3

REPLICA SYMMETRY BREAKING

Let us continue our analysis of the SK model. The free energy of the SK model derived under the ansatz of replica symmetry has the problem of negative entropy at low temperatures. It is therefore natural to investigate the possibility that the order parameter $q_{\alpha\beta}$ may assume various values depending upon the replica indices α and β and possibly the α-dependence of m_α. The theory of replica symmetry breaking started in this way as a mathematical effort to avoid unphysical conclusions of the replica-symmetric solution. It turned out, however, that the scheme of replica symmetry breaking has a very rich physical implication, namely the existence of a vast variety of stable states with ultrametric structure in the phase space. The present chapter is devoted to the elucidation of this story.

3.1 Stability of replica-symmetric solution

It was shown in the previous chapter that the replica-symmetric solution of the SK model has a spin glass phase with negative entropy at low temperatures. We now test the appropriateness of the assumption of replica symmetry from a different point of view.

A necessary condition for the replica-symmetric solution to be reliable is that the free energy is stable for infinitesimal deviations from that solution. To check such a stability, we expand the exponent appearing in the calculation of the partition function (2.16) to second order in $(q_{\alpha\beta} - q)$ and $(m_\alpha - m)$, deviations from the replica-symmetric solution, as

$$\int \prod_{\alpha} \mathrm{d}m_\alpha \prod_{\alpha<\beta} \mathrm{d}q_{\alpha\beta} \exp\left[-\beta N\{f_{\mathrm{RS}} + (\text{quadratic in } (q_{\alpha\beta} - q) \text{ and } (m_\alpha - m))\}\right], \tag{3.1}$$

where f_{RS} is the replica-symmetric free energy. This integral should not diverge in the limit $N \to \infty$ and thus the quadratic form must be positive definite (or at least positive semi-definite). We show in the present section that this stability condition of the replica-symmetric solution is not satisfied in the region below a line, called the *de Almeida–Thouless (AT) line*, in the phase diagram (de Almeida and Thouless 1978). The explicit form of the solution with replica symmetry breaking below the AT line and its physical significance will be discussed in subsequent sections.

3.1.1 *Hessian*

We restrict ourselves to the case $h = 0$ unless stated otherwise. It is convenient to rescale the variables as

$$\beta J\, q_{\alpha\beta} = y^{\alpha\beta}, \ \ \sqrt{\beta J_0}\, m_\alpha = x^\alpha. \tag{3.2}$$

Then the free energy is, from (2.17),

$$[f] = -\frac{\beta J^2}{4} - \lim_{n\to 0}\frac{1}{\beta n}\left\{ -\sum_{\alpha<\beta}\frac{1}{2}(y^{\alpha\beta})^2 - \sum_\alpha \frac{1}{2}(x^\alpha)^2 \right.$$
$$\left. + \log \mathrm{Tr} \exp\left(\beta J \sum_{\alpha<\beta} y^{\alpha\beta} S^\alpha S^\beta + \sqrt{\beta J_0}\sum_\alpha x^\alpha S^\alpha\right)\right\}. \tag{3.3}$$

Let us expand $[f]$ to second order in small deviations around the replica-symmetric solution to check the stability,

$$x^\alpha = x + \epsilon^\alpha, \ \ y^{\alpha\beta} = y + \eta^{\alpha\beta}. \tag{3.4}$$

The final term of (3.3) is expanded to second order in ϵ^α and $\eta^{\alpha\beta}$ as, with the notation $L_0 = \beta J y \sum_{\alpha<\beta} S^\alpha S^\beta + \sqrt{\beta J_0} x \sum_\alpha S_\alpha$,

$$\log \mathrm{Tr}\exp\left(L_0 + \beta J \sum_{\alpha<\beta}\eta^{\alpha\beta} S^\alpha S^\beta + \sqrt{\beta J_0}\sum_\alpha \epsilon^\alpha S^\alpha\right)$$
$$\approx \log \mathrm{Tr}\, \mathrm{e}^{L_0} + \frac{\beta J_0}{2}\sum_{\alpha\beta}\epsilon^\alpha\epsilon^\beta \langle S^\alpha S^\beta\rangle_{L_0} + \frac{\beta^2 J^2}{2}\sum_{\alpha<\beta}\sum_{\gamma<\delta}\eta^{\alpha\beta}\eta^{\gamma\delta}\langle S^\alpha S^\beta S^\gamma S^\delta\rangle_{L_0}$$
$$- \frac{\beta J_0}{2}\sum_{\alpha\beta}\epsilon^\alpha\epsilon^\beta\langle S^\alpha\rangle_{L_0}\langle S^\beta\rangle_{L_0} - \frac{\beta^2 J^2}{2}\sum_{\alpha<\beta}\sum_{\gamma<\delta}\eta^{\alpha\beta}\eta^{\gamma\delta}\langle S^\alpha S^\beta\rangle_{L_0}\langle S^\gamma S^\delta\rangle_{L_0}$$
$$- \beta J\sqrt{\beta J_0}\sum_\delta\sum_{\alpha<\beta}\epsilon^\delta \eta^{\alpha\beta}\langle S^\delta\rangle_{L_0}\langle S^\alpha S^\beta\rangle_{L_0}$$
$$+ \beta J\sqrt{\beta J_0}\sum_\delta\sum_{\alpha<\beta}\epsilon^\delta\eta^{\alpha\beta}\langle S^\delta S^\alpha S^\beta\rangle_{L_0}. \tag{3.5}$$

