Compressible Sherrington–Kirkpatrick spin-glass model

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Abstract

We introduce a Sherrington–Kirkpatrick spin-glass model with the addition of elastic degrees of freedom. The problem is formulated in terms of an effective four-spin Hamiltonian in the pressure ensemble, which can be treated by the replica method. In the replica-symmetric approximation, we analyze the pressure–temperature phase diagram, and obtain expressions for the critical boundaries between the disordered and the ordered (spin-glass and ferromagnetic) phases. The second-order para–ferromagnetic border ends at a tricritical point, beyond which the transition becomes discontinuous. We use these results to make contact with the temperature–concentration phase diagrams of mixtures of hydrogen-bonded crystals.

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1. Introduction

Orientational models with disorder and elastic degrees of freedom have been used to investigate phase transitions in a number of systems, such as the mixed molecular crystal $K(CN)_x Br_{1-x}$ [1]. The work on quadrupolar glass models in the presence of random strain fields, which are supposed to mimic the random mismatching of molecular groups, was reviewed by Binder and Reger [2]. A compressible spherical model, with random bonds and in random fields, has been introduced to account for the peculiar behavior of compositionally disordered perovskites, also known as relaxor ferroelectrics [3]. Disordered Ising models, with random competing interactions and elastic degrees of freedom, have also been used to account for the phase diagram and the glassy transition in mixtures of ferro- and antiferroelectric hydrogen-bonded crystals of the KDP family [4–6]. More recently, random quadrupolar models in the presence of anisotropic strain fields have been studied in the context of nematic liquid crystal elastomers [7]. These investigations on disordered compressible models provided the motivation to introduce a simple compressible Sherrington—Kirkpatrick (SK) Ising spin-glass model

[8, 9], and use standard techniques to obtain the global phase diagram in terms of pressure and temperature.

The investigation of compressible Ising models has a long history [10–12]. Mean-field and renormalization-group calculations indicate that the inclusion of elastic degrees of freedom may change the nature of the continuous Ising transition. An Ising antiferromagnet on the triangular lattice, with properly chosen elastic degrees of freedom, is known to provide a mechanism to explain the formation of striped phases [13, 14]. Although elastic spin models with uniform interactions have been much investigated, disordered compressible spin models are less explored. Nowadays it is feasible to carry out detailed computer simulations for compressible models [15–17], including disordered compressible models, as in the work of Marshall for a compressible Edwards–Anderson Ising spin-glass on a two-dimensional lattice [18, 19]. These works have provided further motivation to study the phase diagram of the simple compressible SK spin-glass model.

We treat the mean-field SK system in the pressure ensemble, which is more adequate to analyze the phase diagram in terms of the intensive field variables, temperature T and pressure p. Using the replica method, the calculation of the free energy is reduced to the minimization of a functional of three sets of replica variables [8]. We obtain a number of results in the replica-symmetric approximation. In particular, we show that the presence of magneto-elastic couplings introduces a simple shift in the border between paramagnetic and spin-glass phases, and that there appears a tricritical point along the para–ferromagnetic border. Also, we perform an analysis of stability of the replica-symmetric solution and locate the de Almeida–Thouless line [20]. In section 4, we consider a compressible two-sublattice SK model to make contact with the experimental phase diagrams of mixtures of ferro- and antiferroelectric hydrogen-bonded crystals.

2. The compressible SK model

The compressible Sherrington–Kirkpatrick spin-glass model is defined by the Hamiltonian

$$\mathcal{H} = -\sum_{1 \leqslant i < j \leqslant N} J_{ij} \left[1 - \gamma \left(v - v_0 \right) \right] S_i S_j - H \sum_{i=1}^{N} S_i + \frac{1}{2} k N \left(v - v_0 \right)^2, \quad (1)$$

where $S_i = \pm 1$, with $i = 1, \ldots, N$, v is the specific volume, $v_0 > 0$ is a constant parameter, γ is the magneto-elastic coupling, H is the external field and $k > 0$ is a uniform elastic constant. As usual, $\{J_{ij}\}$ is a set of independent and identically distributed random variables, with suitably scaled mean values, $\langle J_{ij} \rangle = J_0/N$, and variances, $\langle (J_{ij} - \langle J_{ij} \rangle)^2 \rangle = J^2/N$. Given a configuration $\{J_{ij}\}$, we write the partition function in the pressure ensemble,

