First-Order Phase Transition and Phase Coexistence in a Spin-Glass Model

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We study the mean-field static solution of the Blume-Emery-Griffiths-Capel model with quenched disorder, an Ising-spin lattice gas with random magnetic interaction. The thermodynamics is worked out in the full replica symmetry breaking scheme. The model exhibits a high temperature/low density paramagnetic phase. As temperature decreases or density increases, a phase transition to a full replica symmetry breaking spin-glass phase occurs. The nature of the transition can be either of the second order or, at temperature below a given critical value, of the first order in the Ehrenfest sense, with a discontinuous jump of the order parameter, a latent heat, and coexistence of phases.

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The spin-glass (SG) phase plays a central role in the understanding of disordered and complex systems. The analysis of mean-field models revealed different possible scenarios for the SG phase and the transition to it. Most of the work, however, has been concentrated on just two of them. In order of appearance, the first scenario is described by a full replica symmetry breaking (FRSB) solution characterized by a continuous order parameter function [1], which continuously grows from zero by crossing the transition. The prototype model is the Sherrington-Kirkpatrick (SK) model [2], a fully connected Ising spin model with quenched random magnetic interactions. The second scenario, initially introduced by Derrida [3], provides a transition with a jump in the order parameter to a SG with one step replica symmetry breaking (1RSB). No discontinuity appears, however, in the thermodynamic functions. Actually, at the transition to the 1RSB SG phase, the Edwards-Anderson order parameter can either grow continuously from zero or jump discontinuously to a finite value. The first case includes Potts glasses with three or four states [4], the spherical p-spin spin glass in strong magnetic field [5], and some spherical p-spin spin glasses with a mixture of $p = 2$ and $p > 3$ interactions [6,7]. The latter case includes, instead, Potts glasses with more than four states [4], quadrupolar glasses [4,8], p-spin interaction spin glasses with $p > 2$ [3,9,10], and the spherical p-spin spin glass in weak magnetic field [5]. The models belonging to this second scenario, often referred to as "discontinuous spin glasses" [11], have been widely investigated in the past because of their relevance for the structural glass transition observed in fragile glasses [10,12].

In all cases discussed so far, the transition is *always* continuous in the Ehrenfest sense. To our knowledge, the first case of a spin glass undergoing a genuine first order thermodynamic transition is the so-called Ghatak-Sherrington (GS) model [13]. However, besides the analysis of the replica symmetry (RS) solution, the study of the FRSB solution for this model could be performed only close to the continuous transition (SK-like) down to and including the tricritical point [13,14]. We also recall that an exactly solvable model, a generalization of Derrida's random energy model [3], displaying a first order phase transition to a SG phase with latent heat, was introduced by Mottishaw [15]. However, at difference with the GS model, the SG phase is now 1RSB.

Recently, a generalization of the GS model [13] has been considered in connection with the structural glass transition due to the conjectured existence [16] of a "discontinuous" transition, in the above mentioned sense, to a 1RSB SG phase. This possibility has raised new interest in such a model and its finite dimensions version has been numerically investigated in a search for evidence of a structural glass transition scenario [17].

To clarify this issue and its compatibility with previous results on the GS model, we have investigated the whole phase diagram, deep in the SG phase, for the mean-field quenched disorder variant of the Blume-Emery-Griffiths-Capel (BEGC) model [18], introduced for the λ transition in mixtures of He^3-He^4, which includes the GS model.

There exist two different versions of the model: one is the direct generalization of the BEGC model and uses spin-1 variables $\sigma_i = -1, 0, 1$ on each site i of a lattice [19,20], while the other one is a lattice gas ($n_i = 0, 1$) of spin-1/2 variables ($S_i = -1, 1$) [16,21]. In both cases, the spin variables interact through quenched random couplings. The two formulations are equivalent, at least as far as static properties are concerned. By imposing $\sigma_i \equiv S_i n_i$, the two models can be transformed one into the other, apart from a rescaling of the chemical potential/crystal field [22]. In this Letter, we use the second formulation described by the Hamiltonian [16]

$$\mathcal{H} = -\sum_{i<j} J_{ij} S_i S_j n_i n_j - \frac{K}{N}\sum_{i<j} n_i n_j - \mu \sum_i n_i, \qquad (1)$$

representing an Ising-spin glass lattice gas coupled to a

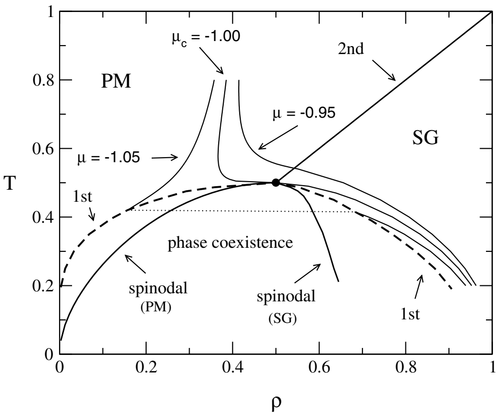

FIG. 1. $T - \rho$ phase diagram for $K = 1$. The dot marks the tricritical point $\mu_c = -1$, $T_c = 1/2$, $\rho_c = 1/2$. See text for discussion.