Here $\langle\cdots\rangle_{L_0}$ denotes the average by the replica-symmetric weight e^{L_0}. We have used the facts that the replica-symmetric solution extremizes (3.3) (so that the terms linear in ϵ^α and $\eta^{\alpha\beta}$ vanish) and that $\mathrm{Tr}\,\mathrm{e}^{L_0} \to 1$ as $n \to 0$ as explained in §2.3.1. We see that the second-order term of $[f]$ with respect to ϵ^α and $\eta^{\alpha\beta}$ is, taking the first and second terms in the braces $\{\cdots\}$ in (3.3) into account,

$$\Delta \equiv \frac{1}{2}\sum_{\alpha\beta}\left\{\delta_{\alpha\beta} - \beta J_0(\langle S^\alpha S^\beta\rangle_{L_0} - \langle S^\alpha\rangle_{L_0}\langle S^\beta\rangle_{L_0})\right\}\epsilon^\alpha\epsilon^\beta$$

$$+\beta J\sqrt{\beta J_0}\sum_{\delta}\sum_{\alpha<\beta}(\langle S^\delta\rangle_{L_0}\langle S^\alpha S^\beta\rangle_{L_0}-\langle S^\alpha S^\beta S^\delta\rangle_{L_0})\epsilon^\delta\eta^{\alpha\beta}$$
$$+\frac{1}{2}\sum_{\alpha<\beta}\sum_{\gamma<\delta}\{\delta_{(\alpha\beta)(\delta\gamma)}-\beta^2J^2(\langle S^\alpha S^\beta S^\gamma S^\delta\rangle_{L_0}$$
$$-\langle S^\alpha S^\beta\rangle_{L_0}\langle S^\gamma S^\delta\rangle_{L_0})\}\,\eta^{\alpha\beta}\eta^{\gamma\delta} \tag{3.6}$$

up to the trivial factor of βn (which is irrelevant to the sign). We denote the matrix of coefficients of this quadratic form in ϵ^α and $\eta^{\alpha\beta}$ by G which is called the *Hessian* matrix. Stability of the replica-symmetric solution requires that the eigenvalues of G all be positive.

To derive the eigenvalues, let us list the matrix elements of G. Since $\langle\cdots\rangle_{L_0}$ represents the average by weight of the replica-symmetric solution, the coefficient of the second-order terms in ϵ has only two types of values. To simplify the notation we omit the suffix L_0 in the present section.

$$G_{\alpha\alpha}=1-\beta J_0(1-\langle S^\alpha\rangle^2)\equiv A \tag{3.7}$$
$$G_{\alpha\beta}=-\beta J_0(\langle S^\alpha S^\beta\rangle-\langle S^\alpha\rangle^2)\equiv B. \tag{3.8}$$

The coefficients of the second-order term in η have three different values, the diagonal and two types of off-diagonal elements. One of the off-diagonal elements has a matched single replica index and the other has all indices different:

$$G_{(\alpha\beta)(\alpha\beta)}=1-\beta^2J^2(1-\langle S^\alpha S^\beta\rangle^2)\equiv P \tag{3.9}$$
$$G_{(\alpha\beta)(\alpha\gamma)}=-\beta^2J^2(\langle S^\beta S^\gamma\rangle-\langle S^\alpha S^\beta\rangle^2)\equiv Q \tag{3.10}$$
$$G_{(\alpha\beta)(\gamma\delta)}=-\beta^2J^2(\langle S^\alpha S^\beta S^\gamma S^\delta\rangle-\langle S^\alpha S^\beta\rangle^2)\equiv R. \tag{3.11}$$

Finally there are two kinds of cross-terms in ϵ and η:

$$G_{\alpha(\alpha\beta)}=\beta J\sqrt{\beta J_0}(\langle S^\alpha\rangle\langle S^\alpha S^\beta\rangle-\langle S^\beta\rangle)\equiv C \tag{3.12}$$
$$G_{\gamma(\alpha\beta)}=\beta J\sqrt{\beta J_0}(\langle S^\gamma\rangle\langle S^\alpha S^\beta\rangle-\langle S^\alpha S^\beta S^\gamma\rangle)\equiv D. \tag{3.13}$$

These complete the elements of G.

The expectation values appearing in (3.7) to (3.13) can be evaluated from the replica-symmetric solution. The elements of G are written in terms of $\langle S^\alpha\rangle=m$ and $\langle S^\alpha S^\beta\rangle=q$ satisfying (2.28) and (2.30) as well as

$$\langle S^\alpha S^\beta S^\gamma\rangle\equiv t=\int \mathrm{D}z\,\tanh^3\beta\tilde{H}(z) \tag{3.14}$$
$$\langle S^\alpha S^\beta S^\gamma S^\delta\rangle\equiv r=\int \mathrm{D}z\,\tanh^4\beta\tilde{H}(z). \tag{3.15}$$

The integrals on the right of (3.14) and (3.15) can be derived by the method in §2.3.1.

3.1.2 *Eigenvalues of the Hessian and the AT line*

We start the analysis of stability by the simplest case of paramagnetic solution. All order parameters m, q, r, and t vanish in the paramagnetic phase. Hence B, Q, R, C, and D (the off-diagonal elements of G) are all zero. The stability condition for infinitesimal deviations of the ferromagnetic order parameter ϵ^α is $A > 0$, which is equivalent to $1 - \beta J_0 > 0$ or $T > J_0$ from (3.7). Similarly the stability for spin-glass-like infinitesimal deviations $\eta^{\alpha\beta}$ is $P > 0$ or $T > J$. These two conditions precisely agree with the region of existence of the paramagnetic phase derived in §2.3.2 (see Fig. 2.1). Therefore the replica-symmetric solution is stable in the paramagnetic phase.

It is a more elaborate task to investigate the stability condition of the ordered phases. It is necessary to calculate all eigenvalues of the Hessian. Details are given in Appendix A, and we just mention the results here.

Let us write the eigenvalue equation in the form

$$G\boldsymbol{\mu} = \lambda\boldsymbol{\mu}, \ \boldsymbol{\mu} = \begin{pmatrix} \{\epsilon^\alpha\} \\ \{\eta^{\alpha\beta}\} \end{pmatrix}. \tag{3.16}$$

The symbol $\{\epsilon^\alpha\}$ denotes a column from ϵ^1 at the top to ϵ^n at the bottom, and $\{\eta^{\alpha\beta}\}$ is for η^{12} to $\eta^{n-1,n}$.

