Amorphous solid state: A locally stable thermodynamic phase of randomly constrained systems

Horacio E. Castillo
CNRS–Laboratoire de Physique Théorique de l'Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France

Paul M. Goldbart
Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080

Annette Zippelius
Institut für Theoretische Physik, Georg August Universität, D-37073 Göttingen, Germany
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The question of the local stability of the (replica-symmetric) amorphous solid state is addressed for a class of systems undergoing a continuous liquid to amorphous-solid phase transition driven by the effect of random constraints. The Hessian matrix, associated with infinitesimal fluctuations around the stationary point corresponding to the amorphous solid state, is obtained. The eigenvalues of this Hessian matrix are all shown to be strictly positive near the transition, except for one—the zero mode associated with the spontaneously broken continuous translational symmetry of the system. Thus the local stability of the amorphous solid state is established. [S0163-1829(99)01641-0]

I. INTRODUCTION

In recent years, a theoretical approach has been developed for the problem of the liquid-amorphous solid phase transition in systems of randomly crosslinked flexible linear macromolecules.[1–4] This approach starts from a semimicroscopic model for the macromolecules, and takes into account explicitly both the thermal fluctuations at nonzero temperature and the quenched disorder due to the random nature of the crosslinking. It is based on the Deam-Edwards formulation of the statistical mechanics of polymer networks,[5] and borrows some concepts and techniques that have in the past been used to study the problem of spin glasses.[6] In the framework of this approach, it is possible to define an order parameter that probes random static particle density fluctuations, and is thus able to detect the transition between the liquid and the amorphous solid state.[1,4]

Along the way, it has been recognized that there exists a class of systems (including, e.g., end-linked flexible and stiff polymers,[7] and crosslinked higher dimensional manifolds[8]) that display identical transitions, and a general Landau theory was formulated to describe this transition.[9] This Landau theory was constructed using only symmetry considerations and the assumption that the phase transition should be continuous (and thus dominated by the long-distance behavior of the system).

By expanding any of the semimicroscopically derived free-energy functionals corresponding to the above-mentioned physical systems in powers of the order parameter and gradients, one recovers this general Landau free-energy functional, up to terms that play no role in the mean-field theory, in the vicinity of the transition. In the study of fluctuations, as we shall show later, these additional terms do not alter the physical picture. The slight difference between the general Landau theory and the microscopically derived theories is due to the fact that, whereas the former theory only allows states that have a disorder-averaged particle density that is spatially homogeneous, in the latter states with spatial inhomogeneities of the density are in principle allowed, but are ultimately suppressed by the repulsive interparticle interactions.

Let us begin by summarizing the results of the mean-field theory of the liquid–amorphous-solid transition driven by random constraints: (i) for densities of constraints smaller than a critical value the system is in the liquid state and all particles are delocalized; (ii) for densities of constraints larger than the critical value the system is in an amorphous solid state, characterized by emerging random static density fluctuations; (iii) at the critical density of constraints there is a continuous phase transition between the liquid and the amorphous solid states; (iv) in the amorphous solid state a positive fraction of the particles is localized around random mean positions and with random rms displacements; (v) in the amorphous solid state, close to the transition, the fraction of localized particles is proportional to the excess of the crosslink density beyond its critical value, and the typical localization length diverges at the transition like the excess crosslink density to the power $-1/2$; (vi) when scaled by the mean value, the statistical distribution of localization lengths is universal near the transition and, consequently, the dependence of the order parameter on the wave vectors also has a universal scaling form.

Although in the amorphous solid state translational invariance and rotational invariance are broken at the microscopic level, because a fraction of the monomers are localized, the average density is uniform, and the system is macroscopically translationally (and rotationally) invariant (MTI).[4] The liquid state is, of course, not only macroscopically but also microscopically translationally and rotationally invariant, as each individual monomer density is uniform over the container. Moreover, as in the case of some of the mean field solutions encountered in spin-glass systems, both the liquid and the amorphous solid states are replica symmetric.[10] However, as will be shown later, the symmetry of these states is even larger, because the replica symmetry combines

with the rotational symmetry (in d-dimensional space) to produce rotational symmetry in a nd-dimensional (i.e., replicated) space.

