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Lattice gas analogue of the Sherrington–Kirkpatrick model: a paradigm for the glass transition

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Abstract. We investigate the connection between the well known Sherrington–Kirkpatrick Ising spin glass and the corresponding lattice gas model by analysing the relation between their thermodynamical functions. We present results of replica approach in the replica-symmetric approximation and discuss its stability as a function of temperature and external source. Then we examine the effects of first-order replica symmetry breaking at zero temperature. Finally, we compare Sherrington–Kirkpatrick results with ours and suggest in which sense the latter could be relevant to a description of the structural glass transition.

1. Introduction

It is well known [1] that the Ising model is equivalent to the lattice gas, a system defined in terms of occupation variables τ taking values 0 and 1. The lattice gas effective Hamiltonian is formally identical to the Ising one [1]. A simple change of variables ($\sigma = 2\tau - 1$) maps each of the two Hamiltonians into the other, provided that the Ising external field is related to the lattice gas chemical potential by $h - J = \frac{1}{2}\mu$. J is the Ising spin-coupling related to the lattice gas site-coupling Φ by $J = \frac{1}{4}\Phi$. This results in a simple relation between the Ising free energy density and the lattice gas pressure: $p = h - \frac{1}{2}J - f$. The two systems therefore have the same phase diagram and the same critical behaviour (real gases and Ising magnets are in the same universality class).

For random systems [2] this whole argument breaks down because the relation between chemical potential and magnetic field involves the quenched couplings. As we shall see, this results in new and unexpected features for the phase diagram of the system.

For neural networks such an inequivalence between spin (± 1) and occupation (0, 1) variables had already been pointed out and analysed, see for example [3] and references therein.

Recently much effort has been devoted to developing a description of the structural glass transition [4–6] within the framework of disordered systems. Many of these models were, however, based on Ising spin variables instead of lattice gas ones, which should be more appropriate for a condensed matter system [1]. For disordered systems the two kinds of variables are not equivalent. To obtain, in a sense, a table of correspondence it would be useful to analyse the properties of a mean-field disordered lattice gas model. This could also show us how the structural glass transition and the liquid–gas one may be described with similar tools [1].

In section 2 we present our model and in section 3 we analyse its ground state. In section 4 we discuss its relation with the Sherrington–Kirkpatrick (SK) model. Section 5 is

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devoted to writing down the saddle-point equations of the replica approach. In section 6 we analyse the low-temperature behaviour of the replica-symmetric approximation and show its *phase diagram*. A condensed version of sections 5 and 6 was originally presented in [7]. In section 7 we discuss the stability of the replica symmetry and look for the De Almeida–Thouless line of the model. Some preliminary results with broken replica symmetry are shown in section 8. Finally, in section 9 we present a comparison of our main results with those of Sherrington and Kirkpatrick and draw some tentative conclusions.

2. The Model

We consider a system of N sites. On each site k is defined an occupation variable τ_k which can take the value 0 or 1. The Hamiltonian of the system is taken to be formally identical to the SK one [9, 10]. The interaction energy between two different (k and l) occupied sites is taken to be ϕ_{kl} and the system is coupled to some external source g. The total effective Hamiltonian is therefore

$$H_\phi[\tau] = -g \sum_{k=1}^{N} \tau_k - \tfrac{1}{2} \sum_{l \neq k} \phi_{kl} \tau_k \tau_l. \tag{1}$$

In magnetic language g would be the external field, while for a lattice gas g is the sum of the chemical potential, the kinetic contribution, and a possible external force term.

The infinite-ranged interaction energies $\{\phi_{kl}\}$ are taken to be quenched independent Gaussian variables with zero mean and variance Φ^2/N. This means that the model should not have, on average, a preference between an ordering transition in two sublattices, as in binary alloys, and gas–liquid transition. For the low-temperature behaviour we could expect at least two regimes. For a strong enough negative g occupied sites should be energetically penalized and we expect, for most of the realizations of the noise, the ground-state energy to be zero and the low-temperature behaviour to be similar to that of a pure system. On the other hand, for a strong enough positive g occupied sites should be energetically favoured and we could expect the low-temperature behaviour of the system to be more similar to that of the SK model. In the following we shall take Φ as our unit of energy and set $\Phi \equiv 1$, so we have

$$P(\phi_{lk}) = \left(\frac{N}{2\pi}\right)^{1/2} \exp\left(-\frac{1}{2} N \phi_{lk}^2\right). \tag{2}$$

Each ϕ_{kl} is taken to be equally distributed and therefore each site interacts with each other. We also set the Boltzmann constant equal to 1, as a consequence T, H, g and ϕ are all dimensionless.

For a given realization of the ϕ's the partition function is

$$Z_\phi(\beta; g) = \sum_{\{\tau\}} \mathrm{e}^{-\beta H\phi[\tau]}. \tag{3}$$

For a lattice gas this would be the grand canonical partition function, because the total number of occupied sites $\sum_k \tau_k$ is not constrained to a specific value. Strictly speaking we should call 'pressure' the thermodynamic potential ($\ln Z$), while the grand canonical independent variable should be the chemical potential. In order to have a more direct comparison with the SK model, and also with other models based on spin variables, we shall however abusively refer to the thermodynamical variables as if they were the canonical ones. In the following we shall therefore call 'free energy density' the thermodynamic potential and refer to g as the 'external field'.

As usual when dealing with quenched disorder, we are interested in evaluating the averaged free energy density

$$f(\beta; g) = -\frac{1}{\beta N} \int P[\phi] \ln Z_\phi \, \mathrm{d}\phi \tag{4}$$

this will be done in the following using the replica approach [2, 8, 9].

3. Ground-state properties

We now discuss in more detail the ground-state picture which was conjectured in the previous section. First, we observe that the energy of the configuration without occupied sites is zero for all realizations of the quenched couplings. We can therefore conclude that the ground-state energy is never positive. Second, we can easily see that the configuration with all occupied sites has an average energy equal to $-gN$, which is exactly the same value obtained for the all-spins-up configuration of the SK model. Combining these two results we obtain, for the (quenched averaged) ground-state energy density, the following upper bound

$$u \leqslant -g\theta(g).$$

A lower bound can be obtained by employing the knowledge of the eigenvalues for a large Gaussian random matrix. Let us call ω_ϕ the maximum eigenvalue of the matrix $[\phi_{lk}]$. For every configuration we can write

$$\sum_{lk} \tau_l \phi_{lk} \tau_k \leqslant \omega_\phi \sum_k (\tau_k)^2.$$

In our case we have $(\tau_k)^2 = \tau_k$ and $\omega = 2$ with probability 1 in the thermodynamic limit. Combining all of this we obtain, for the Hamiltonian (1), the following bound

$$-(1+g) \sum_k \tau_k \leqslant H_\phi[\tau].$$

Taking the minimum of both sides we finally obtain

$$-(1+g)\theta(g+1) \leqslant u.$$

We thus see that for $g \leqslant -1$ the upper and lower bounds saturate and $u = 0$ with probability 1 in the thermodynamic limit. The ground-state configuration is that with no occupied sites. Each configuration with a finite number of occupied sites has the same average energy density in the thermodynamic limit. We therefore conclude that the low-temperature behaviour of the system should be very similar to that of a pure one.