The first eigenvector $\boldsymbol{\mu}_1$ has $\epsilon^\alpha = a$ and $\eta^{\alpha\beta} = b$, uniform in both parts. Its eigenvalue is, in the limit $n \to 0$,

$$\lambda_1 = \frac{1}{2}\left\{A - B + P - 4Q + 3R \pm \sqrt{(A - B - P + 4Q - 3R)^2 - 8(C - D)^2}\right\}. \tag{3.17}$$

The second eigenvector $\boldsymbol{\mu}_2$ has $\epsilon^\theta = a$ for a specific replica θ and $\epsilon^\alpha = b$ otherwise, and $\eta^{\alpha\beta} = c$ when α or β is equal to θ and $\eta^{\alpha\beta} = d$ otherwise. The eigenvalue of this eigenvector becomes degenerate with λ_1 in the limit $n \to 0$. The third and final eigenvector $\boldsymbol{\mu}_3$ has $\epsilon^\theta = a, \epsilon^\nu = a$ for two specific replicas θ, ν and $\epsilon^\alpha = b$ otherwise, and $\eta^{\theta\nu} = c, \eta^{\theta\alpha} = \eta^{\nu\alpha} = d$ and $\eta^{\alpha\beta} = e$ otherwise. Its eigenvalue is

$$\lambda_3 = P - 2Q + R. \tag{3.18}$$

A sufficient condition for $\lambda_1, \lambda_2 > 0$ is, from (3.17),

$$A - B = 1 - \beta J_0(1 - q) > 0, \quad P - 4Q + 3R = 1 - \beta^2 J^2(1 - 4q + 3r) > 0. \tag{3.19}$$

These two conditions are seen to be equivalent to the saddle-point condition of the replica-symmetric free energy (2.27) with respect to m and q as can be verified by the second-order derivatives:

$$A - B = \frac{1}{J_0}\frac{\partial^2 [f]}{\partial m^2}\bigg|_{\mathrm{RS}} > 0, \ P - 4Q + 3R = -\frac{2}{\beta J^2}\frac{\partial^2 [f]}{\partial q^2}\bigg|_{\mathrm{RS}} > 0. \tag{3.20}$$

These inequalities always hold as has been mentioned in §2.3.2.

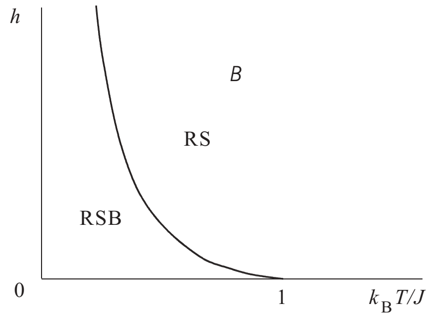

FIG. 3.1. Stability limit of the replica-symmetric (RS) solution in the h–T phase diagram (the AT line) below which replica symmetry breaking (RSB) occurs.

The condition for positive λ_3 is

$$P - 2Q + R = 1 - \beta^2 J^2 (1 - 2q + r) > 0 \tag{3.21}$$

or more explicitly

$$\left(\frac{T}{J}\right)^2 > \int \mathrm{D}z \, \mathrm{sech}^4(\beta J \sqrt{q} z + \beta J_0 m). \tag{3.22}$$

By numerically solving the equations of state of the replica-symmetric order parameters (2.28) and (2.30), one finds that the stability condition (3.22) is not satisfied in the spin glass and mixed phases in Fig. 2.1. The line of the limit of stability within the ferromagnetic phase (i.e. the boundary between the ferromagnetic and mixed phases) is the AT line. The mixed phase has finite ferromagnetic order but replica symmetry is broken there. More elaborate analysis is required in the mixed phase as shown in the next section.

The stability of replica symmetry in the case of finite h with symmetric distribution $J_0 = 0$ can be studied similarly. Let us just mention the conclusion that the stability condition in such a case is given simply by replacing $J_0 m$ by h in (3.22). The phase diagram thus obtained is depicted in Fig. 3.1. A phase with broken replica symmetry extends into the low-temperature region. This phase is also often called the spin glass phase. The limit of stability in the present case is also termed the AT line.

3.2 Replica symmetry breaking

The third eigenvector $\boldsymbol{\mu}_3$, which causes replica symmetry breaking, is called the *replicon mode*. There is no replica symmetry breaking in m_α since the replicon mode has $a = b$ for ϵ^θ and ϵ^ν in the limit $n \to 0$, as in the relation (A.19) or (A.21) in Appendix A. Only $q_{\alpha\beta}$ shows dependence on α and β. It is necessary to clarify how $q_{\alpha\beta}$ depends on α and β, but unfortunately we are not aware of any first-principle argument which can lead to the exact solution. One thus proceeds by trial and error to check if the tentative solution satisfies various necessary conditions for the correct solution, such as positive entropy at low temperatures and the non-negative eigenvalue of the replicon mode.

The only solution found so far that satisfies all necessary conditions is the one by Parisi (1979, 1980). The *Parisi solution* is believed to be the exact solution of the SK model also because of its rich physical implications. The replica symmetry is broken in multiple steps in the Parisi solution of the SK model. We shall explain mainly its first step in the present section.

3.2.1 *Parisi solution*

Let us regard $q_{\alpha\beta}$ $(\alpha \neq \beta)$ of the replica-symmetric solution of the SK model as an element of an $n \times n$ matrix. Then all the elements except those along the diagonal have the common value q, and we may write

$$\{q_{\alpha\beta}\} = \begin{pmatrix} 0 & & & & & \\ & 0 & & q & & \\ & & 0 & & & \\ & & & 0 & & \\ & q & & & 0 & \\ & & & & & 0 \end{pmatrix}. \tag{3.23}$$

In the first step of replica symmetry breaking (1RSB), one introduces a positive integer m_1 $(\leq n)$ and divides the replicas into n/m_1 blocks. Off-diagonal blocks have q_0 as their elements and diagonal blocks are assigned q_1. All diagonal elements are kept 0. The following example is for the case of $n = 6, m_1 = 3$.

$$\left(\begin{array}{ccc|ccc} 0 & q_1 & q_1 & & & \\ q_1 & 0 & q_1 & & q_0 & \\ q_1 & q_1 & 0 & & & \\ \hline & & & 0 & q_1 & q_1 \\ & q_0 & & q_1 & 0 & q_1 \\ & & & q_1 & q_1 & 0 \end{array}\right). \tag{3.24}$$

