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A replica mean field theory for the long range anti-ferromagnetic spin models

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Abstract

We study the long range anti-ferromagnetic Ising spin models defined on one- and two-dimensional lattices by using a replica method for the deterministic spin models. In the long range limit, the replicated partition function reduces to that of the generalized anti-Hebbian model. This suggests that there are a dynamical phase transition and glassy states in the long range anti-ferromagnetic spin models. Results of simulated annealing are also presented.

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1. Introduction

Recently, the study of spin glass models has been extended to spin models without quenched disorder [1]. In addition to glassy states, the dynamical nature of the glass transition has been an attractive subject, since it is not described by the equilibrium statistical mechanics. Many efforts have been made to directly clarify the situation by dynamical approaches [2]. The replica theory is also expected to be useful to find the glassy condensation, which should be described by the replica symmetry breaking (RSB) solution [3–6]. Interestingly, in some infinite range random spin models, glass transitions are successfully identified by the replica method with the marginality condition [4, 7], which was originally suggested by dynamical mean field theory [8]. This idea is quite promising also in the study of deterministic spin models.

The study of the glass transition without quenched disorder is a long standing subject. There have been many studies which address this problem in terms of interacting particles [9]. Another approach will be a formulation by lattice gas models. We imagine a lattice system in which sites are occupied by particles with repulsive long range interactions. By suitable redefinition of interactions, the system will be mapped to an Ising spin model with long range anti-ferromagnetic (AF) interactions. Although the dynamics of particles induces a restricted spin dynamics due to the conservation of the number of particles, the long range AF spin models with conventional spin dynamics will be interesting in themselves. Since these spin systems have affluent frustrations, we expect the low temperature phase to be highly nontrivial and probably glassy. In a previous paper [10], we proposed a step for this problem by studying a spin model suggested by the anti-Hebbian (AH) model [7].

The purpose of this paper is to extend the study to two long range AF spin models defined on one- and two-dimensional lattices. In this introduction, we discuss the structure of energy functions of the long range AF models in terms of the AH model and its generalized version.

The first model is defined on the one-dimensional (1D) lattice of size N with the energy function given by

$$H = \sum_{|\mu|} \mathrm{e}^{-\frac{2|\mu|}{\gamma N}} \left| \sum_i \mathrm{e}^{\sqrt{-1}(2\pi\mu i)/N} S_i/\sqrt{N} \right|^2 = \frac{1}{2}\sum_{ij} J_{ij} S_i S_j \tag{1}$$

where $\sqrt{-1}$ is the imaginary unit, $S_i = \pm 1$ $(i = 1, 2, \ldots, N)$ are Ising spin variables and $\sum_{|\mu|}$ means the sum over $\mu = 0, 1, 2, \ldots, N/2$ to count the different terms once. γ is a small positive parameter such that $\exp(-1/\gamma) \ll 1$. Interactions in (1) are explicitly given by

$$J_{ij} = \frac{\gamma}{1 + (\gamma\pi(i-j))^2} \tag{2}$$

where we take for simplicity the sign of the interactions opposite to that used conventionally. In (1), the terms with $J_{ii} = \gamma$ are included for convenience. Interactions are anti-ferromagnetic and $(\pi\gamma)^{-1}$ characterizes the range of interactions.

The second model is defined on the two-dimensional (2D) lattice of size $N = L \times L$. Spin variables are also of Ising type. Denoting lattice points by $I = (i_x, i_y)$, $(i_x, i_y = 1, 2, \ldots, L)$, Fourier space by $M = (\mu_x, \mu_y)$, $(-L/2 \leqslant \mu_x, \mu_y \leqslant L/2)$, and an inner product of them by $M \cdot I$, the energy function is defined by

$$H_{2D} = \sum_{|\mu|} \mathrm{e}^{-\frac{2M^2}{\delta N}} \left| \sum_I \mathrm{e}^{\sqrt{-1}(2\pi M\cdot I)/L} S_I/\sqrt{N} \right|^2 = \frac{1}{2}\sum_{IJ} J_{IJ} S_I S_J \tag{3}$$

where $M^2 = \mu_x^2 + \mu_y^2$, δ is a small positive number and $\sum_{|\mu|}$ means the sum over $\mu_x = 0, 1, 2, \ldots, L/2$, $\mu_y = -L/2, \ldots, L/2$. Similarly, assuming $\exp(-1/\delta) \ll 1$, we obtain

$$J_{IJ} = \frac{\pi\delta}{2} \exp\left(-\frac{1}{2}\delta\pi^2 |I - J|^2\right) \tag{4}$$

where $|I - J|^2 = (i_x - j_x)^2 + (i_y - j_y)^2$. Due to the assumptions on the parameters, the interactions of these models are long range and the dimensions of the lattice will not matter much in the long range limit.

Both models are suggested by observations on the AH model. The energy function of the AH model is defined by changing the sign of the Hopfield energy function [11, 12]. Here we introduce a slightly generalized version, which has the energy function

$$H_G = \frac{1}{2N} \sum_\mu w_\mu \left(\sum_i \xi_i^\mu S_i \right)^2 \tag{5}$$

where $\xi_i^\mu = \pm 1$ are quenced random variables and weights w_μ are real numbers which will be specified later. We call this kind of spin model a generalized anti-Hebbian (GAH) model. The energy function reduces to that of the AH model by setting $w_\mu = 1$ for $\mu = 1, 2, \ldots, P$ and zero otherwise. In this case, the energy function consists of P constraint terms for N spin variables. Thus the energy function with $P < N$ is zero on the $(N - P)$-dimensional solution space of the constraints if spin variables take continuous values.

The properties of the AH model are summarized as follows. For $P \gg N$, this model is similar to the Sherrington–Kirkpatrick model [13, 14]. For $P < N$, this model is similar to the random orthogonal model [4], that is, it has a dynamical phase transition and glassy low temperature states. This was found by the replica method with the marginality condition and confirmed by simulations. Intuitively, for $P < N$, the states close to the $(N - P)$-dimensional solution space will have very small energy and glassy states for the discrete spin variables. This means that small P gives a large space of glassy states. The properties with small P will basically hold for the GAH model if most of the w_μ are very small or zero.

The energy function of the 1D model (1) is obtained by setting $w_\mu = \exp(-2|\mu|/\gamma N)$ and replacing random linear functions of S_i by the Fourier components of S_i on the one-dimensional lattice. The number of constraints is effectively given by $N\gamma$. The resulting interactions are deterministic and have a range proportional to $1/\gamma$. This range becomes very large in the limit of small number of constraints, which corresponds to the infinite range AF model. This correspondence is a very interesting aspect of these spin models. The energy function of the 2D model (3) is obtained in a similar manner.

