Stability of the replica-symmetric solution of a quadrupolar glass model with random strain fields

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The stability of the replica-symmetric solution of a model recently proposed for describing the glassy properties of mixed alkali halide-cyanide crystals is examined carefully. The limits of stability are determined in terms of the temperature T and the variance parameter Δ of the random strain fields. Analytical results are obtained near the quadrupolar glass (QG) transition for small Δ and the full line of instability in the (T, Δ) plane is obtained numerically. In addition, numerical calculations of the QG order parameter and of the elastic constant C_{44} are given as functions of temperature for various values of Δ.

I. INTRODUCTION

Randomly diluted molecular crystals have recently attracted much experimental and theoretical attention especially in view of their very rich glassy behavior at low temperature (see Refs. 1, 2 and references therein).

Typical examples are the solid ortho-para hydrogen, solid argon-nitrogen mixtures, and mixed alkali-halide-cyanide crystals such as $Na(CN)_xCl_{1-x}$ or $K(CN)_xBr_{1-x}$ which are known to be miscible at all concentrations x. These last systems, to which we are mainly interested, are generally characterized by a cubic structure where the sites of anions are randomly occupied by halide ions and dumbell-shaped CN^- molecular groups which rotate nearly freely. Due to the coupling between translational and orientational degrees of freedom, below a critical concentration x_c, the rotating molecules experience an indirect frustating interaction so that, lowering the temperature below a critical value $T_g(x)$, a special phase occurs where the quadrupolar momenta of the CN^- ions are frozen in random directions. Since the random freezing of the CN^- ions leads to local static lattice deformations, this low-temperature phase, called quadrupolar glass (QG), shows also some properties of a structural glass.[1,2]

A microscopic model of the cyanide glasses was proposed by Michel and Rowe[3] stressing the analogy with the spin-glass phase in disordered magnetic materials.[4] Here, the interaction between randomly distributed CN^- ions originates from linear coupling of translational and rotational degrees of freedom. Subsequently,[5,6] the model was developed and studied including random strain fields as a consequence of a substitutionial disorder. In the theory, the CN^- ions are considered as molecular groups with quadrupolar momenta and no restriction on their orientational states.

An alternative semimicroscopic model, which is a simplified coarse-grained effective version of the previous microscopic one, has been introduced by Vollmayr, Kree, and Zippelius.[7] They assumed the lattice as an anisotropic elastic medium where the randomly interacting CN^- ions have a limited number of orientational states, reducing the problem to the study of the p-state Potts spin-glass model ($p = 3, 4, 5$) with "Potts spins" coupled to the local strain fields.

Quite recently an effective model has been formulated[8] for alkali-halide-cyanide crystals which started from the coarse-graining averaging interactions considered in Ref. 7 but without restrictions on the spatial orientations of the CN^- ions. This model arises from the possibility of integrating over the displacement fields, reducing the original problem to an effective Hamiltonian involving only rotational degrees of freedom of the defects (CN^- ions). So an effective spin-glass-like problem on a rigid lattice is obtained which can be treated using known methods from the theory of spin glasses.[4] In Ref. 8 within the replica-symmetric theory, the general expressions of the Edward-Anderson-like QG order parameter q_{EA} and of the orientation free energy have been obtained. Next, preliminary calculations of the QG order parameter q_{EA} and the elastic constant C_{44} as functions of the temperature have been also performed[9] near the QG transition point under weak disorder conditions.

The main purpose of this paper is to investigate the limits of stability in the phase diagram of the replica-symmetric solution for the previous effective QG model[8] where the random strain fields are present. Moreover, we give also full numerical results for quantities of direct experimental interest such as the QG order parameter and the elastic constant C_{44} as functions of the temperature for different values of the parameter Δ which characterizes the random strain fields. As we shall see, the results appear to be rather in good agreement with experimental data. This will be realized in strict analogy to the de Almeida–Thouless (AT) stability analysis[10] of the replica-symmetric solution for the famous Sherrington-Kirkpatrick spin-glass model[11] and the corresponding one for proton glasses.[12] This appears a quite important tool especially in view of the possible failure of the replica-symmetry breaking Parisi scheme[13] when applied to richer models of disordered systems.[14] Indeed, there has been some previous works

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on the stability of the replica-symmetric solution of continuously orientable units, like QG's. A review of the first mean-field replica-symmetric treatment[15] for QG's and subsequent replica-symmetry breaking scheme applied to these systems[15–17] can be found in Ref. 2.