$$Y = \int_0^\infty \mathrm{d}v \exp(-\beta p v N) \, \mathrm{Tr} \exp(-\beta \mathcal{H}), \quad (2)$$

where p is the pressure, $\beta = 1/(k_B T)$, and the trace is a sum over spin configurations. Performing the volume integration, and discarding irrelevant terms in the thermodynamic limit, we have

$$Y = \exp \left[-\beta N \left(p v_0 - \frac{p^2}{2k} \right) \right] \mathrm{Tr} \exp(-\beta \mathcal{H}_{\mathrm{eff}}), \quad (3)$$

with an effective four-spin Hamiltonian,

$$\mathcal{H}_{\mathrm{eff}} = -\left(1 + \frac{\gamma p}{k} \right) \sum_{i<j} J_{ij} S_i S_j - \frac{\gamma^2}{2kN} \left(\sum_{i<j} J_{ij} S_i S_j \right)^2 - H \sum_i S_i. \quad (4)$$

Using a Gaussian identity, we write the partition function as

$$Y = \exp\left[-\beta N \left(pv_0 - \frac{p^2}{2k}\right)\right] \int_{-\infty}^{+\infty} dx \exp\left(-\frac{N\beta\gamma^2 J^2}{2k} x^2\right)$$

$$\times \operatorname{Tr} \exp\left[\beta \left(1 + \frac{\gamma p}{k} + \frac{J\gamma^2 x}{k}\right) \sum_{i<j} J_{ij} S_i S_j + \beta H \sum_i S_i\right], \tag{5}$$

which is in a more convenient form to be treated by replicas.

According to the replica method,

$$\langle \ln Y \rangle = \lim_{n \to 0} \frac{1}{n} \ln \langle Y^n \rangle, \tag{6}$$

where

$$\langle Y^n \rangle = \exp\left[-\beta N n \left(pv_0 - \frac{p^2}{2k}\right)\right] \int_{-\infty}^{+\infty} \prod_{\alpha=1}^n dx^\alpha \exp\left[-\frac{N\beta\gamma^2 J^2}{2k} \sum_\alpha (x^\alpha)^2\right]$$

$$\times \left\langle \operatorname{Tr}_n \exp\left[\sum_{i<j} J_{ij} \left(\beta \sum_\alpha \xi^\alpha S_i^\alpha S_j^\alpha\right) + \beta H \sum_{i,\alpha} S_i^\alpha\right]\right\rangle, \tag{7}$$

with the definition

$$\xi^\alpha = 1 + \frac{\gamma p}{k} + \frac{J\gamma^2 x^\alpha}{k}. \tag{8}$$

Taking the average over the exchange configurations, and discarding irrelevant terms in the thermodynamic limit, we have

$$\langle Y^n \rangle = \exp\left[-\beta N n \left(pv_0 - \frac{p^2}{2k}\right)\right] \int_{-\infty}^{+\infty} \prod_\alpha dx^\alpha \exp\left[-\frac{N\beta\gamma^2}{2k} \sum_\alpha (x^\alpha)^2\right]$$

$$\times \operatorname{Tr}_n \exp\left[\frac{\beta^2 J^2}{2N} \sum_{\alpha,\beta} \xi^\alpha \xi^\beta \sum_{i<j} S_i^\alpha S_i^\beta S_j^\alpha S_j^\beta + \frac{\beta J_0}{N} \sum_\alpha \xi^\alpha \sum_{i<j} S_i^\alpha S_j^\alpha + \beta H \sum_{i,\alpha} S_i^\alpha\right], \tag{9}$$

which can be rewritten as

$$\langle Y^n \rangle = \exp\left[-\beta N n \left(pv_0 - \frac{p^2}{2k}\right)\right] \int_{-\infty}^{+\infty} \prod_\alpha dx^\alpha \exp\left\{\sum_\alpha \left[-\frac{N\beta J^2\gamma^2}{2k} (x^\alpha)^2\right.\right.$$

