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A replica method for the deterministic spin model with long range interactions

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Abstract
We discuss the spin glass states of the deterministic spin model with long range anti-ferromagnetic interactions. To apply the replica method, the partial statistical summation with fixed overlap parameters is introduced. By this formulation, we find that the replica theory for this model reduces to that of the anti-Hebbian model in the long range limit, suggesting the existence of dynamical phase transition and glassy states. Results of simulated annealing are also presented to confirm these results.

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1. Introduction

In recent years, a lot of efforts have been made to clarify the glassy states of deterministic spin models, which do not have quenched disorder, by using the accumulated results for the random spin models [1]. One of the main interests is focused on the dynamical nature of glass phase transition, which is not reflected in the usual thermodynamic functions. There have been several studies of dynamics to address this problem [2]. On the other hand, the replica method is important to describe the partitioned configuration space, which also characterizes the glassy states. One replica approach is to introduce random spin models to simulate the glassy properties of the deterministic models [3–5]. Another approach is to introduce a small coupling among replicas [6]. By these approaches, it was clarified that some deterministic models really have glassy low temperature states, which are associated with a dynamical phase transition. To clarify the situation in the conventional systems, it will be fruitful to study the familiar spin systems in the light of the studied spin glass models.

In this paper, we first show that some long range anti-ferromagnetic spin models can be viewed as a natural generalization of the anti-Hebbian (AH) model [7], which has glassy states associated with a dynamical phase transition. Secondly, we suggest a replica method for the deterministic spin models to study this model.

The spin model we discuss is defined on the one-dimensional lattice with the energy function given by

$$H = \frac{1}{2}\sum_{ij} J_{ij} S_i S_j \tag{1}$$

with

$$J_{ij} = \frac{\sin \alpha\pi(i-j)}{\pi(i-j)} \tag{2}$$

where $i, j = 1, 2, \ldots, N$, N is the system size and $S_i = \pm 1$ are Ising spin variables located on the lattice sites. α is a positive parameter smaller than 1. The terms with $J_{ii} = \alpha$ are included in (1) for convenience. For simplicity, we define the sign of interactions opposite to the conventional one. Note that the interactions are anti-ferromagnetic for $2k/\alpha < |i-j| < (2k+1)/\alpha$ $(k = 0, 1, \ldots)$ and similar to the RKKY interaction.

Let us introduce this model by starting with the observations on the AH model [7], which is defined by the energy function

$$\begin{aligned} H_A &= \frac{1}{2N}\sum_{ij}\sum_{\mu} \xi_i^{\mu}\xi_j^{\mu} S_i S_j \\ &= \frac{1}{2N}\sum_{\mu}\left(\sum_i \xi_i^{\mu} S_i\right)^2 \end{aligned} \tag{3}$$

where ξ_i^{μ} $(\mu = 1, 2, \ldots, P)$ are quenched random variables which take ± 1 with probability $1/2$. This model has an interesting property. When $P \gg N$, the spin glass phase transition is similar to that of the Sherrington–Kirkpatrick (SK) model [8, 9], while it has a dynamical phase transition for $P/N < 1$. This property is understood by observing the structure of the energy function. That is, the energy function is minimized by the configurations which satisfy $\sum_i \xi_i^{\mu} S_i = 0$ for all μ. This makes an $(N-P)$-dimensional solution space for $P/N < 1$. Although these constraints will not be satisfied exactly by discrete spin variables, the configurations which nearly satisfy these constraints will make a strongly degenerated energy landscape, especially for small P/N, implying there are many glassy states at low temperature. This model can be regarded as a nontrivial generalization of the infinite range anti-ferromagnet, for which $P = 1$.

The observations on the AH model suggest that, to have similar properties, ξ_i^{μ} can be arbitrary as long as they make linear independent functions of S_i. This directly suggests taking the Fourier transformations of S_i as the linear functions, assuming that S_i are located, for example, on the one-dimensional lattice. As a simple realization of this idea, we suggest the energy function which is defined by

$$\begin{aligned} H &= \sum_{|\mu|}\left|\sum_i \mathrm{e}^{\sqrt{-1}(2\pi\mu/N)i} S_i/\sqrt{N}\right|^2 \\ &= \frac{1}{N}\sum_{ij}\sum_{|\mu|} \mathrm{e}^{\sqrt{-1}(2\pi\mu/N)(i-j)} S_i S_j \end{aligned} \tag{4}$$

where $\sqrt{-1}$ stands for an imaginary unit and $\sum_{|\mu|}$ means the sum over $\mu = 0, 1, 2, \ldots, P/2$ with $P < N$. Note that the real part and imaginary part of a Fourier component make two squared linear forms of S_i, giving $P + 1 \sim P$ constraint terms in (4). After performing the μ sum, we obtain the interactions given by (2) with $\alpha = P/N$. We call this model the Fourier component (FC) model. It is quite interesting and suggestive that this model tends to the infinite range anti-ferromagnet as $\alpha \to 0$, just like the AH model. This is a natural consequence of the modelling.

