The nature of the probability distribution function of the local energy in Ising spin glass

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Abstract. The nature of the probability distribution function of the local energy in the $\pm J$ Ising model has been investigated. At finite temperature, it has been derived that the probability distribution function must satisfy several relations at $p = 1/2$ ($p$ is the concentration of the ferromagnetic bond) and at Nishimori-line, respectively on any lattice in any dimension. They relate the probability distribution function corresponding to the local energy lower than $-\tanh(K)$ with that corresponding to the local energy greater than $-\tanh(K)$. ($K$ is the inverse temperature.) The present results at Nishimori-line are, in a sense, generalization of Nishimori’s result about the internal energy obtained by the local gauge transformation. Moreover, from the numerical calculation in the two-dimensional $\pm J$ Ising model, it is found that, in a certain temperature region, the probability distribution function of the local energy has several peaks which are related to the patterns of frustration around a bond of the lattice.

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1. Introduction

To elucidate the nature of random spin systems, especially spin glass systems, has been a subject of a long-standing interest[1-21]. In the random spin systems, when we take one sample, namely, one bond configuration, the local energies of interacting bonds take various values, which change as the sample changes. There have been many works about the energy of spin glass systems, for example, about the ground state energy[7-9], energy barrier[10-12], energy landscape [13-15], low-energy excitation[16,17] for various spin glass systems.

On the other hand, Nishimori[18] derived several rigorous results at a special line in the phase diagram of spin glass systems, which has now been called ”Nishimori-line”. The results were derived mainly by the use of the local gauge transformation, so that they hold for various spin glass models on any lattice in any dimension. The exact internal energy and the upper bound of the specific heat at Nishimori-line were derived. Moreover, a nature of the correlation function was derived, from which it follows that the ferromagnetic order parameter and the spin glass order parameter coincide with

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each other at Nisimori-line, and the ferromagnetic phase boundary has some restriction in the phase diagram[18-20]. Furthermore, it was derived that the correlation-function distribution function must satisfy a certain relation at Nishimori-line[21].

In this paper, we investigate the nature of the probability distribution function of the local energy in the $\pm J$ Ising model. It has been derived that, at finite temperature, the probability distribution function mentioned above must satisfy several relations at $p = 1/2$ and at Nishimori-line, respectively, on any lattice in any dimension. They relate the probability distribution function corresponding to the local energy lower than $-\tanh(K)$ with that corresponding to the local energy greater than $-\tanh(K)$. The present results at Nishimori-line are, in a sense, generalization of Nishimori’s result about the internal energy[18], since the probability distribution function has more information than only the average value.

Moreover, we have numerically calculated the probability distribution functions of the local energy at $p = 1/2$ and at Nishimori-line in the two-dimensional $\pm J$ Ising model, from which we have found that, in a certain temperature region, they have several peaks which are related to the patterns of frustration around a bond of the lattice.

2. The probability distribution function of the local energy

We consider the $\pm J$ Ising model, where the dimension of the lattice, the lattice structure and the range of the interactions may be arbitrary. The Hamiltonian is written as follows:

$$\mathcal{H} = -\sum_{(ij)} \tau_{ij} S_i S_j, \quad (1)$$

where $S_i = \pm 1$, and the summation of $(ij)$ runs over all the interacting pairs. Each $\tau_{ij}$ is determined according to the following probability distribution:

$$P(\tau_{ij}) = p\delta(\tau_{ij} - 1) + (1 - p)\delta(\tau_{ij} + 1). \quad (2)$$

In this paper, we put that $J = 1$ and $k_B = 1$ ($k_B$ is the Boltzmann constant).

Now, we denote the local energy of the interacting bond $(ij)$ in a given bond configuration, $\{\tau\}$, as $e_{ij}(K)$:

$$e_{ij}(K) = -<\tau_{ij} S_i S_j>_K, \quad (3)$$

where $<\cdots>_K$ denotes the thermal average at temperature, $T = 1/K$. Then, the probability distribution function of the local energy, $P_e(x, K, K_p)$, can be written as

$$P_e(x, K, K_p) = [\delta(x - e_{ij}(K))]_{K_p}, \quad (4)$$

where $[\cdots]_{K_p}$ denotes the configurational average at the ferromagnetic bond concentration, $p$. (We define $K_p$ as $\exp(2K_p) = p/(1 - p)$.) In this paper, we do not investigate the nature of $P_e(x, K, K_p)$ directly, but investigate that of a slightly different form, namely,

$$P_e^{(2)}(x, K, K_p) = [\delta(x - (\cosh(2K) + \sinh(2K)e_{ij}(K)))]_{K_p}, \quad (5)$$
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which is related to \( P_e(x, K, K_p) \) as

\[
P_e(x, K, K_p) = \sinh(2K)P_e^{(2)}(\cosh(2K) + \sinh(2K)x, K, K_p).
\] (6)

Here, it is noted that \( P_e(x, K, K_p) \) may take non-zero value in the region, \(-1 \leq x \leq 1\), so that \( P_e^{(2)}(x, K, K_p) \) may take non-zero value in the region, \( \exp(-2K) \leq x \leq \exp(2K)\).

