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Experimental Ising chains: Comparison with theories

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ABSTRACT

It was previously supposed that the one-dimensional Ising model had no long-range order. However, long-range order has since been observed in experimental Ising chains. The author previously showed that there was an error in the traditional solution of the Ising model: redundant terms were included in the partition function. It is now evident that the new solution of the Ising model agrees better with the experimental results. According to this solution, long-range order, inter alia, can exist in experimental Ising chains. Using this solution, one can calculate the length of the segments of the Ising chain much more accurately than the previous theory allowed. Superparamagnetic behaviour of some substances supports the author's arguments.

KEYWORDS

Ising model;
Heisenberg model;
Magnetization;
Partition function;
Superparamagnetism.

INTRODUCTION

Recently, experimental and theoretical studies of experimental one-dimensional Ising models were performed.[1–13] Experiments have revealed the existence of short-range order and long-range ferromagnetic order. The latter result contradicts the prediction of spin lattice models that in an infinite one-dimensional linear chain with short-range interactions long-range ferromagnetic order at non-zero temperature is impossible.[1,2,4,8–12,14,15] Also, according to some formulae for spin lattice models, this chain spontaneously breaks up into domains with different orientation in terms of magnetization and total zero magnetization; according to other formulae for these models, domains cannot exist, so there is an obvious contradiction. In the theory recently developed by the author it is shown that long-range order can exist in this chain and the domains can exist without contradiction. Their length can be calculated much more accurately than with the previous methods. The phenomenon of superparamagnetism supports the author's theory.

THEORY

The exact expression for the correlation length for the one-dimensional Ising model valid at any temperature is:[7,15]

$$\xi = -\frac{1}{\ln(\tanh \beta J)} \quad (1)$$

(in Ref. 7, it is cited as Reference 11). The traditional theory predicts that in the absence of a field at non-zero temperature, the chain can be regarded as a succession of up and down oriented domains, with zero total magnetization. The length of the domains is assumed to be 2ξ[2,4,7,9] or ξ.[6] However, this contradicts another conclusion of the same theory. The exact long-range correlation function of the spins 1 and N, $\Gamma(N)$ for the Ising chain with N spins obtained from this theory is:[14–16]

$$\Gamma(N) = \left[\Gamma(1)\right]^N = \tanh^N(\beta J) \qquad (2)$$

Here $\Gamma(1)$ is the nearest-neighbour correlation function, J is the interaction energy between spins, and $\beta = 1/(kT)$. Eq. (2) predicts that this function of an infinite Ising chain is zero for all non-zero temperatures. If the chain consisted of the domains, then the limit of $\Gamma(N)$ when N tends to infinity would be ± 1. In Ref. 16, the unsoundness of Eq. (2) was also proven.

The most extensive experimental studies of experimental one-dimensional Ising models were performed in Refs. 8, 12. These models constitute chains of the average length of 80 cobalt atoms at a platinum substrate. The interaction between Co atoms is much higher than that between Co and Pt atoms. It was noticed that Co monatomic chains can sustain long- or short-range ferromagnetic order. The short-range order is described thus: 'The observed behaviour is that of a one-dimensional superparamagnetic system, i.e. a system composed by segments, or spin blocks, each containing N_c exchange-coupled Co atoms, whose resultant magnetization orientation is not stable due to thermal fluctuations.' The average length of the Co chains was estimated to be about $N = 80$ atoms. Using numerical fit, N_c was obtained to be 15 atoms.

This result contradicts the traditional solution of the one-dimensional Ising and Heisenberg models: a one-dimensional spin chain of infinite length is characterized by the absence of long-range magnetic order at any non-zero temperature. The authors thus conclude that 'Long-range order in one-dimensional metal chains therefore appears as a metastable state thanks to slow magnetic relaxation.' They also conclude that the short-range order likewise is metastable.

It is necessary to mention that in Ref. 16, another solution of the one-dimensional Ising model was proposed. The magnetization of a uniform Ising chain is determined by the nearest-neighbour correlation function $\Gamma(1)$. Let us suppose that $\Gamma(1) = 0.99$. In this case, two situations are possible. In the first one, the chain has about 99% of the spins up and 1% of those down; this is the long-range order. In the second one, the chain consists of segments directed up and down, each containing about 50 spins. Mathematically, the problem is solved. It has two solutions. One can see that the partition function previously included redundant terms. My theory, however, permits only the terms with $\Gamma(1) = 0.99$ to be included; those with $\Gamma(1)$ unequal to 0.99 cannot be included. For example, the configurations with one third of the spins up have $\Gamma(1) \neq 0.99$ and may not be included.

The nearest-neighbour correlation function is:[14–16]

$$\Gamma(1) = \tanh(\beta J) \qquad (3)$$

Magnetization of the uniform Ising chain is:[16]

$$\sigma = \Gamma(1)^{0.5} = \tanh^{0.5}(\beta J) \qquad (4)$$

in the first situation, and zero in the second one. From the fit performed on the magnetization data at $T = 45$ K, the authors of Ref. 8 obtained $J = 228.7$ K. Using this information, from Eq. (3) one can calculate $\Gamma(1)$ 1.0. In Ref. 12, the value $J = 7.5$ meV was accepted for $T = 45$ K, $kT \approx 4$ meV at this temperature, and $\Gamma(1) \approx 0.95$. The nearest-neighbour correlation function can be calculated also from the following equation:

$$\Gamma(1) = \frac{\sum_{i=1}^{N-1} s_i s_{i+1}}{N-1} \qquad (5)$$

For $N = 80$ and $N_c = 15$, from Eq. (5) one can find $\Gamma(1) \approx 0.87$. There is a rather good agreement with Eq. (3).

Let us calculate the length of domains 2ξ in the Ising model for $\Gamma(1) = 0.99$ by the traditional method. From Eqs. (1) and (3), $2\xi = 200$. There is a huge discrepancy in relation to the correct value, 50. In Ref. 12, 'a theoretical argument due to Landau[17] shows that finite one-dimensional Ising chains with a number of ferromagnetically-coupled spins $N > \exp(2J/kT)$ break up spontaneously into smaller domains'. For $\Gamma(1) = 0.99$, this criterion gives $N_c = 200$, which again is far from the correct value.

Some experimental one-dimensional chains exhibit superparamagnetism,[4–6,8,11–13] that is, they can be only up- or down-oriented. Their magnetization can randomly flip direction under the influence of thermal fluctuations. One can infer that in the description of such systems with statistical mechanics only the up and down state must be included in the partition function, which agrees with the theory developed in Ref. 16: redundant terms were included in the partition function in the previous theory.

CONCLUSIONS

It is evident that the theory developed in Ref. 16 is more useful than that used in Ref. 8: it predicts long-range order as an intrinsic property of a one-dimensional Ising chain (and not as the result of slow dynamics and metastability), the presence of segments in this chain without contradiction, and their size, with much higher accuracy than the previous theories. Superparamagnetism discovered in some one-dimensional systems also supports the conclusions of Ref. 16. In Refs. 18, 19, the results obtained in Ref. 16 received additional confirmation.

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