On the other hand, for a positive g we have $u \leqslant -g$, bound which is saturated in the limit $g \to \infty$. This implies that our system has a (first order?) zero-temperature transition at some g_0 between -1 and 0. We also speculate that for a large enough positive g the low-temperature behaviour of the system should approximate that of the SK model. We note that in the SK case repeating the previous arguments we would obtain $-1-|h| \leqslant u \leqslant -|h|$.

The lower limit for g_0 can be improved using Derrida's argument [11]. Let us define $\Sigma(g, N)$ the average number of configurations with negative energy for a system with N sites

$$\Sigma(g, N) = \int P[\phi] \sum_\tau \theta(-H_\phi[\tau]) \, \mathrm{d}\phi.$$

For a negative g we obtain, in the thermodynamic limit,

$$\sigma \equiv \lim_{N\to\infty} \frac{1}{N} \ln \Sigma(g, N) = \ln 2 - g^2.$$

If $g < -\sqrt{\ln 2}$ we see that $\sigma < 0$ and therefore $\Sigma(g, N) \to 0$ in the thermodynamic limit. Following Derrida [11] we can conclude that for $g < -\sqrt{\ln 2} = -0.8326$ there are almost surely no configurations of negative energy in the thermodynamic limit. Since there is always at least a configuration of zero energy, this must be the ground-state energy. We thus obtain the lower bound $g_0 \geqslant -\sqrt{\ln 2} = -0.8326$ for the transition field at zero temperature.

4. Relation with the Sherrington–Kirkpatrick model

Before proceeding further in our analysis we wish to discuss the connections between the SK model [9] and the previously introduced one. We assume, as for the corresponding homogeneous models [1], that site variables are related by

$$\sigma = 2\tau - 1 \Longleftrightarrow \tau = \tfrac{1}{2}(\sigma + 1). \tag{5}$$

Substituting (5) into the Hamiltonian (1) we obtain

$$-H_\phi \left[\frac{\sigma + 1}{2}\right] = \frac{1}{2} \sum_k \left(g + \frac{1}{4}\Phi_k\right) + \sum_k \left(\frac{1}{2}g + \frac{1}{4}\Phi_k\right) \sigma_k + \frac{1}{8} \sum_{k\neq l} \phi_{kl}\sigma_l\sigma_k \tag{6}$$

where

$$\Phi_k = \sum_l^{l\neq k} \phi_{kl}.$$

We stress that (6) connects a homogeneous (site-independent) field system to a local-field one. In fact, defining a SK effective Hamiltonian with a site-dependent magnetic field

$$H_{J,h}^{(\mathrm{SK})}[\sigma] = -\sum_k h_k\sigma_k - \tfrac{1}{2} \sum_{k\neq l} J_{kl}\sigma_l\sigma_k \tag{7}$$

we can write

$$H_\phi \left[\frac{\sigma + 1}{2}\right] = -\frac{1}{2} \sum \left(g + \frac{1}{4}\Phi_k\right) + \frac{1}{4} H_{\phi,h[\phi]}^{(\mathrm{SK})}[\sigma] \tag{8}$$

and the local magnetic field is correlated to the couplings by

$$h_k[\phi] = 2g + \Phi_k. \tag{9}$$

The change of variables (5) maps our Hamiltonian (1) into a SK-like one, but correlation given by (9) is enough to destroy their equivalence. In fact, summing over configuration, we get for the partition functions

$$Z_\phi(\beta; g) = \exp\left[\frac{1}{2}\beta \sum_k \left(g + \frac{1}{4}\Phi_k\right)\right] Z_\phi^{(\mathrm{SK})}\left(\frac{\beta}{4}; h[\phi]\right] \tag{10}$$

and thus the relation between the free energy densities of the two models leads to

$$f(\beta; g) = -\frac{1}{2}g + \frac{1}{4} \int f_\phi^{(\mathrm{SK})}\left(\frac{\beta}{4}; h[\phi]\right] P[\phi]\,\mathrm{d}\phi. \tag{11}$$

Our system is therefore equivalent to a SK-like one in which the magnetic field is a local random variable correlated with the couplings. The SK averaged free energy is not directly related to ours. Relation (5) is thus not useful in investigating thermodynamics of our model that is not reducible to something known, we have to face it by itself.

5. The replica-symmetric solution

Let us now proceed in applying replica formalism [2] to our system; we have to calculate the averaged nth power of the partition function

$$Z_n = \overline{(Z_\phi)^n} = \int (Z_\phi)^n P[\phi]\,\mathrm{d}\phi. \tag{12}$$

For integer n we get, after performing a Gaussian integration

$$Z_n = \sum_{\{\tau\}} \exp\left[\sum_k \beta g \sum_a \tau_k^a + \frac{\beta^2}{2N}\sum_{k<l}\left(\sum_a \tau_l^a \tau_k^a\right)^2\right].$$

Using the identity

$$2\sum_{k<l}\left(\sum_a \tau_l^a\tau_k^a\right)^2 = \sum_{a,b}\left(\sum_k \tau_k^a\tau_k^b\right)^2 - \sum_k\sum_{a,b}\tau_k^a\tau_k^b \tag{13}$$

which follows from the relation $\tau^2 = \tau$, we can reorder the exponent and obtain

$$Z_n = \sum_{\{\tau\}} \exp\left[\beta\sum_k\left(g\sum_a \tau_k^a - \frac{\beta}{4N}\sum_{a,b}\tau_k^a\tau_k^b\right)\right]\prod_{a,b}\exp\left[\frac{4}{N\beta^2}\left(\frac{\beta^2}{4}\sum_k \tau_k^a\tau_k^b\right)^2\right]. \tag{14}$$

Using Gaussian identities we rewrite (14) as

$$\begin{aligned}Z_n = \sum_{\{\tau\}} \exp&\left[\beta\sum_k\left(g\sum_a \tau_k^a - \frac{\beta}{4N}\sum_{a,b}\tau_k^a\tau_k^b\right)\right]\\ &\times\prod_{a,b}\int\left(\frac{N\beta^2}{4\pi}\right)^{1/2}\exp\left(-\frac{N}{4}\beta^2 Q_{ab}^2 + \frac{1}{2}\beta^2\sum_k Q_{ab}\tau_k^a\tau_k^b\right)\mathrm{d}Q_{ab}.\end{aligned} \tag{15}$$

Reordering the exponentials and defining

$$H_Q[\tau] = -\frac{1}{2}\beta^2\sum_{a,b}\left(Q_{a,b} - \frac{1}{2N}\right)\tau^a\tau^b - \beta g\sum_a \tau^a \tag{16}$$

$$A[Q] = \frac{\beta^2}{4}\sum_{a,b} Q_{ab}^2 - \ln\left[\sum_{\{\tau\}} \mathrm{e}^{-H_Q[\tau]}\right] \tag{17}$$

we finally obtain

$$Z_n(\beta; g) = \left(\frac{N\beta^2}{4\pi}\right)^{n^2/2}\int \mathrm{e}^{-NA[Q]}\,\mathrm{d}^{n^2}Q. \tag{18}$$

The averaged free energy density is given by

$$f(\beta; g) = \lim_{N\to\infty}\lim_{n\to 0} -\frac{1}{\beta n N}\ln Z_n(\beta; g). \tag{19}$$

In the thermodynamic limit the integral can be estimated by maximizing the integrand, and this yields

$$f_n(\beta; g) = \lim_{N\to\infty} -\frac{1}{\beta n N}\ln Z_n(\beta; g) = \frac{1}{\beta n}\inf_Q\{A[Q]\}. \tag{20}$$

The extremum is determined by the saddle-point equation

$$\frac{\partial A}{\partial Q_{ab}} = \frac{\beta^2}{2}Q_{ab} - \frac{\beta^2}{2}\frac{\sum_\tau \tau^a\tau^b\mathrm{e}^{-H_Q[\tau]}}{\sum_\tau \mathrm{e}^{-H_Q[\tau]}} = 0 \tag{21}$$

which may be rewritten as $Q_{ab} = \langle \tau^a \tau^b \rangle_Q$.

