Spin States and Entropy of Ising Spin Glasses

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The relative volume of spin states in the phase space is introduced for the $\pm J$ model of spin glasses. Analysis of its temperature dependence shows that the Nishimori line separates the pure ferromagnetic-like region in the high-temperature side of the ferromagnetic phase from the randomness-dominated region in the low-temperature side. The peak value of the relative volume of the perfect ferromagnetic state is shown to be equivalent to the entropy. Upper and lower bounds on the entropy are derived, which determine the value of the entropy quite precisely.

KEYWORDS: Spin glass, entropy, ferromagnetic phase

§1. Introduction

After a long history of researches, the problem of spin glasses is still essentially unsolved. In particular, there are controversies on the existence and structure of the spin glass phase in finite dimensions. Even our knowledge on the spin states in the ferromagnetic phase is very limited. We focus our attention on this latter problem of the spin states in the ferromagnetic phase in the present contribution.

There are several exact results on the behaviour of Ising spin glasses in finite dimensions. For example, the exact expression of the internal energy on a particular line in the phase diagram is known.[1)] However, such exact results obtained in the early 80s do not give direct information on spin states. It was relatively recently that a useful inequality on the spin orientation within the ferromagnetic phase was derived, which clarified the spin states around the Nishimori line.[2)] We shall elucidate the derivation and significance of this inequality in some detail later.

We then present a formulation of the problem using the relative volume of space that a given spin state occupies in the whole phase space. It will be shown that the peak value of this relative volume is closely related to the entropy on the Nishimori line. We also discuss the lower and upper bounds on the entropy in which the information-theoretical entropy of frustration distribution plays a key role.

§2. Numbers of Up and Down Spins

We review in this section the properties of a basic indicator of the spin state, the difference of the numbers of up and down spins as a function of temperature in the ferromagnetic phase.[2)] Let us consider the $\pm J$ model of Ising spin glasses with the Hamiltonian

$$H = -\sum_{\langle ij \rangle} J_{ij} S_i S_j, \tag{2.1}$$

where the angular brackets denote neighbouring sites on an appropriate lattice such as the square lattice. The distribution of bonds are assumed to be of $\pm J$ type in the present paper; J_{ij} is 1 with probability p and is -1 with probability $1-p$. This distribution of bonds can be conveniently expressed as

$$P(J) = \frac{1}{(2\cosh K_p)^{N_B}} \exp(K_p \sum J_{ij}), \tag{2.2}$$

where K_p is defined by $\exp(-2K_p) = (1-p)/p$ and N_B denotes the number of bonds. The symbol J here denotes the set $\{J_{ij}\}$.

The following quantity to measure the difference between the numbers of up and down spins plays an important role throughout the argument:

$$m_A(T,p) = [\mathrm{sgn}\langle S_i \rangle]. \tag{2.3}$$

Here the outer square brackets denote the configurational average over the distribution of bonds (2.2). The boundary spins are assumed to be fixed up so that the thermal average of a local spin $\langle S_i \rangle$ has a non-trivial value even in finite-size systems. This quantity m_A represents the average number of up spins minus that of down spins per site.

It can be shown that m_A is not a monotonic function of the temperature. This quantity takes its maximum value at a particular temperature satisfying $T = 1/K_p \equiv T(p)$. This temperature is a function of the probability p and defines a line in the phase diagram $T = T(p)$, called the Nishimori line, as shown in Fig. 1.

The relevant inequality is written as

$$m_A(T,p) \le m_A(T(p),p). \tag{2.4}$$

It would be instructive to recall the derivation of eq. (2.4). We first rewrite the definition of m_A using a gauge transformation ($J_{ij} \to J_{ij}\sigma_i\sigma_j$, $S_i \to S_i\sigma_i$):

$$\begin{aligned} m_A(T,p) &= \left[\frac{\langle S_i \rangle_\beta}{|\langle S_i \rangle_\beta|} \right] \\ &= \frac{1}{(2\cosh K_p)^{N_B}} \sum_J e^{K_p \sum J_{ij}} \frac{\sum_S S_i e^{\beta \sum J_{ij} S_i S_j}}{|\sum_S S_i e^{\beta \sum J_{ij} S_i S_j}|} \\ &= \frac{1}{2^N (2\cosh K_p)^{N_B}} \end{aligned}$$