$$\left.\left. + \frac{N\beta^2 J^2}{4} (\xi^\alpha)^2\right]\right\} \operatorname{Tr}_n \exp\left\{\frac{\beta^2 J^2}{2N} \sum_{\alpha<\beta} \xi^\alpha \xi^\beta \left(\sum_i S_i^\alpha S_i^\beta\right)^2\right.$$

$$\left. + \frac{\beta J_0}{2N} \sum_\alpha \xi^\alpha \left(\sum_i S_i^\alpha\right)^2 + \beta H \sum_{i,\alpha} S_i^\alpha\right\}. \tag{10}$$

We now use Gaussian identities to introduce the new set of variables $\{m_\alpha\}$, associated with the magnetization, and $\{q_{\alpha\beta}\}$, associated with the overlap between replicas, so that

$$\langle Y^n \rangle = \int_{-\infty}^{+\infty} \prod_\alpha dx^\alpha \int_{-\infty}^{+\infty} \prod_\alpha dm^\alpha \int_{-\infty}^{+\infty} \prod_{\alpha<\beta} dq^{\alpha\beta} \exp[NG(x^\alpha, m^\alpha, q^{\alpha\beta})], \tag{11}$$

where

$$G(x^\alpha, m^\alpha, q^{\alpha\beta}) = -\beta n \left(p v_0 - \frac{p^2}{2k} \right) - \frac{\beta\gamma^2 J^2}{2k} \sum_\alpha (x^\alpha)^2 + \frac{\beta^2 J^2}{4} \sum_\alpha (\xi^\alpha)^2$$

$$- \frac{\beta^2 J^2}{2} \sum_{\alpha<\beta} \xi^\alpha \xi^\beta (q^{\alpha\beta})^2 - \frac{\beta J_0}{2} \sum_\alpha \xi^\alpha (m^\alpha)^2$$

$$+ \ln \mathrm{Tr} \exp \left(\beta^2 J^2 \sum_{\alpha<\beta} \xi^\alpha \xi^\beta q^{\alpha\beta} S^\alpha S^\beta + \beta J_0 \sum_\alpha \xi^\alpha m^\alpha S^\alpha + \beta H \sum_\alpha S^\alpha \right). \quad (12)$$

In the thermodynamic limit, the free energy comes from

$$g = g(T, p, H) = -\frac{1}{\beta} \lim_{n\to 0} \frac{1}{n} \max G(x^\alpha, m^\alpha, q^{\alpha\beta}), \quad (13)$$

where the maximum should be taken with respect to the three sets of replica variables.

3. Replica-symmetric solution

In the replica-symmetric solution, with $x_\alpha = x$ and $m_\alpha = m$, for all α, and $q_{\alpha\beta} = q$, for all pairs $(\alpha\beta)$, we have

$$-\beta g = -\beta \left(p v_0 - \frac{p^2}{2k} \right) - \frac{\beta\gamma^2 J^2}{2k} x^2 + \frac{\beta^2 J^2}{4} \xi^2 (1-q)^2 - \frac{\beta J_0 \xi}{2} m^2$$

$$+ \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp \left(-\frac{z^2}{2} \right) \ln 2 \cosh[\beta (J\xi q^{1/2} z + J_0 \xi m + H)], \quad (14)$$

with

$$\xi = 1 + \frac{\gamma p}{k} + \frac{J\gamma^2 x}{k}. \quad (15)$$

The equations of state are given by

$$q = \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp \left(-\frac{z^2}{2} \right) \tanh^2[\beta (J\xi q^{1/2} z + J_0 \xi m + H)], \quad (16)$$

$$m = \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp \left(-\frac{z^2}{2} \right) \tanh[\beta (J\xi q^{1/2} z + J_0 \xi m + H)] \quad (17)$$

and

$$x = \frac{\beta J}{2} \xi (1 - q^2) + \frac{J_0}{2J} m^2. \quad (18)$$

We now restrict the analysis to zero field ($H = 0$).