Unfortunately, little has been published about the details of the replica-symmetry-breaking theory for more complex situations (see, however, Ref. 18). It now seems that the mean-field solutions of a number of frustrated models, such as QG's,[2,15] Potts glasses,[2,16,19–21] p-spin interaction spin-glass models,[20] and the random energy model[22] appear to be qualitatively very similar. Nevertheless, doubts on the direct extension of the current spin-glass theory for such more complex randomly frustrated systems are raised. In particular, it has been suggested that QG's (Ref. 15) and Potts glass model[16] are more subtle than conventional spin glasses. Thus it appears to be a quite important problem to give a satisfying solution of such models before confident extention of the analysis to more general frustrated systems. The present investigation on QG's has just to be considered as a contribution towards this direction.

The paper is organized as follows. In Sec. II we introduce the main features of the model, the replica-symmetric solution is presented, and its stability conditions are obtained. Explicit analytical results near the QG phase transition with small values of the control parameter Δ are also given. Section III contains numerical results and a discussion of their connection with experiments.

II. QUADRUPOLAR GLASS MODEL AND STABILITY CONDITIONS OF THE REPLICA-SYMMETRIC SOLUTION

We consider the model defined by the Hamiltonian[8]

$$\tilde{H} = -\frac{1}{2}\sum_{\mathbf{x}\neq\mathbf{y}}\sum_{\lambda,\lambda'=1}^{5} u_{\lambda\lambda'}(\mathbf{x},\mathbf{y})Y_\lambda(\Omega_\mathbf{x})Y_{\lambda'}(\Omega_\mathbf{y}) - \sum_{\mathbf{x}}\sum_{\lambda=1}^{5} h_\lambda(\mathbf{x})Y_\lambda(\Omega_\mathbf{x}) \,, \tag{1}$$

containing only orientational degrees of freedom whose interaction is described in terms of the symmetry-adapted spherical harmonics $Y_\lambda(\Omega_\mathbf{x})(\lambda = 1,\ldots,5)$,[3,5,6,8] where the angles $\Omega_\mathbf{x} \equiv (\theta_\mathbf{x},\varphi_\mathbf{x})$ specify an orientation of a defect at site $\mathbf{x}$ with respect to the cubic crystal axes. In (1), $u_{\lambda,\lambda'}(\mathbf{x},\mathbf{y})$ denote the random orientational couplings and $h_\lambda(\mathbf{x})$ represent the random strain fields at site $\mathbf{x}$. This model appears to be quite relevant for describing the glassy properties of alkali halide-cyanide crystals[8,9] and was obtained by averaging the semimicroscopical coarse-grained Hamiltonian introduced in Ref. 7 on the translational degrees of freedom and assuming the CN^- ions as linear quadrupoles.

Using the replica trick,[4] the free energy of the model can be obtained as

$$F = -k_BT\lim_{n\to 0}\frac{1}{n}\ln Z_n \,, \tag{2}$$

with

$$Z_n = \left[\mathrm{Tr}\; e^{-\sum_{\alpha=1}^{n}\tilde{H}^{(\alpha)}/k_BT}\right]_{\mathrm{av}} \equiv \mathrm{Tr}\; e^{-H_{\mathrm{QG}}/k_BT} \,, \tag{3}$$

where $\mathrm{Tr}\cdots$ denotes an integration over defect orientations, α is the replica index, $[\cdots]_{\mathrm{av}}$ means averaging over the quenched disorder, and H_{QG} is the effective QG Hamiltonian whose explicit expression depends on the probability distribution of the random variables $u_{\lambda\lambda'}(\mathbf{x},\mathbf{y})$ and $h_\lambda(\mathbf{x})$. For Gaussian distributions with zero means and variances J^2/N and Δ^2, respectively, H_{QG} assumes the form