In the second step, the off-diagonal blocks are left untouched and the diagonal blocks are further divided into m_1/m_2 blocks. The elements of the innermost blocks are assumed to be q_2 and all the other elements of the larger diagonal blocks are kept as q_1. For example, if we have $n = 12, m_1 = 6, m_2 = 3$,

$$\left(\begin{array}{c|c} \begin{array}{c|c} \begin{matrix}0&q_2&q_2\\ q_2&0&q_2\\ q_2&q_2&0\end{matrix} & q_1 \\ \hline q_1 & \begin{matrix}0&q_2&q_2\\ q_2&0&q_2\\ q_2&q_2&0\end{matrix} \end{array} & q_0 \\ \hline q_0 & \begin{array}{c|c} \begin{matrix}0&q_2&q_2\\ q_2&0&q_2\\ q_2&q_2&0\end{matrix} & q_1 \\ \hline q_1 & \begin{matrix}0&q_2&q_2\\ q_2&0&q_2\\ q_2&q_2&0\end{matrix} \end{array} \end{array}\right). \tag{3.25}$$

The numbers $n, m_1, m_2, \ldots$ are integers by definition and are ordered as $n \geq m_1 \geq m_2 \geq \cdots \geq 1$.

Now we define the function $q(x)$ as

$$q(x) = q_i \quad (m_{i+1} < x \leq m_i) \tag{3.26}$$

and take the limit $n \to 0$ following the prescription of the replica method. We somewhat arbitrarily reverse the above inequalities

$$0 \leq m_1 \leq \cdots \leq 1 \quad (0 \leq x \leq 1) \tag{3.27}$$

and suppose that $q(x)$ becomes a continuous function defined between 0 and 1. This is the basic idea of the Parisi solution.

3.2.2 *First-step RSB*

We derive expressions of the physical quantities by the first-step RSB (1RSB) represented in (3.24). The first term on the right hand side of the single-body effective Hamiltonian (2.15) reduces to

$$\sum_{\alpha<\beta} q_{\alpha\beta} S^\alpha S^\beta = \frac{1}{2}\left\{ q_0 \left(\sum_{\alpha}^{n} S^\alpha\right)^2 + (q_1 - q_0) \sum_{\text{block}}^{n/m_1} \left(\sum_{\alpha\in\text{block}}^{m_1} S^\alpha\right)^2 - nq_1 \right\}. \tag{3.28}$$

The first term on the right hand side here fills all elements of the matrix $\{q_{\alpha\beta}\}$ with q_0 but the block-diagonal part is replaced with q_1 by the second term. The last term forces the diagonal elements to zero. Similarly the quadratic term of $q_{\alpha\beta}$ in the free energy (2.17) is

$$\lim_{n\to 0} \frac{1}{n} \sum_{\alpha\neq\beta} q_{\alpha\beta}^2 = \lim_{n\to 0} \frac{1}{n}\left\{ n^2 q_0^2 + \frac{n}{m_1} m_1^2 (q_1^2 - q_0^2) - nq_1^2 \right\} = (m_1 - 1) q_1^2 - m_1 q_0^2. \tag{3.29}$$

We insert (3.28) and (3.29) into (2.17) and linearize $(\sum_\alpha S^\alpha)^2$ in (3.28) by a Gaussian integral in a similar manner as in the replica-symmetric calculations.

It is necessary to introduce $1 + n/m_1$ Gaussian variables corresponding to the number of terms of the form $(\sum_\alpha S^\alpha)^2$ in (3.28). Finally we take the limit $n \to 0$ to find the free energy with 1RSB as

$$\beta f_{\text{1RSB}} = \frac{\beta^2 J^2}{4}\left\{(m_1-1)q_1^2 - m_1 q_0^2 + 2q_1 - 1\right\} + \frac{\beta J_0}{2} m^2 - \log 2 - \frac{1}{m_1}\int \mathrm{D}u \log \int \mathrm{D}v \cosh^{m_1} \Xi \tag{3.30}$$

$$\Xi = \beta(J\sqrt{q_0}\,u + J\sqrt{q_1 - q_0}\,v + J_0 m + h). \tag{3.31}$$

Here we have used the replica symmetry of magnetization $m = m_\alpha$.

The variational parameters q_0, q_1, m, and m_1 all fall in the range between 0 and 1. The variational (extremization) conditions of (3.30) with respect to m, q_0, and q_1 lead to the equations of state:

$$m = \int \mathrm{D}u \, \frac{\int \mathrm{D}v \cosh^{m_1}\Xi \tanh \Xi}{\int \mathrm{D}v \cosh^{m_1}\Xi} \tag{3.32}$$

$$q_0 = \int \mathrm{D}u \left(\frac{\int \mathrm{D}v \cosh^{m_1}\Xi \tanh \Xi}{\int \mathrm{D}v \cosh^{m_1}\Xi}\right)^2 \tag{3.33}$$

$$q_1 = \int \mathrm{D}u \, \frac{\int \mathrm{D}v \cosh^{m_1}\Xi \tanh^2 \Xi}{\int \mathrm{D}v \cosh^{m_1}\Xi}. \tag{3.34}$$

Comparison of these equations of state for the order parameters with those for the replica-symmetric solution (2.28) and (2.30) suggests the following interpretation. In (3.32) for the magnetization, the integrand after Du represents magnetization within a block of the 1RSB matrix (3.24), which is averaged over all blocks with the Gaussian weight. Analogously, (3.34) for q_1 is the spin glass order parameter within a diagonal block averaged over all blocks. In (3.33) for q_0, on the other hand, one first calculates the magnetization within a block and takes its product between blocks, an interblock spin glass order parameter. Indeed, if one carries out the trace operation in the definition of $q_{\alpha\beta}$, (2.18), by taking α and β within a single block and assuming 1RSB, one obtains (3.34), whereas (3.33) results if α and β belong to different blocks. The Schwarz inequality assures $q_1 \geq q_0$.

We omit the explicit form of the extremization condition of the free energy (3.31) by the parameter m_1 since the form is a little complicated and is not used later.

When $J_0 = h = 0$, Ξ is odd in u, v, and thus $m = 0$ is the only solution of (3.32). The order parameter q_1 can be positive for $T < T_{\mathrm{f}} = J$ because the first term in the expansion of the right hand side of (3.34) for small q_0 and q_1 is $\beta^2 J^2 q_1$. Therefore the RS and 1RSB give the same transition point. The parameter m_1 is one at T_{f} and decreases with temperature.

