\mu_2)}, \tag{18}$$

where λ_1 and λ_2 are the largest and second-largest eigenvalues of $\mathbf{T}$, and similarly 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 numerical literature.[22]

III. RESULTS AND DISCUSSION

Our calculations are mainly concentrated on two distinct cases. In the first case, the interaction constants J_{AA} and J_{BB} are kept fixed to J and let the other constant J_{AB} vary between zero and $2J$. In the second case $J_{AB}=J_{BB}=J$, where the other constant J_{AA} varies between zero and $2J$.

The calculations of the critical temperature are performed in the classical ($0<\sigma\leqslant 0.5$) and nonclassical ($0.5<\sigma\leqslant 1$) regions. The translational symmetry requires that the scaling range of the interactions, M, in Eq. (6) to be chosen as $N-2$. The eigenvalues of the transfer matrix are calculated with ten digits and the values of $T_{c,N}$ are determined with an accuracy of $10^{-7}J/k$. The extrapolation of the critical temperature is performed for $N=14$, 16, 18. The results of the critical temperature for $J_{AA}=J_{BB}=J_{AB}=J$ are in good agreement with the reported results by Luijten and Blote in the classical region[12] and by Glumac and Uzelac in both the classical and nonclassical regions.[17]

The accuracy of the critical temperature and the critical exponent of the correlation length in the extrapolation procedure depends in a complicated way on the value of σ and the interaction constants. In the FRS method the convergence rate of the fixed points, as well as the accuracy of the extrapolated quantities, decreases as σ is reduced. As the value of the interaction constants, specifically the value of J_{AB} decreases and approaches zero, the range of the interaction reduces from N to $N/2$ and so the accuracy of the results decreases. Because of the mentioned difficulties the significant digits of the data presented in this report are determined from a comparison between the results of the extrapolation procedure for the maximal range of the interaction $N-2$ and N.[17]

The behavior of the critical temperature with respect to the interaction constants has been presented in Figs. 1 and 2 for the first and second cases, respectively. The Figs. 1(a) and 2(a) are the results for the classical and Figs. 1(b) and 2(b) are for the nonclassical region.

As is seen from the figures, for a fixed value of the interaction constants the slope of the curves decreases by increasing σ that is similar to the behavior of the critical temperature with respect to σ. For the first case where $J_{AA}=J_{BB}=J$, the slope of the figures is very large at $J_{AB}\simeq 0$ for large value of σ. It decreases with increasing the interaction constant J_{AB} and approaches rapidly some fixed value. The fast variation of the slope for small value of J_{AB} is obscured as σ decreases, such that for $\sigma=0.1$ it remains almost constant for the whole range of J_{AB}. For the second case where $J_{AB}=J_{BB}=J$, the slope of the curves (as seen in Fig. 2) increases slowly with increasing the interaction constant J_{AA} for the whole range $0\leqslant J_{AA}\leqslant 2J$. The variation of the slope is much pronounced for small value of σ and disappears as σ approaches one.

It seems as though the critical temperature behavior with respect to the interaction constants has originated from the presence of different interactions within the chain. In order to estimate the strength of each interaction, the corresponding contribution of that interaction in the critical temperature is calculated through mean-field approximation.[12] This can be divided into two parts, the interaction between different magnetic sites A and B with distances proportional to the nearest-neighbor distance by an odd number, and the one between similar sites A and A or B and B with the corresponding distances by an even number of the nearest-neighbor distance. Therefore, the critical temperature calculated through the mean-field approximation T_c^{MF} can be written as[12]