$$H_{\mathrm{QG}} = -\frac{J^2}{4k_BTN}\sum_{\mathbf{x}\neq\mathbf{y}}\sum_{\alpha,\alpha'=1}^{n}\hat{q}_{\alpha\alpha'}(\mathbf{x})\hat{q}_{\alpha\alpha'}(\mathbf{y}) - \frac{\Delta^2}{2k_BT}\sum_{\mathbf{x}}\sum_{\alpha,\alpha'=1}^{n}\hat{q}_{\alpha,\alpha'}(\mathbf{x}) \,, \tag{4}$$

where

$$\hat{q}_{\alpha\alpha'}(\mathbf{x}) = (1-\delta_{\alpha,\alpha'})\sum_{\lambda=1}^{5}Y_\lambda(\Omega_\mathbf{x}^{\alpha})Y_\lambda(\Omega_\mathbf{x}^{\alpha'}) \tag{5}$$

and N denotes the number of coarse-grained lattice sites. Now, a Sherrington-Kirkpatrick-like saddle point treatment[4,11] can be applied to the effective problem (4), yielding, for the free energy per site, the expression[8]

$$\frac{F}{N} = J\overline{T}\lim_{n\to 0}\frac{1}{n}\mathcal{H}[q] \,, \tag{6}$$

where

$$\mathcal{H}[q] = \frac{1}{4\overline{T}^2}\sum_{\alpha,\alpha'=1}^{n}q_{\alpha\alpha'}^2 - \ln\left\langle \exp\left[\frac{1}{2\overline{T}^2}\sum_{\alpha,\alpha'=1}^{n}(q_{\alpha\alpha'}^2+\overline{\Delta}^2)\hat{q}_{\alpha\alpha'}\right]\right\rangle_0 . \tag{7}$$

In Eqs. (6) and (7), $\overline{T} = k_BT/J$, $\overline{\Delta} = \Delta/J$, $\hat{q}_{\alpha\alpha'}$ is $\hat{q}_{\alpha\alpha'}(\mathbf{x})$ for any site $\mathbf{x}$, $\langle\cdots\rangle_0 = \int\cdots d\Omega/4\pi$ with $\Omega\equiv(\theta,\varphi)$, and $\hat{q}_{\alpha\alpha'}$ is determined by the self-consistent equation

$$q_{\alpha\alpha'} = \langle\hat{q}_{\alpha\alpha'}\rangle, \tag{8}$$

with

$$\langle\cdots\rangle = \frac{\mathrm{Tr}\left\{e^{\frac{1}{2\overline{T}^2}\sum_{\alpha,\alpha'=1}^{n}(q_{\alpha\alpha'}+\overline{\Delta}^2)\hat{q}_{\alpha\alpha'}}(\cdots)\right\}}{\mathrm{Tr}\left\{e^{\frac{1}{2\overline{T}^2}\sum_{\alpha,\alpha'=1}^{n}(q_{\alpha\alpha'}+\overline{\Delta}^2)\hat{q}_{\alpha\alpha'}}\right\}} . \tag{9}$$

The Edward-Anderson QG order parameter for our model is defined by[8,23]

$$q_{\mathrm{EA}} = \sum_{\lambda=1}^{5}\left[\langle Y_\lambda(\Omega_\mathbf{x})\rangle_T^2\right]_{\mathrm{av}} = \lim_{n\to 0}\frac{1}{n(n-1)}\sum_{\alpha,\alpha'=1}^{n}q_{\alpha,\alpha'} \,, \tag{10}$$

where $\langle\cdots\rangle_T$ denotes the thermal average. For the present model it is also found[8] that the elastic constant C_{44} can be expressed in terms of $q_{\rm EA}$ as

$$C_{44} = C_{44}^0\left[1+\frac{B^2}{20\pi J C_{44}^0 \overline{T}}\left(1-\frac{4\pi}{5}q_{\rm EA}\right)\right]^{-1}, \qquad (11)$$

where the parameter B measures the strength of the coupling of the orientational modes of the T_{2g} symmetry[3] and C_{44}^0 is the bare elastic constant.