The FC model will have some special configurations. We expect that the Fourier components of S_i with small wavelength have very low energy. Most of them do not give the absolute minimum of the energy function due to the discreteness of spin variables. However, there are two exceptions given by $S_i = \pm\cos(\pi \mathrm{i})$, which correspond to crystalline structures. The basin of attraction of them will become larger as the number of constraint terms increases. This is an interesting aspect of the FC model, although we concentrate on the study of glassy states in this paper.

This paper is organized as follows. In section 2, we begin with the high temperature expansion of the FC model to measure the proximity to the AH model. In section 3, we suggest a replica method for the deterministic spin models and apply it to the FC model. The argument in section 2 suggests the perturbation treatment in terms of α for the replicated FC model. This is discussed in section 4, which also provides some simulation results. Section 5 is devoted to some discussions.

2. High temperature expansion of the FC model

The discussion in section 1 suggests that the FC model and the AH model are very similar. In this section, we study the high temperature expansion of both models to clarify this point. This study suggests the perturbation method in terms of α for the FC model. In addition, the formulation in this section will be very helpful to study the replica theory introduced in the next section.

To begin with, we discuss the high temperature expansion for the AH model [7]. The partition function is given by

$$Z_A = \sum_{\{S\}} \exp(-\beta H_A) \tag{5}$$

where $\beta = 1/T$ is an inverse temperature. After the expansion in terms of interactions and the summation over $S_i = \pm 1$, $\ln Z_A$ is expressed as a summation over non-self-intersecting loop diagrams made of interactions. With ξ_i^μ average, which is denoted by $\overline{\cdots}$, a loop of any length becomes proportional to P/N. We then obtain the free energy $f_A = -\overline{\ln Z_A}/\beta N$ given by

$$f_A = -\frac{1}{\beta}\ln 2 + \frac{\alpha}{2\beta}\ln(1+\beta) \tag{6}$$

where $\alpha = P/N$ has the same meaning as the FC model, that is, the ratio between the numbers of constraints and spin variables. The energy and entropy are given by $e_A = \partial\beta f_A/\partial\beta$ and $s_A = \beta(e_A - f_A)$. It is quite interesting that, by this simple result, we find that the entropy s_A becomes negative at some low temperature. This temperature is given by $T_s \sim \exp(-1 - 2\ln 2/\alpha)$ for small α. Since negative entropy for Ising spin is not acceptable, some phase transition should occur above this temperature. Note that T_s is roughly obtained by demanding $Z_A \sim 1$, which implies there are a few configurations contributing to Z_A with nearly zero energy. We can estimate the energy density of these configurations by setting $T = T_s$ in e_A, obtaining $e_A \sim (\alpha/2)\exp(-1 - 2\ln 2/\alpha)$.

Now we discuss the high temperature expansion for the FC model. Actually, collecting all terms of the expansion will not be easy for arbitrary α. In the following, we study this problem by expansion in terms of α. It is convenient to use the Fourier component representations for this purpose. For simplicity, we use the abbreviation $e_i^\mu \equiv \mathrm{e}^{\sqrt{-1}(2\pi\mu/N)i}$ in the following expressions.

Using the Gaussian integrals, the partition function for the FC model is expressed as

$$Z = \sum_{\{S\}} \exp\left(-\frac{1}{2}\beta \sum_{|\mu|} \left|\sqrt{2}\sum_i e_i^\mu S_i/\sqrt{N}\right|^2\right)$$
$$= \sum_{\{S\}} \int \exp\left(-\frac{1}{2}\sum_{|\mu|} |\phi_\mu|^2 + \frac{1}{2}\sqrt{-1}\sqrt{\frac{2\beta}{N}}\sum_i \sum_\mu e_i^\mu \phi_\mu S_i\right) \prod_{|\mu|} \frac{\mathrm{d}\phi_\mu}{2\pi} \quad (7)$$

where $\sum_\mu$ means the summation over $\mu = -P/2, \ldots, P/2$ and ϕ_μ are complex integral variables with $\phi_{-\mu} = \phi_\mu^*$, and $\mathrm{d}\phi_\mu = \mathrm{d}\,\mathrm{Re}\,\phi_\mu\,\mathrm{d}\,\mathrm{Im}\,\phi_\mu$. Note that there is an imaginary unit in the second term in the exponential. This is the common feature of the anti-ferromagnetic-like interactions. After S_i sum, we have

$$Z = 2^N \int \exp(-L\{\phi_\mu\}) \prod_{|\mu|} \frac{\mathrm{d}\phi_\mu}{2\pi} \quad (8)$$

where

$$L\{\phi_\mu\} = \frac{1}{2}\sum_{|\mu|} |\phi_\mu|^2 - \sum_i \ln\cos\sqrt{\frac{\beta}{2N}}\sum_\mu e_i^\mu \phi_\mu$$
$$= \frac{1}{2}(1+\beta)\sum_{|\mu|} |\phi_\mu|^2 + \frac{1}{48N}\beta^2 \sum_{\sum_{k=1}^4 \mu_k = 0} \phi_{\mu_1}\phi_{\mu_2}\phi_{\mu_3}\phi_{\mu_4} + \cdots. \quad (9)$$