Another interesting aspect of these models is that they have low energy crystalline structures constructed by the Fourier components of the smallest wavelength. The basin of attraction of these configurations will become large as the range of interactions becomes short. In the short range limit, only the nearest neighbour interactions survive and crystalline structures will dominate the basin of attraction. The transition to this situation will be quite an interesting subject, although we concentrate on the possible glassy states in this paper.

In spite of the absence of quenched disorder, we expect that, due to the similarity of the energy functions to the AH model, the long range AF models have dynamical phase transitions and glassy states at least for small γ or δ. This transition will not be found in the framework of the equilibrium statistical mechanics. However, the replica method will work well to study these properties as in the AH model.

This paper is organized as follows. In section 2, we discuss the high temperature expansion for the two long range AF models, which will provide the first evidence of phase transition for these models. In section 3, the replica method for the deterministic spin models is reviewed and applied to the long range AF models. In section 4, the results of the replica theory are compared with the simulation results. Section 5 is devoted to some discussions.

2. High temperature expansion for the long range AF models

In this section, we discuss the high temperature expansion for the long range AF models, which will provide the first evidence that the paramagnetic phase should cease to exist at low enough temperature. For this study to parallel that of the AH model, we discuss the expansion in terms of γ or δ. The discussions in this and following sections are mainly focused on the 1D model, but the extension to the 2D model is straightforward. The expansion will be conveniently performed by using Fourier component representation. For simplicity, we use the abbreviations $\mathrm{e}_i^\mu = \mathrm{e}^{\sqrt{-1}(2\pi\mu/N)i}$ and $a_\mu = \mathrm{e}^{-|\mu|/\gamma N}$.

Using the Gaussian integral, the partition function for the long range AF model is expressed as

$$\begin{aligned} Z &= \sum_{\{S\}} \exp\left(-\frac{1}{2}\beta \sum_{|\mu|} \left| \sqrt{2} a_\mu \sum_i e_i^\mu S_i / \sqrt{N} \right|^2 \right) \\ &= \sum_{\{S\}} \int \exp\left(-\frac{1}{2}\sum_{|\mu|} |\phi_\mu|^2 + \frac{1}{2}\sqrt{-1}\sqrt{\frac{2\beta}{N}} \sum_i \sum_\mu a_\mu e_i^\mu \phi_\mu S_i \right) \prod_{|\mu|} \frac{d\phi_\mu}{2\pi} \\ &= 2^N \int \exp(-L\{\phi_\mu\}) \prod_{|\mu|} \frac{d\phi_\mu}{2\pi} \end{aligned} \tag{6}$$

where $\sum_\mu$ means the summation over $\mu = -N/2, \ldots, N/2$, ϕ_μ are complex integral variables with $\phi_{-\mu} = \phi_\mu^*$ and $d\phi_\mu = d\,\mathrm{Re}\,\phi_\mu\, d\,\mathrm{Im}\,\phi_\mu$. $L\{\phi_\mu\}$ is given by

$$L\{\phi_\mu\} = \frac{1}{2}\sum_{|\mu|} |\phi_\mu|^2 - \sum_i \ln\cos\sqrt{\frac{\beta}{2N}} \sum_\mu a_\mu e_i^\mu \phi_\mu. \tag{7}$$

The second term in $L\{\phi_\mu\}$ makes Z small for large β. To evaluate this effect, we expand it in terms of $\sum_\mu a_\mu e_i^\mu \phi_\mu \big/ \sqrt{N}$, which are of order $\sqrt{\gamma}$. We discuss this point later. Then to fourth order, we have

$$L\{\phi_\mu\} = \frac{1}{2}\sum_{|\mu|} \left(1 + \beta a_\mu^2\right) |\phi_\mu|^2 + \frac{1}{48N}\beta^2 \sum_{\sum_{k=1}^4 \mu_k = 0} \prod_k a_{\mu_k} \phi_{\mu_k} + \cdots. \tag{8}$$

The first term in $L\{\phi_\mu\}$ is Gaussian, while the rest are higher order terms of ϕ_μ. The propagators are given by $\langle |\phi_\mu|^2 \rangle = 2\left(1 + \beta a_\mu^2\right)^{-1}$, where $\langle \cdots \rangle$ means an expectation value by the Gaussian part of $L\{\phi_\mu\}$. Performing ϕ_μ integrals and rewriting the μ sum as integrals over μ/N, we obtain the free energy density f, energy density e,

$$\begin{aligned} f &= -\frac{1}{\beta}\ln 2 + \frac{1}{\beta} g(\beta) + \frac{1}{4}\frac{\gamma^2}{\beta} (\ln(1+\beta))^2 + \cdots \\ e &= \frac{1}{2}\frac{\gamma}{\beta}\ln(1+\beta) + \frac{\gamma^2}{2}\frac{\ln(1+\beta)}{(1+\beta)} + \cdots \end{aligned}$$

and entropy $s = \beta(e - f)$ to the second order of γ, where

$$g(x) = \frac{\gamma}{2}\int_0^1 \frac{\ln(1+xt)}{t}\, dt. \tag{9}$$

Numerical study reveals that s becomes negative below a finite low temperature T_s. Using $g(x) \sim (\gamma/4)(\ln x)^2$ for large x, we obtain $T_s \sim \exp(-2\sqrt{\ln 2/\gamma})$ up to some constant to the first order of γ.

For consistency of the expansion, the third term of the free energy should be small compared with the second term. The effective expansion parameter is given by $\beta \sum_\mu a_\mu^2 \langle |\phi_\mu|^2 \rangle / N = 2\gamma \ln(1+\beta)$, which should be smaller than 1. This holds down to temperature $\sim\exp(-1/\gamma)$, which is much lower than T_s for small γ.

For the 2D model, we repeat a similar calculation, where a_μ are replaced by $\exp(-M^2/\delta N)$ and μ sums over $0 \leqslant \mu_x \leqslant L/2$, $-L/2 \leqslant \mu_y \leqslant L/2$. With the assumption $\exp(-1/\delta) \ll 1$, we find that the results for the 2D model are obtained by the replacement of γ by $\delta\pi/2$ in the expressions of the 1D model to the second order of δ.

The existence of T_s is quite an interesting aspect of these AF models, as well as of the AH model. Since negative entropy for an Ising spin system is not acceptable, the above result does not hold below T_s. Physically, small entropy implies that the contributing configurations are very few. Thus T_s may be regarded as some condensation temperature. However, the following remarks should be borne in mind.

