Ferromagnetism in one dimension: Critical temperature

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Ferromagnetism in one dimension is a observation which has been reported in a recent work [Gambardella *et al.*, Nature (London) **416**, 301 (2002)], and it is thought that anisotropy barriers are responsible in that relevant effect. In the present work, transitions between two different magnetic ordering phases are obtained as a result of an alternative approach. The critical temperature has been estimated by the Binder method. Ferromagnetic long-range interactions have been included in a special Hamiltonian through a power law that decays at large interparticle distance r as $r^{-\alpha}$ for $\alpha \geqslant 0$. If the range of interactions decreases ($\alpha \to \infty$), the trend of the critical temperature disappears, but if the range of interactions increases ($\alpha \to 0$), the trend of the critical temperature approaches to the mean field approximation. The crossover between these two limiting situations is discussed.

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Recently, much attention has been paid to structures of lower dimensionality.[1–7] As the space dimension of a physical system decreases, magnetic ordering tends to vanish as fluctuations become relatively more important. In particular, there is no spontaneous magnetization in several one-dimensional models, at any nonzero temperature; for instance, the isotropic spin-s Heisenberg model with finite range exchange interaction[4] and the classical gas model with hard-core and finite range interactions.[8] However, anomalies, such as anisotropy properties as microscopic long-range interactions, are not taken into account at finite temperature.

Regardless, ferromagnetism in one dimension has been recently reported for a monoatomic metal chain of Co constructed on a Pt substrate, with anisotropy barriers.[1] Experimental evidence was found that the monoatomic chains consist of thermally fluctuating segments of ferromagnetically coupled atoms. Chains evolve into a ferromagnetic long-range ordered state owing to the presence of anisotropy barriers below a threshold temperature.[1]

Much effort has been devoted to handling finite and infinite range interactions in computational systems by molecular dynamics and Monte Carlo simulations due to the absence of exact and analytical results. However, some special situations in one dimension can be studied exactly; for instance,

(1) mean field theory (the range of the interactions is infinite) and coupling to first neighbors;[9]

(2) $1/r$ and logarithmic potentials in a periodic media by infinite repetition of a central cell;[10]

(3) hard core classical gas;[8]

(4) isotropic spin-s model;[4]

(5) the thermodynamics of the Casimir force and the excess free energy of d-dimensional spherical model;[11] and

(6) a finite size scaling theory is developed when a particular family of interactions decays slowly with the distance,[12] etc.

In this paper, we present an approach to ferromagnetism in one dimension. More explicitly, the presence of infinite range microscopic interactions induces some important modifications to the thermodynamic properties of systems, some of which have not been yet characterized. Several evidences of a ferromagnetic state have been suggested due to the existence of long-range interactions in some physical systems in one dimension.[5,6,11–18]

The main goal of the present work is to obtain the critical temperature between two states of different magnetic ordering in a spin-$\frac{1}{2}$ Ising linear chain, where the range of interactions is, at least, comparable to the size of the chain. It is well known that there is a state of magnetic ordering in the mean field approximation. This approximation focuses on a single particle and assumes that the most important contribution to the interaction of such a particle with all particles is determined by the mean field due to the other particles. The configuration with lowest energy is one in which the spins are totally aligned. Before, it was emphasized that no magnetic ordering is observed for finite range of interaction (e.g., first neighbors); now, we illustrate the behavior of the system between infinite and finite ranges of interactions through a generic power law decaying as $1/r^{\alpha}$, where r is the distance between two particles and $0 \leqslant \alpha < \infty$ ($\alpha=0$ and $\alpha \to \infty$ close, respectively, to mean field and to independent spin approximations). Hence the main question that we answer in the present work is "How does the critical temperature depend on the range of the interaction?"

First, the critical temperature for a particular case (namely, $\alpha=2$) of this kind of system has been earlier reported by various authors and by the use of several techniques.[19,20] A comparison of results is done in a previous work, see, for instance, Ref. 21. Second, the critical temperature as a function of other values of α (namely, $1 < \alpha \leqslant 3/2$) was reported in Ref. 22. The critical temperature T_c tends to infinite as α tends to 1^+ (this is, $\lim_{\alpha \to 1} T_c \to \infty$) in the thermodynamic limit. In general, a strong dependence on the size of the system has been observed for such a model. Third, the thermodynamic limit is not reached for $\alpha \equiv 1$.