The transition between the spin-glass and the paramagnetic phase comes from the expansions of equations (16) and (18),

$$q = \frac{1}{2\beta^2 J^2 \xi^2} \left(1 - \frac{1}{\beta^2 J^2 \xi^2} \right) + O(q^2)$$

and

$$x = \frac{\beta J \xi}{2} + O(q^2). \quad (19)$$

There is a (positive) solution, $q > 0$, for

$$1 - \frac{1}{\xi \beta J} > 0. \tag{20}$$

Introducing the notation

$$t = \frac{1}{\beta J} = \frac{k_B T}{J}, \tag{21}$$

and using the definition of ξ, given by equation (15), we have the second-order boundary between the paramagnetic and the spin-glass phases,

$$t_{c1} = 1 + \frac{\gamma p}{k} + \frac{J \gamma^2}{2k}. \tag{22}$$

In zero field, the calculation of the para–ferromagnetic transition comes from the analysis of the expansion

$$x = \frac{\beta J}{2} \xi + \frac{J_0}{2J} m^2 + O(q^2), \tag{23}$$

which can be written as

$$\xi \left(1 - \frac{\beta J^2 \gamma^2}{2k} \right) = \left(1 + \frac{\gamma p}{k} \right) + \frac{J_0 \gamma^2}{2k} m^2 + O(q^2). \tag{24}$$

Introducing the dimensionless and more compact notation

$$j_0 = \frac{J_0}{J}, \qquad a = 1 + \frac{\gamma p}{k}, \qquad b = \frac{J \gamma^2}{2k}, \tag{25}$$

equation (24) can be rewritten as

$$\xi \left(1 - \frac{b}{2t} \right) = a + b j_0 m^2 + O(q^2).$$

Inserting this expansion into the equations of state, it is easy to show that

$$1 = \frac{a j_0}{t - b} \left(1 + \frac{j_0 b}{a} m^2 \right) - \frac{1}{3} \left(\frac{a}{t - b} \right)^3 \left(j_0^3 m^2 + 3 q j_0 \right) + O(m^3, q^{3/2}), \tag{26}$$

from which we have the second-order para–ferromagnetic border,

$$t_{c2} = a j_0 + b = \left(1 + \frac{\gamma p}{k} \right) j_0 + \frac{J \gamma^2}{2k}. \tag{27}$$

The transition between the spin-glass and the ferromagnetic phases may be calculated from an analysis of the zero-field susceptibility. It is not difficult to show that this border is given by

$$t_{c3} = b(1 - q^2) + a j_0 (1 - q), \tag{28}$$

where q comes from the equation

$$q = \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp \left(-\frac{z^2}{2} \right) \tanh^2 \left[\frac{a q^{1/2} z}{t - b(1 - q^2)} \right]. \tag{29}$$

In order to investigate the eventual existence of tricritical points, we write the expansions

$$m = \frac{j_0 a m}{t - b} \left(1 + \frac{b}{a} j_0 m^2 \right) - \frac{1}{3} \frac{j_0^3 a^3 m}{(t - b)^3} \left(m^2 + 3 q j_0^{-2} + 3 \frac{b}{a} j_0 m^4 + 9 \frac{b}{a} j_0^{-1} q m^2 \right) + O(m^6, q^3) \tag{30}$$

and

$$q = \left(\frac{j_0 a}{t-b}\right)^2 \left(1 + 2\frac{b}{a}j_0 m^2\right)\left(qj_0^{-2} + m^2\right)$$
$$- \frac{2}{3}\left(\frac{j_0 a}{t-b}\right)^4 \left(3q^2 j_0^{-4} + m^4 + 6qj_0^{-2}m^2\right) + O(m^6, q^3). \tag{31}$$

For $m = 0$, the coefficients of equation (31) indicate that there is no possibility of a tricritical point along the second-order border between the paramagnetic and the spin-glass phases. At the para–ferromagnetic border, however, it is not difficult to locate a tricritical point at

$$p_{tc} = \frac{3J\gamma j_0 \left(j_0^2 - 1\right)}{2\left(j_0^2 + 2\right)} - \frac{k}{\gamma}. \tag{32}$$