As will be discussed in section 3, the free energy obtained in this section can be regarded as a replica symmetry (RS) solution for the paramagnetic phase. The existence of T_s means that this solution is irrelevant below T_s. Thus we should find another solution to describe the low temperature phase, which should appear below a temperature higher than T_s. In short, T_s can be regarded as a property of a simple replica saddle point and we should study a wider space of solutions to describe the low temperature phase.

3. A replica method for the long range AF models

In the previous section, we found that the entropy evaluated by the high temperature expansion becomes zero at finite temperature for the long range AF models just as for the AH model. In this section, we present the replica theory for the long range AF models, which reduces to the replica mean field theory of the GAH model to the first order of γ or δ. We then study the solutions by assuming the RS and RSB ansatz. The results of the replica mean field theory are compared with the simulation results in section 4. For simplicity, we concentrate on the 1D model. The extension to the 2D model is straightforward.

3.1. Replica method without quenched average

We first review the replica method without random averages, which was presented in [10]. The basic idea is to rearrange the summation in the replicated partition function.

Let $H\{S_i\}$ be the energy function. Introducing replica spin variables S_i^ρ $(\rho = 1, 2, \ldots, n)$, the replicated partition function is simply given by

$$Z^n = \sum_{\{S\}} \exp\left(-\beta \sum_{\rho=1}^{n} H\left\{S_i^\rho\right\}\right) \tag{10}$$

where $\beta = 1/T$ is the inverse temperature. The free energy is given by $f = -\ln Z/\beta N$ with $\ln Z = \lim_{n\to 0}(Z^n - 1)/n$. In the case of random spin models, the products $S_i^\rho S_i^\sigma$ arise in the averaged Z^n and they play an important role in finding correlation among replicas.

The basic idea for the replica method without random average is to rearrange the statistical sum in the replicated partition function. We expect that, if there are some configurations which contribute mainly in (10), several replicas will have similar configurations, i.e. condensation among replicas. This suggests performing first a partial statistical sum with fixed correlation among replicas, which will be described by $S_i^\rho S_i^\sigma$. For this purpose, we use the fact that $S_i^\rho S_i^\sigma$ are invariant by the transformation $S_i^\rho \to \eta_i S_i^\rho$, where $\eta_i = \pm 1$ are common among replicas. Thus the partial statistical sum will be achieved by the summation over η_i after the replacement of S_i^ρ by $\eta_i S_i^\rho$ in (10). On the other hand, due to the summation over S_i^ρ, Z^n does not change by this replacement. Thus the summation over $\eta_i = \pm 1$ simply gives $2^N Z^n$. In this way, we obtain

$$Z^n = \frac{1}{2^N} \sum_{\{\eta\}} \sum_{\{S\}} \exp\left(-\beta \sum_{\rho=1}^{n} H\left\{\eta_i S_i^\rho\right\}\right) \tag{11}$$

where $\sum_{\{\eta\}}$ means the sum over all $\eta_i = \pm 1$. In this expression, the summation over η_i with fixed S_i^ρ collects the contributions with fixed $S_i^\rho S_i^\sigma$. The resulting expression will contain the couplings among different replicas and will be treated by the saddle point approximation, if possible.

The following remarks may be helpful in understanding how the η_i sum works. The formulation presented above was originally inspired by the similarity between the diagrams which arise in the usual replica theory and the high temperature expansion [7]. For the original expression (10), this similarity suggests that there may be some prescription which looks like a high temperature expansion and leads to replica theory without using random averages. This is realized by the summation over one replica variable with fixed correlation among replicas. More explicitly, by using the relation

$$\sum_{\rho=1}^{n} H\left\{S_i^\rho\right\} = \sum_{i<j} J_{ij} \sum_{\rho=1}^{n} S_i^\rho S_j^\rho = \sum_{i<j} J_{ij} S_i^1 S_j^1 \sum_{\rho=1}^{n} d_i^\rho d_j^\rho$$

where $d_i^\rho = S_i^1 S_i^\rho$, we can perform the S_i^1 sum with fixed d_i^ρ for (10) in the same way as the high temperature expansion in terms of interactions, yielding a function of d_i^ρ. Note that $S_i^\rho S_i^\sigma = d_i^\rho d_i^\sigma$ with generic replica indices also do not change under this summation. However, to avoid the apparent breaking of symmetry among replicas, we reformulate this procedure by introducing the auxiliary variables η_i and reach the formulation presented in this section. We note that this argument implies that the η_i sum contains the information obtained by the high temperature expansion, which will be obtained by assuming no correlation among replicas. We can get more information by assuming nontrivial correlation among replicas.

3.2. Approximated partition function

To sum η_i in the replicated partition function, it is convenient to use a Fourier representation as the high temperature expansion performed in section 2. After introducing the Gaussian variables ϕ_μ^ρ $(\rho = 1, 2, \ldots, n)$, Z^n for the long range AF model is written as

$$\begin{aligned} Z^n &= \frac{1}{2^N} \sum_{\{\eta,S\}} \exp\left(-\frac{1}{2}\beta \sum_{\rho,|\mu|} \left|\sqrt{2} a_\mu \sum_i \mathrm{e}_i^\mu \eta_i S_i^\rho / \sqrt{N}\right|^2\right) \\ &= \sum_{\{S\}} \int \exp\left(-\frac{1}{2} \sum_{\rho,|\mu|} |\phi_\mu^\rho|^2 + \sum_i \ln\cos\left(\frac{\sqrt{\beta}}{\sqrt{2N}} \sum_{\rho,\mu} a_\mu \phi_\mu^\rho \mathrm{e}_i^\mu S_i^\rho\right)\right) \prod_{\rho,|\mu|} \frac{\mathrm{d}\phi_\mu^\rho}{2\pi}. \end{aligned} \tag{12}$$

We first perform ϕ_i^ρ integrals to obtain $A\{S^\rho\}$, which is defined by

$$\exp A\{S^\rho\} = \int \exp(-L\{S^\rho, \phi^\rho\}) \prod_{\rho,|\mu|} \frac{\mathrm{d}\phi_\mu^\rho}{2\pi} \tag{13}$$

where

$$L\{S^\rho, \phi^\rho\} = \frac{1}{2} \sum_{\rho,|\mu|} |\phi_\mu^\rho|^2 - \sum_i \ln\cos\left(\frac{\sqrt{\beta}}{\sqrt{2N}} \sum_{\rho,\mu} a_\mu \phi_\mu^\rho \mathrm{e}_i^\mu S_i^\rho\right). \tag{14}$$