The first term in the second line of $L\{\phi_\mu\}$ makes a Gaussian part, while there are higher order terms of ϕ_μ. These terms can be treated by perturbation with propagators $\langle|\phi_\mu|^2\rangle = 2(1+\beta)^{-1}$, where the average is done by the Gaussian part of $L\{\phi_\mu\}$. We then obtain the free energy $f \equiv -\ln Z/\beta N$,

$$f = -\frac{1}{\beta}\ln 2 + \frac{\alpha}{2\beta}\ln(1+\beta) + \frac{1}{4}\frac{\alpha^2\beta}{(1+\beta)^2} + \cdots \quad (10)$$

the energy e,

$$e = \frac{1}{2}\frac{\alpha}{1+\beta} + \frac{1}{2}\frac{\alpha^2\beta}{(1+\beta)^3} + \cdots \quad (11)$$

and the entropy $s = \beta(e-f)$ to the second order of α. The effects of the second-order terms are very small for low temperature due to the factor $1/(1+\beta)$. To the first order of α, the expansion reduces to that of the AH model. Just like the AH model, the entropy becomes zero at T_s to the first order of α, which implies that there should be some phase transition above T_s for the FC model at least for small α. In terms of the cosine-functions in (9), they will give a very small value of Z for low temperature and Z substantially becomes of order 1 as $T \to T_s$.

Let us give some remarks on the expansion. When Z is directly expanded in terms of βJ_{ij}, we need to collect all the first- and second-order terms of α to obtain (10). As for the first-order terms, the situation is similar to the AH model. The factor $\ln(1+\beta)$ in the free energy implies that we should collect all contributions of loops made of βJ_{ij} to obtain the first order of α. These terms, after summation over site subscripts, really give the terms proportional to α. For example, denoting the sum over different site subscripts by $\sum'$, we have $\sum' J_{ij}^2/N = \alpha - \alpha^2$, $\sum' J_{ij}J_{jk}J_{ki}/N = \alpha - 3\alpha^2 + 2\alpha^3$, etc. For the FC model, we can sum the leading contributions conveniently by working with Fourier components.

Although there seems no inconsistency in the high temperature expansions down to the point $s = 0$, the study for the AH model revealed that there is a dynamical phase transition far above T_s for small α. This transition can be identified by the replica method with the marginality condition for random spin models. We naturally expect that the same thing happens for the FC model. The problem is how to apply the replica method to the spin models without quenched disorder.

3. Replica method for the FC model

In this section, we first discuss the replica method for the spin model without quenched disorder, and then apply it to the FC model.

For the random spin models, we use the relation $\ln Z = \lim_{n\to 0}(Z^n - 1)/n$ to obtain the sample averages of the free energy $f = -\ln Z/\beta N$. Before the random averages, the replica partition function is simply given by

$$Z^n = \sum_{\{S\}} \exp\left(-\beta \sum_{\rho=1}^{n} H\left\{S_i^\rho\right\}\right) \tag{12}$$

where $H\{S_i\}$ is the energy function of the system and S_i^ρ ($\rho = 1, 2, \ldots, n$) are replica spin variables. In the mean field theory of the random spin models, the averages over randomness with fixed spin variables yield the averaged Z^n as a function of overlap order parameters $\sum_i S_i^\rho S_i^\sigma / N$. Then, the saddle point of $\ln Z^n$ is studied by varying these order parameters. On the other hand, the FC model has no randomness and does not require sample averages. Even in this situation, it is believed that the introduction of replicas will show some signal of condensation states, which may or may not be seen by the usual thermodynamic functions.

The point of our formulation is to perform partial statistical sum which has a given correlation among replicas, which may be described by $S_i^\rho S_i^\sigma$. We first note that $S_i^\rho S_i^\sigma$ are invariant by the simultaneous change $S_i^\rho \to -S_i^\rho$ for all replicas. This strongly suggests that we will obtain the same result if we perform some partial statistical sum in Z^n with fixed $S_i^\rho S_i^\sigma$ without doing random averages.

