No or Diffuse Phase-Transition With Temperature in One-dimensional Ising Model?

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No or diffuse phase-transition with temperature in one-dimensional Ising model?

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Abstract

For nearly a century since Ising model was proposed in 1925, it is agreed that there is no phase-transition with temperature in the one-dimensional based on no global-spontaneous-magnetization in whole temperature region. In this letter, the exact calculation of local-spontaneous-magnetization shows that a diffuse phase-transition with temperature occurs in one-dimensional Ising model. In addition, although diffuse phase-transition phenomenon is common in the systems of heterogeneous-components and small-sizes etc., there is no accurate prediction of corresponding theoretical models so far, so the present works lay the theoretical foundation of this kind of phase-transition.

In the nearly 100 years since Ising model (IM)$^1$, one of the most important microscopic models of phase-transition$^{2-8}$, was proposed in 1925, it is agreed that there is no temperature dependent phase-transition in the one-dimensional. This is because the global-spontaneous-magnetization of the model system is zero in whole temperature range, i.e. there is no global-spontaneous-magnetization$^{1,2}$ as shown in the Supplementary Information (SI).

However, the absence of global-spontaneous-magnetization does not deny the existence of short-range local-spontaneous-magnetization in one-dimensional-IM (1D-IM). In this paper, the local-spontaneous-magnetization with temperature and size in the model is calculated accurately, and the results show that 1D-IM has a diffuse phase-transition with temperature$^9$-13. In other words, our conclusion subverts the century consensus in this model.

Results

The Hamiltonian ($H_{1D-IM}$) of one-dimensional Ising model (1D-IM) is,

$$H_{1D-IM} = \lim_{N \to \infty} \left[ -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} \right]$$

in which $\sigma_i$ is the ith spin and $\sigma_i = \pm 1$, $J$ the interaction energy constant between the nearest-neighbor spins, and $N$ the total number of spins in the model system (Fig. S1).

In the model, the local magnetic moment ($s^r_l$) including $l$ nearest-neighbor spins is,

$$s^r_l \equiv \mu \sum_{i=0}^{l-1} \sigma_{r+i}$$

where $\mu$ is the magnetic moment of a spin, and $r$ expresses an arbitrary reference site.
Fig. 1. For series $T$, (A) local-spontaneous-magnetization ($m^l_s$) and (B) relative local-spontaneous-magnetization ($\delta^l_s$) vs local spin number ($l$) in one-dimensional Ising model.

To describe the temperature dependence of the amplitude of $s^l_i$ (excluding the orientations corresponding to its signs) in this paper, the local-spontaneous-magnetization ($m^l_s$) is defined as (see SI and METHODS),

$$m^l_s \equiv \frac{1}{l} \lim_{n \to \infty} \frac{1}{Z_n} \sum_{\sigma_i=\pm 1, \cdots, \sigma_n=\pm 1} (s^l_i)^2 \exp \left[ \frac{J}{k_B T} \sum_{i=1}^{n-1} \sigma_i \sigma_{i+1} \right]$$

$$= \frac{\mu}{l} \sqrt{2 \left[ \frac{l - \gamma^l}{1 - \gamma} - \frac{\gamma(1 - \gamma^{l-1})}{(1 - \gamma)^2} \right]} - l \tag{3}$$

here $k_B$ is Boltzmann constant, $T$ the temperature of the heat bath in which the one-dimensional spin chain is located, $Z_n$ the partition function of the spin orientation ensemble of 1D-IM (SI), and $n$ the spin number of the subsystems in the ensemble (Fig. S1), and $\gamma \equiv \tanh \left( \frac{J}{k_B T} \right)$.

Obviously, $m^\infty_s$ is the global stochastic magnetization when $l \to \infty$. From Eq. 3, we can get that $m^\infty_s = 0$ except $T \to 0$, which is consistent with the past result$^{12}$.

Fig. 1A shows $m^l_s$ vs $l$ for series $T$, and it can be seen that: (i) At high temperature (e.g. $T = 5.00J/k_B$), $m^l_s$ decreases rapidly with increasing $l$, which indicates that the spatial scale
of local-spontaneous-magnetization is small; and (ii) At low temperature (e.g. $T = 0.15J/k_B$), $m_s^l \rightarrow \mu$ in a large range of $l$, which states clearly that the local-spontaneous-magnetization regions not only has a large spatial scale, but also almost all the spins in the regions have the same orientation.