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

The studies of the high temperature expansion suggest studying $A\{S^\rho\}$ by perturbation in terms of γ. Noting that $\Phi_i = \sum_{\rho,\mu} a_\mu \phi_\mu^\rho \mathrm{e}_i^\mu S_i^\rho \big/ \sqrt{N}$ are of order $\sqrt{\gamma}$, we expand the expression in terms of Φ_i and obtain

$$L\{S^\rho, \phi^\rho\} = \frac{1}{2} \sum_{\rho,|\mu|} \left|\phi_\mu^\rho\right|^2 + \frac{\beta}{4} \sum_i \Phi_i^2 + \frac{\beta^2}{48} \sum_i \Phi_i^4 + \cdots \tag{15}$$

to the fourth order of Φ_i. The second-order term of Φ_i contains diagonal and off-diagonal terms of μ. Some inspections imply that the off-diagonal terms give second and higher order terms of γ, as well as the fourth-order terms of Φ_i. Thus, to the first order of γ, we obtain

$$L_1\{S^\rho, \phi^\rho\} = \frac{1}{2} \sum_{\rho,|\mu|} \left|\phi_\mu^\rho\right|^2 + \frac{1}{2}\beta \sum_{\rho\sigma} \sum_{|\mu|} a_\mu^2 \phi_\mu^\rho \phi_{-\mu}^\sigma q_{\rho\sigma} \tag{16}$$

where $q_{\rho\sigma} = \sum_i S_i^\rho S_i^\sigma \big/ N$, including $q_{\rho\rho} = 1$. Using this expression, we obtain

$$A_1\{S^\rho\} = -\mathrm{Tr} \sum_{|\mu|} \ln\left(1 + \beta q a_\mu^2\right) \tag{17}$$

where Tr means a trace over the replica indices. Rewriting the μ sum as integrals over μ/N, we reach the expression given by

$$A_1\{S^\rho\} = -\frac{1}{2} N\gamma \,\mathrm{Tr} \int_0^1 \frac{\ln(1 + \beta q t)}{t}\, \mathrm{d}t. \tag{18}$$

This expression defines the replica mean field theory since the action is expressed only by the overlap matrix q.

For the 2D model, we repeat the same procedure. After some calculations, we obtain (18) with γ replaced by $\pi\delta/2$. The expressions obtained for both models imply that the two AF models are described by the same replica mean field theory at least to the first order of γ or δ.

At this stage, it is convenient to introduce the GAH model which gives (18) by the usual replica theory. By the discussion in appendix, we find

$$H_G = \frac{1}{2N} \sum_\mu a_{\mu/2}^2 \left(\sum_i \xi_i^\mu S_i \right)^2 \tag{19}$$

where the subscript $\mu/2$ is to count the constraint terms with a certain weight correctly.

The study in this section suggests that the glass transition of the long range AF models can be studied by the replica mean field theory for the GAH model for small parameters. This implies that the details of the lattice structure become irrelevant in the limit of long range interactions, as often happens in statistical physics.

3.3. Marginally stable RSB solution

The replica study of the GAH model can be done in the same way as the random orthogonal model [4] and the AH model [7]. The study on the AH model suggests that the GAH model also has two kinds of one-step RSB solutions for small parameters. One is the usual solution, which is defined by the extremum condition on the saddle point function and referred to as static RSB. The other is the marginally stable RSB solution. We are especially interested in the latter, which is expected to describe the dynamical phase transition and glass states. In this subsection, we review these solutions.

The replica partition function for the GAH model is given by

$$Z_1^n = \sum_{\{S\}} \exp - N \,\mathrm{Tr}\, g(\beta q) \tag{20}$$

where $g(x)$ is given by (9). This expression is evaluated by the saddle point approximation, which is reviewed in the appendix, where the definitions of the saddle point variables $q_{\rho\sigma}$ and $\lambda_{\rho\sigma}$ are also presented. The free energy, which should be extremized, is given by $f = -\lim_{n\to 0}\left(Z_1^n - 1\right)/n\beta N$.

We first give some remarks on the RS solutions, which are defined by $q_{\rho\sigma} = q$ for $\rho \neq \sigma$. The trivial RS solution $q = 0$ gives the same expression of free energy as the high temperature expansion to the first order of γ. This solution is not physically acceptable below T_s as discussed in section 2. As shown in the appendix, the RS solution with $q \neq 0$ appears below an extremely low temperature $T_{\mathrm{RS}} \sim \exp(-1/\gamma)$, which is lower than T_s for small γ. This situation may look strange, but in case of the AH model with $P/N < 1$, there is no RS solution with $q \neq 0$ down to zero temperature. The positive but very small T_{RS} may be due to the exponential decay of the weights w_μ. Since the instability of the paramagnetic phase below T_s has no physical meaning, we concentrate on the solutions whose transition takes place above T_s.

The one-step RSB ansatz 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. The value of m should satisfy $0 < m < 1$ to describe the fragmented configuration space properly. By this ansatz, the free energy reduces to

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

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 given by the extremum condition $\partial f/\partial q_1 = 0, \partial f/\partial \lambda_1 = 0$ and $\partial f/\partial m = 0$. This solution appears below the temperature T_{RSB} which is higher than but very close to $T_s \cdot q_1$ is very close to 1.0 down to lower temperature. This solution is stable with respect to small changes of the saddle point variables at least near T_{RSB}. We expect that this solution represents the absolute minimum state of the GAH model.

Interestingly, as pointed out in the literature [4, 7], the results of simulated annealing are not described by the static RSB solution but by the marginally stable RSB solution. It is expected that the random condensation states, including spin glasses, are characterized by marginal stability of the saddle point [1, 14]. This is also suggested by the dynamical mean field theory [8]. As discussed in the appendix, the marginally stable RSB solution for the GAH model is defined by the condition

$$1 - g\mu = 0 \tag{22}$$

where

$$\mu = -\frac{\int \cosh^m(\sqrt{\lambda_1}z)\cosh^{-4}(\sqrt{\lambda_1}z)\,\mathrm{D}z}{\int \cosh^m(\sqrt{\lambda_1}z)\,\mathrm{D}z} \tag{23}$$

$$g = 2\beta^2 g''(\beta x_0) \tag{24}$$

in addition to $\partial f/\partial q_1 = 0$ and $\partial f/\partial \lambda_1 = 0$. Numerical studies reveal that the marginally stable RSB appears below a moderate temperature, which is denoted by T_g, and the energy for this solution is nearly constant below T_g as presented in the next section.

To summarize this section, we present the γ-dependence of T_{RS}, T_s and T_g in figure 1. Although these characteristic temperatures decrease as γ decreases, T_g becomes much higher than T_s for small γ. In the next section, we present some simulation results of the 1D and 2D AF models, as well as the numerical studies of the marginally stable RSB solutions of the GAH model.