3. The nature of the probability distribution function of the local energy

In this section, we investigate the nature of the probability distribution function of the local energy, \( P_e^{(2)}(x, K, K_p) \), at \( p = 1/2 \) and at Nishimori-line, respectively.

Firstly, we can derive the following identity:

\[
P_e^{(2)}(x, K, K_p) = [\cosh(2K_p) + \sinh(2K_p)e_{ij}(K_p)]\delta(x - \frac{1}{\cosh(2K) + \sinh(2K)e_{ij}(K)})]_{K_p}.
\] (7)

(For the detailed derivation of equation (7), see the appendix.)

Next, we integrate both terms of equation (7) from \( a \) to \( b \) (\( a \) and \( b \) are arbitrary real numbers, which satisfy \( \exp(-2K) \leq a < b \leq \exp(2K) \)): namely,

\[
\int_{a}^{b} P_e^{(2)}(x, K, K_p)dx = \int_{a}^{b} [\cosh(2K_p) + \sinh(2K_p)e_{ij}(K_p)]\delta(x - \frac{1}{\cosh(2K) + \sinh(2K)e_{ij}(K)})]_{K_p}dx = \int_{1/a}^{1/b} [\cosh(2K_p) + \sinh(2K_p)e_{ij}(K_p)]\delta(\frac{1}{x} - \frac{1}{\cosh(2K) + \sinh(2K)e_{ij}(K)})]_{K_p}^{\frac{dx}{x^2}} = \int_{1/a}^{1/b} [\cosh(2K_p) + \sinh(2K_p)e_{ij}(K_p)]\delta(x - (\cosh(2K) + \sinh(2K)e_{ij}(K))]_{K_p}dx,
\] (8)

where we use the following property of \( \delta \)-function to derive the last term:

\[
\delta(\frac{1}{x} - \frac{1}{a}) = x^2\delta(x - a).
\] (9)

Equation (8) is the basic identity, which we use to derive the properties of the probability distribution function of the local energy.

First, we investigate the case, \( p = 1/2 \). At \( p = 1/2 \), \( K_p = 0 \), so that equation (8) becomes

\[
\int_{a}^{b} P_e^{(2)}(x, K, 0)dx = \int_{1/a}^{1/b} [\delta(x - (\cosh(2K) + \sinh(2K)e_{ij}(K))]_{0}dx = \int_{1/b}^{1/a} P_e^{(2)}(x, K, 0)dx
\] (10)

Changing the variable \( x \) into \( x^{-1} \) of rhs of equation (10), we also obtain

\[
\int_{a}^{b} P_e^{(2)}(x, K, 0)dx = \int_{a}^{b} x^{-2}P_e^{(2)}(x^{-1}, K, 0)dx.
\] (11)
For investigating the direct form of $P_e^{(2)}(x, K, K_p)$, we define the following averaged distribution function, $\{P_e^{(2)}(x, K, K_p)\}_\Delta$:

$$\{P_e^{(2)}(x, K, K_p)\}_\Delta = \frac{1}{\Delta} \int_x^{x+\Delta} P_e^{(2)}(x, K, K_p) dx,$$

where $\Delta$ is an arbitrary finite value which satisfies $x + \Delta \leq \exp(2K)$. Then, equation (11) can be written as:

$$\{P_e^{(2)}(x, K, 0)\}_\Delta = \{x^{-2}P_e^{(2)}(x^{-1}, K, 0)\}_\Delta.$$  (13)

We can take the value, $\Delta$, as an arbitrarily small but finite value. In this sense, we can conclude that the value of $P_e^{(2)}(x, K, 0)$ coincides with that of $x^{-2}P_e^{(2)}(x^{-1}, K, 0)$ at any finite temperature. Equations (10), (11) and (13) are the main results at $p = 1/2$. In a word, these equations are the conditions which relates the value of the probability distribution function at $x$ with that at $1/x$. As the temperature changes, the distribution function of the local energy itself may change, however, the distribution function must satisfy the above relations at any finite temperature on any lattice in any dimension.