spin reservoir. The symmetric couplings J_{ij} are quenched Gaussian random variables of zero mean and variance $\overline{J_{ij}^2} = J^2/N$. The overline denotes average with respect to disorder. Limiting cases of the model are the SK model [2] ($\mu/J \to \infty$), the site frustrated percolation model [23] ($K = -J, J/\mu \to \infty$), and the GS model ($K = 0$). To keep the level of the presentation as general as possible, we avoid technical details and report only the main results for the phase diagrams of the three relevant cases of the GS model ($K = 0$), the frustrated Ising lattice gas ($K = -J$), and the case of attracting particle-particle interaction ($K = J$). We set $J = 1$.

Applying the standard replica method, the FRSB solution in the SG phase is described by the order parameter function [1]

$$q(x) = \int_{-\infty}^{\infty} dy P(x, y) m(x, y)^2, \tag{2}$$

and the density of occupied sites by

$$\rho = \int_{-\infty}^{\infty} dy P(1, y) \frac{\cosh \beta J y}{e^{-\Theta_1} + \cosh \beta J y}, \tag{3}$$

where $\Theta_1 \equiv (\beta J)^2 [\rho - q(1)]/2 + \beta(\mu + K\rho)$, and $m(x, y)$ and $P(x, y)$ [24] are solutions of

$$\dot{m}(x, y) = -\frac{\dot{q}}{2} m''(x, y) + \dot{\Delta}(x)\, m(x, y)\, m'(x, y), \tag{4}$$

$$\dot{P}(x, y) = \frac{\dot{q}(x)}{2} P''(x, y) + \dot{\Delta}(x)[P(x, y) m(x, y)]', \tag{5}$$

with boundary conditions $m(1, y) = \sinh(\beta y)/[e^{-\Theta_1} + \cosh(\beta y)]$, $P(0, y) = \exp\{-y^2/[2q(0)]\}/\sqrt{2\pi q(0)}$.

The functions $m(x, y)$ and $P(x, y)$ are, respectively, the local magnetization and local field probability distribution at "time scale" $x \in [0, 1]$ [24], while $\Delta(x)$ is Sompolinsky's anomaly [25]. The "dot" denotes partial derivative with respect to x while the "prime" the one with respect to y. All thermodynamic quantities can be written in terms of the above functions. Defining $\tilde{K} \equiv K + \beta J/2$, the internal energy density u and the entropy density s read

$$u = -\frac{\tilde{K}}{2}\rho^2 - \mu\rho + \frac{\beta J^2}{2} q(1)^2 + \int_0^1 dx q(x) \dot{\Delta}(x), \tag{6}$$

$$s = -\rho\Theta_1 - \frac{(\beta J)^2}{4}[\rho - q(1)]^2 + \int_{-\infty}^{\infty} dy P(1, y) \times \{\log[2 + 2e^{\Theta_1}\cosh(\beta J y)] - \beta J y m(1, y)\}. \tag{7}$$

We have solved the coupled equations (2)–(5) in Parisi's gauge $\dot{\Delta} = -\beta J x \dot{q}(x)$ using the pseudospectral method introduced in Ref. [26]. Analyzing the stability of the RS solution one gets the critical lines

$$1 - (\beta J \rho)^2 = 0, \tag{8}$$

$$1 - \beta\tilde{K}(1 - \rho)\rho = 0, \tag{9}$$

above which the only solution is the paramagnetic (PM) solution $\rho = 1/[1 + e^{-\Theta_1}]$, $q(x) \equiv 0$ for $x \in [0, 1]$, stable for any value of K. In the $T - \rho$ plane, they are,

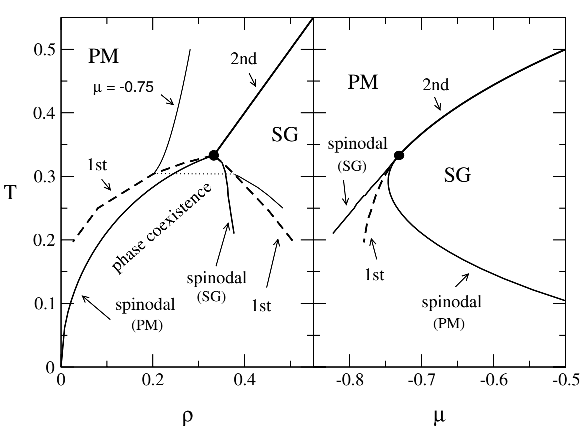

FIG. 2. $T - \rho$ and $T - \mu$ phase diagrams for $K = 0$. A line at constant $\mu = -0.75 < \mu_c$ is shown in the $T - \rho$ plane.