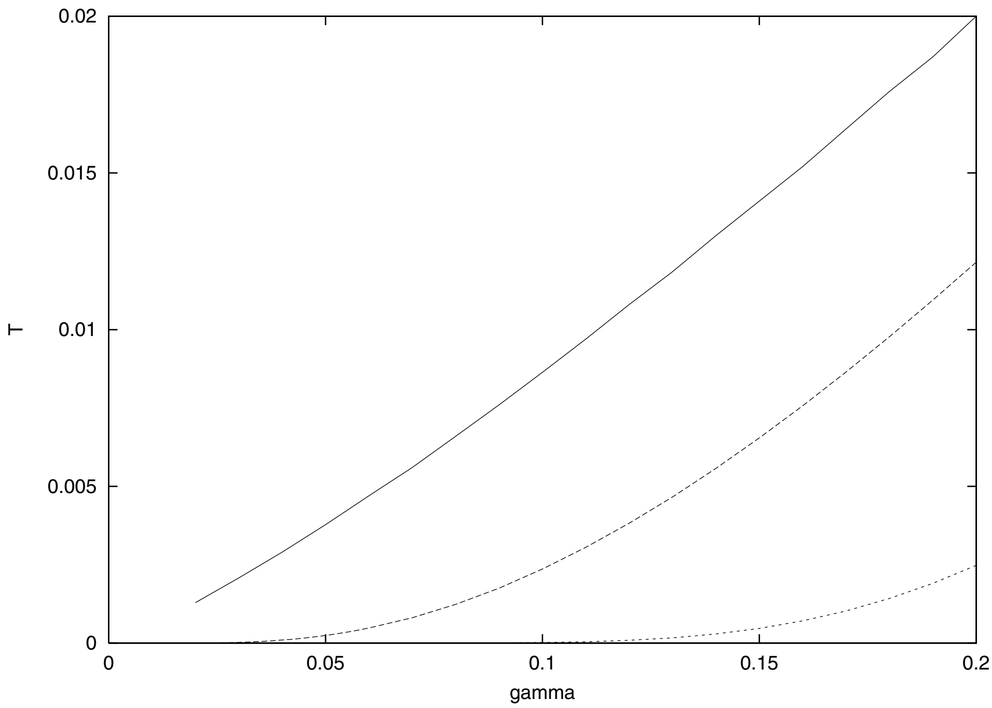

Figure 1. γ-dependence of three characteristic temperatures of the GAH model, $T_{\rm RS}$, T_s and T_g (from bottom).

4. The results of simulated annealing

This section is devoted to the presentation of simulation results. Spin variables are assumed to obey the Monte Carlo (MC) dynamics, where spin flips are performed sequentially according to the probabilities controlled by the change of energy. For comparison with the results of the replica method, we restrict ourselves to small γ and δ. The boundary conditions are simply assumed to be open, that is, the interactions are only determined by the line length between the two sites on the lattice. We are especially interested in the temperatures at which the properties of dynamics change, which may be regarded as the onset of condensation states.

By studying several runs of simulated annealing for 1D and 2D models, we found that the behaviour of the energy is similar to that of the AH model and other spin models which show a glass transition. Basically, the energy decreases as the temperature decreases in the high temperature region and ceases to decrease around a certain temperature, which is much higher than T_s. Around this temperature, the acceptance rate of spin flips decreases drastically and the Edward–Anderson order parameter increases to 1.0 rapidly. This means that the annealing configurations freeze below this temperature. The resulting configurations seem to be random and uncorrelated. The energies at low temperature depend on the initial configurations. In addition, the averages of these depend on the number of MC steps at each temperature, i.e. an annealing schedule, especially when it is not large enough.

In figures 2 and 3, the results of simulated annealing for the 1D model are represented by dots with error bars for $\gamma = 0.025$ and 0.05 respectively, and in figures 4 and 5 for the 2D model with corresponding $\delta = 2\gamma/\pi$. The full curves represent the results of the high temperature expansion and the marginally stable RSB solutions for the GAH model, which give

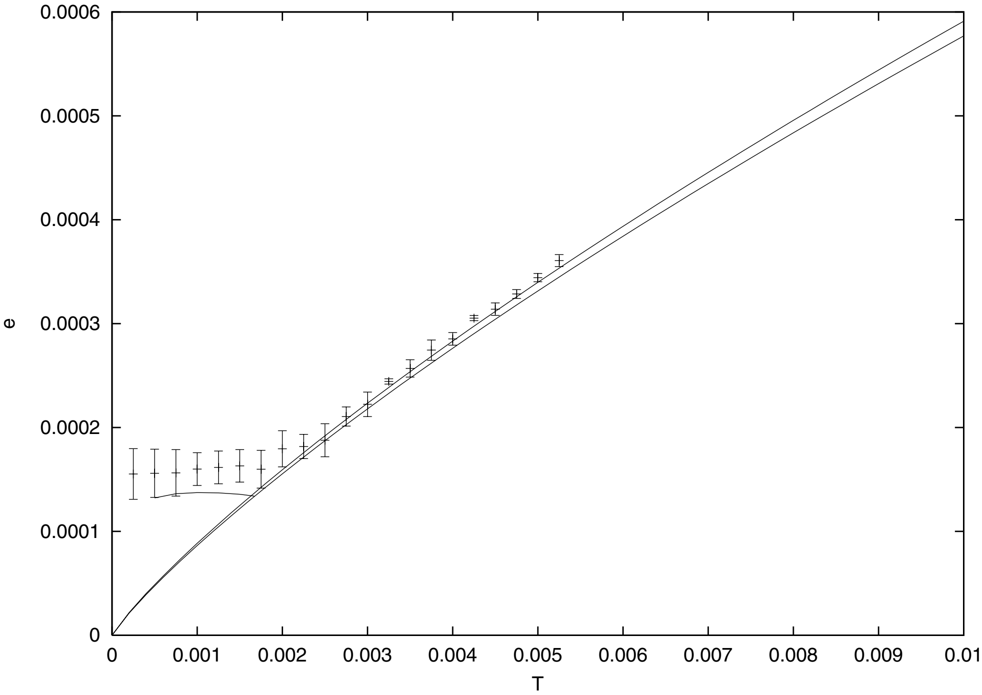

Figure 2. T-dependence of energies for the 1D model with $\gamma = 0.025$, $N = 500$. Dots with error bars represent the energies obtained by five runs of simulated annealing. The number of MC steps at each temperature is 10^4. The full curves are obtained using the results of high temperature expansion of the first and second orders of γ, and marginally stable RSB of the GAH model for $T < T_g = 0.001\,67$.