Using $P_e(x, K, K_p)$, equation (13) is written by the following form:

$$\{P_e(x - (-\tanh(K)), K, 0)\}_\Delta = \left\{ \frac{1}{(1 + \sinh(2K))(x - (-\tanh(K)))^2} P_e\left( -\frac{x - (-\tanh(K))}{1 + \sinh(2k)(x - (-\tanh(K)))}, K, 0 \right) \right\}_\Delta,$$

which becomes a rather complicated form, from which, however, we can see that equation (14) is a condition which relates the probability distribution function corresponding to the local energy lower than $-\tanh(K)$ with that corresponding to the local energy greater than $-\tanh(K)$.

Next, we investigate the nature of the probability distribution function of the local energy at Nishimori-line. At Nishimori-line, $K_p = K$, so that equation (8) becomes

$$\int_a^b P_e^{(2)}(x, K, K) dx$$

$$= \int_{1/b}^{1/a} [(\cosh(2K) + \sinh(2K)e_{ij}(K))\delta(x - (\cosh(2K) + \sinh(2K)e_{ij}(K)))_K dx$$

$$= \int_{1/b}^{1/a} [x\delta(x - (\cosh(2K) + \sinh(2K)e_{ij}(K)))_K dx$$

$$= \int_{1/b}^{1/a} xP_e^{(2)}(x, K, K) dx.$$  (15)

Also, we obtain

$$\int_a^b P_e^{(2)}(x, K, K) dx = \int_a^b x^{-3}P_e^{(2)}(x^{-1}, K, K) dx.$$  (16)

For the averaged distribution function, it can be derived that

$$\{P_e^{(2)}(x, K, K)\}_\Delta = \{x^{-3}P_e^{(2)}(x, K, K)\}_\Delta.$$  (17)
4. The property of the local energy at $p = 1/2$ and at Nishimori-line

In this section, we derive several properties of the local energy at $p = 1/2$ and at Nishimori-line, using the results of the preceding section.

For the configurational average of the local energy at Nishimori-line, from equation (15), we obtain

$$[\cosh(2K) + \sinh(2K)e_{ij}(K)]_K = \int_{\exp(-2K)}^{\exp(2K)} xP_e(x, K, K)dx = 1,$$

from which, it is easily calculated that

$$[e_{ij}(K)]_K = -\tanh(K), \quad (19)$$

which was first derived by Nishimori[18]. At $p = 1/2$, by the similar procedure, it can be derived that

$$[e_{ij}(K)]_0 \geq -\tanh(K). \quad (20)$$

Next, putting $a = \exp(-2K)$ and $b = 1$ in equation (10) at $p = 1/2$, we obtain

$$\int_{\exp(-2K)}^{1} P_e(x, K, 0)dx = \int_{1}^{\exp(2K)} P_e(x, K, 0)dx. \quad (21)$$

Using $P_e(x, K, K_p)$, equation (21) can be written as

$$\int_{-\tanh(K)}^{1} P_e(x, K, 0)dx = \int_{1}^{\exp(2K)} P_e(x, K, 0)dx. \quad (22)$$

On the other hand, at Nishimori-line, from equation (15), we obtain

$$\int_{-\tanh(K)}^{1} P_e(x, K, K)dx \geq \int_{1}^{\exp(2K)} P_e(x, K, K)dx. \quad (23)$$

The above results are interesting, since, at Nishimori-line, the configurational average of the local energy coincides with $-\tanh(K)$ at any temperature, while, at $p = 1/2$, the probability that the local energy, $e_{ij}(K)$, takes the value smaller than $-\tanh(K)$ always coincides with one that $e_{ij}(K)$ takes the value larger than $-\tanh(K)$ at any temperature. Furthermore, these results hold on any lattice structure in any dimension.