We first consider saddle points that are symmetric under the replica group [2]. Setting $Q_{ab} = q + b\delta_{ab}$ we can write $\sum_{ab} Q_{ab}\tau^a\tau^b = q(\sum_a \tau^a)^2 + b\sum_a \tau_a$ and $\sum_{ab} Q_{ab}^2 = n(q+b)^2 + n(n-1)q^2$. Substitution into (17) and extraction of the $n \to 0$ limit then yields

$$f = \tfrac{1}{4}\beta b(2q+b) - (2\pi\beta^2)^{-1/2}\int_{-\infty}^{\infty} \ln[1 + \mathrm{e}^{\beta(\alpha + z\sqrt{q})}]\mathrm{e}^{-\frac{1}{2}z^2}\,\mathrm{d}z. \tag{22}$$

In equation (22) we set $\alpha = g + \frac{1}{2}\beta b$, and the matrix elements satisfy the coupled equations

$$\begin{aligned} \rho \equiv q + b &= (2\pi)^{-1/2}\int [1 + \mathrm{e}^{-\beta(\alpha+z\sqrt{q})}]^{-1}\mathrm{e}^{-\frac{1}{2}z^2}\,\mathrm{d}z \\ q &= (2\pi)^{-1/2}\int [1 + \mathrm{e}^{-\beta(\alpha+z\sqrt{q})}]^{-2}\mathrm{e}^{-\frac{1}{2}z^2}\,\mathrm{d}z. \end{aligned} \tag{23}$$

As can be seen following the line of [9, 10] the physical significance of ρ and q is

$$\rho = \overline{\langle\tau\rangle} \qquad q = \overline{\langle\tau\rangle^2} \tag{24}$$

where, following the notations of [2], a bar denotes the average over quenched disorder.

For $\beta = 0$ we have $\rho = \frac{1}{2}$ and $q = \frac{1}{4}$, as we expect from their physical significance. In the high-temperature regime we can solve (23) by expansion in powers of β, and this yields

$$\begin{aligned} \rho &= \tfrac{1}{2} + \tfrac{1}{4}\beta g + \tfrac{1}{32}\beta^2 \\ q &= \tfrac{1}{4} + \tfrac{1}{4}\beta g + \tfrac{1}{16}(\tfrac{3}{4} + g^2)\beta^2. \end{aligned}$$

6. Low-temperature results

At zero temperature we can perform a detailed analytic study of the saddle-point equations. In this limit equation (23) leads to

$$\begin{aligned} q &= (2\pi)^{-1/2}\int_{-\infty}^{\alpha/\sqrt{q}} \mathrm{e}^{-\frac{1}{2}z^2}\,\mathrm{d}z \equiv \mathrm{erf}\left(\frac{\alpha}{\sqrt{q}}\right) \\ \gamma_0 &\equiv \lim_{T\to 0}\beta(\rho - q) = (2\pi q)^{-1/2}\mathrm{e}^{-\alpha^2/2q}. \end{aligned} \tag{25}$$

The equation for ρ is the same as that for q, indeed for $T \to 0$ we have $\rho = q + \gamma T$ and thus $\alpha = g + \frac{1}{2}\gamma_0$.

For $g < 0$ there always is a solution of (25) with $q = 0$, $\gamma_0 = 0$ and $\alpha \equiv g$. To look for solutions with $q \neq 0$ let us define $x \equiv \mathrm{erf}^{-1}(q) = \alpha/\sqrt{q}$, then we obtain

$$\begin{aligned} \rho &= q = \mathrm{erf}(x) \\ \alpha &= x\sqrt{\mathrm{erf}(x)} \\ \gamma_0 &= [2\pi\,\mathrm{erf}(x)]^{-1/2}\mathrm{e}^{-\frac{1}{2}x^2} \\ g &= \alpha - \tfrac{1}{2}\gamma_0 = x\sqrt{\mathrm{erf}(x)} - \tfrac{1}{2}[2\pi\,\mathrm{erf}(x)]^{-1/2}\mathrm{e}^{-1/2x^2} \end{aligned} \tag{26}$$

we can therefore express all relevant quantities as functions of parameter x. From the last of (26) (see figure 1) we can see that each value of g in the range $-0.702\,42 < g < 0$ corresponds to two values of x, both lower than 0.308 59. Summarizing, if $g < -0.702\,42$ or $g > 0$ we have a single solution of (25) for each value of g, but if $-0.702\,42 < g < 0$ we have three solutions, and in order to pick out the physical one we have to impose the continuity of the free energy density as a function of external field (see figure 2). We thus

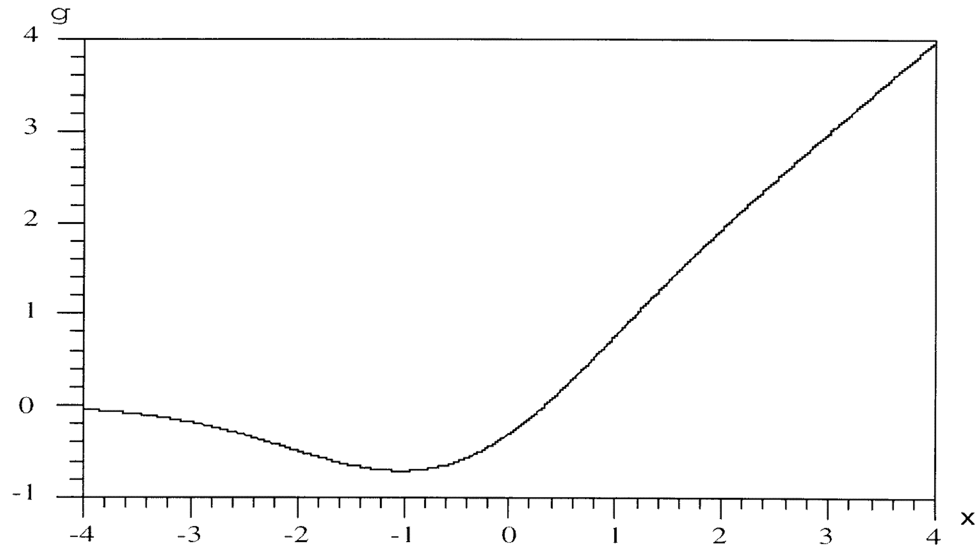

Figure 1. External field g versus parameter x ($x \equiv \mathrm{erf}^{-1}(q)$) as results from the last equation of (26).