3.2.3 *Stability of the first step RSB*

The stability of 1RSB can be investigated by a direct generalization of the argument in §3.1. We mention only a few main points for the case $J_0 = h = 0$. It is sufficient to treat two cases: one with all indices $\alpha, \beta, \gamma, \delta$ of the Hessian elements within the same block and the other with indices in two different blocks.

If α and β in $q_{\alpha\beta}$ belong to the same block, the stability condition of the replicon mode for infinitesimal deviations from 1RSB is expressed as

$$\lambda_3 = P - 2Q + R = 1 - \beta^2 J^2 \int \mathrm{D}u \frac{\int \mathrm{D}v \cosh^{m_1 - 4} \Xi}{\int \mathrm{D}v \cosh^{m_1} \Xi} > 0. \tag{3.35}$$

For the replicon mode between two different blocks, the stability condition reads

$$\lambda_3 = P - 2Q + R = 1 - \beta^2 J^2 \int \mathrm{D}u \left(\frac{\int \mathrm{D}v \cosh^{m_1 - 1} \Xi}{\int \mathrm{D}v \cosh^{m_1} \Xi} \right)^4 > 0. \tag{3.36}$$

According to the Schwarz inequality, the right hand side of (3.35) is less than or equal to that of (3.36), and therefore the former is sufficient. Equation (3.35) is not satisfied in the spin glass phase similar to the case of the RSB solution. However, the absolute value of the eigenvalue is confirmed by numerical evaluation to be smaller than that of the RS solution although λ_3 is still negative. This suggests an improvement towards a stable solution. The entropy per spin at $J_0 = 0, T = 0$ reduces from $-0.16\,(= -1/2\pi)$ for the RS solution to -0.01 for the 1RSB. Thus we may expect to obtain still better results if we go further into replica symmetry breaking.

3.3 Full RSB solution

Let us proceed with the calculation of the free energy (2.17) by a multiple-step RSB. We restrict ourselves to the case $J_0 = 0$ for simplicity.

3.3.1 *Physical quantities*

The sum involving $q_{\alpha\beta}^2$ in the free energy (2.17) can be expressed at the Kth step of RSB (K-RSB) as follows by counting the number of elements in a similar way to the 1RSB case (3.29):

$$\begin{aligned} &\sum_{\alpha \neq \beta} q_{\alpha\beta}^l \\ &= q_0^l n^2 + (q_1^l - q_0^l) m_1^2 \cdot \frac{n}{m_1} + (q_2^l - q_1^l) m_2^2 \cdot \frac{m_1}{m_2} \cdot \frac{n}{m_1} + \cdots - q_K^l \cdot n \\ &= n \sum_{j=0}^{K} (m_j - m_{j+1}) q_j^l, \end{aligned} \tag{3.37}$$

where l is an arbitrary integer and $m_0 = n, m_{K+1} = 1$. In the limit $n \to 0$, we may use the replacement $m_j - m_{j+1} \to -\mathrm{d}x$ to find

$$\frac{1}{n}\sum_{\alpha\neq\beta} q_{\alpha\beta}^l \to -\int_0^1 q^l(x)\mathrm{d}x. \tag{3.38}$$

The internal energy for $J_0 = 0, h = 0$ is given by differentiation of the free energy (2.17) by β as[2]

$$E = -\frac{\beta J^2}{2}\left(1 + \frac{2}{n}\sum_{\alpha<\beta} q_{\alpha\beta}^2\right) \to -\frac{\beta J^2}{2}\left(1 - \int_0^1 q^2(x)\mathrm{d}x\right). \tag{3.39}$$

The magnetic susceptibility can be written down from the second derivative of (2.17) by h as

$$\chi = \beta\left(1 + \frac{1}{n}\sum_{\alpha\neq\beta} q_{\alpha\beta}\right) \to \beta\left(1 - \int_0^1 q(x)\mathrm{d}x\right). \tag{3.40}$$

It needs some calculations to derive the free energy in the full RSB scheme. Details are given in Appendix B. The final expression of the free energy (2.17) is

$$\beta f = -\frac{\beta^2 J^2}{4}\left\{1 + \int_0^1 q(x)^2\mathrm{d}x - 2q(1)\right\} - \int \mathrm{D}u\, f_0(0, \sqrt{q(0)}u). \tag{3.41}$$

Here f_0 satisfies the *Parisi equation*

$$\frac{\partial f_0(x,h)}{\partial x} = -\frac{J^2}{2}\frac{\mathrm{d}q}{\mathrm{d}x}\left\{\frac{\partial^2 f_0}{\partial h^2} + x\left(\frac{\partial f_0}{\partial h}\right)^2\right\} \tag{3.42}$$

to be solved under the initial condition $f_0(1,h) = \log 2\cosh\beta h$.

3.3.2 *Order parameter near the critical point*

It is in general very difficult to find a solution to the extremization condition of the free energy (3.41) with respect to the order function $q(x)$. It is nevertheless possible to derive some explicit results by the Landau expansion when the temperature is close to the critical point and consequently $q(x)$ is small. Let us briefly explain the essence of this procedure.

When $J_0 = h = 0$, the expansion of the free energy (2.17) to fourth order in $q_{\alpha\beta}$ turns out to be

$$\begin{aligned}\beta f = \lim_{n\to 0}\frac{1}{n}\bigg\{&\frac{1}{4}\left(\frac{T^2}{T_\mathrm{f}^2} - 1\right)\mathrm{Tr}\, Q^2 - \frac{1}{6}\mathrm{Tr}\, Q^3 \\ &- \frac{1}{8}\mathrm{Tr}\, Q^4 + \frac{1}{4}\sum_{\alpha\neq\beta\neq\gamma} Q_{\alpha\beta}^2 Q_{\alpha\gamma}^2 - \frac{1}{12}\sum_{\alpha\neq\beta} Q_{\alpha\beta}^4\bigg\},\end{aligned} \tag{3.43}$$

where we have dropped q-independent terms. The operator Tr here denotes the diagonal sum in the replica space. We have introduced the notation $Q_{\alpha\beta} =$

[2] The symbol of configurational average $[\cdots]$ will be omitted in the present chapter as long as it does not lead to confusion.