$T_g = 0.001\,67$ with $e = 0.000\,134$ for $\gamma = 0.025$ and $T_g = 0.003\,78$ with $e = 0.000\,527$ for $\gamma = 0.05$. Qualitatively, the simulation results show fair agreement with the high temperature expansion and the results of replica theory, although the energies obtained by simulations tend to be larger than those obtained theoretically. There may be two reasons for this; one is the small number of MC steps at each temperature and the other is the small system size. System-size effect seems very large for the 2D model due to the large open boundary. Even with these aspects, T-dependence of energies, including the break points, seems to be described well by the replica theory.

As discussed in section 1, the long range AF models have crystalline states, which are given by $S_i = \pm(-1)^i$ for the 1D model and $S_I = \pm(-1)^{i_x+i_y}$ for the 2D model. By increasing the temperature, we can study the melting of these states. In figures 3 and 5, the temperature dependence of energies is presented for respective values of parameters. The initial configurations have small positive energies probably due to the finite system sizes. As the temperature increases, the energies do not change until T_g and start increasing rather rapidly slightly above T_g, tending to the values in the high temperature region. This clearly shows the melting of the AF configurations.

Having these results, we conclude that, at least for small γ or δ, results of simulated annealing for the long range AF are well described by the high temperature expansions down to T_g and the marginally stable RSB solutions below T_g. This implies that we are observing glass transitions of the long range AF spin models.

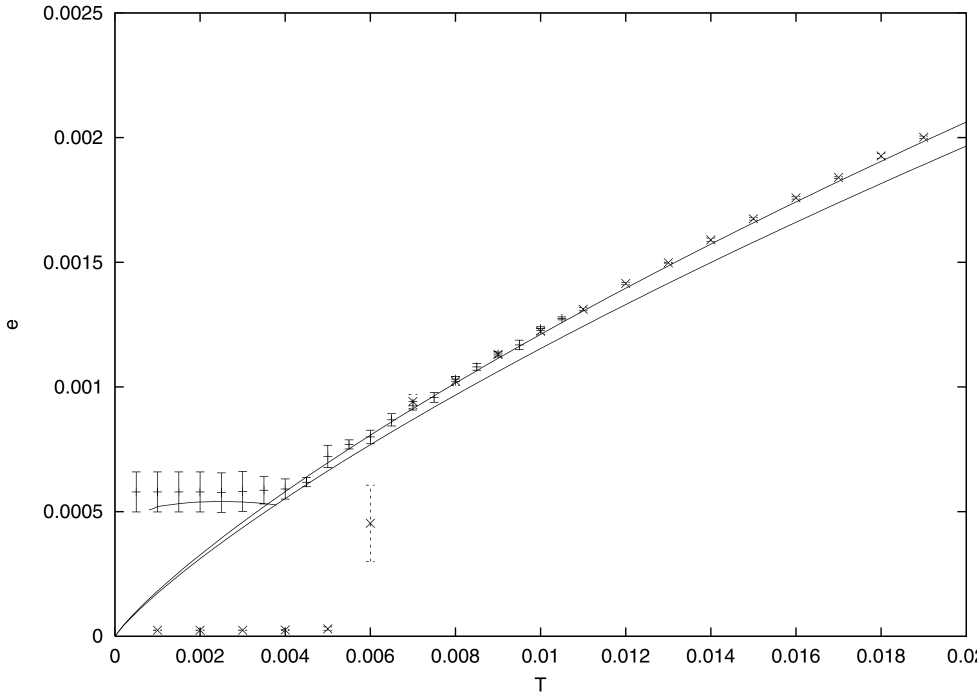

Figure 3. Same as figure 2 but for $\gamma = 0.05$ and $T_g = 0.003\,78$. The crosses with broken error bars represent the melting of the crystalline state of the 1D model with initial temperature $T = 0.001$. The number of MC steps at each temperature is 10^4.

5. Discussion

In this paper, we have studied two long range AF spin models by the replica method which does not require random averages. These models are motivated by observations on the AH model, which is characterized by P constraint terms in the energy function. When these constraints are generalized to Fourier components of spin variables with suitable weights, the energy functions become those of long range AF models. The ranges of interactions are proportional to the inverse of the effective number of constraints.

Although the long range AF models introduced in this way are not fully described by the replica mean field theory, we can study them to the first order of the inverse of the interaction range, e.g. γ in the framework of replica mean field theory. As γ tends to 0, the model tends to the infinite range AF model, which shows no phase transition at finite temperature. For small but finite γ, the situation changes dramatically. By high temperature expansion, we found that there is a finite temperature T_s below which the entropy becomes negative and the replica theory suggests that there is a glass transition at T_g far above T_s. The simulated annealing gives consistent results. We expect that these properties will hold generally in the long range AF Ising spin models since the idea of modelling is not restricted to the situations considered in this paper.

The basic picture of the glassy phase of spin models has already been suggested in the literature [1, 3–5]. The existence of two characteristic temperatures $T_{\mathrm{RSB}} \sim T_s$ and T_g is common among the studied models. We expect that T_{RSB} would be a phase transition point to the absolute minimum state if the annealing configurations could move over all configuration

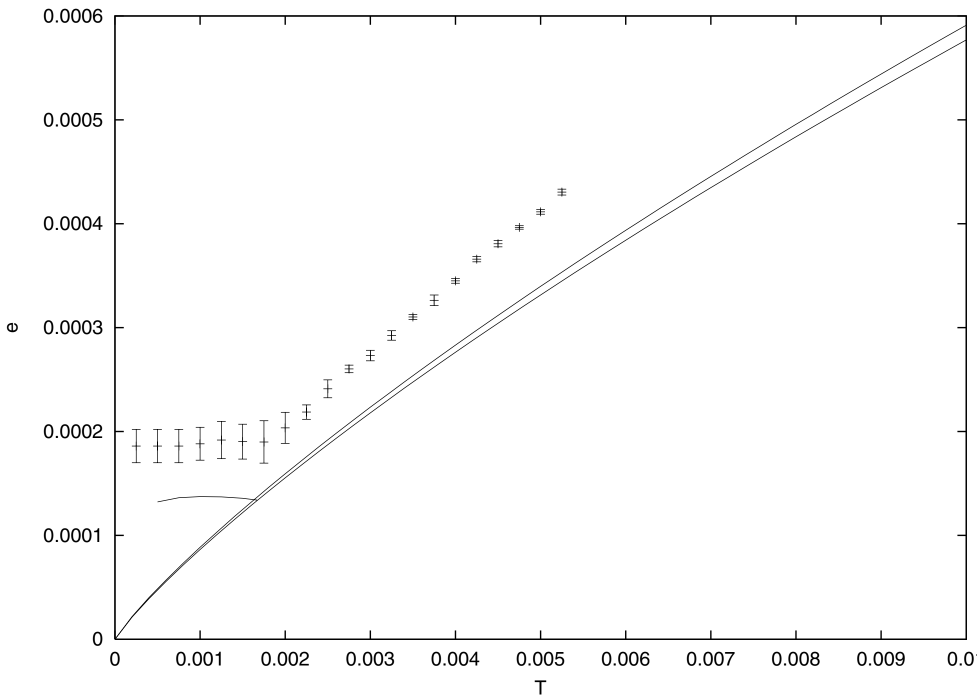

Figure 4. The results of simulated annealing for the 2D model with $\delta = 2 \times 0.025/\pi$ and $L = 20$. Full curves are the same as in figure 2.