Let us turn to the Hessian matrix associated with the replica-symmetric solutions of $-\beta g$. There is a total of 13 distinct elements in the $n \to 0$ limit, seven of which come from derivatives involving the x^α variables. As in the standard SK model, the paramagnetic phase is always stable, and the eigenvector subspace is generated by three classes of vectors, which have the general form

$$\vec{\mu} = \begin{pmatrix} \{\phi^\alpha\} \\ \{\epsilon^\alpha\} \\ \{\eta^{(\alpha\beta)}\} \end{pmatrix}, \qquad \alpha, \beta = 1, \ldots, n, \tag{33}$$

where $\{\phi^\alpha\}$, $\{\epsilon^\alpha\}$ and $\{\eta^{(\alpha\beta)}\}$ are column vectors with n, n and $n(n-1)/2$ elements, respectively [20]. The eigenvalue spectrum is obtained straightforwardly following the same steps as the rigid model. In the ordered region, the change of sign of the transverse eigenvalue leads to an instability. The de Almeida–Thouless line is given by

$$\left(\frac{k_B T}{J}\right)^2 = (a + 2bx)^2 \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \text{sech}^4[\beta(a + 2bx)(Jq^{1/2}z + J_0 m)], \tag{34}$$

where $H = 0$, and m, q and x are the equations of state.

4. Conclusions

It is interesting to draw a typical phase diagram in terms of temperature $t = k_B T/J$ and the ratio $j_0 = J_0/J$ (in zero field). The dotted lines in figure 1 are the well-known replica-symmetric second-order boundaries, with the addition of the de Almeida–Thouless (AT) instability line, for the rigid SK model (with no magneto-elastic coupling). The location of these borders and of the AT line is shifted in the presence of a magneto-elastic coupling. The spin-glass and ferromagnetic regions are broadened as a result of a decrease of the effective energy of the system due to the magneto-elastic coupling, as seen in equation (4). The solid and dashed lines were drawn for the parameter values $a = 1 + \gamma p/k = 1.5$ and $b = J\gamma^2/2k = 0.5$. For these particular values of pressure and elastic parameters, the second-order boundary between the paramagnetic and the ferromagnetic phases, given by $t = 1/2 + 3j_0/2$, ends at a tricritical point, at $j_0 = 2$, beyond which there is a (dashed) line of first-order transitions. These are typical results for the compressible SK model in the replica-symmetric approximation.

With the exception of the well-known corrections in the spin-glass region [9], in analogy to the treatment of the rigid SK model, the form of the effective four-spin Hamiltonian in the pressure ensemble does not indicate any drastic qualitative changes of the phase diagrams even if we go beyond the simple replica-symmetric approximation.
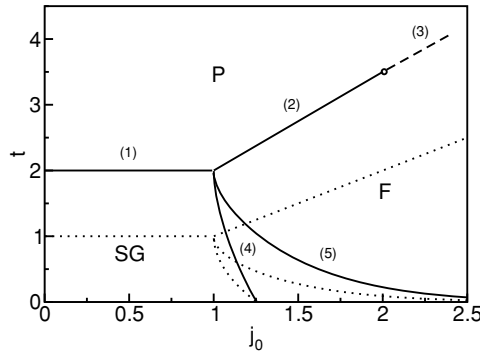
Figure 1. Comparison between the $t - j_0$ phase diagrams of the rigid (dotted lines) and compressible (solid lines) SK models. We indicate the paramagnetic (P), spin-glass (SG), and ferromagnetic (F) phases. Solid lines (1)–(4) are the boundaries coming from the replica-symmetric solution of the compressible SK model. Solid line (5) is the AT instability border. There is a tricritical point separating the continuous (solid line) and first-order (dashed line) P-F border of the compressible SK model.

