A proper choice of the Ising model order parameter

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The impossibility of a phase transition in one-dimensional (1D) systems with short-range interactions has been established after the publication of the Mermin-Wagner theorem. Nonetheless, many theoretical works have pursued such a transition under different arguments. The development of heteroepitaxy techniques ushered in the manufacturing of continuous, extreme low dimensional metal matrices on non magnetic substrates, allowing experimental characterization and theoretical studies of 1D magnetic systems. For instance, the experimental observation of an 1D chain of Co atoms deposited on a Pt surface enduring a ferromagnetic phase at a temperature around 15 K seems to contradict classical theoretical predictions whether there are true thermodynamic phase transitions in 1D systems with short range interactions. Some attempts to explain this apparent discrepancy have been made. Curilef et al. investigated the critical temperature of the Ising model including a long-range term through a power law that decays over large interparticle distances. However they made no comparisons to the results of Ref. In its turn Li and Liu proposed a Heisenberg model with a large magnetic anisotropy and an additional external magnetic field to describe a monatomic chain of Co. Afterwards, Vinhigni et al developed a combined experimental and theoretical study to explain the behavior of the magnetization of 1D magnetic systems, using the Heisenberg model with an anisotropic term, solved by the transfer matrix technique. Recently a study was performed on the magnetic properties of an 1D Au-Co chain on a copper surface using the density functional theory and kinetic Monte Carlo (KMC). They performed a KMC simulation of a 1D chain of Heisenberg anisotropic magnets taking the module of the magnetization as the order parameter. They found a phase transition at non zero temperature. The authors argued that this does not violate the Mermin-Wagner theorem due to the nonzero anisotropic term.

The foregoing works treated an 1D magnetic chain using a Heisenberg Hamiltonian with an additional anisotropic or a long-range term. Notwithstanding the first approximation for an 1D magnetic system should be the Ising model, for which we have now a new scenario. Well-established theories should be revisited. In 1966, Kadanoff determined the scaling laws for a second order phase transition of the Ising model based on a Widom’s argument on the consequences of considering the free energy as a homogeneous function of parameters describing the proximity to the critical point, such as $\epsilon = (T - T_c)/T_c$. He assumed that a large lattice can be divided into smaller ones of still larger sizes, but much smaller than the system correlation length. The zeroth order approximation is based on the assumption that the free energy of an isolated system of side $L$ is an analytical function for $\epsilon$, but singular for the system size. Kadanoff considered two possibilities for the specific heat divergence which is given by $\epsilon^{-\alpha}$. The first one assumes the exponent $\alpha \neq 0$ and the second one $\alpha = 0$, the latter representing the 2D Ising model since the results obtained with $\alpha = 0$ corroborate the experiments. Hence, we can state that in a second-order phase transition the specific heat is an analytical function of temperature and singularities occur as the system size increases.

Another important issue is the Landau’s theory of second-order phase transitions, which is based on a continuous transition from an ordered state to a disordered one. A second-order phase transition may be related to some symmetry property, such as the Curie point where a ferromagnetic substance passes into the paramagnetic phase. To describe this phase transition, Landau defined an order parameter as a quantity that assumes nonzero values (positive or negative) for an ordered phase.
and zero for the disordered one. Furthermore, he proposed that the singularity is observed when the thermodynamic potential is expanded in terms of the order parameter. For a magnetic system the property that has such a behavior is the magnetization which is moreover proportional to the system size.

The standard model to study second-order phase transitions was proposed by Wilhelm Lenz in the doctoral work of his student Ernst Ising to describe the behavior of a magnetic material in one dimension. Their solution showed that at zero magnetic field a second order phase transition occurs only at \( T = 0 \).