After several inspections, we found that the statistical sum with fixed $S_i^\rho S_i^\sigma$ is conveniently performed by introducing the replacements of S_i^ρ by $\eta_i S_i^\rho$, where $\eta_i = \pm 1$, which are common among replicas. Since $S_i^\rho S_i^\sigma$ do not change by η_i, the terms in Z^n with the same $S_i^\rho S_i^\sigma$ change mutually by various η_i. To perform a partial statistical sum over them, it is natural to extend the statistical sum to that over $\eta_i = \pm 1$. To count the terms correctly, we use the fact that Z^n is invariant by η_i due to the summation over S_i^ρ. Thus we can write

$$Z^n = \frac{1}{2^N} \sum_{\{\eta\}} \sum_{\{S\}} \exp\left(-\beta \sum_{\rho=1}^{n} H\left\{\eta_i S_i^\rho\right\}\right) \tag{13}$$

where $\sum_{\{\eta\}}$ means the sum over all $\eta_i = \pm 1$. Then the η_i sum is performed first with fixed S_i^ρ, resulting in the desired partial statistical sum. This summation will correspond to the configuration sum with fixed $S_i^\rho S_i^\sigma$ in the original Z^n without η_i. Note that the introduction of η_i has nothing to do with the symmetry of the energy function. We simply change the order of summation in Z^n by using η_i. Note also that, at this point, it is not clear if the result is expressed by the site sum of $S_i^\rho S_i^\sigma$. This depends on the nature of the problem.

Let us perform the η_i sum for the FC model. Formally the η_i sum is very similar to the high temperature expansion. For the FC model, it is convenient to follow the procedure presented in section 2. We first express each term in (13) as an integral over Gaussian variables ϕ_μ^ρ with $\rho = 1, 2, \ldots, n$ in the same way as (7), and then the summation over η_i is performed.

In this way, we can obtain the replicated partition function given by

$$Z^n = \frac{1}{2^N} \sum_{\{\eta\},\{S\}} \exp\left(-\frac{1}{2}\beta \sum_{\rho,|\mu|} \left| \sqrt{2} \sum_i e_i^\mu \eta_i S_i^\rho \Big/ \sqrt{N} \right|^2 \right)$$
$$= \sum_{\{S\}} \int \exp\left\{ -\frac{1}{2} \sum_{\rho,|\mu|} |\phi_\mu^\rho|^2 + \sum_i \ln\cos\left(\frac{\sqrt{\beta}}{\sqrt{2N}} \sum_{\rho,\mu} \phi_\mu^\rho e_i^\mu S_i^\rho \right) \right\} \prod_{\rho,|\mu|} \frac{\mathrm{d}\phi_\mu^\rho}{2\pi}. \tag{14}$$

This is the basic formula for the following argument. We should note that this is just another expression of (12) with the interactions (2). Integral over ϕ_μ^ρ is performed by the expansion in terms of α in a similar way as the high temperature expansion. We will discuss this point in the next section.

4. Marginally stable RSB and simulation results

In this section, we discuss Z^n to the first order of α and study the resulting expression by the saddle point approximation. The simulation results for the FC model are also presented to compare with the replica results.

There remain two steps to give the saddle point equations for our problem. We first perform ϕ_i^ρ integrals to obtain $A\{S^\rho\}$, which is defined by

$$\exp A\{S^\rho\} = \int \exp(-L\{S^\rho, \phi^\rho\}) \prod_{\rho,|\mu|} \frac{\mathrm{d}\phi_\mu^\rho}{2\pi} \tag{15}$$

where

$$L\{S^\rho, \phi^\rho\} = \frac{1}{2} \sum_{\rho,|\mu|} |\phi_\mu^\rho|^2 - \sum_i \ln\cos\left(\frac{\sqrt{\beta}}{\sqrt{2N}} \sum_{\rho,\mu} \phi_\mu^\rho e_i^\mu S_i^\rho \right).$$

Then the partition function $Z^n = \sum_S \exp(A\{S^\rho\})$ will be evaluated by the saddle point approximation, if possible.

Now let us discuss the expression of $A\{S^\rho\}$. We first note that the value of $\Phi_i = \sum_{\rho,\mu} \phi_\mu^\rho e_i^\mu S_i^\rho$ will be proportional to $\sqrt{P}$. Thus, it is natural to discuss $A\{S^\rho\}$ by perturbation in terms of α. The results will confirm this idea. By expanding $L\{S^\rho, \phi^\rho\}$ in terms of Φ_i, we obtain

$$L\{S^\rho, \phi^\rho\} = \frac{1}{2} \sum_{\rho,|\mu|} |\phi_\mu^\rho|^2 + \frac{\beta}{4N} \sum_i \Phi_i^2 + \frac{\beta^2}{48N^2} \sum_i \Phi_i^4 + \cdots. \tag{16}$$