It is well known that in the spin-glass case the early replica-symmetric spin-glass solution[10] for the Sherrington-Kirkpatrick model was later found to be locally unstable at temperatures below the critical temperature by de Almeida and Thouless,[11] and was superseded by the replica symmetry-breaking solution[12] discovered by Parisi, with its elegant interpretation in terms of symmetry-unrelated pure equilibrium states.[13] This replica symmetry-breaking solution has a non-negative entropy at all temperatures and is locally marginally stable.[14]

By analogy with the spin-glass case, and considering also the fact that random topological constraints can, in principle, lead to a partitioning of the configuration space of three-dimensional macromolecular systems into ergodic regions that are not connected by symmetry operations,[1,4] it would not be entirely surprising if in systems undergoing a liquid–amorphous-solid transition under the effect of random constraints, the replica symmetric stationary point of the free energy corresponding to the amorphous solid state turned out to be unstable and had to be superseded by a less symmetric solution of the mean-field equations.

However, the Deam-Edwards distribution[5,4] used to model the disorder favors sets of constraint locations that are associated with highly probable configurations of the unconstrained system. Thus, although frustration may in principle be present, the disorder distribution tends to discourage it.[15]

The purpose of this paper is to show that the mean-field amorphous solid state is, in fact, locally stable, at least near the transition. More specifically, the Hessian matrix that describes changes of the free-energy functional for infinitesimal fluctuations around the stationary point corresponding to the amorphous solid state is computed, and it is shown that, to linear order in the excess crosslink density, all its eigenvalues are strictly positive, except for a nd degenerate zero mode associated with the spontaneous breaking of the continuous translational symmetry of the system. In order to do this, we construct a description for the space of fluctuations around the stationary point that allows the eigenvalue problem for the Hessian matrix in replicated space to be reduced, in essence, to an integral eigenvalue equation in one dimension.

The rest of this paper is organized as follows: In Sec. II we compute the Hessian matrix for the Landau free-energy functional around the amorphous solid state, and make use of the continuous symmetry of the problem to identify a basis set that significantly simplifies the eigenvalue equation for the Hessian. In Sec. III we find positive lower bounds for all the eigenvalues of the Hessian, except for the zero mode that is present due to the spontaneously broken symmetry. In Sec. IV we extend these results to allow for fluctuations in the particle density in the case of the microscopically derived free-energy functional for randomly crosslinked macromolecules. Finally, in Sec. V we present our conclusions.

II. LANDAU THEORY: HESSIAN MATRIX

In this section we first summarize briefly the basics of the general Landau theory of the liquid–amorphous-solid phase transition, as presented in Ref. 9, and later derive expressions for the Hessian matrix for the free-energy functional in this theory.

A. Brief review of the Landau theory

In a system characterized by static random density fluctuations, the appropriate order parameter is[1,4,9]

$$\overline{\Omega}_{\mathbf{k}^1,\mathbf{k}^2,\cdots,\mathbf{k}^g} \equiv \left[\frac{1}{N} \sum_{j=1}^{N} \langle e^{i\mathbf{k}^1\cdot\mathbf{c}_j}\rangle_\chi \langle e^{i\mathbf{k}^2\cdot\mathbf{c}_j}\rangle_\chi \cdots \langle e^{i\mathbf{k}^g\cdot\mathbf{c}_j}\rangle_\chi \right], \tag{2.1}$$

where N is the total number of particles, $\mathbf{c}_i$ (with $i=1,\ldots,N$) is the (d-dimensional) position vector of particle i, the wave vectors $\mathbf{k}^1,\mathbf{k}^2,\ldots,\mathbf{k}^g$ are arbitrary, $\langle\cdots\rangle_\chi$ denotes a thermal average for a particular realization χ of the disorder, $[\cdots]$ represents averaging over the disorder, and g is a positive number.

We make the Deam-Edwards assumption[5] that the statistics of the disorder is determined by the correlations of the unconstrained system. Under the Deam-Edwards assumption, obtaining disorder averages with the replica technique amounts to working with the $n\to 0$ limit of systems of $n+1$, as opposed to n, replicas. The additional replica, labeled by $\alpha=0$, represents the degrees of freedom of the original system before adding the constraints or, equivalently, describes the constraint distribution.