The replica-symmetric solution for our problem[8] can be obtained setting $q_{\alpha\alpha'} = q$ ($\alpha \neq \alpha'$) in the previous equations. In this case one has a $q_{\rm EA} = q$ solution of the self-consistent Eqs. (8) and (9). Our objective here is just to determine the stability condition of the replica-symmetric solution.

For this, as usual in the spin-glass theory,[4,10] one must require that, in the limit $n \to 0$, the eigenvalues of the Hessian,

$$G_{(\alpha\beta),(\gamma\delta)}(q) = \left.\frac{\partial^2\mathcal{H}[q]}{\partial q_{\alpha\beta}\partial q_{\gamma\delta}}\right|_{\{q_{\alpha\alpha'}=q\}}, \qquad (12)$$

must be positive. Similarly, as in the spin-glass problem,[10] the elements of the matrix (12) have the form

$$\begin{aligned} G_{(\alpha\beta),(\alpha\beta)} &= 1-\frac{1}{\overline{T}^2}\left[\langle\hat q^2_{\alpha\beta}\rangle-\langle\hat q_{\alpha\beta}\rangle^2\right], \\ G_{(\alpha\beta),(\alpha\gamma)} &= -\frac{1}{\overline{T}^2}\left[\langle\hat q_{\alpha\beta}\hat q_{\alpha\gamma}\rangle-\langle\hat q_{\alpha\beta}\rangle\langle\hat q_{\alpha\gamma}\rangle\right] \qquad (\beta\neq\gamma), \\ G_{(\alpha\beta),(\gamma\delta)} &= -\frac{1}{\overline{T}^2}\left[\langle\hat q_{\alpha\beta}\hat q_{\gamma\delta}\rangle-\langle\hat q_{\alpha\beta}\rangle\langle\hat q_{\gamma\delta}\rangle\right] \qquad (\alpha\neq\beta\neq\gamma\neq\delta). \end{aligned} \qquad (13)$$

Using Eqs. (5) and (9), in the limit $n \to 0$, one obtains

$$\langle\hat q_{\alpha\beta}\rangle = \frac{1}{(2\pi)^{5/2}}\int\prod_{\lambda=1}^{5}d\xi_\lambda e^{-\frac12\sum_{\lambda=1}^5\xi_\lambda^2}\sum_{\lambda=1}^{5}m_\lambda^2(\vec\xi), \qquad (14)$$

$$\langle\hat q^2_{\alpha\beta}\rangle = \frac{1}{(2\pi)^{5/2}}\int\prod_{\lambda=1}^{5}d\xi_\lambda e^{-\frac12\sum_{\lambda=1}^5\xi_\lambda^2}\sum_{\lambda,\lambda'=1}^{5}\left[\overline{T}\chi_{\lambda\lambda'}(\vec\xi)+m_\lambda(\vec\xi)m_{\lambda'}(\vec\xi)\right]^2, \qquad (15)$$

$$\langle\hat q_{\alpha\beta}\hat q_{\alpha\gamma}\rangle = \frac{1}{(2\pi)^{5/2}}\int\prod_{\lambda=1}^{5}d\xi_\lambda e^{-\frac12\sum_{\lambda=1}^5\xi_\lambda^2}\sum_{\lambda,\lambda'=1}^{5}\left[\overline{T}\chi_{\lambda\lambda'}(\vec\xi)+m_\lambda(\vec\xi)m_{\lambda'}(\vec\xi)\right] \times m_\lambda(\vec\xi)m_{\lambda'}(\vec\xi), \qquad (16)$$

$$\langle\hat q_{\alpha\beta}\hat q_{\gamma\delta}\rangle = \frac{1}{(2\pi)^{5/2}}\int\prod_{\lambda=1}^{5}d\xi_\lambda e^{-\frac12\sum_{\lambda=1}^5\xi_\lambda^2}\left(\sum_{\lambda=1}^{5}m_\lambda^2(\vec\xi)\right)^2, \qquad (17)$$

where

$$m_\lambda(\vec\xi) = \langle Y_\lambda(\Omega)\rangle_{\vec\xi}, \qquad (18)$$

$$\chi_{\lambda\lambda'}(\vec\xi) = \frac{1}{\overline{T}}\left[\langle Y_\lambda(\Omega)Y_{\lambda'}(\Omega)\rangle_{\vec\xi}-m_\lambda(\vec\xi)m_{\lambda'}(\vec\xi)\right], \qquad (19)$$