Previously, no results have been reported for $\alpha \leqslant 1$. In this work, we propose a model for this kind of system which allows one to calculate the critical temperature by standard methods in the thermodynamic limit for $0 \leqslant \alpha < \infty$. We carry out a numerical study through Monte Carlo procedure and we report direct results from our model, which considers information on the range of interactions.

We describe the model by the following Hamiltonian:

$$H = -\sum_{i,j=1}^{n} J(i-j)s_i s_j, \tag{1}$$

where $s_i = \pm 1\ \forall i$ and $(i-j)$ is the distance between two sites and n is the number of particles in every cell.

$$J(K) = \frac{1}{2}\sum_{l=-L}^{l=L} \frac{J_\alpha^L(n)}{|nl+K|^\alpha} \tag{2}$$

where

$$(2L+1)n = N \tag{3}$$

is the total number of particles in $2L+1$ repetition of a central configuration,

$$J_\alpha^L(n) = \frac{J}{2^\alpha}\frac{1-\alpha}{N^{1-\alpha}-1} = \begin{cases} \dfrac{1-\alpha}{2^\alpha}J/N^{1-\alpha} & \text{if } \alpha < 1 \\ \dfrac{1}{2}J/\ln N & \text{if } \alpha = 1, \end{cases} \tag{4}$$

where J is a positive parameter, $J_\alpha^L(n)$ measures the strength of the coupling that depends on the size n of the system, and $J_\alpha^L(n) \to (\alpha-1)J/2^\alpha$ if $\alpha > 1$.[23]

We consider a computational cell in one dimension with size n and we apply periodic boundary conditions through infinite replications of a central cell. Recently, the problem related to the periodic boundary conditions in systems with microscopic long-range interactions has attracted the attention of several authors (see, for instance, Refs. 21, 22, and 24–26). We apply periodic boundary conditions in a similar way which was recently discussed.[22] However, this way was already introduced by Curilef.[27]

Thermodynamics describes the behavior of systems with many degrees of freedom after they have reached a state of thermal equilibrium. Furthermore, their thermodynamic state can be specified in terms of a few parameters called state variables. At equilibrium, thermodynamic properties impose that macroscopic observables $[f(n)]$ be linear homogeneous functions of n (number of particles), this is $f(n) = nf_n$, where $f_n = f(n)/n$ and $f(\lambda n) = \lambda f(n)$ for very large n.[9,28] At this point, it is important to emphasize that by choosing the Hamiltonian of Eq. (1) (that contains ferromagnetic interactions that decay as a $1/r^\alpha$ law) we can find two facts.

(1) The nice property, about observables as a linear homogeneous function of n, is verified for thermodynamic functions, e.g., the internal energy.

(2) In a possible test of the linearity of thermodynamic observables; this is, $f(n) = f(\lambda n)/\lambda$, the factor $(2L+1)$ can be related to the parameter λ from Eq. (3).

As a consequence of the previous properties, we expect a weak dependence on the size of the system for results that arise from this model.

In the present computational study, we carry out on a linear chain with $L = 10^6$ and n between 10^2 and 10^3, to give effective sizes of the chain of the order from 10^8 to 10^9 particles according to Eq. (3), and several values of α. Standard techniques are taken into account to compute its normalized autocorrelation function $C(t)$, $C(t) \sim 1\%$, due to the large fluctuations near the critical point.

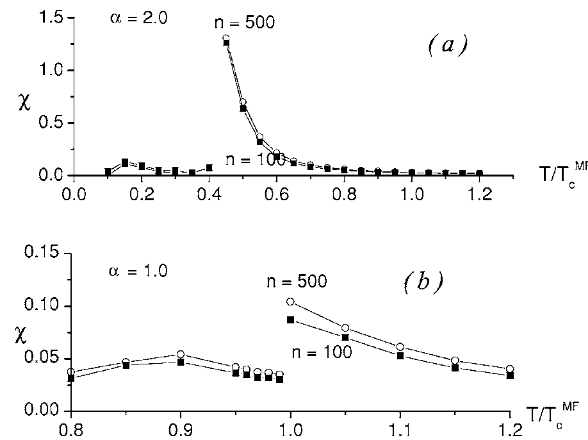

FIG. 1. The susceptibility as a function of the temperature T is depicted by (a) $\alpha = 2$ and (b) $\alpha = 1$, the values of n are indicated in the figure.