5. Numerical calculation of the probability distribution function

Now, we show the examples how the above feature holds in the two-dimensional square-lattice $\pm J$ Ising model with only nearest neighbour interactions. By the transfer matrix method, we have calculated the values of $e_{ij}(K)$ in $L \times L$ lattice ($L = 11$) for $10^7$ bond configurations, from which we have estimated $\{P_e^{(2)}(x, K, K_p)\}_\Delta$ at $p = 1/2$ and at Nishimori-line for $\Delta = (\exp(2K) - \exp(-2K))/1000$. Figures 1 and 2 are the results of the above procedure at $K = 0.75$ at $p = 1/2$ and at Nishimori-line, respectively. We have confirmed that equations (13) and (17) definitely hold within the statistical errors.
In the figures, we can see that the averaged probability distribution function, \( \{P_e^{(2)}(x, K, K_p)\}_\Delta \), has three peaks at \( p = 1/2 \), and one peak and two shoulders at Nishimori-line. In the two-dimensional square lattice \( \pm J \) Ising model, the number of the patterns of frustration of two plaquettes around a certain bond of the lattice is three if we take into account only the number of frustration plaquettes, and each bond configuration belongs to one of the three patterns. We have confirmed that each peak or shoulder corresponds to the contribution from one of the three patterns of frustration. As the temperature decreases, each peak broadens, and at sufficient low temperature, it is found that \( \{P_e^{(2)}(x, K, K_p)\}_\Delta \) has only one peak. More detailed numerical properties of the probability distribution function of the local energy is reported in a separated paper in the future.

6. Conclusions

We have investigated the nature of the probability distribution function of the local energy in Ising spin glass.

We have derived that, in the \( \pm J \) Ising model, the probability distribution function, \( P_e^{(2)}(x, K, K_p)(P_e(x, K, K_p)) \), must satisfy several relations at finite temperature on any lattice in any dimension at \( p = 1/2 \) and at Nishimori-line, respectively. They relate the probability distribution function corresponding to the local energy lower than \( -\tanh(K) \) with that corresponding to the local energy greater than \( -\tanh(K) \). The present results at Nishimori-line are generalization of Nishimori’s result[18] about the internal energy, since the probability distribution function has more information than only the average value.

Moreover, from the numerical calculation, we have found that, in a certain temperature region, the probability distribution function of the local energy has several peaks which are related to the patterns of frustration around a certain bond in the lattice. More detailed numerical properties are reported in the near future.

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Appendix A. Derivation of equation (7)

In this appendix, we briefly explain the derivation of equation (7).

First, we denote the partition function of the system in a given bond configuration, \( \{\tau\} \) as;

\[
Z(K, K') = \sum_{\{s\}} \exp(\sum_{lm \neq ij} K_{lm}s_l s_m + K'_{ij}s_i s_j),
\]  

(A.1)
where we denote the temperature at bond \((ij)\) separately. Also, we introduce the notation, \([\cdots]_{K_p,K'_p}\):

\[
[\cdots]_{K_p,K'_p} = \frac{1}{(2 \cosh(K_p))^{N_B-1} 2 \cosh(K'_p)} \sum_{\tau} \exp(K_p \sum_{lm \neq ij} \tau_{lm} + K'_p \tau_{ij}) \cdots ,
\]

(A.2)

where \(N_B\) is the numbers of bonds, and we denote the ferromagnetic bond concentration of bond \((ij)\) separately. Of course, if \(K'_p = K_p\), the notation mentioned above coincides with the standard one:

\[
[\cdots]_{K_p,K_p} = [\cdots]_{K_p}.
\]

(A.3)

It is easily obtained that

\[
\cosh(2K) + \sinh(2K)e_{ij}(K) = \frac{Z(K,-K)}{Z(K,K)}.
\]

(A.4)

Then, it yields that

\[
P_e^{(2)}(x, K, K_p) = [\delta(x - (\cosh(2K) + \sinh(2K)e_{ij}(K)))]_{K_p}
\]

\[
= [\delta(x - \frac{Z(K,-K)}{Z(K,K)})]_{K_p,K_p}
\]

(A.5)

The last term of the above equation is invariant when we change the sign of \(K\) and \(K_p\) at bond \((ij)\) simultaneously, since it means that we just take the summation of \(\tau_{ij}(= \pm 1)\) reversely; namely,

\[
P_e^{(2)}(x, K, K_p)
\]

\[
= [\delta(x - \frac{Z(K,K)}{Z(K,-K)})]_{K_p,K_p}
\]

\[
= [\exp(-2K_p \tau_{ij})\delta(x - \frac{1}{Z(K,-K)})]_{K_p,K_p}
\]

\[
= [\delta(x - \frac{1}{\cosh(2K) + \sinh(2K)e_{ij}(K)})]_{K_p,K_p}
\]

(A.6)

where we use the local gauge transformation to derive the last term. Thus, we obtain equation (7).

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Figure captions

Figure 1. The averaged probability distribution function, \( \{P^{(2)}_e(x, K, 0)\}_\Delta \), at \( K = 0.75 \) at \( p = 1/2 \).
Figure 2. The averaged probability distribution function, \( \{P^{(2)}_e(x,K,K)\}_\Delta \), at \( K = 0.75 \) at Nishimori-line.