with

$$\langle\cdots\rangle_{\vec\xi} = \frac{\langle e^{\frac{(q+\overline{\Delta}^2)^{1/2}}{\overline{T}}\sum_{\lambda=1}^5\xi_\lambda Y_\lambda(\Omega)}(\ldots)\rangle_0}{\langle e^{\frac{(q+\overline{\Delta}^2)^{1/2}}{\overline{T}}\sum_{\lambda=1}^5\xi_\lambda Y_\lambda(\Omega)}\rangle_0} \qquad (20)$$

and $\vec\xi = \{\xi_\lambda;\lambda=1,\ldots,5\}$. Notice that, Eq. (14), with $\langle q_{\alpha\beta}\rangle = q$ [see Eq. (8)], determines the QG order parameter within the replica-symmetric theory.

Now, following strictly the procedure of Ref. 10, we see that the matrix (12) has, in the limit $n \to 0$, the two eigenvalues

$$\lambda_1 = 1-\frac{1}{\overline{T}^2}\left[\langle\hat q^2_{\alpha\beta}\rangle-4\langle\hat q_{\alpha\beta}\hat q_{\alpha\gamma}\rangle+3\langle\hat q_{\alpha\beta}\hat q_{\gamma\delta}\rangle\right], \qquad (21)$$

$$\lambda_2 = 1-\frac{1}{\overline{T}^2}\left[\langle\hat q^2_{\alpha\beta}\rangle-2\langle\hat q_{\alpha\beta}q_{\alpha\gamma}\rangle+\langle\hat q_{\alpha\beta}\hat q_{\gamma\delta}\rangle\right]. \qquad (22)$$

The use of the expressions (15)–(17) shows immediately that $\lambda_1 > \lambda_2$ so that the stability condition for the replica-symmetric solution is $\lambda_2 > 0$ or, explicitly,

$$\frac{1}{(2\pi)^{5/2}}\int\prod_{\lambda=1}^{5}d\xi_\lambda e^{-\frac12\sum_{\lambda=1}^5\xi_\lambda^2}\sum_{\lambda,\lambda'=1}^{5}\chi^2_{\lambda\lambda'}(\vec\xi) < 1. \qquad (23)$$

Equation (23) expresses the complicated relation between $\overline{\Delta}$ and $\overline{T}$ to be satisfied in order that the replica symmetric-solution for the QG order parameter,

$$q = \frac{1}{(2\pi)^{5/2}}\int\prod_{\lambda=1}^{5}d\xi_\lambda e^{-\frac12\sum_{\lambda=1}^5\xi_\lambda^2}\sum_{\lambda=1}^{5}\langle Y_\lambda(\Omega)\rangle^2_{\vec\xi}, \qquad (24)$$

is a stability value for the argument of the free energy density (6).

From Eqs. (23) and (24) it is possible to obtain a line of instability $\overline{\Delta} = \overline{\Delta}(\overline{T})$ in the plane $(\overline{T}, \overline{\Delta})$ which is analogous to the known AT instability line[10] for the Sherrington-Kirkpatrick solution of a spin glass.[4,11] Its exact analytic expression is, of course, prohibitive and the problem is accessible only numerically. Postponing the numerical results to the next section, here we investigate analytically the limits of stability for our glassy problem near the QG transition point ($q \ll 1$) under the condition $\overline{\Delta} \ll 1$.