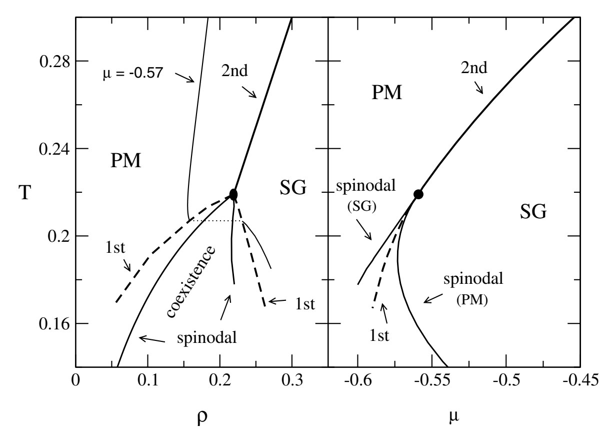

FIG. 3. $T - \rho$ and $T - \mu$ phase diagrams for $K = -1$. In the $T - \rho$ plane the line at constant $\mu = -0.57 < \mu_c$ is plotted.

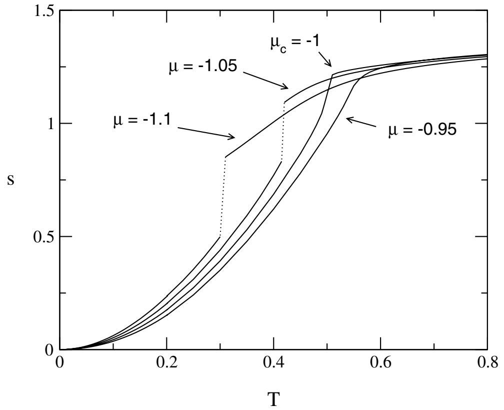

FIG. 4. Entropy density as a function of temperature for $K = 1$. For $\mu < \mu_c = -1$ the entropy is discontinuous at the transition temperature.

respectively, the straight line and the left branch of the spinodal line shown in Figs. 1–3 (for $K = 1, 0, -1$, respectively). The two lines meet at the tricritical point

$$T_c = \rho_c = \frac{-3/2 + K + \sqrt{K^2 - K + 9/4}}{2K}, \qquad (10)$$

$$\mu_c = -\frac{1}{2} - \rho_c\left[K + \log\left(\frac{1}{\rho_c} - 1\right)\right]. \qquad (11)$$

By crossing the critical line (8) above the tricritical point ($\rho > \rho_c, T > T_c, \mu > \mu_c$), the system undergoes a continuous phase transition of the SK-type to a FRSB SG phase, with a nontrivial continuous order parameter function $q(x)$ which smoothly grows from zero.

Below the tricritical point, the scenario is completely different with a transition from the PM phase to a FRSB SG phase with $q(x)$ which discontinuously jumps from zero to a nontrivial (continuous) function. At the critical temperature the entropy is discontinuous (see Fig. 4) and, hence, a latent heat is involved in the transformation, implying that the transition is of the first order in the Ehrenfest sense. The transition line is determined by the free energy balance between the PM and the SG phase [15], and it is shown as a broken line in the phase diagrams. The line (9) where the PM solution becomes unstable, and the equivalent line from the SG side, are the *spinodal* lines. This can be better appreciated in the $\mu - \rho$ plane. From Fig. 5 we indeed see that the isothermal lines cross the instability lines with zero derivative and, hence, a diverging compressibility $\kappa = (1/\rho^2)\partial\rho/\partial\mu$ occurs.

It can be shown that the first order transition line can be determined in the $\mu - \rho$ plane from the isothermal and spinodal lines by using a Maxwell construction. In the region between the first order transition line and the spinodal line, the pure phase is metastable. Below the spinodal lines (in the $T - \rho$ plane) no pure phase can

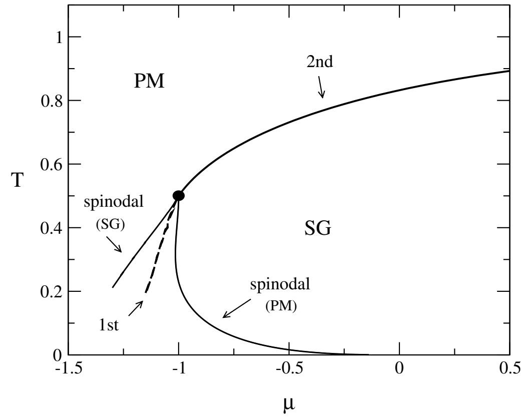

FIG. 6. $T - \mu$ phase diagram for $K = 1$.