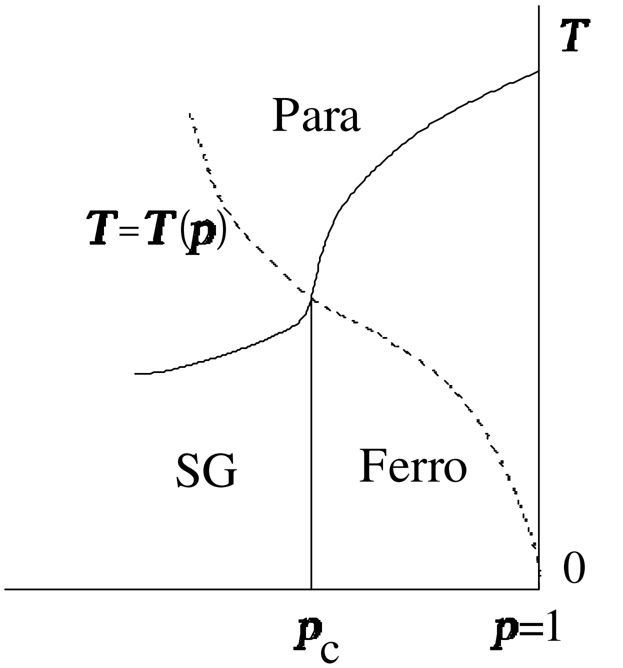

Fig. 1. The phase diagram of the $\pm J$ model and the Nishimori line.

$$\times \sum_J \sum_{\sigma'} e^{K_p \sum J_{ij}\sigma'_i\sigma'_j} \langle\sigma_i\rangle_{K_p} \frac{\langle S_i\rangle_\beta}{|\langle S_i\rangle_\beta|}, \tag{2.5}$$

where $\langle\ldots\rangle_\beta$ denotes the thermal average at inverse temperature $\beta = 1/T$. By taking the absolute value of the final expression, we obtain

$$\begin{aligned} & m_A(T,p) \\ & \le \frac{1}{2^N(2\cosh K_p)^{N_B}} \sum_J \sum_{\sigma'} e^{K_p \sum J_{ij}\sigma'_i\sigma'_j} |\langle\sigma_i\rangle_{K_p}| \\ & = \left[\frac{\langle S_i\rangle_{K_p}}{|\langle S_i\rangle_{K_p}|}\right] = m_A(T(p),p). \end{aligned} \tag{2.6}$$

The last line can be verified by using that $|\langle\sigma_i\rangle_{K_p}| = \langle\sigma_i\rangle^2_{K_p}/|\langle\sigma_i\rangle_{K_p}| = \langle\sigma_i\rangle_{K_p}\langle S_i\rangle_{K_p}/|\langle S_i\rangle_{K_p}|$ and comparing with (2.5).

Since the difference of the numbers of up and down spins is equal to the twice of the number of up spins minus a constant, the relation (2.4) implies that the number of up spins as a function of the temperature reaches its maximum value at $T = T(p)$ under the boundary condition of up spins. Therefore, as the temperature is lowered beyond $T = T(p)$, the spin orientation becomes less ordered in the sense that the number of up spins decreases in spite of the up-spin boundary condition. This behaviour is counter-intuitive because one naively expects that more and more ordered states dominate at lower temperatures.

One should remember that the magnetization defined without the 'sgn' symbol in (2.3) is probably a monotonic function of the temperature. As the temperature decreases, thermal fluctuations die out and the magnitude of an up spin, $\langle S_i \rangle (>0)$, would increase. This could well lead to an increase of magnetization even when the *number* of up spins decreases.

These observations motivated us to further investigate the spin states in the ferromagnetic phase using different ideas.

§3. Bayesian Interpretation

Before we proceed to the presentation of new ideas, it is useful to explain an interpretation of the inequality (2.4) in the context of error-correcting codes.[3,4] If we regard the $\pm J$ model as an error-correcting code, m_A is identified with the mean bitwise overlap of the decoded message with the original message.[2] This means that maximization of m_A gives the best decoded message from the viewpoint of minimization of bitwise errors. With this fact in mind, we show that the inequality (2.4) is derived naturally from the Bayes formula.