In the replica formalism, the order parameter takes the form[1,4,9]

$$\overline{\Omega}_{\hat{k}} \equiv \left\langle \frac{1}{N} \sum_{i=1}^{N} \exp(i\hat{k}\cdot\hat{c}_i) \right\rangle_{n+1}^{\mathrm{P}}. \tag{2.2}$$

Here, hatted vectors denote replicated collections of (d-dimensional) vectors, viz., $\hat{v}\equiv(\mathbf{v}^0,\mathbf{v}^1,\ldots,\mathbf{v}^n)$, their scalar product being $\hat{v}\cdot\hat{w}\equiv\Sigma_{\alpha=0}^{n}\mathbf{v}^\alpha\cdot\mathbf{w}^\alpha$, and $\langle\cdots\rangle_{n+1}^{\mathrm{P}}$ denotes an average for an effective pure (i.e., disorder-free) system of $n+1$ coupled replicas of the original system. We use the terms *one-replica sector* (1rs) and *higher replica sector* (hrs) to refer to replicated vectors with, respectively, exactly one and more than one replica α for which the corresponding vector $\mathbf{k}^\alpha$ is nonzero.

In the Landau theory the order parameter in the one-replica sector represents spatial variations in the disorder-averaged mean particle density, and is always assumed to be strictly zero.

In the stationary point approximation, the disorder-averaged free energy f (per particle and space dimension) is given by[6,16,17]

$$f = \lim_{n\to 0} \min_{\{\Omega_{\hat{k}}\}} \mathcal{F}_n(\{\Omega_{\hat{k}}\}), \tag{2.3}$$

with the Landau free-energy functional given by

$$nd\mathcal{F}_n(\{\Omega_{\hat{k}}\}) = \sum_{\hat{k}}{}' \left(-\epsilon + \frac{|\hat{k}|^2}{2} \right) |\Omega_{\hat{k}}|^2 - \sum_{\hat{k}_1\hat{k}_2\hat{k}_3}{}' \Omega_{\hat{k}_1}\Omega_{\hat{k}_2}\Omega_{\hat{k}_3}\delta_{\hat{k}_1+\hat{k}_2+\hat{k}_3,\hat{0}}. \tag{2.4}$$

Here ϵ is the control parameter, and is proportional to the amount by which the constraint density exceeds its value at the transition. The symbol $\overline{\Sigma}$ denotes a sum over replicated wave vectors $\hat{k}$ in the higher replica sector.

For $\epsilon<0$, the stationary point equations for the free-energy functional of Eq. (2.4) only have the solution $\overline{\Omega}_{\hat{k}} = \delta_{\hat{k},\hat{0}}$, corresponding to the liquid state. For $\epsilon>0$, there are two solutions, one ($\overline{\Omega}_{\hat{k}} = \delta_{\hat{k},\hat{0}}$) corresponding to the liquid state and a second one corresponding to an amorphous solid state, given by

$$\overline{\Omega}_{\hat{k}} = (1-q)\,\delta_{\hat{k},\hat{0}} + q\,\delta_{\tilde{\mathbf{k}},\mathbf{0}}\,\omega(\sqrt{2\hat{k}^2/\epsilon}),$$

$$q = 2\epsilon/3,$$

$$\omega(k) = \int_0^\infty d\theta\,\pi(\theta) e^{-k^2/2\theta}. \tag{2.5}$$

Here, the quantity q is the ratio of the number of localized particles to the total number of particles (i.e., the *localized fraction*), $\pi(\theta)$ is a universal scaling function that characterizes the distribution $p(1/\xi^2)$ of the (inverse square) localization lengths ξ for the localized particles, through $p(1/\xi^2) = (2/\epsilon)\,\pi(2/\epsilon\xi^2)$, and we use the definition $\tilde{\mathbf{k}} \equiv \Sigma_{\alpha=0}^{n} \mathbf{k}^\alpha$. The factor $\delta_{\tilde{\mathbf{k}},\mathbf{0}}$ encodes the property of macroscopic translation invariance (MTI) for the amorphous solid state, i.e., the fact that the state is invariant under common translations of all the replicas, or, in more physical terms, that the particles are localized around randomly located points that have a homogeneous probability of being found anywhere in the volume of the system. The scaling function $\pi(\theta)$ satisfies the stationarity condition

$$\frac{\theta^2}{2}\frac{d\pi}{d\theta} = (1-\theta)\,\pi(\theta) - \int_0^\theta d\theta'\,\pi(\theta')\,\pi(\theta-\theta'), \tag{2.6}$$

together with the normalization condition

$$1 = \int_0^\infty d\theta\,\pi(\theta). \tag{2.7}$$

This normalization condition directly follows from the fact that the order parameter of Eq. (2.2) has to be unity at the origin of replicated wave-vector space.[3,4] It is worth noticing that in the limit $\epsilon \to 0$ the above parametrization of $\overline{\Omega}$ reduces continuously to the order parameter $\overline{\Omega}_{\hat{k}} = \delta_{\hat{k},\hat{0}}$ for the liquid state, as it should.