The 1D Ising model is widespread in literature, with the Hamiltonian given by

\[
\mathcal{H}_L = -J \sum_{i=1}^{L} \sigma_i \sigma_{i+1} - H \sum_{i=1}^{L} \sigma_i,
\]

where \( \sigma_i \) is a lattice variable that can assume the values \( \pm 1 \), which are associated with the spins, \( J \) is the coupling constant that fixes the energy scale, \( H \) is the external magnetic field, and \( L \) is the number of sites. The magnetization per site of the system is given by

\[
m = \frac{1}{L} \sum_{i=1}^{L} \sigma_i.
\]

The order parameter must indicate the transition of a particular ordered state to a disordered one. Taking the magnetization as the order parameter and \( H \neq 0 \) we have that its value per site in the ground state configuration is conditioned to the field sign, being \( m_+ = 1 \) when the field is positive and \( m_- = -1 \) when negative. If \( H = 0 \) there is a singularity where both phases have the same probability. This situation is the same as described by Landau for a first order transition, i.e. an equilibrium between two phases. Calculating the mean magnetization at \( T = 0 \) we have

\[
\langle m \rangle = m_+ P_{\uparrow \uparrow \uparrow} + m_- P_{\downarrow \downarrow \downarrow},
\]

where \( P_{\uparrow \uparrow \uparrow} \) (\( P_{\downarrow \downarrow \downarrow} \)) denotes the probability of a configuration with all spins up (down). Substituting the values of \( m_+ \) and \( m_- \) we obtain \( \langle m \rangle = 0 \). At high temperatures the most probable configurations are those which energies match \( k_B T \) and in the limit \( T \to \infty \) they are configurations where \( \mathcal{H}_L = 0 \), the maximum energy. For these configurations the magnetization is zero since the number of positive and negative spins is the same. Hence, if \( H = 0 \), the magnetization does not behave as an order parameter in the study of a second order phase transition in the 1D Ising model, since it does not distinguish an ordered configuration from a disordered one.

Otherwise, if we choose as the order parameter the module of the magnetization per site

\[
|m| = \frac{1}{L} \left| \sum_{i=1}^{L} \sigma_i \right|,
\]

such that \( |m_+| = |m_-| = 1 \), then we obtain at \( T = 0 \)

\[
\langle |m| \rangle = P_{\uparrow \uparrow \uparrow} + P_{\downarrow \downarrow \downarrow} = 1,
\]

whereas for a disordered configuration we get \( \langle |m| \rangle = 0 \).

Now if we write the Hamiltonian in terms of this order parameter

\[
\tilde{\mathcal{H}} = -J \sum_{i=1}^{L} \sigma_i \sigma_{i+1} - |H| \sum_{i=1}^{L} \sigma_i,
\]

then we can calculate a partition function \( \tilde{Z} \) using \( \tilde{\mathcal{H}} \) such that when \( H = 0 \) it will yield reliable results. In this case the solution via transfer matrix becomes unfeasible, because the module in the second term is not factorable. Since an exact solution for an infinite lattice in this case is not available, what can be done is the direct calculation of the partition function for small sizes.

Defining \( E_j \) and \( M_j \) as

\[
E_j = \sum_{i=1}^{L} \sigma_i \sigma_{i+1} \quad \text{and} \quad M_j = \sum_{i=1}^{L} \sigma_i,
\]

where the index \( j \) denotes a particular configuration, we can write \( \tilde{\mathcal{H}} = -J E_j - |H|M_j \) and the partition function may be written as

\[
\tilde{Z} = \sum_j e^{\beta (JE_j + H|M_j|)},
\]

where the sum runs over all possible configurations. In terms of the joint density of states \( g_L(E, M) \) for a finite lattice of size \( L \)

\[
\tilde{Z}_L = \sum_{E=-L}^{L} \sum_{M=-L}^{L} g_L(E, M) e^{\beta (JE + H|M|)}
\]

\[
= \sum_{E=-L}^{L} \sum_{M=0}^{L} g_L(E, M) e^{\beta (JE + HM)},
\]

where

\[
g_L(E, M) = \begin{cases} g_L(E, -M) + g_L(E, M), & \text{if } M \neq 0; \\ g_L(E, M), & \text{if } M = 0. \end{cases}
\]

It is worth noting that the Mermin-Wagner theorem does not apply to this case, since its demonstration assumes that the partition function can be factored.