The *a posteriori* probability of the original message $\{S_i\}$ given the output $\{J_{ij}\}$ of the binary symmetric channel is given by the Bayes formula as

$$P(S|J) = \frac{P(J|S)P(S)}{\sum_S P(J|S)P(S)} = \frac{\exp(K_p \sum J_{ij} S_i S_j)}{\sum_S \exp(K_p \sum J_{ij} S_i S_j)}. \tag{3.1}$$

We have assumed that the source messages are generated uniformly and thus the prior $P(S)$ is a constant. The code bits are $J_{ij} = S_i S_j$; with probability $1-p$ (which is related to the coefficient K_p), they have their signs flipped by channel noise.

Let us now focus our attention to the marginal distribution of the ith bit:

$$P(S_i|J) = \sum_{S \backslash S_i} P(S|J). \tag{3.2}$$

The Bayes-optimal strategy is to choose the decoded result for S_i that maximizes $P(S_i|J)$. In other words, the decoded result will be 1 if $P(S_i = 1|J) > P(S_i = -1|J)$ and is -1 otherwise. This idea is equivalent to accepting the sign of the thermal average $\langle S_i \rangle_{K_p}$ because $\langle S_i \rangle_{K_p}$ is positive if and only if $P(S_i = 1|J) > P(S_i = -1|J)$ and is negative otherwise.

Since this method maximizes the bitwise marginal probability which is written in terms of a Boltzmann factor with the inverse temperature K_p, the bitwise overlap of the decoded result with the original message should acquire its best possible value at $T = T(p) = 1/K_p$. Thus $m_A(T,p)$ satisfies (2.4). Nothing looks mysterious and it may even seem trivial that m_A has its maximum at this temperature. However, this Bayesian interpretation does not give an explicit clue to a better understanding of the spin states at various temperatures in the ferromagnetic phase. The non-monotonic behaviour of the spin orientation as a function of temperature still remains counter-intuitive, at least to us. We therefore proceed to a different analysis using the volume of phase space and entropy.

§4. Volume of States

Since the spin state becomes most 'ferromagnetic-like' at $T = T(p)$ according to the inequality (2.4), it should be useful to see the behaviour of the relative volume of the perfect ferromagnetic state in the whole phase space defined by

$$
\begin{aligned}
P_{\rm F}(T,p) &= \left[\log \frac{e^{\beta \sum J_{ij}}}{\sum_S e^{\beta \sum J_{ij} S_i S_j}}\right] \\
&= \beta(2p-1)N_B - [\log Z(\beta)].
\end{aligned} \tag{4.1}
$$

The average over the bond distribution is taken after the operation of logarithm so that the configurational average is carried out for an extensive quantity as is usual the case in random systems.

The relative volume $P_{\rm F}(T,p)$ reaches its maximum as a function of temperature at $T = T(p)$ as can be verified by differentiation of (4.1) with respect to β, using that for $T = T(p)$ one has[1)]

$$
\left[\langle \sum J_{ij} S_i S_j \rangle\right] = (2p-1)N_B. \tag{4.2}
$$

It is also possible to check that P_F really has a maximum, not a minimum, at $T = T(p)$ from convexity of the free energy. Equation (4.1) further suggests that the maximum value of $P_{\rm F}$ is equal to $-S$, minus of the thermodynamic entropy if we note that (4.2) indicates that the internal energy is equal to $-(2p-1)N_B$ at $T = T(p)$. Therefore, the entropy on the Nishimori line $T = T(p)$ directly reflects the relative weight of the perfect ferromagnetic state.

It is quite straightforward to generalize the above analysis to an arbitrary spin configuration $\{\sigma_i\}$. The relative volume of a configuration $\{\sigma_i\}$ is

$$
\begin{aligned}
P_\sigma(T,p) &= \left[\log \frac{e^{\beta \sum J_{ij}\sigma_i\sigma_j}}{\sum_S e^{\beta \sum J_{ij} S_i S_j}}\right] \\
&= (2p-1)\beta \sum \sigma_i\sigma_j - [\log Z(\beta)].
\end{aligned} \tag{4.3}
$$

This quantity has its maximum as a function of the temperature at some $T = T_\sigma$ larger than $T(p)$. To see this, we differentiate both sides of (4.3) by β and set the result equal to 0 to find

$$
[\langle \sum J_{ij} S_i S_j \rangle] = (2p-1)\sum \sigma_i\sigma_j. \tag{4.4}
$$

Let us note here that the left-hand side is proportional to the internal energy and is therefore a monotonic function of the temperature. And it is trivial that $\sum \sigma_i\sigma_j < N_B$ unless $\{\sigma_i\}$ is a perfect ferromagnetic state. Then T_σ satisfying (4.4) is found to be larger than $T(p)$ satisfying (4.2).