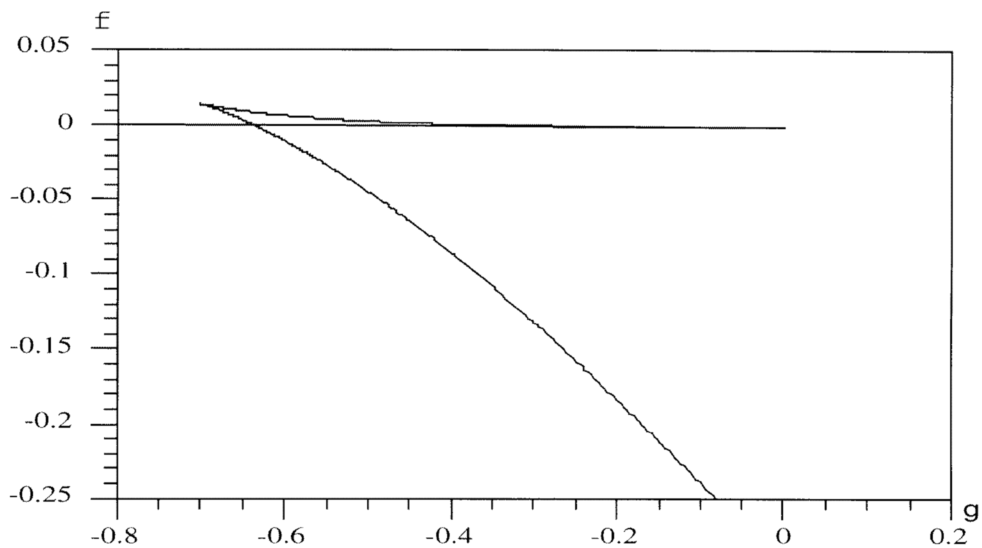

Figure 2. Free energy density versus external field, at zero temperature, in the replica-symmetric solution. The transition point is where the two lower branches cross each other. The higher branch is an unstable solution.

find a *first-order phase transition* in the point $g_0 = -0.636\,33$ where the two lower branches of f cross each other. The transition point is determined by the condition $\gamma_0(g_0) = -g_0$. In figure 3 we show ρ $(= q)$ as a function of external field. As expected it is discontinuous on the transition point.

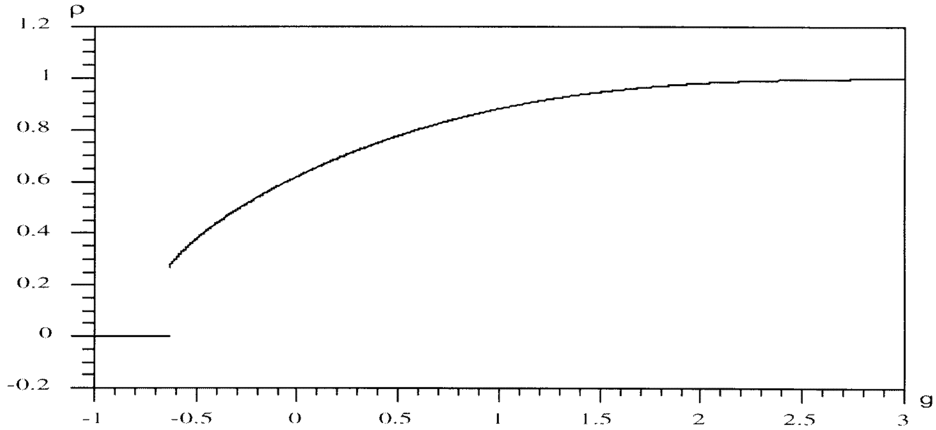

Figure 3. Replica symmetric order parameter ρ $(= q)$ at $T = 0$ as a function of external field.

Next we look at the thermodynamical functions, the internal energy and entropy densities are given by

$$
\begin{aligned}
u &= -(g + \gamma_0)\rho \\
s &= -\tfrac{1}{4}\gamma_0^2 .
\end{aligned}
\tag{27}
$$

The entropy (27) is negative in the range $g > g_0$, where γ_0 is different from zero, so we should expect the replica symmetry to be broken in this region. We stress that, in contrast to the SK case, we have a region in which the replica-symmetric solution remains physical down to zero-temperature. The maximum absolute value of the zero-temperature entropy is at $g = g_0^+$, where it takes the value 0.101, and it strongly decreases for higher values of g (e.g. $s = -0.011$ at $g = 1$).

For $\beta \gg 1$ the solution of (23) can behave in two different ways. In the range $g < g_0$, where q_0 $(\equiv q(T; g)|_{T=0})$ and $\gamma_0(g)$ are identically zero, we find that all their temperature derivatives vanish for $T \to 0$, q vanishes as $\mathrm{e}^{\beta g}$ $(g < 0)$ and γ $(\equiv \beta(\rho - q))$ as $\beta \mathrm{e}^{\beta g}$. Otherwise if $g > g_0$, they depend linearly on T, indeed we obtain

$$
\begin{aligned}
q &= q_0 - \frac{q_0\gamma_0(q_0 + \frac{1}{2}\gamma_0\alpha_0)}{(q_0 + \frac{1}{2}\gamma_0\alpha_0)^2 + \frac{1}{4}\gamma_0(q_0 - \alpha_0^2)} T \\
\gamma &= \gamma_0 + \frac{\frac{1}{2}\gamma_0^2(q_0 - \alpha_0^2)}{(q_0 + \frac{1}{2}\gamma_0\alpha_0)^2 + \frac{1}{4}\gamma_0(q_0 - \alpha_0^2)} T \\
\rho &= q + \gamma T .
\end{aligned}
$$

We have also numerically solved (by iteration) equations (23) for several values of T and g, the results of which are plotted in figure 4. We find a line of first-order phase transitions. Such a line ends in a second-order transition point for $T \simeq 0.22$ and $g \simeq -0.7$, as attested by figure 5 where the linear response function $\chi = \partial\rho/\partial g$ (the 'susceptibility') is plotted versus temperature for $g = -0.7$. The line of first-order transitions is the full curve plotted in the phase diagram of figure 6.

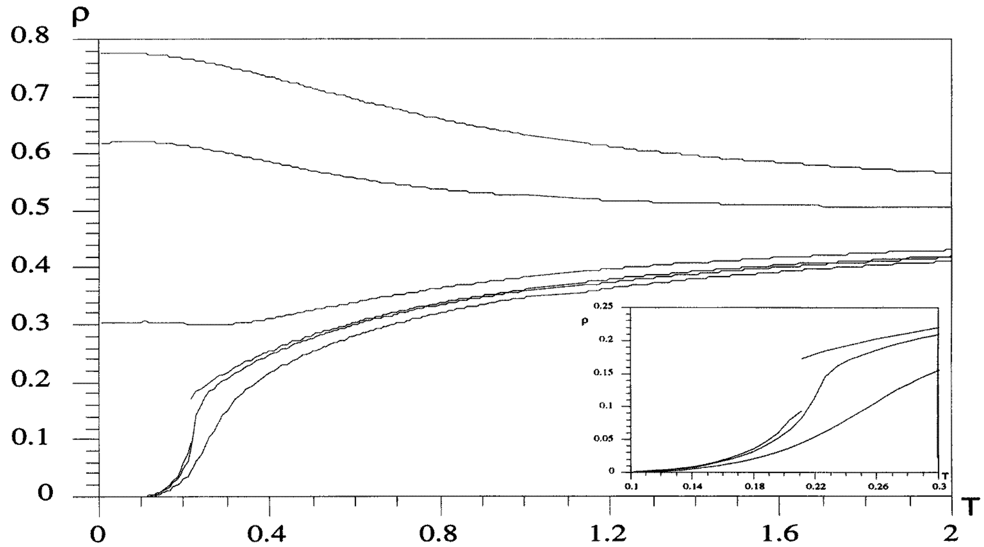

Figure 4. Replica symmetric order parameter ρ as a function of temperature for several values of external field. From top to bottom the values of g are 0.5, 0, −0.6, −0.68, −0.7 and −0.75. The embedded picture represents a magnification of the region around the transition.