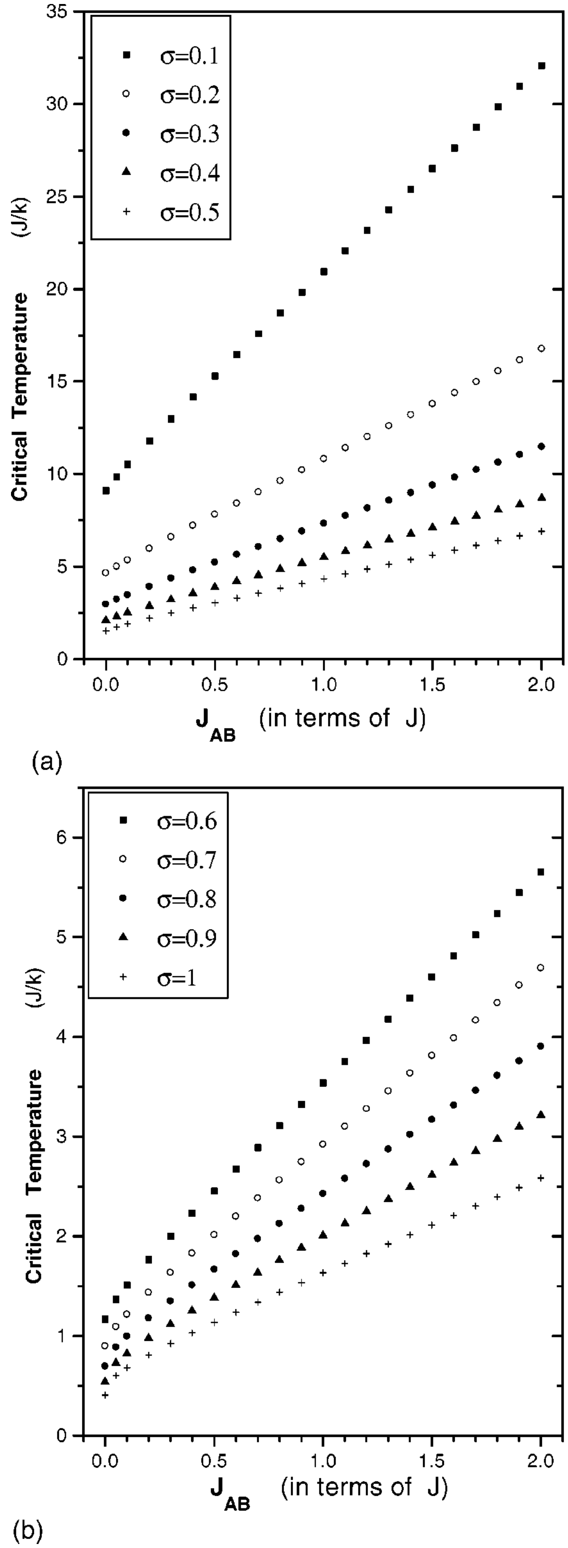

FIG. 1. The critical temperature as a function of the interaction constant J_{AB} where $J_{AA}=J_{BB}=J$ (a) for the classical region $0<\sigma\leqslant 0.5$ and (b) for the nonclassical region $0.5<\sigma\leqslant 1$.

$$T_c^{MF}(AB)=2\sum_{n=odd\ \ no.}\frac{J_{AB}}{n^{1+\sigma}}=2J_{AB}(1-2^{-(1+\sigma)})\zeta(1+\sigma), \tag{19}$$