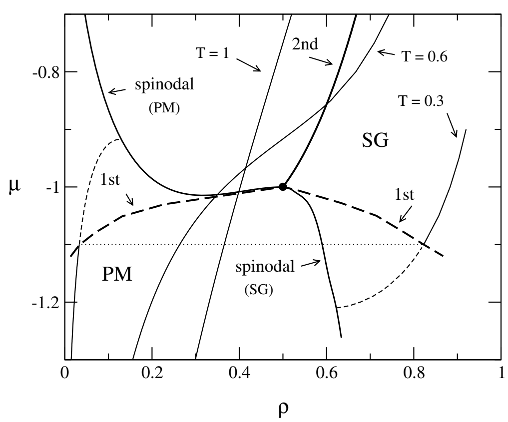

FIG. 5. $\mu - \rho$ phase diagram for $K = 1$. Three isothermal lines are plotted, two above and one below the tricritical temperature $T_c = 1/2$. For $T = 0.3$ also the metastable branches are shown, both in the RS PM phase and in the FRSB SG phase. They reach the spinodal lines with zero derivative. In this plane of conjugated thermodynamic variables, a Maxwell construction can be explicitly performed.

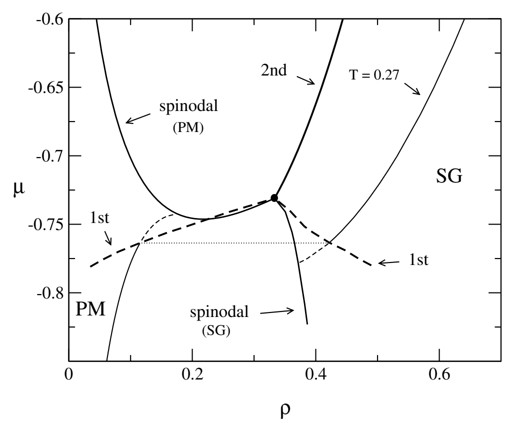

FIG. 7. $\mu - \rho$ phase diagram for $K = 0$. The dot marks the tricritical point $\mu_c = -0.731$, $T_c = \rho_c = 1/3$. The isothermal at $T = 0.27$ is plotted, together with its metastable parts (dotted line) both in the SG and in the PM phase.

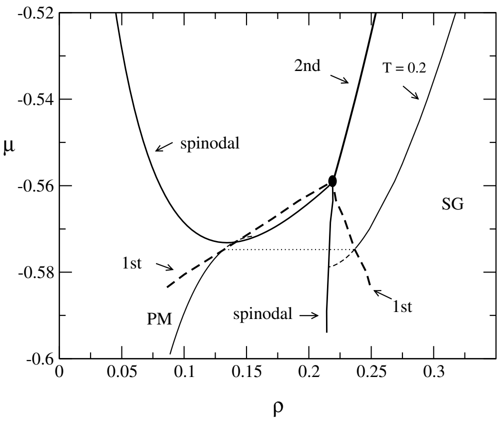

FIG. 8. $\mu - \rho$ phase diagram for $K = -1$, with isothermal at $T = 0.2$. The dot marks the tricritical point $\mu_c = -0.559$, $T_c = \rho_c = 0.219$.

exist and the system is in a mixture of PM and SG phase (*phase coexistence*). Finally, the phase diagram in the $T - \mu$ plane, for $K = 1$, is shown in Fig. 6.

By varying K the scenario remains qualitatively unchanged. The only effect of a strong repulsive particle-particle interaction is to increase the phase diagram zone where the empty system ($\rho = 0$) is the only stable solution. In order to find further phases, e.g., an antiquadrupolar phase [16], a generalization of the present analysis to a two component magnetic model [27], including quenched disorder, has to be carried out [28]. In Figs. 2, 3, 7, and 8 we show the phase diagrams for $K = 0$, the GS model [13], and $K = -1$ the frustrated lattice gas [17].

In conclusion, we have discussed the complete phase diagram of the disordered BEGC model in the mean-field limit, solving the FRSB equations in the whole SG phase with the pseudospectral method developed in Ref. [26]. Our results rule out the possibility of a 1RSB phase: the SG phase is *always* of FRSB type. The transition between the PM phase and the SG phase can be either of the SK-type or, below the tricritical temperature, a first order thermodynamic phase transition. In the latter case, as in the gas-liquid transition, a latent heat is involved in the transformation. Moreover, for a certain range of parameters (between the spinodal lines), no pure phase is achievable, not even as a metastable one, and the two phases coexist.

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