$(\beta J)^2 q_{\alpha\beta}$. Only the last term is relevant to the RSB. It can indeed be verified that the eigenvalue of the replicon mode that determines stability of the RS solution is, by setting the coefficient of the last term to $-y$ (which is actually $-1/12$),

$$\lambda_3 = -16y\theta^2, \tag{3.44}$$

where $\theta = (T_\mathrm{f} - T)/T_\mathrm{f}$. We may thus neglect all fourth-order terms except $Q^4_{\alpha\beta}$ to discuss the essential features of the RSB and let $n \to 0$ to get

$$\beta f = \frac{1}{2}\int_0^1 \mathrm{d}x \left\{ |\theta| q^2(x) - \frac{1}{3} x q^3(x) - q(x)\int_0^x q^2(y)\mathrm{d}y + \frac{1}{6} q^4(x) \right\}. \tag{3.45}$$

The extremization condition with respect to $q(x)$ is written explicitly as

$$2|\theta| q(x) - x q^2(x) - \int_0^x q^2(y)\mathrm{d}y - 2q(x)\int_x^1 q(y)\mathrm{d}y + \frac{2}{3} q^3(x) = 0. \tag{3.46}$$

Differentiation of this formula gives

$$|\theta| - x q(x) - \int_x^1 q(y)\mathrm{d}y + q^2(x) = 0 \quad \text{or} \quad q'(x) = 0. \tag{3.47}$$

Still further differentiation leads to

$$q(x) = \frac{x}{2} \quad \text{or} \quad q'(x) = 0. \tag{3.48}$$

The RS solution corresponds to a constant $q(x)$. This constant is equal to $|\theta|$ according to (3.46). There also exists an x-dependent solution

$$q(x) = \frac{x}{2} \quad (0 \le x \le x_1 = 2q(1)) \tag{3.49}$$

$$q(x) = q(1) \quad (x_1 \le x \le 1). \tag{3.50}$$

By inserting this solution in the variational condition (3.46), we obtain

$$q(1) = |\theta| + \mathcal{O}(\theta^2). \tag{3.51}$$

Figure 3.2 shows the resulting behaviour of $q(x)$ near the critical point where θ is close to zero.

3.3.3 *Vertical phase boundary*

The susceptibility is a constant $\chi = 1/J$ near the critical point T_f because the integral in (3.40) is $1 - T/T_\mathrm{f}$ according to (3.49)–(3.51). It turns out in fact that this result remains valid not only near T_f but over the whole temperature range below the critical point. We use this fact to show that the phase boundary between the spin glass and ferromagnetic phases is a vertical line at $J_0 = J$ as in Fig. 2.1 (Toulouse 1980).

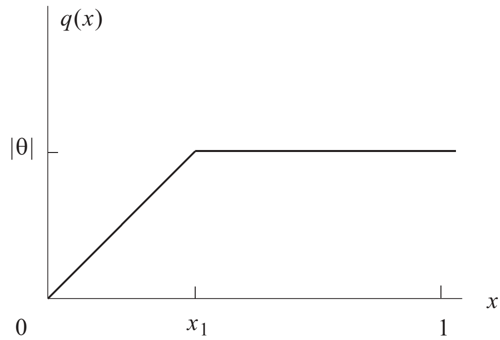

FIG. 3.2. $q(x)$ near the critical point

The Hamiltonian of the SK model (2.7) suggests that a change of the centre of distribution of J_{ij} from 0 to J_0/N shifts the energy per spin by $-J_0 m^2/2$. Thus the free energy $f(T, m, J_0)$ as a function of T and m satisfies

$$f(T, m, J_0) = f(T, m, 0) - \frac{1}{2} J_0 m^2. \tag{3.52}$$

From the thermodynamic relation

$$\frac{\partial f(T, m, 0)}{\partial m} = h \tag{3.53}$$

and the fact that $m = 0$ when $J_0 = 0$ and $h = 0$, we obtain

$$\chi^{-1} = \left(\frac{\partial m}{\partial h} \bigg]_{h \to 0} \right)^{-1} = \frac{\partial^2 f(T, m, 0)}{\partial m^2} \bigg]_{m \to 0}. \tag{3.54}$$

Thus, for sufficiently small m, we have

$$f(T, m, 0) = f_0(T) + \frac{1}{2} \chi^{-1} m^2. \tag{3.55}$$

Combining (3.52) and (3.55) gives

$$f(T, m, J_0) = f_0(T) + \frac{1}{2} (\chi^{-1} - J_0) m^2. \tag{3.56}$$

This formula shows that the coefficient of m^2 in $f(T, m, J_0)$ vanishes when $\chi = 1/J_0$ and therefore there is a phase transition between the ferromagnetic and non-ferromagnetic phases according to the Landau theory. Since $\chi = 1/J$ in the whole range $T < T_{\rm f}$, we conclude that the boundary between the ferromagnetic and spin glass phases exists at $J_0 = J$.

Stability analysis of the Parisi solution has revealed that the eigenvalue of the replicon mode is zero, implying marginal stability of the Parisi RSB solution. No other solutions have been found with a non-negative replicon eigenvalue of the Hessian.

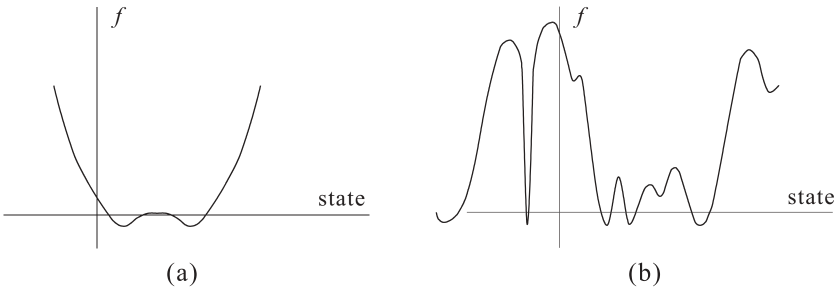

FIG. 3.3. Simple free energy (a) and multivalley structure (b)

3.4 Physical significance of RSB

The RSB of the Parisi type has been introduced as a mathematical tool to resolve controversies in the RS solution. It has, however, been discovered that the solution has a profound physical significance. The main results are sketched here (Mézard *et al.* 1987; Binder and Young 1986).