We now make contact with previous work for mixtures of ferroelectric and antiferroelectric hydrogen-bonded crystals of the KDP family. A disordered Ising model in a random field, with the inclusion of elastic degrees of freedom, has been used to investigate the glassy transition in $Rb_{1-x}(NH_4)_x H_2 AsO_4$, known as RADA [6]. Also, the phase diagram of $Rb_{1-x}(NH_4)_x H_2 PO_4$ (RADP), in terms of temperature T and concentration x, has been drawn on the basis of a cluster calculation for a model of Ising pseudo-spins [4, 5]. The rubidium crystals, $RbH_2 PO_4$ (RDP) and $RbH_2 AsO_4$ (RDA), display a ferroelectric transition, at about 150 K, similar to the well-known ferroelectric phase transition in the isomorphous $KH_2 PO_4$ (KDP) crystals. The ammonium crystals, $NH_4 H_2 AsO_4$ (ADA) and $NH_4 H_2 PO_4$ (ADP), display a strong first-order antiferroelectric transition. At the mean-field level, the description of the T–x phase diagrams requires the consideration of two sublattices. We thus use a two-sublattice compressible SK model, given by the Hamiltonian

$$\mathcal{H} = - \sum_{i \in A, j \in B} J_{ij}[1 - \gamma(v - v_0)]S_i S_j + \frac{1}{2}kN(v - v_0)^2, \tag{35}$$

where the sum refers to all distinct pairs of spins belonging to different sublattices, A and B. The random variables $\{J_{ij}\}$ are associated with a Gaussian distribution, with suitably scaled moments, $\langle J_{ij} \rangle = J_0/N$, and $\langle (J_{ij} - \langle J_{ij} \rangle)^2 \rangle = J^2/N$, where we choose

$$J_0 = x J_R - (1 - x) J_A, \tag{36}$$

and make $J^2 \to J^2 x(1 - x)$, in order to mimic ferroelectric ($x = 1$) and antiferroelectric ($x = 0$) transitions. Two-sublattice Sherrington–Kirkpatrick models, even in the presence of random fields, have been studied in connection with transitions from antiferromagnetic to spin-glass phases [21–24]. The addition of elastic degrees of freedom, according to the steps of the previous sections, suggests a typical phase diagram as sketched in figure 2. With a convenient choice of the parameters, it is possible to predict an elastically induced first-order transition from the paraelectric to the antiferroelectric phase for $x \approx 1$, turning into second order for smaller values of concentration, and which is in qualitative agreement with the experimental findings. The glassy transition can still be understood within the framework of the rigid SK models, with the well-known instability of the replica-symmetric solution in
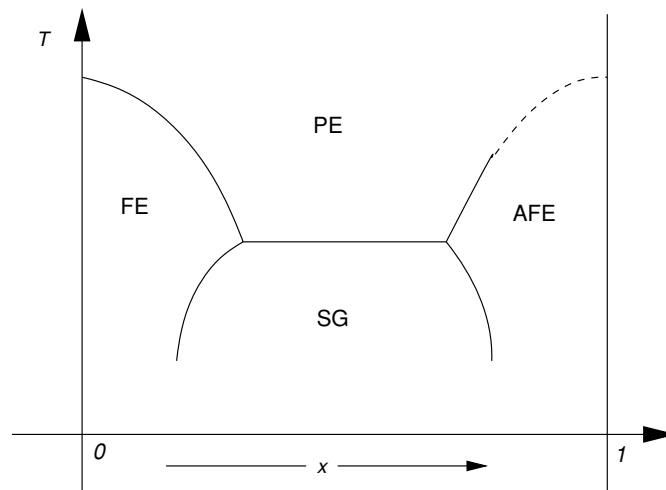
Figure 2. Schematic phase diagram for the two-sublattice compressible SK model for RADP in terms of temperature T and composition x. We indicate paraelectric, ferroelectric, antiferroelectric and glassy regions. Solid lines represent continuous transitions. The dashed line is a first-order transition.

the low-temperature region. It is important to remark that the inclusion of Gaussian random fields is not capable of explaining a first-order transition, in contrast to the predictions of the proposed compressible model [24, 25]. In fact, first-order transitions are associated with either a double-delta distribution of random fields [24, 26] or with the consideration of certain discrete quadrupolar-glass and Potts-glass models [2].

Acknowledgments

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