The second term consists of the terms which are diagonal and off-diagonal with respect to μ. The diagonal terms make

$$L_1\{S^\rho, \phi^\rho\} = \frac{1}{2} \sum_{\rho,|\mu|} |\phi_\mu^\rho|^2 + \frac{\beta}{2N} \sum_{\rho\sigma} \sum_{|\mu|} \phi_\mu^\rho \phi_{-\mu}^\sigma \sum_i S_i^\rho S_i^\sigma. \tag{17}$$

As discussed in the appendix, the off-diagonal Gaussian terms in Φ_i^2 and higher order terms of Φ_i give the second and higher order terms of α to $A\{S^\rho\}$. This is because more than one free subscript μ remains to be summed in these contributions. We then obtain to the first order of α

$$A_1\{S^\rho\} = -\tfrac{1}{2} N\alpha \operatorname{Tr} \ln(1 + \beta q) \tag{18}$$

where $q_{\rho\sigma} = \sum_i S_i^\rho S_i^\sigma \big/ N$ with $q_{\rho\rho} = 1$. This is the same expression as the AH model, which implies that the FC model is described by the AH model to the first order of α even at low temperature.

As discussed in [7], the study of Z^n with $A_1\{S^\rho\}$, denoted by Z_1^n, can be performed in the same way as that of the random orthogonal model [4]. We briefly describe the main results here. By introducing

$$
\begin{aligned}
1 &= \prod_{\rho<\sigma} \int \delta\left(Nq_{\rho\sigma} - \sum_i S_i^\rho S_i^\sigma\right) N\,\mathrm{d}q_{\rho\sigma} \\
&= \prod_{\rho<\sigma} \int \exp\left\{\lambda_{\rho\sigma}\left(Nq_{\rho\sigma} - \sum_i S_i^\rho S_i^\sigma\right)\right\} \frac{N\,\mathrm{d}\lambda_{\rho\sigma}\,\mathrm{d}q_{\rho\sigma}}{2\pi\mathrm{i}}
\end{aligned}
$$

we obtain

$$
Z_1^n = \iint \exp\{-N\beta n f(\lambda_{\rho\sigma}, q_{\rho\sigma})\} \prod_{\rho<\sigma} \frac{N\,\mathrm{d}\lambda_{\rho\sigma}\,\mathrm{d}q_{\rho\sigma}}{2\pi\mathrm{i}} \tag{19}
$$

where

$$
\beta n f(\lambda_{\rho\sigma}, q_{\rho\sigma}) = \mathrm{Tr}g(\beta q) + \frac{1}{2}\sum_{\rho\neq\sigma} \lambda_{\rho\sigma} q_{\rho\sigma} - \ln \sum_{\{S\}} \exp \frac{1}{2} \sum_{\rho\neq\sigma} \lambda_{\rho\sigma} S^\rho S^\sigma \tag{20}
$$

with $g(x) = (\alpha/2)\ln(1+x)$.

By studying this expression, we found that there is no replica symmetry solution for $\alpha < 1$. On the other hand, there are two types of one-step replica symmetry breaking (RSB) solution, which is defined by $q_{\rho\sigma} = q_1, \lambda_{\rho\sigma} = \lambda_1$ in $m \times m$ diagonal blocks and $q_{\rho\sigma} = 0, \lambda_{\rho\sigma} = 0$ elsewhere. In this ansatz, the matrix q has eigenvalue $1 - q_1 + mq_1$ with degeneracy n/m and eigenvalue $1 - q_1$ with degeneracy $n - n/m$. The free energy then reduces to

$$
\begin{aligned}
\beta f = \frac{1}{2}\alpha &\left\{\frac{1}{m}\ln(1+\beta x_m) + \left(1 - \frac{1}{m}\right)\ln(1+\beta x_0)\right\} \\
&+ \frac{1}{2}(m-1)\lambda_1 q_1 + \frac{1}{2}\lambda_1 - \frac{1}{m}\ln\int 2^m \cosh^m(\sqrt{\lambda_1} z)\,\mathrm{D}z
\end{aligned} \tag{21}
$$

where $\mathrm{D}z = \exp(-z^2/2)\,\mathrm{d}z/\sqrt{2\pi}$ and $x_m = 1 - q_1 + mq_1$, $x_0 = 1 - q_1$.

The static RSB solution is defined by $\partial f/\partial q_1 = 0$, $\partial f/\partial\lambda_1 = 0$ and $\partial f/\partial m = 0$. For small α, this solution appears at very low temperature, which is close to T_s, where the high temperature entropy becomes zero. This solution is stable with respect to the small changes of order parameters and is expected to represent the absolute minimum state of the AH model.