These arguments indicate that the perfect ferromagnetic state occupies the largest relative volume at $T = T(p)$, and the relative volume shrinks as the temperature is further decreased. All other states reach the maximum relative volume at higher temperatures. The relative volumes of all states shrink at low temperatures, in particular when $T < T(p)$. This situation is depicted in Fig. 2.

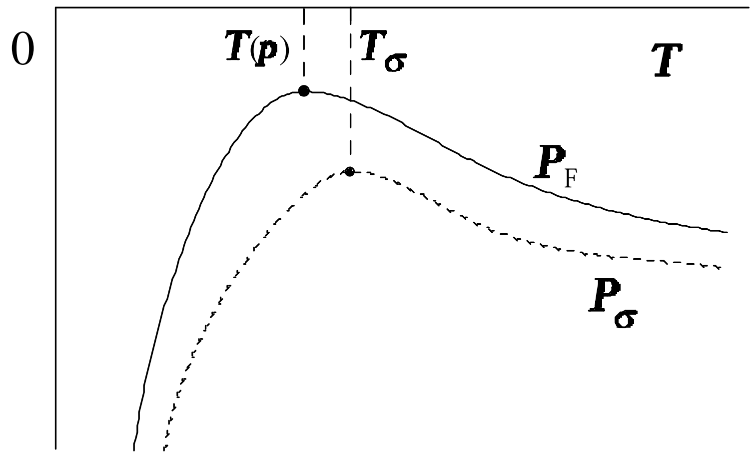

Fig. 2. The relative volume of states as a function of temperature.

Therefore, as the temperature is decreased beyond $T(p)$, any specific spin state $\{\sigma_i\}$ given independently of the bond configuration loses its average relative volume in the phase space. This means that, at $T < T(p)$, the thermodynamically relevant spin states directly reflect the randomly given configuration of bonds. They differ significantly from one bond configuration to another, while any specific spin state independent of the bond configuration is unlikely to be relevant at lower temperatures. This is the reason that P_{F} and P_σ decrease below $T(p)$.

In contrast, in the region $T > T(p)$, the perfect ferromagnetic state gradually comes to dominate the phase space with decrease of the temperature. In this sense, this higher temperature range has a character similar to the non-random ferromagnetic system while the lower temperature region $T < T(p)$ is strongly affected by randomness.

These observations do not necessarily mean that the line $T = T(p)$ is a phase boundary. As a renormalization-group analysis suggests,[5] it would in general be a crossover line between the two regions dominated by the ferromagnetic fixed point and a random fixed point. It is nevertheless true that the spin state changes remarkably, if unaccompanied by thermodynamic singularities, at $T(p)$. The non-monotonic behaviour of the difference between the numbers of up and down spins, m_A, directly reflects this crossover.

§5. Bounds on the Entropy

Analysis of the previous section shows that the entropy serves as an important indicator of spin states at $T(p)$ where the pure ferromagnetic-like and randomness-dominated regions cross over. It is however very difficult to calculate the entropy exactly. We instead estimate upper and lower bounds.

5.1 Lower bound

A lower bound on the entropy is derived from comparison of the free energy with the information-theoretical entropy of the probability distribution of frustration. For this purpose, we introduce the entropy of bond configuration by

$$H(J) = -\sum_J P(J) \log P(J), \tag{5.1}$$

where

$$P(J) = \frac{1}{2^N (2\cosh K_p)^{N_B}} \sum_\sigma e^{K_p \sum J_{ij}\sigma_i\sigma_j} \tag{5.2}$$

is the probability distribution of bond configuration summed up over all configurations with the same distribution of frustration. For example, when J denotes the ferromagnetic configuration ($J_{ij} = 1$, $\forall\langle ij\rangle$), the summation over σ in (5.2) corresponds to the sum of all probability weights of frustration-free (*i.e.* Mattis-like) bond configurations. As a consequence, $P(J)$ has the same value for all frustration-free bond configurations.