For this purpose, in terms of the shifted QG parameter $\tilde{q} = q + \overline{\Delta}^2 \ll 1$, we first calculate the quantities $\chi_{\lambda\lambda'}(\vec{\xi})$ and $m_\lambda(\vec{\xi})$ in Eqs. (23) and (24) with an accuracy up to terms proportional to $\tilde{q}$ and $\tilde{q}^{1/2}$, respectively. From (20) it is easy to see that

$$\langle Y_\lambda(\Omega) Y_{\lambda'}(\Omega)\rangle_{\vec{\xi}} = \frac{\delta_{\lambda,\lambda'}}{4\pi} + \frac{\tilde{q}^{1/2}}{\overline{T}} \sum_{\lambda_1=1}^{5} \langle Y_\lambda(\Omega) Y_{\lambda'}(\Omega) Y_{\lambda_1}(\Omega)\rangle_0 \xi_{\lambda_1} + \frac{\tilde{q}}{2\overline{T}^2}\left[\sum_{\lambda_1,\lambda_2=1}^{5} \langle Y_\lambda(\Omega) Y_{\lambda'}(\Omega) Y_{\lambda_1}(\Omega) Y_{\lambda_2}(\Omega)\rangle_0 \xi_{\lambda_1}\xi_{\lambda_2} - \frac{\delta_{\lambda,\lambda'}}{16\pi^2}\sum_{\lambda_1=1}^{5} \xi_{\lambda_1}^2\right] + \mathcal{O}\left(\tilde{q}^{3/2}\right) , \tag{25}$$

where use was made of the relations

$$\langle Y_\lambda(\Omega)\rangle_0 = 0 \ , \quad \langle Y_\lambda(\Omega) Y_{\lambda'}(\Omega)\rangle_0 = \frac{\delta_{\lambda,\lambda'}}{4\pi} . \tag{26}$$

Similarly, for $m_\lambda(\vec{\xi})$ we find

$$m_\lambda(\vec{\xi}) = \frac{\tilde{q}^{1/2}}{4\pi\overline{T}}\xi_\lambda + \mathcal{O}(\tilde{q}) . \tag{27}$$

Then, for $\chi_{\lambda\lambda'}(\vec{\xi})$ defined by Eq. (19), we obtain

$$\chi_{\lambda\lambda'}(\vec{\xi}) = \frac{1}{\overline{T}}\left\{\frac{\delta_{\lambda\lambda'}}{4\pi} + \frac{\tilde{q}^{1/2}}{\overline{T}} \sum_{\lambda_1=1}^{5} \langle Y_\lambda(\Omega) Y_{\lambda'}(\Omega) Y_{\lambda_1}(\Omega)\rangle_0 \xi_{\lambda_1} + \frac{\tilde{q}}{2\overline{T}^2}\left[\sum_{\lambda_1,\lambda_2=1}^{5} \langle Y_\lambda(\Omega) Y_{\lambda'}(\Omega) Y_{\lambda_1}(\Omega) Y_{\lambda_2}(\Omega)\rangle \xi_{\lambda_1}\xi_{\lambda_2} - \frac{\delta_{\lambda\lambda'}}{16\pi^2}\sum_{\lambda_1=1}^{5} \xi_{\lambda_1}^2 - \frac{1}{8\pi^2}\xi_\lambda\xi_{\lambda'}\right] + \mathcal{O}(\tilde{q}^{3/2})\right\} . \tag{28}$$

Using this equation and the relations[3,5–8]

$$\sum_{\lambda=1}^{5} Y_{\lambda=1}^2(\Omega) = \frac{5}{4\pi} ,$$

$$\sum_{\lambda\lambda'\lambda_1=1}^{5} \langle Y_\lambda(\Omega) Y_{\lambda'}(\Omega) Y_{\lambda_1}(\Omega)\rangle_0^2 = \frac{50}{448\pi^3}, \tag{29}$$

the stability condition (23) becomes

$$\frac{\overline{T}_g^2}{\overline{T}^2}\left[1 - \frac{\tilde{q}}{7\pi\overline{T}^2} + O(\tilde{q}^2)\right] < 1 , \tag{30}$$

where, as we shall see, $\overline{T}_g = \sqrt{5}/4\pi$ is the scaled QG transition temperature in the absence of random strain fields.