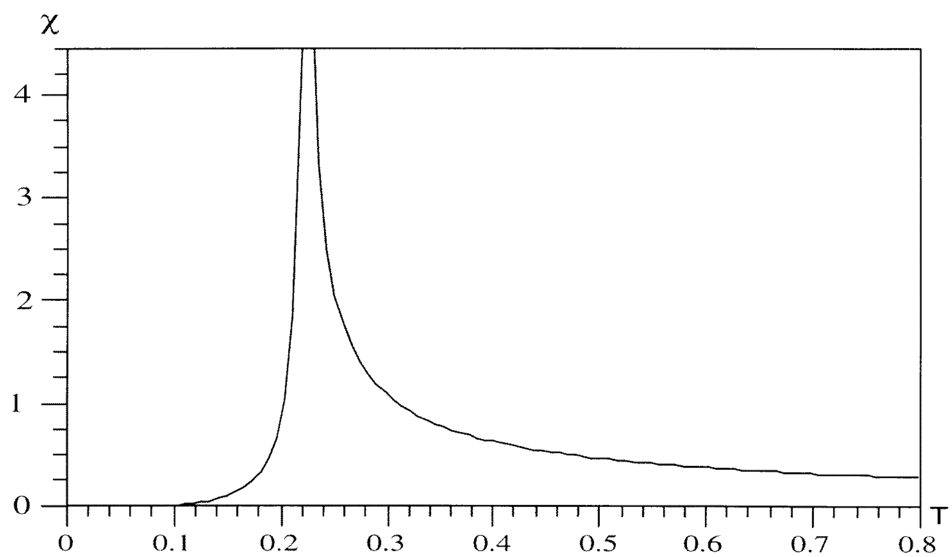

Figure 5. Linear response function $\chi = \partial\rho/\partial g$ ('susceptibility') as a function of temperature for $g = -0.7$.

7. Study of stability

As we pointed out in the previous section, the replica-symmetric ansatz for the saddle-point equations (21) can lead to unphysical results at low temperature. This should be considered as a signal [2] of replica symmetry breaking. To check this conjecture we have to calculate the eigenvalues of the Hessian of (17), this will be done in this section following the lines

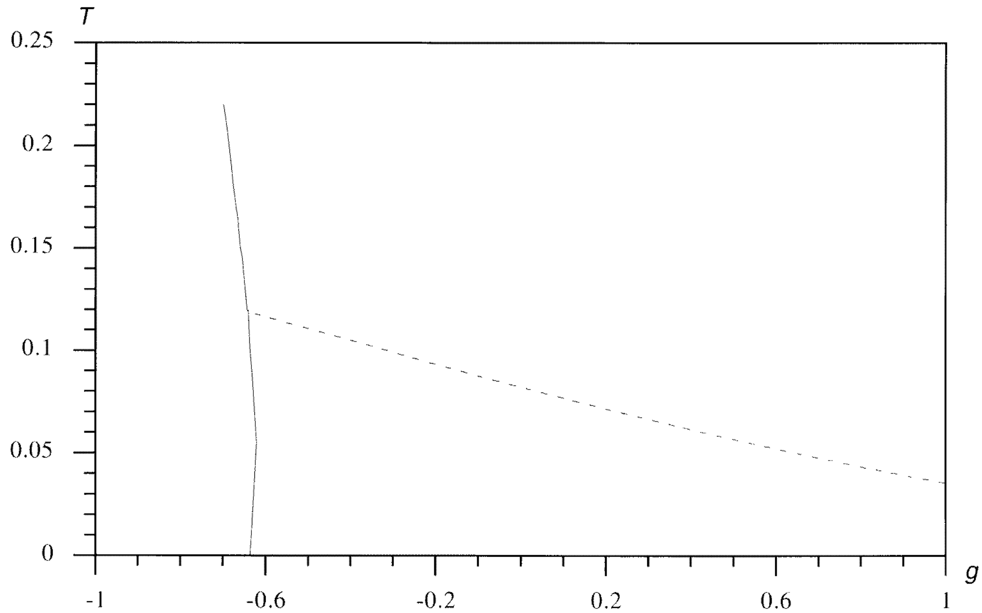

Figure 6. Phase diagram for the replica-symmetric solution in the $(g; T)$ plane. The full curve is a line of first-order phase transitions which ends in a second-order transition point. The broken curve is the stability boundary of the replica-symmetric solution. The region under the instability line is the glassy phase.

of [12] but with two main differences. The first refers to the fact that we have $\overline{\phi} = 0$ but the diagonal part of the matrix Q_{ab} is different from zero and plays the same role as the magnetization 'vector' of [9, 10, 12] where $\overline{J} = J_0 \neq 0$. The second difference is that we never impose *a priori* Q_{ab} to be a symmetric matrix. Actually the only term in $A[Q]$ depending on the antisymmetric part of Q_{ab} is $\mathrm{tr}Q^2$, its contribution could be integrated out and has no physical significance but allowing for its presence permits a more compact and elegant notation. We can indeed treat the diagonal and the off-diagonal parts of Q_{ab} in the same way. However, we shall see that the saddle point is (as it should be) always a symmetric matrix and stable against antisymmetric perturbation.

The Hessian of $A[Q]$ is

$$H_{ab}^{cd} = \frac{\partial^2 A}{\partial Q_{ab} \partial Q_{cd}} = \frac{1}{2}\beta^2 \delta_{ac}\delta_{bd} + \Gamma_{ab}^{cd}$$

where we have set

$$\Gamma_{ab}^{cd} = \tfrac{1}{4}\beta^4[\langle \tau^a \tau^b \rangle_Q \langle \tau^c \tau^d \rangle_Q - \langle \tau^a \tau^b \tau^c \tau^d \rangle_Q]$$

and the elements of Γ have the following symmetries

$$\Gamma_{ab}^{cd} = \Gamma_{ba}^{cd} = \Gamma_{ab}^{dc} = \Gamma_{cd}^{ab}.$$

Remembering that $\tau^2 = \tau$, and substituting the replica-symmetric ansatz for the saddle point, we have the following different matrix elements for Γ

$$\Gamma_{aa}^{aa} = \tfrac{1}{4}\beta^4[\langle \tau^a \rangle_Q^2 - \langle \tau^a \rangle_Q] = \tfrac{1}{4}\beta^4(\rho^2 - \rho)$$

$$\Gamma_{aa}^{cc} = \tfrac{1}{4}\beta^4[\langle \tau^a \rangle_Q \langle \tau^c \rangle_Q - \langle \tau^a \tau^c \rangle_Q] = \tfrac{1}{4}\beta^4(\rho^2 - q)$$