Another RSB solution is defined by replacing $\partial f/\partial m = 0$ with the marginality condition $1 - g\mu = 0$, where

$$
g = -\frac{\alpha\beta^2}{(1+\beta x_0)^2} \qquad \mu = -\frac{\int \cosh^m(\sqrt{\lambda_1} z)\cosh^{-4}(\sqrt{\lambda_1} z)\,\mathrm{D}z}{\int \cosh^m(\sqrt{\lambda_1} z)\,\mathrm{D}z}.
$$

This condition corresponds to the marginal stability of the spin dynamics and it is expected to describe the glassy states [3, 4, 10]. In the AH model with small α, the solution with $0 < m < 1$ appears at the moderate temperature T_g, which is much higher than T_s. Below T_g, this RSB solution gives the energy which depends on temperature very weakly down to rather low temperature. For both solutions, the expectation value of energy is given by

$$
e = \frac{\alpha}{2}\left\{\frac{1}{m}\frac{x_m}{1+\beta x_m} + \left(1 - \frac{1}{m}\right)\frac{x_0}{1+\beta x_0}\right\} \tag{22}
$$

which reduces to the energy of high temperature expansion for $q_1 = 0$ and $m = 1$.

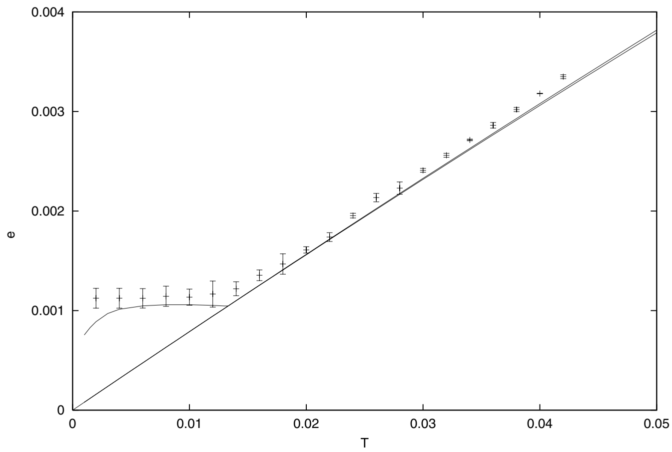

Figure 1. T-dependence of energy for $\alpha = 0.5/\pi$. The simulation results for the FC model are presented by points with error bars, which show the standard deviations for five annealing runs. $N = 500$. MC steps at each temperature is 10^4. Full curves show the energies obtained by the high temperature expansion to the first and second orders of α, and marginal RSB for the AH model, which appears below $T_g = 0.0133$.

Let us present some simulation results for the FC model. To avoid being commensurate with lattice, we control $\alpha\pi$ in the numerical simulations. By observing many runs of simulated annealing, we found that the expectation value of energy decreases nearly in accordance with the result of high temperature expansion at moderate temperature, and around a certain temperature, it ceases to decrease. In this narrow temperature region, the acceptance rate of spin flips decreases drastically and the Edward–Anderson order parameter $\sum_i \langle S_i \rangle_M^2 / N$ rapidly increases to 1.0, while $\sum_i \langle S_i \rangle_M / N$ remains nearly zero, where $\langle \cdots \rangle_M$ means the averages over Monte Carlo (MC) steps at each temperature. The spin configurations obtained in this way look really random and uncorrelated with each other. However, we also monitor $\sum_i \langle S_i \rangle_M \cos(\pi \mathrm{i})/N$, which are also found to be very small for the studied small α down to zero temperature. Although we should clarify that the obtained states really show randomness in the deterministic model, we concentrate on the temperature dependence of the energy, for which analytic results by the AH model are available.

Figures 1 and 2 show the temperature dependence of energy obtained by simulated annealing for the FC model with $\alpha\pi = 0.5$ and 1.0, respectively. The figures also show the results of the high temperature expansion for e and those of marginal one-step RSB which are obtained for the AH model. The replica study of the AH model gives $T_g = 0.0133$ with $e = 0.001\,05$ for $\alpha = 0.5/\pi$ and $T_g = 0.0313$ with $e = 0.004\,83$ for $\alpha = 1.0/\pi$. These values seem to be consistent with the simulation results.