space even below T_g. We suspect that this will be achieved by enumerating all configurations to calculate the partition function. The existence of T_g far above T_{RSB} implies that, before the temperature reaches the static RSB transition point, the annealing configurations are trapped dynamically in the partitioned configuration space. Our studies imply that the replicated partition function, when it is treated properly, gives a signal of this partitioning also for the deterministic spin models. However, at very low temperature, we should note two aspects. First, the Gaussian approximation for Z^n should be replaced by something else for $\beta \to \infty$. The resulting theory may be out of the replica mean field theory. Secondly, the one-step RSB ansatz does not seem to be correct at very low temperature, since it does not describe the behaviour of energy down to zero temperature [7]. These points remain to be studied.

Strictly speaking, glass transitions should be studied by dynamical approaches, as was done for the Ising perceptron problem [8]. Recent studies of the dynamical mean field method for the random spin model imply that, below the glass transition, the time correlation function shows a plateau on a short thermal timescale, which is described by the Edward–Anderson order parameter, and starts to decrease on a much larger timescale [1]. We suppose that this behaviour is reflected by the replica solutions, i.e. no relevant RS but one-step RSB with zero off-block elements. However, as discussed in [4], we should be careful about the meaning of the resulting free energies. Theoretical studies of spin dynamics are highly desirable for the long range AF models, as well as numerical studies of large timescale dynamics.

In this paper, we restrict ourselves to the situation of very long range interactions. To study the spin models with short range interactions, we need to extend the study to the large parameter region. We have performed simulations up to $\gamma = 0.1$ and corresponding δ in the same way as in section 4 and found qualitatively different behaviour of energies, that

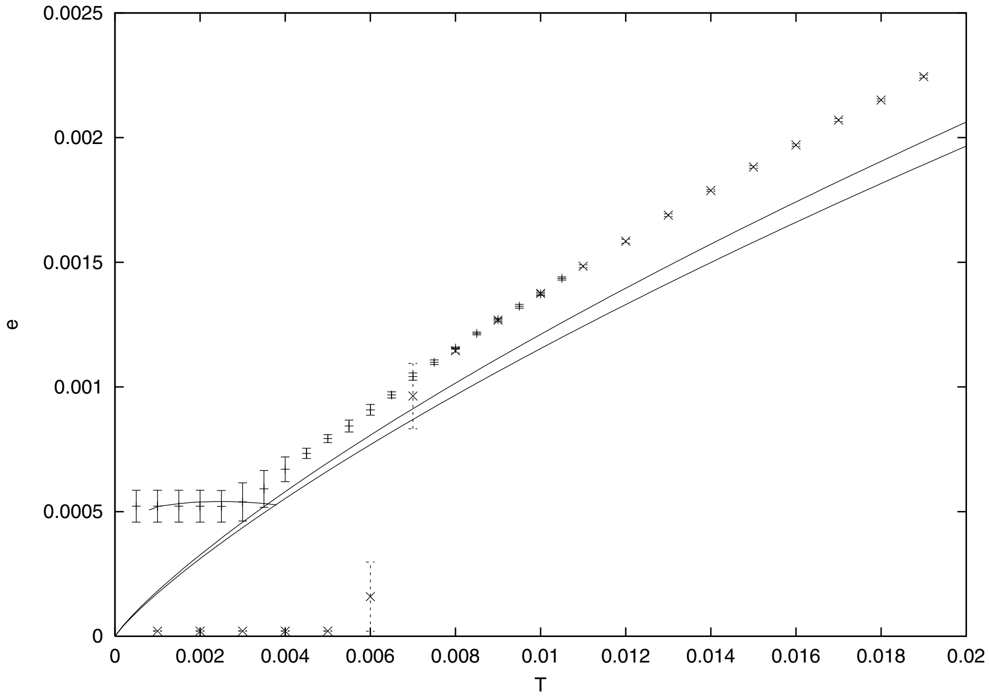

Figure 5. The results of simulated annealing for the 2D model with $\delta = 2 \times 0.05/\pi$ and $L = 20$. The full curves are the same as in figure 3. The crosses with broken error bars represent the melting of crystalline states for the 2D model.

is, the energies start to become smaller than the high temperature expansion around a temperature higher than T_g. It is interesting that this temperature is close to the melting temperature of the AF configurations. We suspect that the annealing configurations are affected by short scale anti-ferromagnetic correlation for this γ. In the short range limit, the models reduce to the spin models with nearest neighbour interactions, which have been studied well in statistical physics. In 2D short range models, it is known that there is a second-order phase transition to crystalline states. The crossover between the crystalline transition and glass transition will be an interesting subject in 2D and higher dimensional moderate range AF Ising models.

Although the replica method suggested in this and the previous paper is restricted to Ising spin models, the basic idea will be generalized to other models, including other types of dynamical variables. Although we should be careful about suitable order parameters and the relevance of the partial statistical sum, it will be quite interesting to study the system of interacting particles using this idea.

Appendix

In this appendix, we first discuss the proper GAH model to describe the long range AF models and then present some reviews of the replica theory, including the RS solution and the marginally stable condition of the one-step RSB solution.

Let us first discuss the GAH model which describes the long range AF models. The energy function (1) has two constraint terms for each μ, which come from the real and imaginary parts of the linear functions. This suggests introducing the energy function of the GAH model given by

$$H_G = \frac{1}{2N}\sum_\mu a_\mu^2 \left\{ \left(\sum_i \xi_i^{2\mu} S_i\right)^2 + \left(\sum_i \xi_i^{2\mu+1} S_i\right)^2 \right\} \tag{A.1}$$

where $a_\mu = \exp(-\mu/\gamma N)$. For large N, this expression reduces to

$$H_G = \frac{1}{2N}\sum_\mu a_{\mu/2}^2 \left(\sum_i \xi_i^{\mu} S_i\right)^2 \tag{A.2}$$

which will give the same action as long range AF models give by the usual replica method.