The information-theoretical entropy $H(J)$ is related to the free energy $F(T,p)$ at $T = T(p)$ by the following relation

$$H(J) = \beta F(T(p),p) + N\log 2 + N_B \log\cosh K_p \tag{5.3}$$

$$= -S(T(p),p) - \beta(2p-1)N_B + N\log 2$$
$$+ N_B \log 2\cosh K_p. \tag{5.4}$$

This relation is derived from comparison of the definitions (5.1) and (5.2) with the free energy

$$-\beta F(T,p) = \sum_J \frac{e^{K_p\sum J_{ij}}}{(2\cosh K_p)^{N_B}} \log \sum_S e^{\beta\sum J_{ij}S_iS_j}$$
$$= \frac{1}{2^N(2\cosh K_p)^{N_B}} \sum_J\sum_\sigma e^{K_p\sum J_{ij}\sigma_i\sigma_j}$$
$$\times \log\sum_S e^{\beta\sum J_{ij}S_iS_j}. \tag{5.5}$$

The second equation comes from a gauge transformation.

Equation (5.4) shows that an upper bound on the information-theoretical entropy $H(J)$ leads to a lower bound on the thermodynamic entropy S at $T = T(p)$. To estimate an upper bound on

$H(J)$, it is useful to define the probability distribution of frustration $\{\pi\}$ by

$$P(\pi) = 2^N P(J). \tag{5.6}$$

The factor 2^N reflects the fact that there are 2^N different bond configurations with the same distribution of frustration; thus there are only 2^{N-N_B} different configurations of the frustration distribution π. If we specialize to the case of hypercubic lattices, π is specified by the values of all the plaquette 'spins' $\pi_\Box = J_{12}J_{23}J_{34}J_{41}$; there are $N - N_B$ of those. An upper bound on $H(J)$ is then obtained by maximization of the information-theoretical entropy:

$$\begin{aligned} H(J) &= -\sum_J P(J)\log P(J) \\ &= -\sum_\pi P(\pi)\log P(\pi) + N\log 2 \\ &\le (N_B - N)H_2(\tanh^4 K_p) + N\log 2, \end{aligned} \tag{5.7}$$

where

$$H_2(x) = -\frac{1+x}{2}\log\frac{1+x}{2} - \frac{1-x}{2}\log\frac{1-x}{2}. \tag{5.8}$$

The inequality in (5.7) has been derived by maximization of $H(\pi)$ under the constraint that the average of each plaquette spin over $P(\pi)$ is given by $[\pi_\Box] = \tanh^4 K_p$. Comparison of (5.7) with (5.4) leads to the final expression of a lower bound of the thermodynamic entropy

$$\begin{aligned} S(T(p),p) \ge &-\beta(2p-1)N_B + N_B\log 2\cosh K_p \\ &+(N-N_B)H_2(\tanh^4 K_p). \end{aligned} \tag{5.9}$$

5.2 Upper bound

An upper bound on the entropy is obtained from the Jensen inequality combined with a variational method. The following inequality holds for a general function $f(J)$ of bond variables:

$$\begin{aligned} -\beta F(T,p) &= \left[\log\sum_S e^{\beta\sum J_{ij}S_iS_j + f(J)}\right] - [f(J)] \\ &\le \log[\sum_S e^{\beta\sum J_{ij}S_iS_j+f(J)}] - [f(J)] \end{aligned} \tag{5.10}$$

according to the Jensen inequality. Let us now choose

$$f(J) = h\sum_{\langle ij\rangle} J_{ij} \tag{5.11}$$

and restrict our attention to the case of $T = T(p)$. Since the exact energy is known at $T = T(p)$, an upper bound on the entropy is obtained by minimization of the right-hand side of (5.10) with respect to h.

The average over the bond randomness in the argument of the logarithmic function of (5.10) can be carried out relatively simply and the entropy is found to be bounded as

$$S(T(p),p) \le \min_h \Big\{ N_B \log A + \log Z_0(\tilde{K}) - N_B \log 2\cosh K_p \\ -N_B h \tanh K_p \big\}\,, \qquad (5.12)$$

where we have rewritten $h+K_p$ as h, and A and $\tilde{K}$ are defined by

$$2\cosh(K+h) = Ae^{\tilde{K}}, \quad 2\cosh(K-h) = Ae^{-\tilde{K}}. \qquad (5.13)$$

The partition function Z_0 is that of the non-random Ising model.