It remains to solve the self-consistent equation (24) for small q or $\tilde{q}$. This can be realized as before by expanding the right hand side of Eq. (24) into a power series of $\tilde{q}$ up to terms of the order $\tilde{q}^2$. In terms of $\tau = (\overline{T}_g - \overline{T})/\overline{T}_g \ll 1$, assumed to be of the same order of $\overline{\Delta}$, we find

$$\tilde{q} = \frac{28\pi}{9}\overline{T}_g^2\left[\tau + \left(\tau^2 + \frac{9}{28\pi}\frac{\overline{\Delta}^2}{\overline{T}_g^2}\right)^{1/2}\right] . \tag{31}$$

Inserting this expression for $\tilde{q}$ into Eq. (30), the stability condition, with an accuracy to linear terms in τ, reads

$$\overline{\Delta} > \frac{5}{4}\sqrt{\frac{7}{\pi}}\tau \approx 1.866\ \tau . \tag{32}$$

Notice that, for $\overline{\Delta} = 0$, the stability condition is fulfilled only for $\tau < 0$, i.e., $T > T_g = \frac{\sqrt{5}}{4\pi}J/k_B$, where $q = \tilde{q} \equiv 0$ [see Eq. (31)]. Thus, decreasing the temperature with $\overline{\Delta} = 0$, a sharp continuous transition to the QG phase ($q \neq 0$) occurs but, here, the replica-symmetric solution is unstable. In the presence of the random strain fields the phase transition is smeared out, the replica-symmetric solution is stable below T_g, and near T_g the stability limit for $\overline{\Delta} \ll 1$ is expressed by the equation

$$\overline{\Delta} = 1.866\tau . \tag{33}$$

It is worth noting that a similar scenario exists in the Ising spin-glass model with random longitudinal field[12] for proton glasses where the stability limit for $\overline{\Delta} \ll 1$ is given by $\overline{\Delta} = 0.534\tau$. A comparison with (33) shows that the range of stability for the replica-symmetric solution at a given $\overline{\Delta}$ is about 3.5 times larger for proton glasses than for quadrupolar ones.

III. NUMERICAL SOLUTION AND DISCUSSION

As mentioned before, the complexity of the equations describing QG systems let us obtain analytical results for physical quantities only for small values of the involved parameters. Therefore particular relevance, expecially from the experimental point of view, is assumed by numerical predictions on the corresponding quantities for realistic values of the parameters.

In Fig. 1 the full behavior of the QG Edwards-Anderson order parameter $q_{\mathrm{EA}} = q$ as function of the reduced temperature $\overline{T}$ is plotted for seven different values of $\overline{\Delta}$. As a support to the present model for QG's, the form of the temperature dependence of q for $\overline{\Delta} \neq 0$ is very similar to that of the quadrupolar Edwards-Anderson order parameter determined from the ^{23}Na satellite distribution's second moment data for $\mathrm{Na(CN)}_x\mathrm{Cl}_{1-x}$ systems[23] and from elastic diffuse intensity neutron scattering.[24] It is also worth noting that a comparison of our numerical results with the corresponding ones of Ref. 12 confirms the strict analogy existing between alkali halide-cyanide crystals and mixed hydrogen-bonded ferro- and antiferroelectric crystals such as $\mathrm{Rb}_{1-x}(\mathrm{NH}_4)_x\mathrm{H}_2\mathrm{PO}_4$.

The temperature behavior of the elastic constant C_{44}, as given by Eq. (11) in terms of q, is shown in Fig. 2 for the same values of $\overline{\Delta}$ used for numerical results in Fig. 1. Here we have assumed $B^2/(20\pi J C_{44}^0) = 0.1$ from experimental data.[23–27] The numerical results show clearly that the sharp minimum, which appears at $\overline{T}_g$ for $\overline{\Delta} = 0$, is flattened in the presence of the random strain field and this effect becomes more and more apparent with increasing $\overline{\Delta}$. Also, for this quantity, the characteristic form as a function of temperature agrees with the experimental measurements.[23–27]

The results of Figs. 1 and 2 give clear evidence for the smearing of the sharp QG transition at $(T_g, \Delta = 0)$ caused by random local strain fields. This aspect of the effective model (1) has been verified by various experimental methods[1,23–27] and in particular by nuclear magnetic resonance.[1,23]