Let us look at the simulation results more closely. In the high temperature region, the annealing energies are slightly higher than (11) systematically for $\alpha = 0.5/\pi$. We suspect that this is due to the large system size dependence for small α caused by the long range nature of interactions. In fact, figure 2 for $\alpha = 1.0/\pi$ shows a better agreement in the high temperature region. Note that the factor $(1 + \beta)^{-1}$ contained in higher order terms is very small for these temperatures. We have studied the number of MC steps of each temperature from 10^3 to 10^4. For the temperature around and below T_g, numerical e depends on the number of MC steps of each temperature and initial configurations in high temperature. Numerical e at low

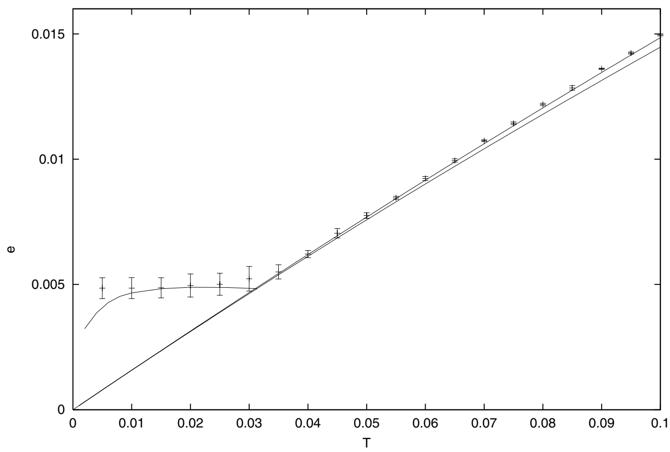

Figure 2. Same as figure 1 but for $\alpha = 1.0/\pi$ and $T_g = 0.0313$.

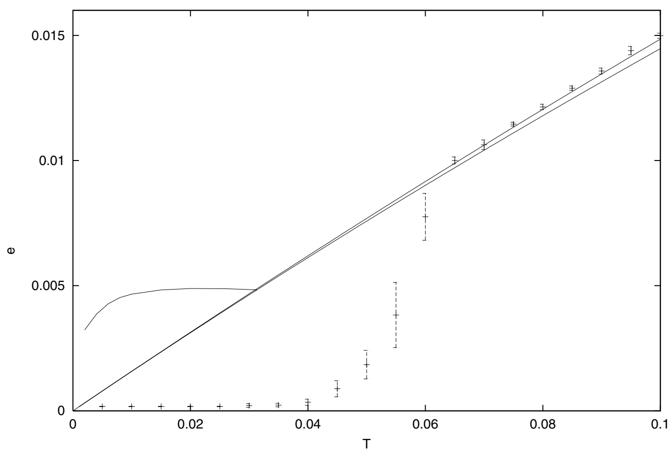

Figure 3. Simulation of increasing temperature for $\alpha = 1.0/\pi$. The initial configuration at $T = 0.005$ is assumed to be the crystalline state given in the text. The average is over the five runs created by different random number sequences. $N = 500$ and MC steps at each temperature is 10^3. Full lines are the same as figure 2.

temperature tends to be large for a small number of MC steps and decrease to the same value as the number increases. These phenomena are typical for glass phase transitions.

Figure 3 shows another interesting phenomenon in the FC model. As discussed in section 1, this model has crystalline state $S_i = \cos(\pi i)$. Assuming this configuration at very low temperature, we can observe 'melting' of this by increasing the temperature step by step. Figure 3 shows the temperature dependence of the averaged energy of the resulting configurations. The initial configuration has a small positive energy probably due to the finite system size. As the temperature increases, the crystalline state starts melting slightly above T_g, and goes to the paramagnetic phase in the narrow range of temperature.

To summarize, the simulation results strongly suggest that there is a phase transition at finite temperature in the FC model at least for small α. We may safely say that the transition points and temperature dependence of energy are well described by the RSB solution with the marginality condition of the AH model, which is viewed as an approximated FC model. All these results suggest that we are observing a glass transition of the long range anti-ferromagnetic spin model.

5. Discussion

In this paper, we have studied the dynamical phase transition and glassy states of the deterministic spin model defined on the one-dimensional lattice, which is called the FC model. This model is inspired by the studies on the AH model. To apply the replica method, we introduced a partial statistical sum for the replicated partition function. With this formulation, we found that the FC model reduces to the AH model for small α. The simulation results for the FC model are consistent with the marginal RSB solution obtained by the AH model.

The AH model and the FC model are regarded as nontrivial generalizations of the infinite range anti-ferromagnetic model, which has only one constraint term in the energy function. When the number of constraint terms P is of order N but smaller than N, a remarkable situation arises, i.e. a glass transition. For the FC model, the range of interactions is inversely proportional to the number of constraint terms on the Fourier components. The model remains tractable for small P/N in the framework of replica mean field theory. Although the resulting picture on glass transitions was already found several years ago, it is interesting that a similar property holds in the FC model, which looks rather simple and conventional.

To study the glassy states of the spin model without quenched disorder, we have introduced a replica method in which the partial statistical sum is performed with fixed $S_i^\rho S_i^\sigma$. If the statistical sum in Z^n is performed independently for each replica, we simply obtain n times the free energy evaluated by the high temperature expansion. But the situation essentially changes under the partial statistical sum, by which the stage of thermodynamic limit will be changed. This procedure seems general and probably applicable to models with other types of dynamical variable, although we need to find a suitable order parameter to describe the glassy states.