Replica theory for this model is studied in the same way as the AH model. Averaging over quenched randomness, which is denoted by $\overline{\cdots}$, gives

$$\overline{Z_G^n} = \exp\left\{-\frac{1}{2}\,\mathrm{Tr}\sum_\mu \ln\left(1+\beta a_{\mu/2}^2 q\right)\right\} \tag{A.3}$$

where q in this expression is an order parameter matrix. By introducing the integral representations for delta functions and the expression

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

we obtain

$$\overline{Z_G^n} = \iint \exp\{-N\beta n f(\lambda_{\rho\sigma}, q_{\rho\sigma})\}\prod_{\rho<\sigma}\frac{N\,\mathrm{d}\lambda_{\rho\sigma}\,\mathrm{d}q_{\rho\sigma}}{2\pi\mathrm{i}} \tag{A.4}$$

where

$$\beta n f(\lambda_{\rho\sigma}, q_{\rho\sigma}) = \mathrm{Tr}\, g(\beta q) + \frac{1}{2}\sum_{\rho\neq\sigma}\lambda_{\rho\sigma}q_{\rho\sigma} - \ln\sum_{\{S\}}\exp\frac{1}{2}\sum_{\rho\neq\sigma}\lambda_{\rho\sigma}S^\rho S^\sigma \tag{A.5}$$

where $g(x)$ is given by (9).

With the one-step RSB ansatz, matrix q has eigenvalue $1-q_1+mq_1$ with degeneracy n/m and eigenvalue $1-q_1$ with degeneracy $n-n/m$. We then obtain (21).

Let us discuss RS saddle points, which are defined by $q_{\rho\sigma} = q$, $\lambda_{\rho\sigma} = \lambda$ for $\rho\neq\sigma$. The free energy reduces to

$$\beta f = \beta q g'(\beta(1-q)) + g(\beta(1-q)) + \frac{1}{2}\lambda(1-q) - \int \ln 2\cosh(\sqrt{\lambda}x)\,\mathrm{D}x. \tag{A.6}$$

The saddle point equations are given by

$$q = \int \tanh^2(\sqrt{\lambda}x)\,\mathrm{D}x \qquad \lambda = -2\beta^2 q g''(\beta(1-q)).$$

We first note that the trivial RS soultion $q=0$ gives

$$f = -\frac{1}{\beta}\ln 2 + \frac{1}{\beta}g(\beta).$$

This equals the high temperature free energy of the long range AF model to the first order of γ. Assuming that q continuously appears from zero, we obtain

$$1 = \gamma \left\{ \ln(1+\beta) - \frac{\beta}{1+\beta} \right\} \tag{A.7}$$

for the transition temperature $T_{\rm RS}$ of $q \neq 0$ RS solution. For γ small enough, we obtain $T_{\rm RS} \sim \exp(-1/\gamma)$.

The derivation of the marginality condition for one-step RSB has been discussed in appendices in [4, 7]. Here we briefly review them. Let $g(x) = \sum_k c_k x^k$. By setting $q_{\rho\sigma} = q^0_{\rho\sigma} + \delta q_{\rho\sigma}$ and $\lambda_{\rho\sigma} = \lambda^0_{\rho\sigma} + \delta\lambda_{\rho\sigma}$ in (A.5), where $q^0_{\rho\sigma}$ and $\lambda^0_{\rho\sigma}$ are one-step RSB saddle points, the change of (A.5) is given by

$$\beta n \delta^2 f = \frac{1}{2} \sum_{(\rho\sigma)(\kappa\tau)} G_{(\rho\sigma)(\kappa\tau)} \delta q_{\rho\sigma} \delta q_{\kappa\tau} + \sum_{(\rho\sigma)} \delta q_{\rho\sigma} \delta\lambda_{\rho\sigma} + \frac{1}{2} \sum_{(\rho\sigma)(\kappa\tau)} F_{(\rho\sigma)(\kappa\tau)} \delta\lambda_{\rho\sigma} \delta\lambda_{\kappa\tau} \tag{A.8}$$

to the second order of deviations, where

$$G_{(\rho\sigma)(\kappa\tau)} = \frac{\partial^2\, \mathrm{Tr}\, g(\beta q)}{\partial q_{\rho\sigma} \partial q_{\kappa\tau}} = \sum_k c_k \beta^k 2k \frac{\partial (q^{k-1})_{\rho\sigma}}{\partial q_{\kappa\tau}}$$

$$F_{(\rho\sigma)(\kappa\tau)} = \langle S_\rho S_\sigma \rangle \langle S_\kappa S_\tau \rangle - \langle S_\rho S_\sigma S_\kappa S_\tau \rangle$$

where $\langle \cdots \rangle$ is the expectation value with the weight $\exp\left(\frac{1}{2}\right) \sum_{\rho\neq\sigma} \lambda^0_{\rho\sigma} S^\rho S^\sigma$. The marginally stable condition is given by setting to zero the eigenvalue of replicon modes, which have the same structure as the de Almeida–Thouless (AT) instability of the RS solution [15]. The matrix elements related to these modes have four replica indices which belong to the same sub-blocks of the RSB ansatz. There are three different values depending on the combination: $(\rho = \kappa, \sigma = \tau)$, $(\rho = \kappa, \sigma \neq \tau)$ and $(\rho \neq \kappa, \tau \neq \sigma)$. The respective elements are denoted by P, Q and R for $F_{(\rho\sigma)(\kappa\tau)}$ and P', Q' and R' for $G_{(\rho\sigma)(\kappa\tau)}$. For these matrices, the replicon modes have the eigenvalues $\mu = P - 2Q + R$ and $g = P' - 2Q' + R'$, respectively. Taking into account the coupling $\sum_{(\rho\sigma)} \delta q_{\rho\sigma} \delta\lambda_{\rho\sigma}$, we obtain the marginality condition $1 - g\mu = 0$.

The explicit form for μ is given by (23) for the one-step RSB with zero off-diagonal blocks. To evaluate g, we write

$$\frac{\partial (q^{k-1})_{\rho\sigma}}{\partial q_{\kappa\tau}} = \sum_{l=0}^{k-2} \left\{ (q^{k-2-l})_{\rho\kappa} (q^l)_{\tau\sigma} + (q^{k-2-l})_{\rho\tau} (q^l)_{\kappa\sigma} \right\}$$

and express the matrix elements by the eigenvalues of q. After a straightforward calculation, we obtain (24).

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