In Fig. \( n \) we depict the possible configurations for a \( L = 4 \) lattice, from which we can write the partition function for this lattice size as

\[
\tilde{Z}_4 = \tilde{g}_4(4, 4) e^{4\beta H} e^{4\beta J} + \tilde{g}_4(0, 2) e^{2\beta H}
\]

\[
+ \tilde{g}_4(0, 0) + \tilde{g}_4(-4, 0) e^{-4\beta J}
\]

\[
= 2 e^{4\beta H} e^{4\beta J} + 8 e^{2\beta H} + 4 + 2 e^{-4\beta J},
\]

where \( \tilde{g}_4(E, M) \) is the number of configurations with dimensionless interaction energy \( E \) and order parameter \( M \). One can see that \( \tilde{g}_4(4, 4) = 2, \tilde{g}_4(0, 2) = 8, \)
$$E = 4 \quad g(4, 4) = 1 \quad g(4, -4) = 1$$
$$M = 4$$

$$E = 0$$
$$M = 2$$
$$g(0, 2) = 4 \quad g(0, -2) = 4$$

$$E = 0$$
$$M = 4$$
$$g(0, 0) = 4$$

$$E = -4$$
$$M = 0$$
$$g(-4, 0) = 2$$

FIG. 1. Spin configurations for \(L = 4\). The first represents two configurations, the second eight, and so forth. \(g(E, M)\) enumerates the states considering the magnetization as the order parameter, while \(\tilde{g}(E, M)\) represents the degeneracy when the order parameter is the module of the magnetization.

\(\tilde{g}_4(0, 0) = 4\) and \(\tilde{g}_4(-4, 0) = 2\), where the first term corresponds to the ordered states, the second one to the configurations with one unpaired spin and the remaining to configurations with two unpaired spins, in which case they may be neighbors or not, corresponding to the terms \(\tilde{g}_4(0, 0)\) and \(\tilde{g}_4(-4, 0)\), respectively.

Using the same counting process for \(L = 8\) we obtain

$$\tilde{Z}_8 = 2e^{8\beta H}e^{8\beta J} + 16e^{6\beta H}e^{4\beta J} + e^{4\beta H}(16e^{4\beta J} + 40) + e^{2\beta H}(16e^{4\beta J} + 64 + 32e^{-4\beta J}) + 8e^{4\beta J} + 36 + 24e^{-4\beta J} + 2e^{-8\beta J}. \quad (9)$$

Taking the free energy as \(\tilde{F}_L = -k_B T \ln \tilde{Z}_L\), we obtain the magnetization as \(\tilde{M}_L = \lim_{H \to 0} (\frac{\partial \tilde{F}_L}{\partial H})\), yielding

$$\tilde{M}_4 = 4 \frac{1 + 2e^{-4\beta J}}{1 + 6e^{-4\beta J} + e^{-8\beta J}} \quad (10)$$

and

$$\tilde{M}_8 = 8 \frac{1 + 12e^{-4\beta J} + 18e^{-8\beta J} + 4e^{-12\beta J}}{1 + 28e^{-4\beta J} + 70e^{-8\beta J} + 28e^{-12\beta J} + e^{-16\beta J}}. \quad (11)$$

Inspecting the numerators and denominators of the two quantities above we see that they can be described by the following series

$$N = \sum_{k=0}^{L/2} \left( \frac{L}{k} \right) e^{-4k\beta J} \quad (12)$$

$$D = \sum_{k=0}^{L/2} \left( \frac{L}{2k} \right) e^{-4k\beta J} \quad (13)$$

where \(\lfloor \cdot \rfloor\) denotes the largest integer not greater than the argument and \(L\) should be a power of 2.

In order to confirm these predictions, we carried out entropic sampling simulations for \(L = 4, 8, 256, 512,\) and 1024 to construct the joint density of states. Entropic sampling simulations are based on the Wang-Landau method[13] where we introduced some changes to improve accuracy and help saving CPU time[14–16]. We halt the simulations when the sixteenth Wang-Landau level \((f_{15})\) becomes flat. Once the joint density of states is available we can obtain the canonical averages as

$$\langle E^k M^l \rangle_{T,H} = \frac{\sum_{E,M=-L}^{L} E^k M^l g(E,M)e^{-\beta(-JE-HM)}}{\sum_{E,M=-L}^{L} g(E,M)e^{-\beta(-JE-HM)}}, \quad (14)$$

$$k, l = 0, 1, 2, \ldots,$$

which are present in the estimate of thermodynamic quantities as mean energy, magnetization, heat capacity, susceptibility and cumulants.