Studies of the higher order terms of α will reveal the properties of the moderate range FC model. The brief study presented in the appendix implies that there appear complicated terms made of $q_{\rho\sigma}$ and the products of S_i^ρ even in the second order of α. A similar situation was already found in the models with finite connectivity [11, 12]. The studies accumulated for these models may be helpful to know more about the FC model.

The idea that we have described to make the FC model is very general. In this paper, we adopted a simple truncation of Fourier components to do an analysis as close as possible to the AH model. The oscillation of interactions is due to the truncation of the Fourier components. There will be another choice to weight the constraint terms of the energy function, which will induce another spin models mainly characterized by spatially varying anti-ferromagnetic interactions. Such models will be studied in a similar way if we can find a proper expansion parameter. We may even generalize the model to higher dimensional lattice by introducing a suitable Fourier representation. Studies in this direction may reveal that there is some universality in the spin models with long range anti-ferromagnetic interactions.

Appendix

In this appendix, we briefly discuss the off-diagonal and fourth-order terms of ϕ_i^ρ in $L\{S^\rho, \phi^\rho\}$ and show that they give the second-order terms of α.

The second-order term of Φ_i in (16) contains

$$L_{\mathrm{off}} = -\frac{\beta}{4N}\sum_i\sum_{\rho\sigma}\sum_{\mu\neq-\nu}\phi_\mu^\rho\phi_\nu^\sigma e_i^\mu e_i^\nu S_i^\rho S_i^\sigma. \tag{A.1}$$

The leading contribution to $A\{S\}$ of this term reads

$$\frac{1}{2}\langle L_{\mathrm{off}}^2\rangle = \left(\frac{\beta}{4N}\right)^2\sum_{\rho\sigma\gamma\delta}\sum_{\mu\neq-\nu,ij} g_\mu^{\rho\gamma} g_\nu^{\sigma\delta} e_i^\mu e_i^\nu e_j^{-\mu} e_j^{-\nu} S_i^\rho S_i^\sigma S_j^\gamma S_j^\delta \tag{A.2}$$

where $g_\mu^{\rho\sigma} = \langle\phi_\mu^\rho\phi_{-\mu}^\sigma\rangle = 2(1+\beta q)^{-1}_{\rho\sigma}$, where the averages are by $L_1\{S^\rho,\phi^\rho\}$. The summation over μ and ν gives a factor proportional to P^2. Collecting P and N, we have a factor $N\alpha^2$ in $\langle L_{\mathrm{off}}^2\rangle$.

The contribution from the fourth order of Φ_i reads

$$-\langle L_4\rangle = -\frac{\beta^2}{16N^2}\sum_i\sum_{\rho\sigma\gamma\delta}\sum_{\mu\nu} g_\mu^{\rho\sigma} g_\nu^{\gamma\delta} e_i^\mu e_i^{-\mu} e_i^\nu e_i^{-\nu} S_i^\rho S_i^\sigma S_i^\gamma S_i^\delta. \tag{A.3}$$

Similarly, there is a factor $e_i^\mu e_i^{-\mu} e_i^\nu e_i^{-\nu} = 1$ with two free subscripts μ,ν. This gives also a factor P^2, making $N\alpha^2$ in $\langle L_4\rangle$. The number of free subscripts will increase in higher order terms of Φ_i.

References

[1] For a recent review, see Young A P (ed) 1998 *Spin Glasses and Random Fields* (Singapore: World Scientific)
[2] Chandra P, Feigelman M V and Ioffe L B 1996 *Phys. Rev. Lett.* **76** 4805 and references therein
[3] Marinari E, Parisi G and Ritort F 1994 *J. Phys. A: Math. Gen.* **27** 7615
[4] Marinari E, Parisi G and Ritort F 1994 *J. Phys. A: Math. Gen.* **27** 7647
[5] Bouchaud J P and Mézard M 1994 *J. Physique* I **4** 1109
[6] Monasson R 1995 *Phys. Rev. Lett.* **75** 2847
[7] Nokura K 1998 *J. Phys. A: Math. Gen.* **31** 7447
[8] Sherrington D and Kirkpatrick S 1975 *Phys. Rev. Lett.* **35** 1792
[9] Mézard M, Parisi G and Virasoro M A 1987 *Spin Glass Theory and Beyond* (Singapore: World Scientific)
[10] Horner H 1992 *Z. Phys. B* **86** 291
[11] Kanter I and Sompolinsky H 1987 *Phys. Rev. Lett.* **58** 164
[12] Monasson R 1998 *J. Phys. A: Math. Gen.* **31** 513