Discussion

According to Landau theory\cite{14}, the order parameter is the essential to phase-transition, which characterizes the relative change of the low to high temperature phase. Therefore, in order to describe the relative variation of $m_s^l$ to $m_s^l(T \rightarrow \infty)$, the relative local-spontaneous-magnetization ($\delta_s^l$) is introduced here,

$$\delta_s^l \equiv \frac{m_s^l - m_s^l(T \rightarrow \infty)}{\mu} \quad (4)$$

In fact, $m_s^l(T \rightarrow \infty)$ represents the autocorrelation ($\sigma_i^2$) of a spin (Eq. 3 and M5 in METHODS), and of course has nothing to do with the phase transition process.

At series $T$, $\delta_s^l$ vs $l$ is shown in Fig. 1B, which indicates that for all temperatures, $\delta_s^l$ has a single diffuse peak as a function of $l$. In this paper, the maximum value of $\delta_s^l$ is expressed as Fig. 2. (A) characteristic spontaneous magnetization ($\eta_c$) and its characteristic spatial size ($l_c$), as well as (B) $-\partial \eta_c/\partial t$ and heat capacity per spin ($c_s$) in 1D-IM vs reduced temperature ($t \equiv k_BT/J$). Inset of Fig. 2A shows static susceptibility ($\chi^B_s$) per spin vs $t$ for a series of external magnetic fields ($B$).
77 $\eta_c$, and the corresponding value of $l$ as $l_c$. Obviously, $\eta_c$ and $l_c$ can be used as the
78 characteristic parameters to describe the local-spontaneous-magnetization and its spatial size,
79 so here $\eta_c$ is called the characteristic spontaneous magnetization and $l_c$ the characteristic
80 spatial size of $\eta_c$ in 1D-IM. Moreover, the dispersion of the $\delta^1$ peak shows that both the size
81 of the local-spontaneous-magnetization regions and its internal magnetization have obvious
82 distributions.
83
84 $\eta_c$ and $l_c$ vs $T$ (Fig. 2A) show that with decreasing $T$: (i) $\eta_c$ first increases slowly, then
85 rapidly, and slowly again. It should be noted that at high temperature, $\eta_c$ is still not zero (e.g.
86 $\eta_c = 0.10$ when $T = 3.82/\text{k}_B$). In addition, $\eta_c \to 1$ at nonzero low temperature (e.g. $\eta_c =
87 0.9999$ for $T = 0.07/\text{k}_B$); and (ii) $l_c$ first increases slowly and then rapidly. For example,
88 $l_c = 4$ when $T = 3.82/\text{k}_B$, and $l_c = 10^3$ for $T = 0.07/\text{k}_B$ (if the lattice parameter of 1D-
89 IM is assumed to be 0.5 nanometers, the characteristic size of the local-spontaneous-
90 magnetization region will reach the macroscopic ~ 5 centimeters). These results state clearly
91 that in 1D-IM, there exists a diffuse transition between the nanoscale regions of small
92 spontaneous magnetization at high temperature and the macroscopic domains of large
93 spontaneous magnetization at low temperature.
94
95 By comparing the order parameters$^{10-13}$, heat capacity$^{15-17}$, and domain structure
96 evolution$^{18-20}$ of existing diffuse phase-transition, with the diffuse variation of $\eta_c$, the diffuse
97 peak$^{1,2}$ of heat capacity ($c_s$) per spin (SI and Fig. 2B), and the diffuse transition between the
98 nanoscale regions of local-spontaneous-magnetization to the macroscopic domains as a
99 function of $T$, it can be concluded that a diffuse phase-transition with temperature occurs in
100 1D-IM.
101
102 According to the method of reference$^{21}$, the temperature corresponding to the maximum
103 of $-\frac{\partial \eta_c}{\partial T}$ is defined as the characteristic temperature ($T_p$) of diffuse phase-transition in 1D-IM,
104 and it is obtained $T_p = 0.32/\text{k}_B$ (Fig. 2B). It should be pointed out that $T_p$ is lower than the
105 peak temperature ($T_d = 0.83/\text{k}_B$) of $c_s$. For second-order or continuous phase-transition, the
106 peak temperatures of heat capacity and the negative of the differential of order parameter to $T$
107 are equal to each other$^{14,22,23}$, so the authors thinks that the difference between $T_p$ and $T_d$ just
108 reflects the dispersion of the diffuse phase-transition. In order to describe this dispersion, the
109 dispersion degree ($\varphi$) of the diffuse phase-transition is proposed as,
110
111 $\varphi \equiv \frac{T_d - T_p}{T_d + T_p} = 0.44$  \hspace{1cm} (5)
112
113 It is worth noting that the static susceptibility ($\chi_s$) per spin in 1D-IM (inset of Fig. 2A and
114 SI) always increases rapidly with decreasing $T^{1,2}$, instead of the $\lambda$-type peak of second-order
115 phase-transition$^{14}$, which is thought to be one of the key evidences that no phase-transition with
116 temperature exist in this model.
117
118 In order to further explore the micro mechanism of the above characteristic of $\chi_s$, the
119 static susceptibility ($\chi_s^B$) per spin in 1D-IM as a function of $T$ in a fixed external magnetic field
120 ($B$ ) is calculated (SI), as shown in the inset of Fig. 2A. We can see that for finite small $B$, there
121 is a single diffuse peak of $\chi_s^B$ with $T$, and the peak temperature moves to high temperature
122 with the increase of $B$. This is due to that very small $B$ can saturate the magnetization of 1D-IM at
123 low temperature (as shown in Fig. S2, the saturation $B \sim 10^{-9}/\mu$ for $T = 0.10/\text{k}_B$), while
124 the saturated magnetization leads to a smaller value $\chi_s^B$. Because the saturation magnetization
125 corresponds to the single domain state of the model, the increase of $\chi_s$ at low temperature is
126 caused by the movement of domain walls$^{24,25}$. 