Let us now discuss the symmetry properties of the Landau free-energy functional. Under independent translations of all the replicas, i.e., $\mathbf{c}_i^\alpha \to \mathbf{c}_i^\alpha + \mathbf{a}^\alpha$, the replica order parameter, Eq. (2.2), transforms as

$$\Omega_{\hat{k}} \to \Omega'_{\hat{k}} = e^{i\hat{k}\cdot\hat{a}}\,\Omega_{\hat{k}}. \tag{2.8}$$

For later reference, let us calculate the change in the order parameter for the case of small displacements of the replicas:

$$\delta\Omega_{\hat{k}} \equiv \Omega'_{\hat{k}} - \Omega_{\hat{k}} = i\,\hat{k}\cdot\hat{a}\,\Omega_{\hat{k}} + \mathcal{O}(a^2). \tag{2.9}$$

Under independent rotations of the replicas, defined by $\mathbf{c}_i^\alpha \to \mathbf{c}'^{\alpha}_i = R^\alpha \mathbf{c}_i^\alpha$, and $\hat{R}\hat{v} \equiv \{R^0\mathbf{v}^0, \ldots, R^n\mathbf{v}^n\}$, where each R^α is a rotation matrix in d dimensions, the order parameter transforms as

$$\Omega_{\hat{k}} \to \Omega'_{\hat{k}} = \Omega_{\hat{R}^{-1}\hat{k}}. \tag{2.10}$$

By inserting the transformed order parameter for either of the above operations into the free-energy functional Eq. (2.4), we see that in both cases

$$nd\mathcal{F}_n(\{\Omega'_{\hat{k}}\}) = nd\mathcal{F}_n(\{\Omega_{\hat{k}}\}), \tag{2.11}$$

i.e., that the Landau free energy is invariant under *independent* translations and rotations of the replicas.

Anticipating the conclusions of this paper, that the liquid state, which becomes unstable when ϵ is increased through zero, is replaced by a stable amorphous solid state for $\epsilon>0$, we now pause to compare some aspects of this phase transition with their counterparts in simple models of the paramagnet-to-ferromagnet phase transitions [e.g., the $O(N)$ symmetric vector ϕ^4 model]. We shall refer to Fourier components of fields as *modes*, and shall consider the mean-field level of description. At high temperatures (for magnetism) and low constraint densities (for amorphous solidification) the equilibrium value of all modes is zero. As the relevant control parameter is changed through its critical value, a band of modes, including those of the longest wavelength, become linearly unstable, the longer the wavelength the stronger the instability. In both settings, magnetism and amorphous solidification, stability is recovered by the acquisition of a nonzero equilibrium value by one or more of the modes. For magnetism, there is a *zero* wave-vector mode, which is the most unstable mode, and by giving it the appropriate nonzero equilibrium value, this mode *and all others* are restabilized (i.e., are no longer *un*stable, as discussed below, there should and does remain one marginally stable Goldstone mode). For amorphous solidification, restabilization is more intricate. There is no fluctuating zero wave-vector mode in the theory to be given a nonzero equilibrium value. Instead, the most unstable modes have the smallest allowed nonzero wave vectors. If these modes become nonzero, as some of them do, there is no symmetry dictated ''selection rule'' prohibiting them from acting as ''sources'' for certain other modes, and thus not just one but a large family of modes become nonzero, not only including modes that were formerly unstable. (This may be regarded as an analog of domain-wall formation in wave-vector space.) There is one further subtlety to the amorphous solidification case: to give a nonzero equilibrium value to modes that reside in the one replica sector would be extremely energetically costly and, from the viewpoint of the Landau theory, is ruled out (via an implicit linear constraint on the order parameter). This requirement is satisfied by giving a nonzero equilibrium value only to modes that are MTI, because such modes are prohibited, on symmetry grounds, from acting as sources for modes in the one replica sector. Thus stability is restored not by giving one unstable mode a nonzero value, and not by giving only the unstable modes a nonzero value, but by giving a sheet of modes (some unstable and some stable) a nonzero value.