3.4.1 *Multivalley structure*

In a ferromagnet the free energy as a function of the state of the system has a simple structure as depicted in Fig. 3.3(a). The free energy of the spin glass state, on the other hand, is considered to have many minima as in Fig. 3.3(b), and the barriers between them are expected to grow indefinitely as the system size increases. It is possible to give a clear interpretation of the RSB solution if we accept this physical picture.

Suppose that the system size is large but not infinite. Then the system is trapped in the valley around one of the minima of the free energy for quite a long time. However, after a very long time, the system climbs the barriers and reaches all valleys eventually. Hence, within some limited time scale, the physical properties of a system are determined by one of the valleys. But, after an extremely long time, one would observe behaviour reflecting the properties of all the valleys. This latter situation is the one assumed in the conventional formulation of equilibrium statistical mechanics.

We now label free energy valleys by the index a and write $m_i^a = \langle S_i \rangle_a$ for the magnetization calculated by restricting the system to a specific valley a. This is analogous to the restriction of states to those with $m > 0$ (neglecting $m < 0$) in a simple ferromagnet.

3.4.2 $q_{\rm EA}$ *and* $\overline{q}$

To understand the spin ordering in a single valley, it is necessary to take the thermodynamic limit to separate the valley from the others by increasing the barriers indefinitely. Then we may ignore transitions between valleys and observe the long-time behaviour of the system in a valley. It therefore makes sense to define the order parameter $q_{\rm EA}$ for a single valley as

$$q_{\rm EA} = \lim_{t\to\infty} \lim_{N\to\infty} \left[\langle S_i(t_0) S_i(t_0+t)\rangle\right]. \tag{3.57}$$

This quantity measures the similarity (or overlap) of a spin state at site i after a long time to the initial condition at t_0. The physical significance of this quantity suggests its equivalence to the average of the squared local magnetization $(m_i^a)^2$:

$$q_{\rm EA} = \left[\sum_a P_a \,(m_i^a)^2\right] = \left[\sum_a P_a \frac{1}{N}\sum_i (m_i^a)^2\right]. \tag{3.58}$$

Here P_a is the probability that the system is located in a valley (*a pure state*) a, that is $P_a = {\rm e}^{-\beta F_a}/Z$. In the second equality of (3.58), we have assumed that the averaged squared local magnetization does not depend on the location.

We may also define another order parameter $\overline{q}$ that represents the average over all valleys corresponding to the long-time observation (the usual statistical-mechanical average). This order parameter can be expressed explicitly as

$$\overline{q} = \left[(\sum_a P_a m_i^a)^2\right] = \left[\sum_{ab} P_a P_b m_i^a m_i^b\right] = \frac{1}{N}\left[\sum_{ab} P_a P_b \sum_i m_i^a m_i^b\right], \tag{3.59}$$

which is rewritten using $m_i = \sum_a P_a m_i^a$ as

$$\overline{q} = [m_i^2] = [\langle S_i\rangle^2]. \tag{3.60}$$

As one can see from (3.59), $\overline{q}$ is the average with overlaps between valleys taken into account and is an appropriate quantity for time scales longer than transition times between valleys.

If there exists only a single valley (and its totally reflected state), the relation $q_{\rm EA} = \overline{q}$ should hold, but in general we have $q_{\rm EA} > \overline{q}$. The difference of these two order parameters $q_{\rm EA} - \overline{q}$ is a measure of the existence of a *multivalley structure*. We generally expect a continuous spectrum of order parameters between $\overline{q}$ and $q_{\rm EA}$ corresponding to the variety of degrees of transitions between valleys. This would correspond to the continuous function $q(x)$ of the Parisi RSB solution.

3.4.3 *Distribution of overlaps*

Similarity between two valleys a and b is measured by the overlap q_{ab} defined by

$$q_{ab} = \frac{1}{N}\sum_i m_i^a m_i^b. \tag{3.61}$$

This q_{ab} takes its maximum when the two valleys a and b coincide and is zero when they are completely uncorrelated. Let us define the distribution of q_{ab} for a given random interaction $\boldsymbol{J}$ as

$$P_J(q) = \langle \delta(q - q_{ab})\rangle = \sum_{ab} P_a P_b \delta(q - q_{ab}), \tag{3.62}$$

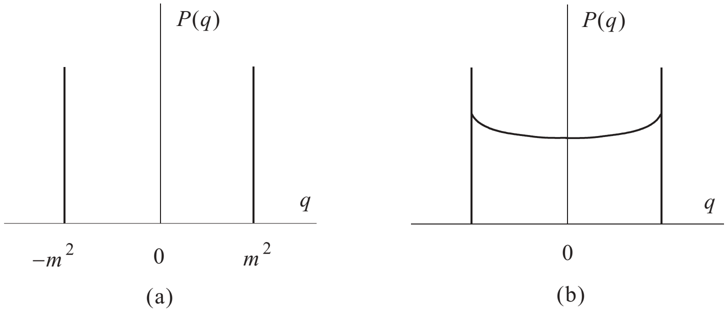

FIG. 3.4. Distribution function $P(q)$ of a simple system (a) and that of a system with multivalley structure (b)

and write $P(q)$ for the configurational average of $P_J(q)$:

$$P(q) = [P_J(q)]. \tag{3.63}$$

In a simple system like a ferromagnet, there are only two different valleys connected by overall spin reversal and q_{ab} assumes only $\pm m^2$. Then $P(q)$ is constituted only by two delta functions at $q = \pm m^2$, Fig. 3.4(a). If there is a multivalley structure with continuously different states, on the other hand, q_{ab} assumes various values and $P(q)$ has a continuous part as in Fig. 3.4(b).