The borderline of the stability is given by the simultaneous solution of Eq. (24) and the equality assumed in (23). In Fig. 3, the instability line is plotted in the $(\overline{T}, \overline{\Delta})$plane. It plays a role similar to that of the AT line in spin glasses in a homogeneous field[10] and in proton glasses;[12] i.e., for all values $(\overline{T}, \overline{\Delta})$ above the line the replica-symmetric solution is stable. Below this line, only a solution with replica-symmetry breaking (to be determined) may provide a correct description of the QG

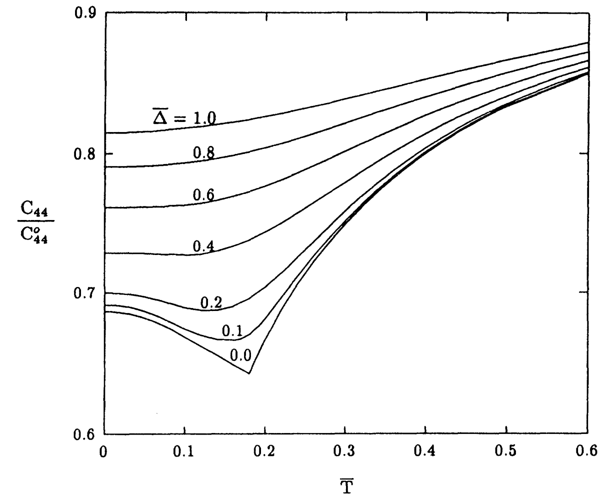

FIG. 2. Elastic constant C_{44} scaled by the bare one C_{44}^0 plotted vs $\overline{T} = k_B T/J$ for various values of the random strain field parameter $\overline{\Delta} = \Delta/J$.

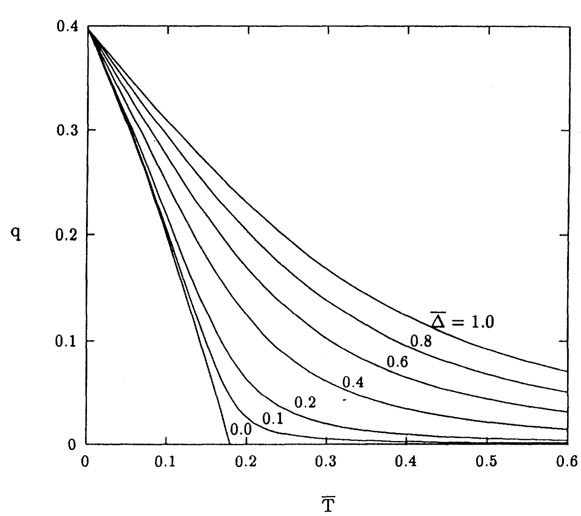

FIG. 1. Replica-symmetric solution for the QG order parameter plotted vs $\overline{T} = k_B T/J$ for various values of the random strain field parameter $\overline{\Delta} = \Delta/J$.

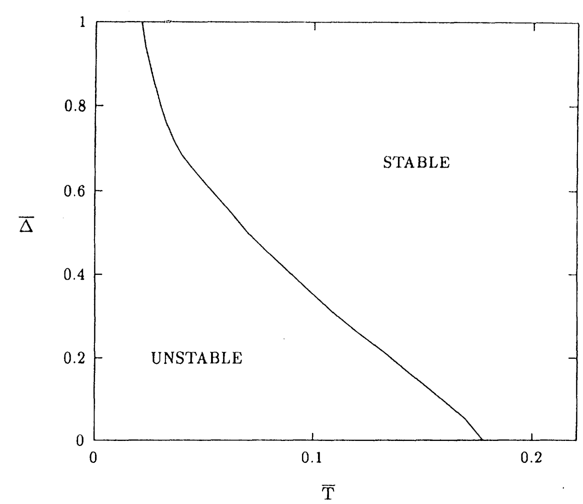

FIG. 3. Phase diagram showing the limit of stability of the replica-symmetric solution for quadrupolar glasses in the presence of random strain fields.

phase properties.

Of course, our results for too low a temperature cannot be applied to alkali-halide-cyanide crystals. In such a case, indeed, bipolar effects become important and our model is not sufficient to describe correctly the properties of these materials. However, knowledge of the full instability line and of all the predictions based on the semimicroscopic model (1) may be in any case of interest for more general aspects of QG theory.

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