4
In particular, because the measurement magnetic field used in experiments is always finite, the susceptibility peak (inset of Fig. 2A) will appear in 1D-IM as long as the experimental measurement is carried out. In other words, the continuously increasing characteristic of the theoretically predicted $\chi_s (\chi_s B=0)$ with decreasing $T$ cannot be measured directly, which is only an ideal value.

Although diffuse phase-transition is common in component-heterogeneous\textsuperscript{10-13,26-29} and small-size\textsuperscript{30-32} systems, there is no accurate calculation of the corresponding theoretical model so far\textsuperscript{21}. Therefore, the exact results in this paper lay the theoretical foundation of this kind of phase-transition.

Weiss mean-field theory\textsuperscript{33} is always thought to be not suitable for 1D-IM because it predicts that there is a phase-transition with $T$ in this system. The present and relevant\textsuperscript{2,22,23} results show that this theory is valid for IM of all dimensions in judging whether there exists phase-transition, although its predicting phase-transition behaviors, such as the transition temperature and the subtle characteristics of order parameter and heat capacity, are different from the exact solutions\textsuperscript{2,22,23}. It also shows that Weiss-type mean-field approximation\textsuperscript{21} is an effective and feasible method for Ising-category models of phase-transition which are too complex and difficult to get their exact solutions.

Traditionally, the description to 1\textsuperscript{st} and 2\textsuperscript{nd}-order phase-transitions is based on global-order-parameter (such as global-spontaneous-magnetization and global-spontaneous-polarization etc.)\textsuperscript{1,2,14,33}, but it cannot describe the spatially heterogeneous behavior of the order-parameter corresponding to the diffuse-phase-transition in component-heterogeneous\textsuperscript{10-13,26-29} and small-size\textsuperscript{30-32} systems. Obviously, as the scale of the local-order-parameter proposed in Ref.\textsuperscript{21} and this paper tends to infinity, it becomes the global-order-parameter. So, local-order-parameter can provide a unified description of 1\textsuperscript{st} and 2\textsuperscript{nd}-order phase-transitions as well as diffuse-phase-transition.

**Methods**

The method to calculate the local-spontaneous-magnetization ($m^l_1$) in 1D-IM is as the follows.

The Hamiltonian ($H_n$) of the subsystem (Fig. S1) without external magnetic field is,

$$H_n = -J \sum_{i=1}^{n-1} \sigma_i \sigma_{i+1}$$  \hspace{1cm} (M1)

and the partition function ($Z_n$) of the spin orientation ensemble (Fig. S1) is,

$$Z_n \equiv \sum_{\sigma_1=\pm1, \cdots, \sigma_n=\pm1} \exp \left[ v \sum_{i=1}^{n-1} \sigma_i \sigma_{i+1} \right] = \cosh^{n-1}(v)Q_n$$  \hspace{1cm} (M2)

In which,

$$Q_n \equiv \sum_{\sigma_1=\pm1, \cdots, \sigma_n=\pm1} \prod_{i=1}^{n-1} (1 + \gamma \sigma_i \sigma_{i+1}) = 2^n$$  \hspace{1cm} (M3)