$$\Gamma_{ab}^{aa} = \tfrac{1}{4}\beta^4[\langle \tau^a \tau^b \rangle_Q \langle \tau^a \rangle_Q - \langle \tau^a \tau^b \rangle_Q] = \tfrac{1}{4}\beta^4(q\rho - q)$$

$$\Gamma_{ab}^{cc} = \tfrac{1}{4}\beta^4[\langle\tau^a\tau^b\rangle_Q\langle\tau^c\rangle_Q - \langle\tau^a\tau^b\tau^c\rangle_Q] = \tfrac{1}{4}\beta^4(q\rho - \rho_3)$$
$$\Gamma_{ab}^{ab} = \tfrac{1}{4}\beta^4[\langle\tau^a\tau^b\rangle_Q^2 - \langle\tau^a\tau^b\rangle_Q] = \tfrac{1}{4}\beta^4(q^2 - q)$$
$$\Gamma_{ab}^{ad} = \tfrac{1}{4}\beta^4[\langle\tau^a\tau^b\rangle_Q\langle\tau^a\tau^d\rangle_Q - \langle\tau^a\tau^b\tau^d\rangle_Q] = \tfrac{1}{4}\beta^4(q^2 - \rho_3)$$
$$\Gamma_{ab}^{cd} = \tfrac{1}{4}\beta^4[\langle\tau^a\tau^b\rangle_Q\langle\tau^c\tau^d\rangle_Q - \langle\tau^a\tau^b\tau^c\tau^d\rangle_Q] = \tfrac{1}{4}\beta^4(q^2 - \rho_4)$$

where explicitly written replica labels are different. In the $n \to 0$ limit, the required expectation values are

$$\langle\tau^a\rangle_{Q^*} = Q^*_{aa} = \rho$$
$$\langle\tau^a\tau^b\rangle_{Q^*} = Q^*_{ab} = q$$
$$\langle\tau^a\tau^b\tau^c\rangle_{Q^*} \equiv \rho_3 = (2\pi)^{-1/2}\int [1 + \mathrm{e}^{-\beta(\alpha+z\sqrt{q})}]^{-3}\mathrm{e}^{-\frac{1}{2}z^2}\,\mathrm{d}z$$
$$\langle\tau^a\tau^b\tau^c\tau^d\rangle_{Q^*} \equiv \rho_4 = (2\pi)^{-1/2}\int [1 + \mathrm{e}^{-\beta(\alpha+z\sqrt{q})}]^{-4}\mathrm{e}^{-\frac{1}{2}z^2}\,\mathrm{d}z.$$

The eigenvalues equation for the Hessian H_{ab}^{cd}

$$\sum_{c,d} H_{ab}^{cd}\eta_{cd} = \lambda\eta_{ab} \tag{28}$$

has, for general n, four classes of eigenvectors with no more than six distinct eigenvalues. Antisymmetric eigenvectors ($\eta_{ba} = -\eta_{ab}$) give the eigenvalue $\lambda_0 = \frac{1}{2}\beta^2$ which (as we should expect) is always positive. Eigenvectors that are symmetric matrices, and invariant under the replica group, give two eigenvalues that, in the $n \to 0$ limit, are

$$\lambda_{1,2} = \tfrac{1}{2}\beta^2 + \tfrac{1}{8}\beta^4(8\rho_3 - 6\rho_4 - q - \rho) \pm \tfrac{1}{8}\beta^4\sqrt{(8\rho_3 - 6\rho_4 - 3q + \rho)^2 - 16(\rho_3 - q)^2}. \tag{29}$$

Symmetric eigenvectors ($\eta_{ba} = \eta_{ab}$) that are invariant under interchange of all but one of the replicas give, for general n, two more eigenvalues $\lambda_{3,4}$ that for $n \to 0$ reduce to the previous ones. There are finally symmetric eigenvectors that are invariant under interchange of all but two replicas. For $n \to 0$ these give rise to the eigenvalue

$$\lambda_5 = \tfrac{1}{2}\beta^2[1 + \beta^2(2\rho_3 - \rho_4 - q)]. \tag{30}$$

In the high-temperature regime the eigenvalues λ_1 and λ_2 are found to be, despite the hermiticity of the Hessian matrix, complex conjugate. This should not be too surprising because we are working in a space where the norm is not positive definite ($\lim_{n\to 0}\frac{1}{n}\mathrm{tr}Q^2 = \rho^2 - q^2$). However, as could be seen by considering the Gaussian approximation to the integral in (18), we believe that the stability of the solution is determined by their (common) real part, which is always positive. At lower temperatures these eigenvalues are real and never negative, they are found to vanish linearly on the second-order transition point. This means that this saddle point is stable against *replica-symmetric* perturbation.

The eigenvalues λ_0 λ_3 and λ_4 are not relevant and thus the stability of this solution against replica symmetry breaking perturbations is determined by the eigenvalue λ_5. This eigenvalue is always real, to study its sign it is useful to define $\Lambda_5 = 2T^3\lambda_5$, so we obtain

$$\Lambda_5 = T - \frac{1}{8}(2\pi q)^{-\frac{1}{2}}\int \frac{\mathrm{e}^{-\frac{(\alpha+2Tu)^2}{2q}}}{\cosh^4 u}\,\mathrm{d}u. \tag{31}$$

The low-temperature limit then follows in a straightforward way, and we find

$$\lim_{T\to 0}\Lambda_5 = -\tfrac{1}{6}(2\pi q)^{-1/2}\mathrm{e}^{-\frac{\alpha^2}{2q}} = -\tfrac{1}{6}\gamma_0.$$

It is therefore apparent that, if $g \geqslant g_0$, λ_5 must become negative at low enough temperatures. The *replica-symmetric* saddle point is unstable and the replica symmetry is *spontaneously broken*. The line of instability, obtained by numerical evaluation, is the broken curve shown in figure 6 we stress the presence of a region in which the replica symmetry remains *exact* down to zero temperature.

8. Zero-temperature results with first-order replica symmetry breaking

Once stated that the replica symmetry can be broken, we looked for saddle points that are not invariant under the replica group. As a first step we analysed the zero-temperature behaviour of the solution given by the ansatz proposed in [13, 14]. We divide the n replicas in $\nu \equiv n/m$ groups, each of m replicas, and we take the matrix elements of Q as follows

$$\begin{aligned} &Q_{ab} = \rho = q + d + b \qquad \text{if } a = b \\ &Q_{ab} = q_1 = q + d \qquad \text{if } a \neq b \qquad \text{but } I(a/m) = I(b/m) \\ &Q_{ab} = q_0 \equiv q \qquad \text{if } I(a/m) \neq I(b/m) \end{aligned} \tag{32}$$

where I is the function introduced in [13], $I(x) = \min\{n \in N : n \geqslant x\}$. With this position we have $\mathrm{tr}Q^2 = n[\rho^2 + (m-1)q_1^2 + (n-m)q_0^2]$, and the effective Hamiltonian (16) reads

$$H_Q[\tau] = -\beta\alpha \sum_{a=1}^{n} \tau^a - \tfrac{1}{2}\beta^2 q_0 \left(\sum_{a=1}^{n} \tau^a \right)^2 - \tfrac{1}{2}\beta^2 d \sum_{l=1}^{\nu} \left(\sum_{k(a)=l} \tau^a \right)^2 \tag{33}$$

where $k(a) = I(a/m)$ and as previously we set $\alpha = g + \frac{1}{2}\beta b$.