for A-B interaction and

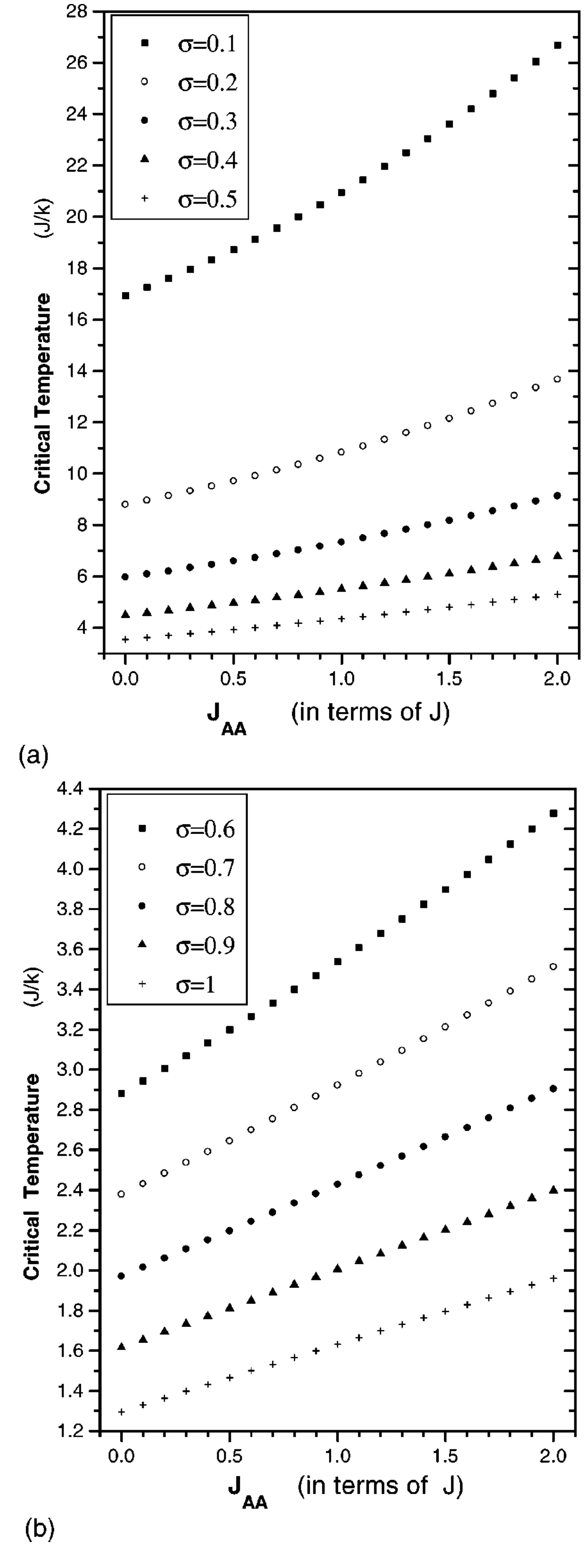

FIG. 2. The critical temperature as a function of the interaction constant J_{AA} where $J_{AB}=J_{BB}=J$ (a) for the classical region $0<\sigma\leqslant 0.5$ and (b) for the nonclassical region $0.5<\sigma\leqslant 1$.

$$T_c^{MF}(AA)=2\sum_{n=even\ \ no.}\frac{J_{AA}}{n^{1+\sigma}}=J_{AA}2^{-\sigma}\zeta(1+\sigma), \tag{20}$$

for A-A interaction and similarly for B-B. ζ is the Riemann zeta function. Therefore we have

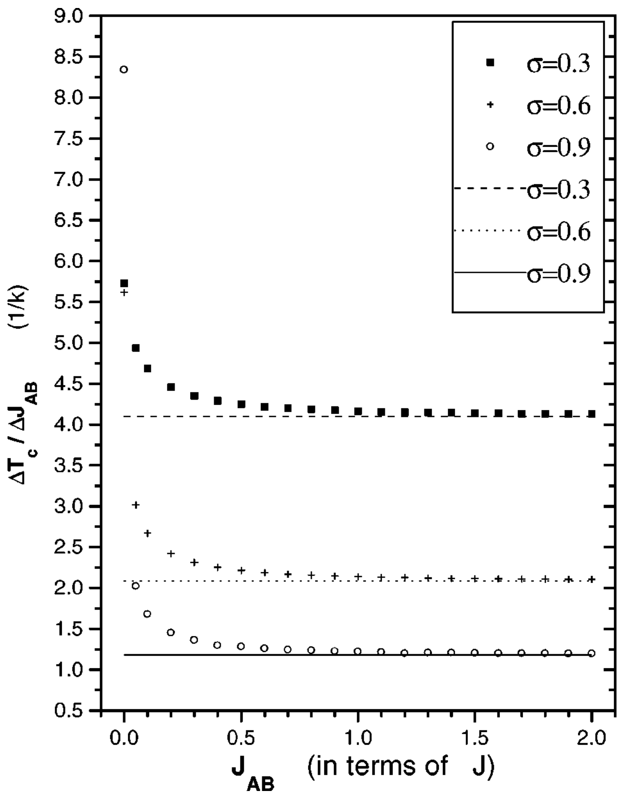

FIG. 3. The slope of the critical temperature, $\Delta T_c/\Delta J_{AB}$, as a function of the interaction constant J_{AB}. The points present the case where $J_{AA}=J_{BB}=J$ and the lines indicate the condition while $J_{AA}=J_{BB}=0$.

$$\frac{T_c^{MF}(AB)}{T_c^{MF}(AA)}=\frac{J_{AB}}{J_{AA}}(2^{1+\sigma}-1). \tag{21}$$

For $J_{AA}=J_{AB}$, this ratio is larger than 1 for all values of $\sigma>0$. (It is equal to 1 for $\sigma=0$ and 3 for $\sigma=1$). As J_{AB} approaches zero, the system become equivalent to two identical chains and behaves exactly the same as the case where $J_{AB}=J_{AA}=J_{BB}=J$ and the nearest-neighbor distances are doubled. Therefore, we have

$$T_c(J_{AA}=J_{BB}=J,J_{AB}=0)=\frac{T_c(J_{AB}=J_{AA}=J_{BB}=J)}{2^{1+\sigma}}. \tag{22}$$

The calculated results for the critical temperature at $J_{AB}=0$ and $J_{AB}=J$ both in the classical and nonclassical regions (see Fig. 1) are in good agreement with Eq. (22).