Now, we estimate the magnetic susceptibility as a function of temperature from the magnetization fluctuation,

$$\chi(T) = \begin{cases} \dfrac{N}{k_B T}(\langle s^2\rangle_n - \langle |s|\rangle_n^2) & \text{for } T < T_c \\ \dfrac{N}{k_B T}\langle s^2\rangle_n & \text{for } T > T_c, \end{cases} \tag{5}$$

where T_c is the critical temperature, $\langle s\rangle = 0$ for $T > T_c$. In Fig. 1, we depict a set of curves for the magnetic susceptibility as a function of a reduced temperature T/T_c^{MF}, where $T_c^{MF} = J_\alpha^L(n)/k_B$, where k_B is the Boltzmann constant. Ranges of interactions are given by (a) $\alpha = 2$ and (b) $\alpha = 1$, and sizes of the central cell are shown for $n = 100$ and 500, for $L = 10^6$. The total number of particles is given by Eq. (3). We believe that the trend of the magnetic susceptibility $\chi(T)$ suggests a discontinuity in Fig. 1. We relate to it a change of phase of the magnetic ordering. We represent data from simulations by circles and the linear interpolation, among circles, by lines in Fig. 1. We expect the trend of the magnetic susceptibility takes a behavior similar to the mean field approximation; this is because the magnetic susceptibility has an infinite jump at the critical temperature.

In the following, we estimate the specific heat as a function of the temperature from the energy fluctuation, which is given by

$$C(T) = \frac{N}{T^2}(\langle H^2\rangle_n - \langle H\rangle_n^2). \tag{6}$$

In Fig. 2, we depict the typical trend of specific heat. Again, we carry out numerical calculations for several values of n and α; namely, $n = 100, 500$ and $\alpha = 1, 2$. In addition, we observe a discontinuity for the specific heat at critical temperature.

In general, the phase transition can be characterized by several ways. A suitable approach to define the critical point in the finite system is the Binder method.[29] We expect a

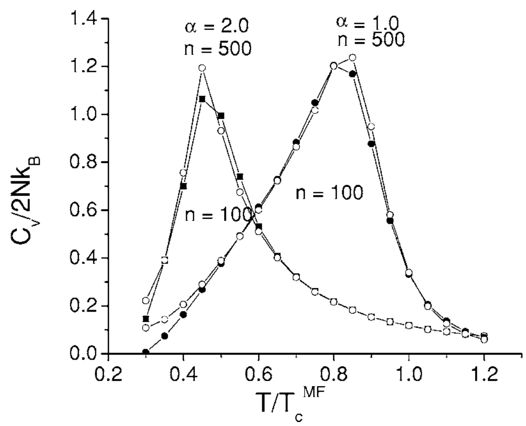

FIG. 2. The specific heat as a function of the temperature T is shown. The trend of these functions shows also a discontinuity. The values of $\alpha=1,2$ and $n=100,500$ are indicated in the figure.

standard behavior of phase diagrams for this kind of system. The Binder cumulant of fourth order is defined as

$$U_n = 1 - \frac{\langle s^4\rangle_n}{3\langle s^2\rangle_n^2}. \quad (7)$$

Cumulants U_n as a function of the temperature are intersected in a common point for several sizes of system n. This point is the critical temperature which depends on values of the parameter α. The typical behavior of the Binder cumulant U_n (or equivalent quantity $g_n=-3U_n$ called the renormalized coupling constant[30]) is rather stable under critical temperature; however, fluctuations can be important above the critical point. This property allows one to distinguish the critical point by a very simple graphical criterion.

In Fig. 3, we depict the critical temperature as a function of $1/\alpha$ for the magnetic ordering transition in the thermodynamic limit. We include error bars to represent a deviation of

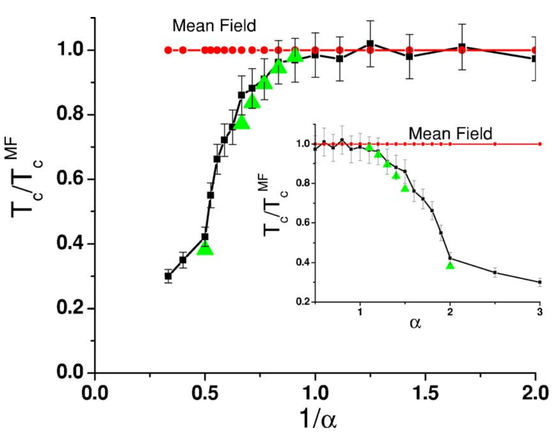

FIG. 3. (Color online) The critical temperature as a function of $1/\alpha$, the inverse of the range of the microscopic interaction, is depicted. The trend of T_c goes to zero when $1/\alpha\to 0$, namely $\alpha\to\infty$. In the inset is shown the trend of T_c as a function of α. Error bars represent a deviation of the 7% or less at each point of results. The critical temperature known from previous works (Refs. 16 and 21) is represented by solid triangles.