Using standard properties of Gaussian integrals, and setting $g_\sigma(x) = (2\pi\sigma)^{-1/2} \mathrm{e}^{-x^2/2\sigma}$, we find in the $n \to 0$ limit

$$f = \frac{1}{4}\beta[\rho^2 + (m-1)q_1^2 - mq_0^2] - \frac{1}{\beta m} \int g_{q_0}(z) \ln[I_m(\alpha + z; d)]\, \mathrm{d}z \tag{34}$$

where

$$I_m(x; d) = \int [1 + \mathrm{e}^{\beta(x+y)}]^m g_d(y)\, \mathrm{d}y. \tag{35}$$

Substituting the ansatz (32) into the saddle-point equations (21) we find, in the $n \to 0$ limit, the following equations for ρ, q_1 and q_0

$$\begin{aligned} \rho &= \int g_{q_0}(z - \alpha) \frac{\int [1 + \mathrm{e}^{\beta(z+y)}]^{m-1} \mathrm{e}^{\beta(z+y)} g_d(y)\, \mathrm{d}y}{I_m(z; d)}\, \mathrm{d}z \\ q_1 &= \int g_{q_0}(z - \alpha) \frac{\int [1 + \mathrm{e}^{\beta(z+y)}]^{m-2} \mathrm{e}^{2\beta(z+y)} g_d(y)\, \mathrm{d}y}{I_m(z; d)}\, \mathrm{d}z \\ q_0 &= \int g_{q_0}(z - \alpha) \left[\frac{\int [1 + \mathrm{e}^{\beta(z+y)}]^{m-1} \mathrm{e}^{\beta(z+y)} g_d(y)\, \mathrm{d}y}{I_m(z; d)} \right]^2 \mathrm{d}z. \end{aligned} \tag{36}$$

To determine if the correct saddle point has to be a maximum or minimum of equation (34) we note that $\lim_{n\to 0} \frac{1}{n}\mathrm{tr}Q^2 = \rho^2 - (1-m)q_1^2 - mq_0^2$. Therefore, for $0 \leqslant m \leqslant 1$, we should expect the saddle point to be a minimum with respect to ρ (diagonal parameter) and a maximum with respect to q_1 and q_0 (off-diagonal parameters). Because m is also a parameter for the off-diagonal part of Q_{ab} we speculate that f should be maximized with respect to it [2].

In order to work out the $T \to 0$ limit of equation (36) let us consider the internal energy density

$$u = -g\rho - \tfrac{1}{2}\beta b(\rho + q_1) - \tfrac{1}{2}\beta m d(q_0 + q_1).$$

To keep u finite as $\beta \to \infty$ we set $b = \gamma T$ and $m = \mu T$, and we expect that γ and μ remain finite as $T \to 0$. Indeed in this limit equation (36) leads to

$$\begin{aligned}
\gamma &= \int \frac{g_d(z) g_{q_0}(\alpha + z)}{\operatorname{erf}\left(\frac{z}{\sqrt{d}}\right) + \mathrm{e}^{-\mu(z-\frac{1}{2}\mu d)} \operatorname{erf}\left(\frac{\mu d - z}{\sqrt{d}}\right)} \,\mathrm{d}z \\
\rho \equiv q + d &= \int \frac{\mathrm{e}^{-\mu(z-\frac{1}{2}\mu d)} \operatorname{erf}\left(\frac{\mu d - z}{\sqrt{d}}\right)}{\operatorname{erf}\left(\frac{z}{\sqrt{d}}\right) + \mathrm{e}^{-\mu(z-\frac{1}{2}\mu d)} \operatorname{erf}\left(\frac{\mu d - z}{\sqrt{d}}\right)} g_{q_0}(\alpha + z) \,\mathrm{d}z \\
q &= \int \left[\frac{\mathrm{e}^{-\mu(z-\frac{1}{2}\mu d)} \operatorname{erf}\left(\frac{\mu d - z}{\sqrt{d}}\right)}{\operatorname{erf}\left(\frac{z}{\sqrt{d}}\right) + \mathrm{e}^{-\mu(z-\frac{1}{2}\mu d)} \operatorname{erf}\left(\frac{\mu d - z}{\sqrt{d}}\right)} \right]^2 g_{q_0}(\alpha + z) \,\mathrm{d}z.
\end{aligned} \tag{37}$$

In the same limit the free energy density (34) then becomes

$$f = \frac{1}{4} \left[2\gamma(q + d) + \mu d(2q + d) \right] - \frac{1}{\mu} \int g_q(\alpha + z) \ln\left[I_m(-z; d) \right] \mathrm{d}z \tag{38}$$

where

$$\lim_{T \to 0} I_m(-z; d) = \operatorname{erf}\left(\frac{z}{\sqrt{d}} \right) + \mathrm{e}^{-\mu(z-\frac{1}{2}\mu d)} \operatorname{erf}\left(\frac{\mu d - z}{\sqrt{d}} \right). \tag{39}$$

Equations (37) have been numerically solved by iteration with μ held fixed, next the resulting free energy (38) has been maximized with respect to μ using a standard IMSL† routine. Such a numerical solution of the saddle-point problem gives the results plotted in figures 7–9 as functions of g. We note that the transition point is shifted from $g_0 = -0.636\,33$ to $g_0 \simeq -0.6250$ and the discontinuity of q (0.27) is split in 0.28 for ρ and 0.22 for q_0. We also note that the values of γ are about a factor of 4 smaller than those obtained in the replica-symmetric approximation.

9. Discussion, conclusions and outlook

In this paper we have investigated the thermodynamical properties of a lattice gas model with infinite-ranged random interactions. We have discussed its relation with the SK model and showed that the *averaged thermodynamical functions* of the two systems are not directly related to each other.

In the SK case, the zero-field Hamiltonian has a *global Z_2 symmetry* and all relevant thermodynamical functions are either even or odd in the external field. The SK model can have a first-order phase transition, as a function of magnetic field, only if a strong enough ferromagnetic part (i.e. a non-zero mean) is added to the random coupling. Such a transition is indeed related to the breaking of the global Z_2 symmetry induced (as in the homogeneous case) by a ferromagnetic coupling. Moreover, at each value of the external field, the SK replica symmetric solution always becomes unstable at low enough temperatures.

It is apparent how our picture is different from the usual one. We have considered the case of purely random (zero-mean) interactions and our Hamiltonian has no Z_2 symmetry. Nevertheless, the *replica-symmetric solution* of our system exhibits a line of first-order phase transition points ending with a second-order transition point. This feature is robust to *replica symmetry breaking*, indeed the second-order transition point lies outside the unstable region

† International Mathematical and Statistical Library. Information on this collection of subroutines and functions is available at http://www.vni.com/products/ct/