For a large value of σ, where the coupling between the chains is stronger than the interaction within the chains, the critical temperature around $J_{AB}\simeq 0$ rapidly increases and approaches a linear behavior for large value of J_{AB}. As σ decreases, the interaction between the chains and within the chains approach the same order and therefore the slope remains almost the same in the whole range of J_{AB}. For $\sigma=0.1$, where the interactions are almost in the same order, the linear dependence of the critical temperature on J_{AB} is clearly observed.

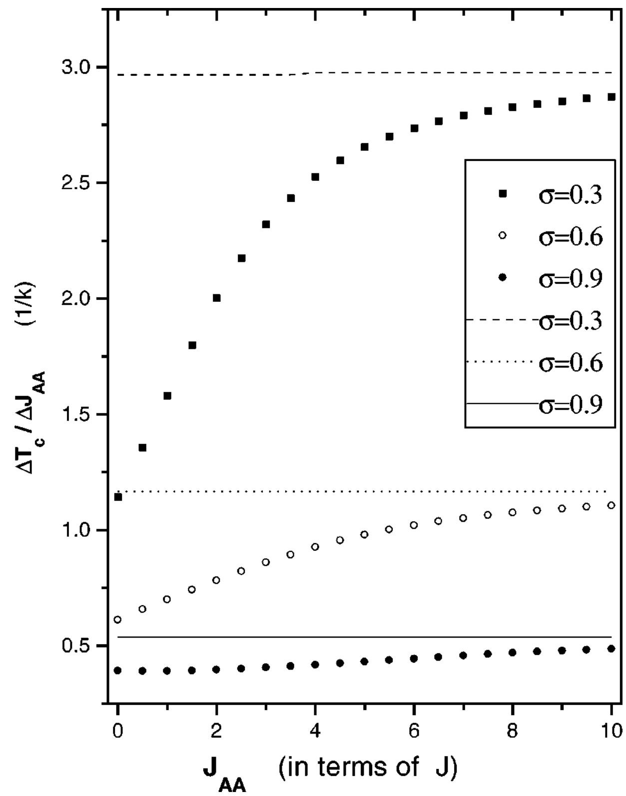

FIG. 4. The slope of the critical temperature, $\Delta T_c/\Delta J_{AA}$, as a function of the interaction constant J_{AA}. The points present the case where $J_{AB}=J_{BB}=J$ and the lines indicate the condition while $J_{AB}=J_{BB}=0$.

It is interesting to note that the slope of the critical temperature as a function of the interaction constant in both cases approaches a limiting value that is the same as the case where the other two interaction constants are zero. In order to observe this behavior more precisely, the slope of the critical temperature with respect to J_{AB} for both $J_{AA}=J_{BB}=J$ and $J_{AA}=J_{BB}=0$ (where the slope is constant) for three different values of σ in both the classical and nonclassical regions are plotted in Fig. 3 (the slope $\Delta T_c/\Delta J_{AB}$ is calculated for $\Delta J_{AB}=0.01J$ at each point). As is seen in the figure, the slope of the curves approaches rapidly its final limit as J_{AB} increases. The rapid change of the slope is more pronounced for large values of σ that indicates how fast the *A*-*B* interaction for large σ exceeds the other two interactions. The calculation shows that the difference between the slope at $J_{AB}=J$ and the corresponding limiting value is less than 3% for all three different values of σ.

The same calculation is also performed for the second case where the slope of the critical temperature as a function of J_{AA} for $J_{AB}=J_{BB}=J$ and $J_{AB}=J_{BB}=0$ is investigated. In this case, the variation of the slope is much slower than the first one. Therefore in order to see the behavior more clearly, the range of investigation is expanded to $J_{AA}=10J$ as shown in Fig. 4. It is seen that for small value of σ, where the *A*-*A* interaction is close to the other two interactions, the variation of the slope is relatively large so that the difference between the slope at $J_{AA}=10J$ and the limiting value is 3.5% for $\sigma=0.3$, which is smaller than 5.3% and 9.5% for $\sigma=0.6$ and 0.9, respectively.