Numerical minimization of the right-hand side of (5.12) gives the result shown in Fig. 3 in the case of the square lattice. The lower bound from the previous subsection is also shown, along with

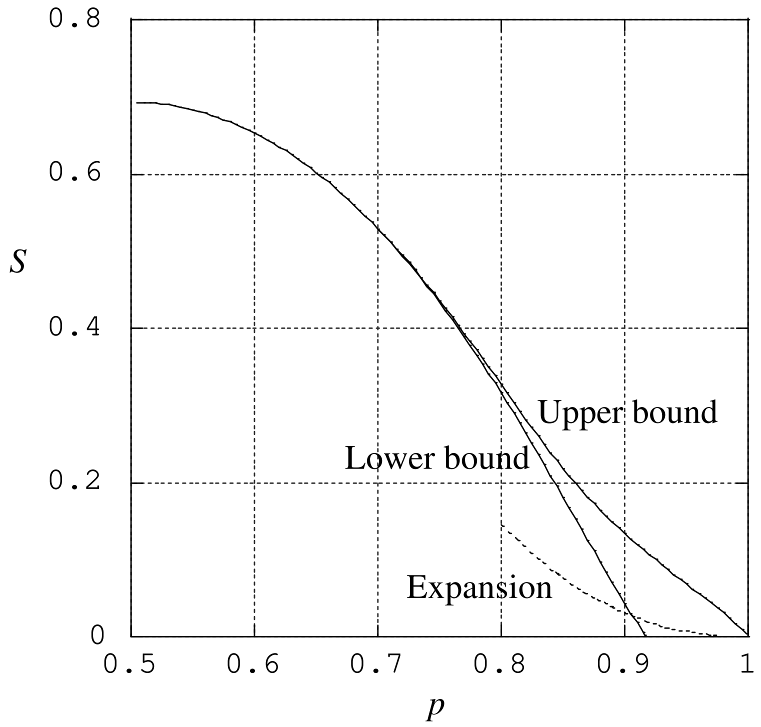

Fig. 3. Bounds on the entropy for the square lattice. The dotted line shows the leading term of an expansion around $p=1$.

the leading term of an expansion around $p=1$ (Nishimori and Sollich, unpublished)

$$S(T(p),p) \approx 3N_B \log 2 \cdot (1-p)^2. \qquad (5.14)$$

We observe that the entropy is bounded very tightly in the high temperature region. Systematic improvements along the line of Morita and Kühn[6,7] should further improve the upper bound.

§6. Discussion

We have tried to clarify the spin states in the ferromagnetic phase of the $\pm J$ Ising model of spin glasses. The first hint was given by an inequality on the number of up spins as a function of temperature. The average number of up spins first increases as the temperature is lowered and reaches a maximum on the Nishimori line. Then it turns to a decrease at lower temperatures. In this sense the lower temperature region may be regarded to be less ordered than the high-temperature region. This non-trivial behaviour does not necessarily imply a reentrant transition to a non-ferromagnetic phase; a reentrant transition is characterized by disappearance of magnetization below a certain temperature, while in the present context it is likely that the magnetization actually grows: The increase in the *magnitude* $\langle S_i \rangle$ of up spins ($\langle S_i \rangle > 0$) can offset the decrease in the *number* of up spins.

The fact that the number of up spins reaches a maximum on the Nishimori line is understood relatively naturally from a Bayesian point of view. In fact, some of the other properties of the $\pm J$ model derived by the method of gauge transformation can be re-derived within the Bayesian framework.[4] However, as far as the $\pm J$ model is concerned the Bayesian approach does not yield new results on spin states beyond those known from the gauge transformation method.

We therefore turned to another point of view using the relative volume of a spin state in the phase space. It was shown that the region above the Nishimori line in the ferromagnetic phase is similar to the pure ferromagnetic system from the behaviour of the relative volume. In contrast, in the low temperature region, thermodynamically relevant spin states directly reflect the random bond configuration. This observation is quite consistent with the result from the inequality on the number of up spins. It was also shown that the relative volume of the perfect ferromagnetic state on the Nishimori line is equal to the minus of the entropy. Thus the entropy carries important information on the weight of the perfect ferromagnetic state.

We then derived upper and lower bounds on the entropy using the maximum-entropy method and the Jensen inequality. Very precise bounds resulted at least in the high-temperature region. Further refinement of the variational method should improve the upper bound in the low-temperature side.

All in all, we feel that we now have a better – though still not quite perfect – understanding of spin states in the ferromagnetic phase of the $\pm J$ model. Most of the arguments developed here are very generic and apply to any lattice. Further progress may well require ideas which make use of the properties of particular lattices, but we nevertheless hope that the present contribution may contribute some useful building blocks for such developments.

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