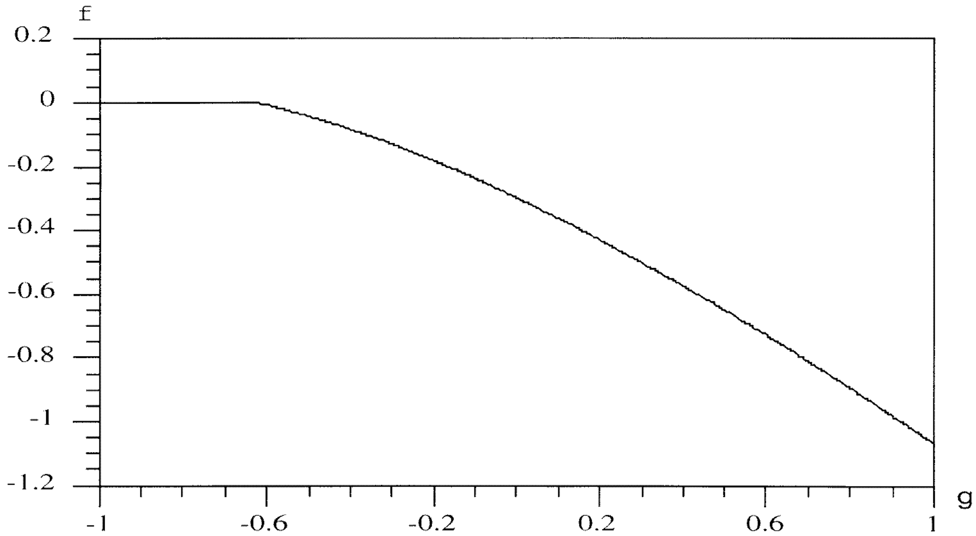

Figure 7. Free energy density versus external field, at zero temperature, with first-order replica-symmetry breaking. The first-order transition point is at $g = -0.625$.

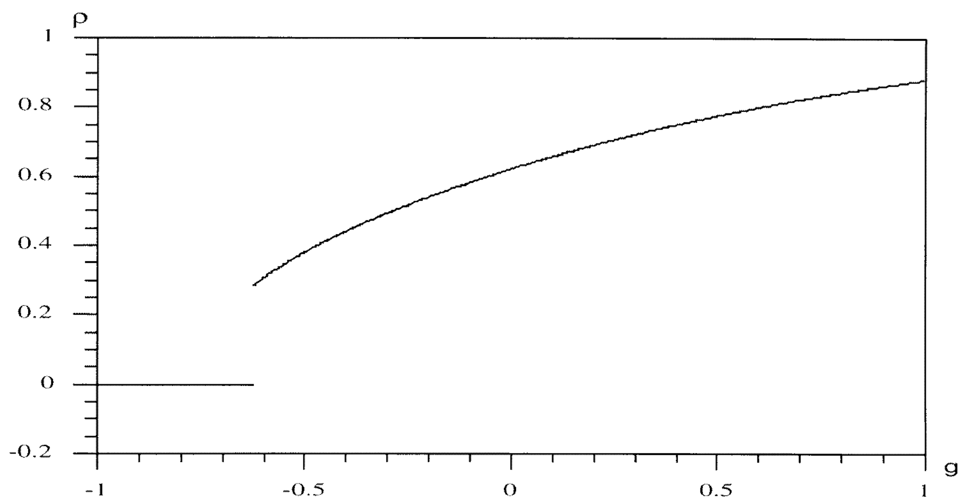

Figure 8. Solution with first-order replica-symmetry breaking. Diagonal order parameter ρ ($= q_1$) at $T = 0$ versus external field.

and we only expect that the transition line should be deflected on the instability boundary. Two phases coexist along the transition line and, as we have stressed, in one of them the replica symmetry is *exact down to zero temperature.* We believe that this is a consequence of the fact that in such a phase the system should behave like a homogeneous one.

To have a possible physical interpretation of the obtained phase diagram it is useful to return to a more conventional framework for lattice gases [1]. The effective Hamiltonian (1) describes a system of mutually avoiding particles, in a discrete space, interacting with a two-body potential ϕ_{kl}. In this context g is closely related to the chemical potential and the thermodynamic potential (4) is the negative of the pressure. The parameters ρ and q are

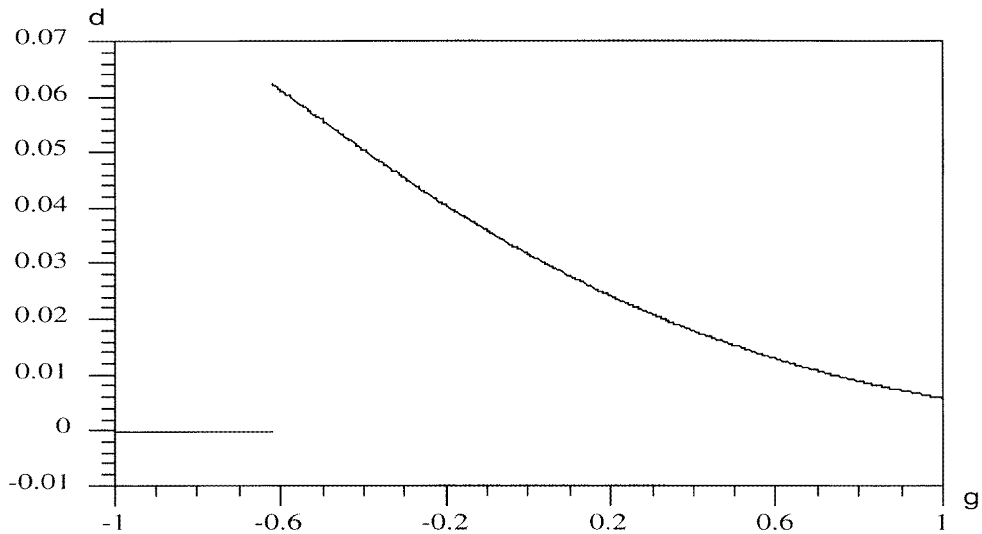

Figure 9. Solution with first-order replica-symmetry breaking. Symmetry breaking parameter d ($= q_1 - q_0$) as a function of external field at zero temperature.

respectively the quenched averages of particle density and of its square. When a first-order transition occurs there are two coexisting phases, the low-density one is to be interpreted as the gas phase, while the other is the liquid one. In our model the gas phase is that which is replica stable at all temperatures. On the other hand, at sufficiently low temperatures, the replica symmetry breaks inside the liquid phase giving a glassy state. With this picture in mind, a part of the line of first-order transitions could be interpreted as glass in equilibrium with its vapour.

We thus have a simple and soluble mean-field model accounting (in a conventional and so far well-understood way [1]) for both a liquid–gas transition and a glassy regime. Given the supposed similarity of the replica symmetry broken phase with the one of the SK model, this model should retain those qualitative features that spin glasses have been observed to share with real glasses. This could be regarded as an intriguing paradigm for capturing the structural glass transition in the framework of replica theory.

We obviously cannot take too literally such an idyllic picture because the lattice gas is a very crude model of a fluid. On the other hand, we know that the lattice gas (even if it is not in any way a realistic model for a fluid) and real gases do belong to the same universality class. As an example, we recall that the homogeneous infinite-ranged lattice gas (equivalent to the mean-field Ising model) has the same critical properties of the van der Waals equation. Therefore, in the spirit of universality, we can hope that, at least at the mean-field level, our model lies in the same universality class of real glasses.

There is a flaw in this. We have analysed a model with quenched (random) disorder included *by hand*. Structural glasses instead do not necessarily have random interactions in their Hamiltonians. In several recent publications (see, e.g. [4–6]) the main effort was first to present a system, *without random interactions*, which behaves in a glassy way, and next try to construct a disordered model which mimics the starting one. Here we have to go in the opposite direction. We have a good candidate of random system, the way of proposing a corresponding deterministic one will be presented elsewhere [15].

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