3.4.4 *Replica representation of the order parameter*

Let us further investigate the relationship between the RSB and the continuous part of the distribution function $P(q)$. The quantity $q_{\alpha\beta}$ in the replica formalism is the overlap between two replicas α and β at a specific site

$$q_{\alpha\beta} = \langle S_i^\alpha S_i^\beta \rangle. \tag{3.64}$$

In the RSB this quantity has different values from one pair of replicas $\alpha\beta$ to another pair. The genuine statistical-mechanical average should be the mean of all possible values of $q_{\alpha\beta}$ and is identified with $\overline{q}$ defined in (3.59),

$$\overline{q} = \lim_{n\to 0} \frac{1}{n(n-1)} \sum_{\alpha\neq\beta} q_{\alpha\beta}. \tag{3.65}$$

The spin glass order parameter for a single valley, on the other hand, does not reflect the difference between valleys caused by transitions between them and therefore is expected to be larger than any other possible values of the order parameter. We may then identify $q_{\rm EA}$ with the largest value of $q_{\alpha\beta}$ in the replica method:

$$q_{\rm EA} = \max_{(\alpha\beta)} q_{\alpha\beta} = \max_x q(x). \tag{3.66}$$

Let us define $x(q)$ as the accumulated distribution of $P(q)$:

$$x(q) = \int_0^q \mathrm{d}q' P(q'), \quad \frac{\mathrm{d}x}{\mathrm{d}q} = P(q). \tag{3.67}$$

Using this definition and the fact that the statistical-mechanical average is the mean over all possible values of q, we may write

$$\overline{q} = \int_0^1 q' \mathrm{d}q' P(q') = \int_0^1 q(x)\mathrm{d}x. \tag{3.68}$$

The two parameters q_{EA} and $\overline{q}$ have thus been expressed by $q(x)$. If there are many valleys, $q_{\alpha\beta}$ takes various values, and $P(q)$ cannot be expressed simply in terms of two delta functions. The order function $q(x)$ under such a circumstance has a non-trivial structure as one can see from (3.67), which corresponds to the RSB of Parisi type. The functional form of $q(x)$ mentioned in §3.3.2 reflects the multivalley structure of the space of states of the spin glass phase.

3.4.5 *Ultrametricity*

The Parisi RSB solution shows a remarkable feature of *ultrametricity*. The configurational average of the distribution function between three different states

$$P_J(q_1, q_2, q_3) = \sum_{abc} P_a P_b P_c \delta(q_1 - q_{ab})\delta(q_2 - q_{bc})\delta(q_3 - q_{ca}) \tag{3.69}$$

can be evaluated by the RSB method to yield

$$[P_J(q_1, q_2, q_3)] = \frac{1}{2} P(q_1)x(q_1)\delta(q_1 - q_2)\delta(q_1 - q_3)$$
$$+\frac{1}{2}\left\{P(q_1)P(q_2)\Theta(q_1 - q_2)\delta(q_2 - q_3) + (\text{two terms with } 1, 2, 3 \text{ permuted})\right\}.$$

Here $x(q)$ has been defined in (3.67), and $\Theta(q_1 - q_2)$ is the step function equal to 1 for $q_1 > q_2$ and 0 for $q_1 < q_2$. The first term on the right hand side is non-vanishing only if the three overlaps are equal to each other, and the second term requires that the overlaps be the edges of an isosceles triangle ($q_1 > q_2, q_2 = q_3$). This means that the distances between three states should form either an equilateral or an isosceles triangle. We may interpret this result as a tree-like (or equivalently, nested) structure of the space of states as in Fig. 3.5. A metric space where the distances between three points satisfy this condition is called an ultrametric space.

3.5 TAP equation

A different point of view on spin glasses is provided by the equation of state due to Thouless, Anderson, and Palmer (TAP) which concerns the local magnetization in spin glasses (Thouless *et al.* 1977).

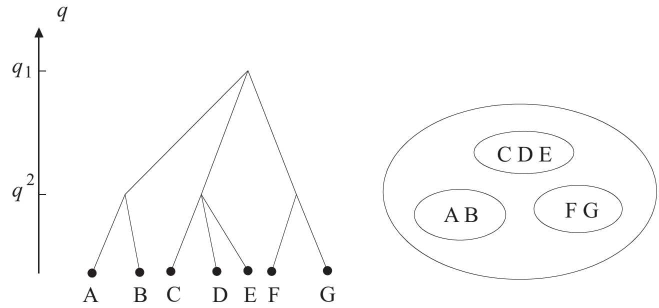

FIG. 3.5. Tree-like and nested structures in an ultrametric space. The distance between C and D is equal to that between C and E and to that between D and E, which is smaller than that between A and C and that between C and F.

3.5.1 *TAP equation*

The local magnetization of the SK model satisfies the following *TAP equation*, given the random interactions $\boldsymbol{J} = \{J_{ij}\}$:

$$m_i = \tanh \beta \left\{ \sum_j J_{ij} m_j + h_i - \beta \sum_j J_{ij}^2 (1 - m_j^2) m_i \right\}. \tag{3.70}$$

The first term on the right hand side represents the usual internal field, a generalization of (1.19). The third term is called the *reaction field of Onsager* and is added to remove the effects of self-response in the following sense. The magnetization m_i affects site j through the internal field $J_{ij} m_i$ that changes the magnetization of site j by the amount $\chi_{jj} J_{ij} m_i$. Here

$$\chi_{jj} = \left. \frac{\partial m_j}{\partial h_j} \right|_{h_j \to 0} = \beta (1 - m_j^2). \tag{3.71}$$

Then the internal field at site i would increase by

$$J_{ij} \chi_{jj} J_{ij} m_i = \beta J_{ij}^2 (1 - m_j^2) m_i. \tag{3.72}$$

The internal field at site i should not include such a rebound of itself. The third term on the right hand side of (3.70) removes this effect. In a usual ferromagnet with infinite-range interactions, the interaction scales as $J_{ij} = J/N$ and the third term is negligible since it is of $\mathcal{O}(1/N)$. In the SK model, however, we have $J_{ij}^2 = \mathcal{O}(1/N)$ and the third term is of the same order as the first and second terms and cannot be neglected. The TAP equation gives a basis to treat the spin glass problem without taking the configurational average over the distribution of $\boldsymbol{J}$.