Let,

$$X_i \equiv \lim_{n \to \infty} \frac{1}{Z_n} \sum_{\sigma_1=\pm1, \cdots, \sigma_n=\pm1} (s_i^f)^2 \exp \left[ v \sum_{i=1}^{n-1} \sigma_i \sigma_{i+1} \right]$$  \hspace{1cm} (M4)

and according to,
\[(s_t^2) = \mu^2 \left\{ l + 2 \sum_{i=1}^{l-1} \sigma_{r+i-1}^1 \sigma_{r+i}^1 + \sum_{i=2}^{l-1} \sigma_{r+i-2}^1 \sigma_{r+i}^1 + \cdots + \sum_{i=l-1}^{l-1} \sigma_{r+l-1}^1 \sigma_{r+l-1}^1 \right\} \]  

(M5)

we obtain,

\[
X_t = \mu^2 \left[ l + 2 \sum_{k=1}^{l-1} (l-k) \zeta_k \right] \]  

(M6)

where \(\zeta_k\) is the correlation function between \(\sigma_r\) and \(\sigma_{r+k}\), i.e.

\[
\zeta_k \equiv \lim_{n \to \infty} \frac{1}{Q_n} \sum_{\sigma_i = \pm 1, \ldots, \sigma_n = \pm 1} \sigma_r \sigma_{r+k} \exp \left[ \nu \sum_{i=1}^{n-1} \sigma_i \sigma_{i+1} \right] 
\]

(M7)

Based on,

\[
I_0 \equiv \sum_{\sigma_r = \pm 1} (1 + \gamma \sigma_{r-1} \sigma_r)(1 + \gamma \sigma_r \sigma_{r+1}) \sigma_r 
\]

(M8)

\[
I_1 \equiv \sum_{\sigma_{r+1} = \pm 1} I_1 (1 + \gamma \sigma_{r+1} \sigma_{r+2}) 
\]

(M9)

\[
I_k \equiv \sum_{\sigma_{r+k} = \pm 1} I_{k-1} (1 + \gamma \sigma_{r+k} \sigma_{r+k+1}) \sigma_{r+k} 
\]

(M10)

we get,

\[
\zeta_k = \lim_{n \to \infty} \frac{1}{Q_n} \sum_{\sigma_i = \pm 1, \ldots, \sigma_{r-1} = \pm 1, \sigma_{r+k+1} = \pm 1} I_k \prod_{i=1}^{r-2} (1 + \gamma \sigma_i \sigma_{i+1}) \prod_{i=r+k+1}^{n-1} (1 + \gamma \sigma_i \sigma_{i+1}) 
\]

(M11)

\[
= \gamma^k 
\]

From Eq.M6 and M11, we obtain,

\[
X_t = \mu^2 \left[ l + 2 \sum_{k=1}^{l-1} (l-k) \gamma^k \right] 
\]

(M12)

Here, \(\sum_{k=1}^{l-1} (l-k) \gamma^k\) is the well-known arithmetic-geometric series, and,

\[
X_t = \mu^2 \left\{ 2 \left[ (l - 1) - \gamma (1 - \gamma^{l-1}) \right] - l \right\} 
\]

(M13)

Therefore,

\[
m_t^l = \frac{\mu}{l} \left[ 2 \left[ (l - 1) - \gamma (1 - \gamma^{l-1}) \right] - l \right] 
\]

(M14)

and obviously,

\[
m_t^l (T \to \infty) = \frac{\mu}{l^{1/2}} 
\]

(M15)

Data availability
The data that support the plots and other findings of this paper are available from the corresponding author upon a reasonable request.

**Code availability**

The code is available from the corresponding author upon a reasonable request.