TABLE I. Comparison of our estimation of the critical temperature to previous results in the literature (Ref. 16).

α	T_c (this work)	$T_c=(1-\alpha)/2^\alpha\ K_c$
1.1	0.9689	0.9797309
1.2	0.9625	0.9438766
1.3	0.9101	0.8951426
1.4	0.8813	0.8367191
1.5	0.86	0.7714285

7% or less for the obtained values at each point of the critical temperature. Additionally, we include an inset in Fig. 3 to show the same fact for $0\leqslant\alpha\leqslant 3$. Both pictures are included to emphasize the following features about critical temperature.

(1) It is close to the mean field one for $\alpha\to 0$.

(2) It is lesser than the critical temperature given by the mean field approximation for $\alpha > 1$.

(3) It falls to zero for the short-range interaction regime (e.g., nearest neighbor) as it is expected.

(4) It is depicted as a function of $1/\alpha\to 0$ to remark that goes to zero while $\alpha\to\infty$.

(5) It is depicted as the crossover between two known limiting cases.

(6) It is recovered by the present model the known results for particular values of α; namely, $\alpha=1.1$, 1.2 1.3, 1.4, and 1.5 (Ref. 21) and $\alpha=2$.[22]

We can compare the critical temperature with earlier results presented in the literature. We have chosen Ref. 16 because the authors have made an exhaustive search of the critical couplings K_c as a function of α and compare their values to others.[31] In order to compare our critical temperatures to precedent results, it is necessary to make a simple transformation from Eq. (4) for $N\to\infty$ given by $T_c=(1-\alpha)/2^\alpha\ K_c$. The comparison is in Table I. In a similar way, for $\alpha=2$, our critical temperature is 0.4221 and we can compare it to a previous value 0.3816 obtained from Ref. 21. In Fig. 3, we represent the known critical temperature from previous works[16,21] by solid triangles.

In general, according to Table I, our estimation for the critical temperature is greater than the value obtained by the other authors previously. We expect that in the limit of short-range interactions $T_c\to 0$, the lower value could be more acceptable. Simulations for larger systems had been carried out in order to obtain accurate results in one dimension.[16] However, the numerical work is much more costly due to the enormous number of particles in systems ($n=300\,000$), in contrast to the method which has been implemented here, few particles in a cell and a big number of repetitions over all space. If replicas of the central cell increase, the time of computation does not practically suffer changes, because such time only depends on the number of particles on the central cell. Sometimes, computation facilities are not sufficient for filling the demands of resources that make simulations of many-body systems; then, it is very important to resort to an alternative numerical way.

On one hand, a simple theoretical argument given by Reichl[9] shows that a finite Ising chain in one dimension with a number of ferromagnetically coupled spins cannot exhibit a phase transition. If the external magnetic field goes to zero the order parameter $\langle s \rangle$ tends also to zero. Hence no spontaneous nonzero value of the order parameter is possible. On the other hand, another simple theoretical argument given by the same author[9] shows that the mean field theory predicts a phase transition at a finite temperature for a lattice in one dimension. Both arguments are not opposite between them. In the present point of view, the mean field theory (e.g., $\alpha=0$) approaches the case of every spin that interacts with each other without discriminating over the sites and an Ising chain is the limit whose interactions are very short ranged (e.g., $\alpha=\infty$). In this work, we discussed the crossover between both limiting cases, with a system of finite ferromagnetically coupled spins that obeys the Hamiltonian given by Eq. (1).

In summary, thermodynamic systems with interactions for $\alpha \leqslant 1$ are characterized by nonlinear homogeneous observables. We suggest in Eq. (4) the scaling $J/J_\alpha^L(n)$ to remove the nonlinearity from thermodynamic observables and we use that scaling to define the Hamiltonian in Eq. (1). Thus, if we suppose that the scaling represents the number of nearest neighbor spins, then the size of the system (the total number of spins in the chain) is always greater than the scaling for $0<\alpha \leqslant 1$. Both values, nearest neighbor and size of the system, are coincident for $\alpha=0$. In this way, we expected that a proper thermodynamic limit could be defined for $\alpha \leqslant 1$. The scaling is defined and revised by several authors (see, for instance, Ref. 5 and references therein). With such considerations, we can repeat the mean field approximation and we hope that its critical temperature comes to be exact in this problem. In addition, it is known that the most important problem about the thermodynamic behavior related to the systems with long-range interactions is the strong dependence on the size of systems. It is thought that no standard thermodynamic equilibrium is reached. In this work, we have presented a possible way to solve such a problem, for that reason, it is crucial to make a suitable choice of the Hamiltonian. Thermodynamic quantities do depend weakly on the size of the system as a result of the choice of the Hamiltonian suggested in Eqs. (1)–(4).