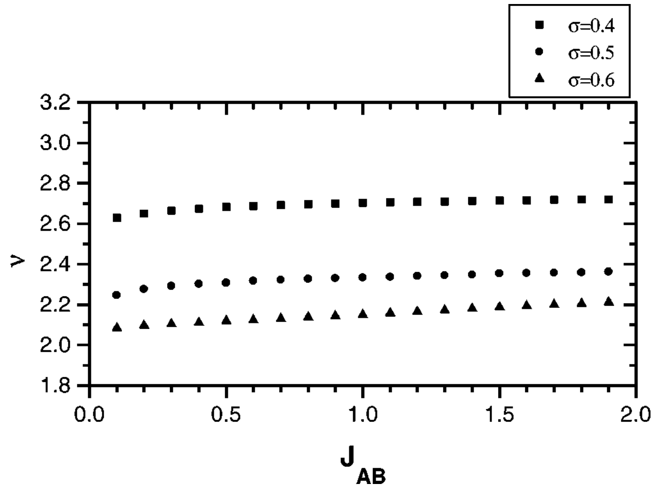

FIG. 5. The critical exponent of the correlation length as a function of the interaction constant J_{AB} where $J_{AA}=J_{BB}=J$ for different values of σ in the classical and the nonclassical regions.

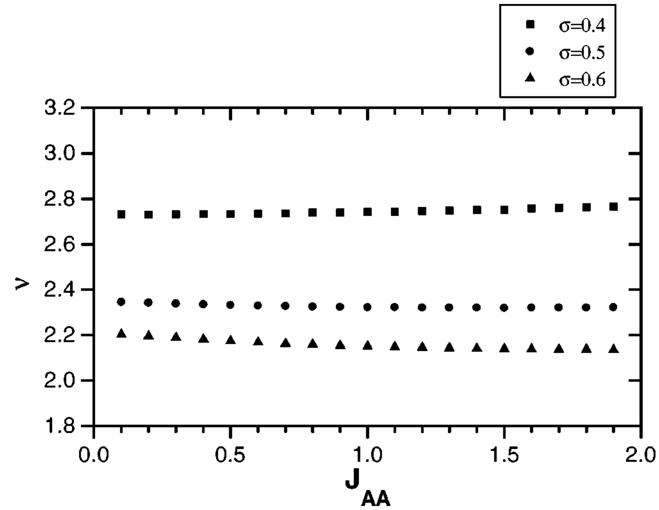

FIG. 6. The critical exponent of the correlation length as a function of the interaction constant J_{AA} where $J_{AB}=J_{BB}=J$ for different values of σ in the classical and the nonclassical regions.

The behavior of the critical exponent of the correlation length as a function of interaction constants J_{AA} and J_{AB} is studied in the classical and the nonclassical regions. Since the ν_Ns are determined by Eq. (7), where the derivative of the correlation length is involved, the accuracy of the results reduces to six or five significant digits. The extrapolated results are obtained by using Eq. (8) in the nonclassical region and by the relation $\nu_N^{-1}=B+A(M/N)^x$ in the classical region as suggested by the pioneers of the FRS method.[7] The results as a function of the interaction constants J_{AB} and J_{AA} are presented in Figs. 5 and 6, respectively. The calculations are performed for three different values of σ in the classical ($\sigma=0.4$) and the nonclassical ($\sigma=0.6$) regions and at the border $\sigma=0.5$. As is seen from Figs. 5 and 6, the critical exponent ν is independent of the interaction constants J_{AB} and J_{AA} with a good approximation and also is in good agreement with the results given for homogeneous chains by the other authors.[3,16,12] It should be mentioned that the small variation of ν (less than 6%) with respect to the interaction constants is mainly caused by the uncertainty in the method of calculation. As mentioned before, the uncertainty depends on the interaction constants and it is more pronounced for the case where the effect of A-B interaction is considered.

IV. CONCLUSION

The phase diagram of a magnetic Ising chain consisting of two different sites at alternating locations, with a long-range interaction in the form of $1/r^{1+\sigma}$ was investigated. The numerical analysis was performed using the FRS technique and developing a suitable transfer matrix. Regarding the two different kinds of interaction involved in the chain, the behavior of the critical temperature of the system as a function of each interaction constants (J_{AA},J_{AB}) was investigated. In order to understand the behavior of the system more precisely, the slope of the critical temperature as a function of each interaction constants was also studied. The results indicate that for the case where $J_{AA}=J_{BB}=J$, the interactions between different sites become rapidly dominant over the other interactions with a rate that depends on the value of σ. However, for the other case where $J_{AB}=J_{BB}=J$, the process is quite slow with a rate that still depends on the value of σ. Therefore, using the mean-field approximation, the contribution of each interaction in the critical temperature as a function of σ was also estimated. The results of the calculation show that the variation of the critical temperature with respect to σ is mainly caused by different types of interactions within the chain.

The study of the critical exponent of the correlation length indicates that the exponent is independent of the interaction constants in both the classical and nonclassical regions with a good approximation.

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