The joint density of states for a lattice of size \(L\) can be used in Eq. (14). Also, setting \(k = 0, l = 1\) and taking |\(M|\) before \(g_L(E, M)\), we obtain via simulations the same magnetizations for these lattice sizes for \(H = 0\) as

$$\langle |M| \rangle_{T,L} = \frac{\sum_{E=-L}^{L} \sum_{M=-L}^{L} |M| g_L(E, M)e^{\beta J E}}{\sum_{E=-L}^{L} \sum_{M=-L}^{L} g_L(E, M)e^{\beta J E}}. \quad (15)$$

In Fig. 2 we display the analytical results with lines and those of the simulations with dots for \(L = 4, 8, 256, 512,\) and 1024, assuming \(J = 1\). One can see that they match with great accuracy. It is also clear from the behavior of these magnetizations that the system displays finite-size effects, suggesting a finite-size scaling study. It is important to note that for lattice sizes greater than 8 the simulations corroborate our conjectures on the series pointed out above. The analytical expression of the partition function for \(L > 8\) and not a power of 2 is unfeasible. Nonetheless, the simulations are free to go ahead to as large and diverse lattices as necessary. Following Refs. [17, 18] we can define a set of thermodynamic

FIG. 2. Magnetization as function of temperature exhibiting a clear finite-size scaling behavior. The lines represent the analytical results, and the dots the simulated ones. The error bars are smaller than the symbols.
We performed simulations for exponent $\nu$ temperature. We thus see that the proper choice of the order parameter instead of the magnetization as the order parameter instead of the magnetization which on the average does not distinguish the ordered state from the disordered one, reveals the existence of a second order phase transition with a finite and well-defined critical temperature for the 1D Ising model, in contrast to the belief that such a transition would be impossible, as stated by the Mermin-Wagner theorem. However, as explained above, we see that it does not apply to the present case, once the factorization of the partition function becomes impossible when we take the module of the magnetization as the order parameter instead of the magnetization itself.

Our results open up a wide range of opportunities to understand phase transitions in one dimension and may have potential ramifications and applications, leading subsequently to possible advances in a much broader context.

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quantities related to logarithmic derivatives of the magnetization that scales as

$$V_j \approx \frac{1}{\nu} \ln L + V_j(tL^{1/\nu})$$

(16)

for $j = 1, 2, ..., 6$, where $t = (T - T_c)/T_c$ is the reduced temperature.

These cumulants allow to estimate the critical exponent $\nu$ before determining the critical temperature. We performed simulations for $L = 256, 320, 384, 448, 512, 640, 768, 896, 1024, \text{ and } 1152$ with $n = 24, 24, 20, 20, 20, 16, 16, 16, 12, \text{ and } 12$ independent runs for each size, respectively. In Fig. 3 we depict the behavior of these quantities, obtaining $1/\nu = 0.34159(72)$ as the mean value of the slopes of the six best fitting straight lines, yielding $\nu = 1/(1/\nu) = 1/(1/\nu)^2 \Delta(1/\nu) = 2.9274(33)$. Now, with the correlation length critical exponent $\nu$ well determined we can use the finite-size scaling relation

$$T_c(L) = T_c + aL^{1/\nu},$$

(17)

where $a$ is a constant, then allowing the determination of $T_c$ for an infinite lattice. This relation is valid for the quantities $\chi, D_{K_2}, D_{K_3}, D_{K_4}, \text{ and } U_4$, defined in Refs. [17, 18]. For an infinite lattice ($L \to \infty$) we obtain five estimates for the critical temperature, the mean value yielding $T_c = 0.171008(63)$.

Our result can be compared with the experimental result reported in Ref. [6], where a transition temperature of $15 \pm 5$ K was obtained with the definition of the value of $2J = 15$ meV for the coupling constant. We then obtained our critical temperature as $T_c = 0.171008(63)J/k_B = 14.8835(55)$ K, where $k_B = 8.6173324(78) \times 10^{-5}$ eV/K in excellent agreement with the experiment.

We thus see that the proper choice of the order parameter for the 1D Ising model as the module of the magnetization, and not simply as the magnetization which on the average does not distinguish the ordered state from the disordered one, reveals the existence of a second order phase transition with a finite and well-defined critical temperature for the 1D Ising model, in contrast to the belief that such a transition would be impossible, as stated by the Mermin-Wagner theorem. However, as explained above, we see that it does not apply to the present case, once the factorization of the partition function becomes impossible when we take the module of the magnetization as the order parameter instead of the magnetization itself.

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