Finally, in the study and characterization of the phase transition and critical phenomena for systems with arbitrary range interactions, advances and suggestions are always very important to find appropriated models for calculating typical physical quantities.

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[1] P. Gambardella, A. Dallmeyer, K. Maiti, M. C. Malagoli, W. Eberhardt, K. Kern, and C. Carbone, Nature (London) **416**, 301 (2002).
[2] J. Dorantes-Davila and G. M. Pastor, Phys. Rev. Lett. **81**, 208 (1998).
[3] J. Shen, R. Skomski, M. Klaua, H. Jenniches, S. S. Manoharan, and J. Kirschner, Phys. Rev. B **56**, 2340 (1997).
[4] N. D. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).
[5] S. A. Cannas and F. Tamarit, Phys. Rev. B **54**, R12661 (1996).
[6] I. F. Herbut, Phys. Rev. B **58**, 971 (1998).
[7] P. Gambardella, M. Blanc, H. Brune, K. Kuhnke, and K. Kern, Phys. Rev. B **61**, 2254 (2000).
[8] L. van Hove, Physica (Amsterdam) **16**, 137 (1950).
[9] L. Riechl, *A Modern Course in Statistical Mechanics*, 2nd ed. (Wiley, New York, 1998).
[10] S. Curilef, Physica A **344**, 456 (2004).
[11] H. Chamati and D. M. Dantchev, Phys. Rev. E **70**, 066106 (2004).
[12] H. Chamati and N. S. Tonchev, Mod. Phys. Lett. B **17**, 1187 (2003); J. Phys. A **33**, L187 (2000).
[13] R. Mainieri, Phys. Rev. A **45**, 3580 (1992).
[14] E. Luijten and H. W. J. Blöte, Phys. Rev. Lett. **76**, 1557 (1996).
[15] E. Luijten and H. Messingfeld, Phys. Rev. Lett. **86**, 5305 (2001).
[16] E. Luijten and H. W. J. Blöte, Phys. Rev. B **56**, 8945 (1997).
[17] J. O. Vigfusson, Phys. Rev. B **34**, 3466 (1986).
[18] J. A. Cuesta and A. Sanchez, J. Stat. Phys. **115**, 869 (2004).
[19] P. W. Anderson and J. Yuval, J. Phys. C **4**, 607 (1971).
[20] J. F. Nagle and J. C. Bonner, J. Phys. C **3**, 352 (1970).
[21] E. Luijten, *Computer Simulation Studies in Condensed-Matter Physics XII* (Springer, Heidelberg, 2000), p. 86.
[22] S. Cannas, C. Lapilli, and D. Stariolo, Int. J. Mod. Phys. C **15**, 115 (2004).
[23] For a discussion of the behavior of this kind of expressions see, for instance, Ref. 5 and references therein. We remark that it has been originally proposed as a nonextensive scaling. An alternative model is studied here.
[24] J. Lekner, Physica A **157**, 826 (1989); **176**, 485 (1991).
[25] N. Groenbech-Jensen, Int. J. Mod. Phys. C **6**, 873 (1996).
[26] H. Fangohr, A. Price, S. Cox, P. de Groot, G. Daniell, and K. Thomas, J. Comput. Phys. **162**, 372 (2004).
[27] S. Curilef, Int. J. Mod. Phys. C **11**, 629 (2000).
[28] D. Ruelle, *Statistical Mechanics* (Imperial College Press and World Scientific, Singapore, 1999).
[29] K. Binder and D. W. Heermann, *Monte Carlo Simulation in Statistical Physics An Introduction*, 4th ed. (Springer, New York, 2002).
[30] M. N. Barber, R. B. Pearson, D. Toussaint, and J. L. Richardson, Phys. Rev. B **32**, 1720 (1985).
[31] The reader can be addressed to Table III of Ref. 16 and to see previous results for K_c.