**References**

1. Ising, E. Report on the theory of ferromagnetism. Z. Phys. 31, 253-258 (1925).
2. McCoy, B. M. & Wu, T. T. The two-dimensional Ising model. (Dover Publications, Inc., Mineola, New York, 2014).
3. Li, Y. Ising model for strings. Nat. Phys. 16, 1006 (2020).
4. Young, J. T., Gorkshov, A. V., Foss-Feig, M. & Magrebi, M. F. Nonequilibrium Fixed Points of Coupled Ising Models. Phys. Rev. X. 10, (2020).
5. Christiansen, H., Majumder, S., Henkel, M. & Janke, W. Aging in the Long-Range Ising Model. Phys. Rev. Lett. 125, (2020).
6. Walker, N., Tam, K. & Jarrell, M. Deep learning on the 2-dimensional Ising model to extract the crossover region with a variational autoencoder. Sci. Rep. 10, (2020).
7. Wang, B., Hu, F., Yao, H. & Wang, C. Prime factorization algorithm based on parameter optimization of Ising model. Sci. Rep. 11, (2021).
8. Smolenskii, G. A., Isupov, V. A., Agranovskaya, A. I. & Krainik, N. N. New ferroelectrics of complex composition. Sov. Phys. Sol. Stat. 2, 2651-2654 (1961).
9. Kimura, T., Tomioka, Y., Kumai, R., Okimoto, Y. & Tokura, Y. Diffuse phase transition and phase separation in Cr-doped Nd12Ca12MnO3: A relaxor ferromagnet. Phys. Rev. Lett. 83, 3940-3943 (1999).
10. Granzow, T., Woike, T., Wohlecke, M., Imlau, M. & Kleemann, W. Change from 3D-Ising to random field-Ising-model criticality in a uniaxial relaxor ferroelectric. Phys. Rev. Lett. 92, 65701 (2004).
11. Gehring, P. M. et al. Reassessment of the Burns temperature and its relationship to the diffuse scattering, lattice dynamics, and thermal expansion in relaxor Pb(Mg1/3Nb2/3)O3. Phys. Rev. B. 79, 224109 (2009).
12. Stock, C. et al. Interplay between static and dynamic polar correlations in relaxor Pb(Mg1/3Nb2/3)O3. Phys. Rev. B. 81, 144127 (2010).
13. Landau, L. Zur Theorie der Phasenumwandlungen II. Phys. Z. Soviet Union. 545, 26-35 (1937).
14. Moriya, Y., Kawaji, H., Tojo, T. & Atake, T. Specific-heat anomaly caused by ferroelectric nanoregions in Pb(Mg1/3Nb2/3)O3 and Pb(Mg1/3Ta2/3)O3 relaxors. Phys. Rev. Lett. 90, 205901 (2003).
15. Kleemann, W., Dec, J., Shvartsman, V. V., Kutnjak, Z. & Braun, T. Two-dimensional Ising model criticality in a three-dimensional uniaxial relaxor ferroelectric with frozen polar nanoregions. Phys. Rev. Lett. 97, 65702 (2006).
16. Tachibana, M., Sasame, K., Kawaji, H., Atake, T. & Takayama-Muromachi, E. Thermal signatures of nanoscale inhomogeneities and ferroelectric order in [PbZn1/3Nb2/3O3]x[PbTiO3]1-x. Phys. Rev. B. 80, 94115 (2009).
17. Burns, G. & Scott, B. A. Index of refraction in dirty displacive ferroelectrics. Sol. State Commun. 13, 423-426 (1973).
18. Shvartsman, V. V. & Lupascu, D. C. Lead-free relaxor ferroelectrics. J. Am. Cera. Soc. 95, 1-26 (2012).
19. Shvartsman, V. V., Dkhil, B. & Kholkin, A. L. Mesoscale domains and nature of the relaxor state by piezoresponse force microscopy. Annu. Rev. Mater. Res. 43, 423-449 (2013).
20. Zhang, L. L. & Huang, Y. N. Theory of relaxor-ferroelectricity. Sci. Rep. 10, 50601 (2020).
21. Onsager, L. Crystal statistics I: A two-dimensional model with an order-disorder transition. Phys. Rev. 65, 117-149 (1944).
22. Yang, C. N. The spontaneous magnetization of a 2-dimensional Ising model. Phys. Rev. 85, 808-815 (1952).
23. Huang, Y. N., Wang, Y. N. & Shen, H. M. Internal-friction and dielectric loss related to domain-walls. Phys. Rev. B. 46, 3290-3295 (1992).
24. Huang, Y. N. et al. Domain freezing in potassium dihydrogen phosphate, triglycine sulfate, and CuAlZnNi. Phys. Rev. B. 55, 16159-16167 (1997).
25. Cross, L. E. Relaxor ferroelectrics. Ferroelectrics. 76, 241-267 (1987).
26. Kumar, A. et al. Atomic-resolution electron microscopy of nanoscale local structure in lead-based relaxor ferroelectrics. Nat. Mat. 20, (2021).
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Author contributions

Y-N.H. and L-L.Z. conceived this article together. Y-N.H. calculated the local-spontaneous-magnetization. L.Z. did the numerical calculations and made plots.

Competing interests

Authors declare that they have no competing interests.

Additional information

All data are available in the main text or the supplementary information.
Figures

Figure 1

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Figure 2

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