B. Hessian matrix elements

Consider any variation $\{\delta\Omega_{\hat{k}}\}$ of the $\{\Omega_{\hat{k}}\}$ around a stationary point $\{\overline{\Omega}_{\hat{k}}\}$. To first order in $\{\delta\Omega_{\hat{k}}\}$, the variation of the free-energy functional is, of course, zero. We see from Eq. (2.4) that the second order variation is[18]

$$\delta^{(2)}[nd\mathcal{F}_n(\{\Omega_{\hat{k}}\})]=\overline{\sum_{\hat{k}}}\left(-\epsilon+\frac{|\hat{k}|^2}{2}\right)|\delta\Omega_{\hat{k}}|^2-3\times\overline{\sum_{\hat{k}_1\hat{k}_2\hat{k}_3}}\delta_{\hat{k}_1+\hat{k}_2+\hat{k}_3,\hat{0}}\,\overline{\Omega}_{\hat{k}_1}\delta\Omega_{\hat{k}_2}\delta\Omega_{\hat{k}_3}. \tag{2.12}$$

Now consider expanding around the liquid state for any value of ϵ. In this case, the second variation reduces to

$$\delta^{(2)}[nd\mathcal{F}_n(\{\Omega_{\hat{k}}\})]=\overline{\sum_{\hat{k}}}\left(-\epsilon+\frac{|\hat{k}|^2}{2}\right)|\delta\Omega_{\hat{k}}|^2, \tag{2.13}$$

which evidently indicates that the liquid is stable for $\epsilon<0$ and unstable for $\epsilon>0$. For $\epsilon>0$ the only candidate we know of for a stable thermodynamic state is the amorphous solid. From now on we focus only on that state.

By inserting the value of the order parameter, Eq. (2.5), into the three wave-vector sum in Eq. (2.12), we obtain

$$\begin{aligned}&\overline{\sum_{\hat{k}_1\hat{k}_2\hat{k}_3}}\delta_{\hat{k}_1+\hat{k}_2+\hat{k}_3,\hat{0}}\delta_{\tilde{\mathbf{k}}_1,\mathbf{0}}\frac{2\epsilon}{3}\omega(\sqrt{2\hat{k}_1^2/\epsilon})\delta\Omega_{\hat{k}_2}\delta\Omega_{\hat{k}_3}\\&=\overline{\sum_{\hat{k}_2\hat{k}_3}}\delta_{\tilde{\mathbf{k}}_2+\tilde{\mathbf{k}}_3,\mathbf{0}}\frac{2\epsilon}{3}\omega\left(\sqrt{\frac{2}{\epsilon}(\hat{k}_2+\hat{k}_3)^2}\right)\delta\Omega_{\hat{k}_2}\delta\Omega_{\hat{k}_3}\\&\quad-\frac{2\epsilon}{3}\overline{\sum_{\hat{k}}}|\delta\Omega_{\hat{k}}|^2.\end{aligned} \tag{2.14}$$

Thus we can rewrite the second variation in terms of the Hessian matrix $H_{\hat{q},\hat{q}'}$:

$$\delta^{(2)}[nd\mathcal{F}_n(\{\Omega_{\hat{q}}\})]=\overline{\sum_{\hat{q},\hat{q}'}}H_{\hat{q},\hat{q}'}\delta\Omega_{\hat{q}}\delta\Omega_{-\hat{q}'}, \tag{2.15}$$

where we have defined $H_{\hat{k},\hat{l}}$ by

$$H_{\hat{k},\hat{l}}\equiv\frac{1}{2!}\frac{\delta^2[nd\mathcal{F}_n]}{\delta\Omega_{\hat{k}}\delta\Omega_{-\hat{l}}}. \tag{2.16}$$

(For later convenience, we have chosen a definition that differs from the standard one by a factor of 1/2.) More explicitly, we have

$$H_{\hat{k},\hat{l}}=\delta_{\hat{k},\hat{l}}\left(\epsilon+\frac{\hat{k}^2}{2}\right)-\delta_{\tilde{\mathbf{k}},\tilde{\mathbf{l}}}2\epsilon\int_0^\infty d\theta\,\pi(\theta)e^{-(\hat{k}-\hat{l})^2/\epsilon\theta}+\mathcal{O}(\epsilon^2). \tag{2.17}$$

As it is adequate to be concerned with matrix elements to leading (i.e., first) order in ϵ, we shall neglect higher orders from now on.

C. Change of basis

In order to simplify the diagonalization of the Hessian, we are going to exploit the symmetries of the problem. As a direct consequence of the invariance of the free-energy functional under translations and the MTI property of the amorphous solid state, the matrix element $H_{\hat{k},\hat{l}}$ of the Hessian only connects wave vectors $\hat{k}$ and $\hat{l}$ such that $\tilde{\mathbf{k}}=\tilde{\mathbf{l}}$. This already reduces the complexity of the problem by making the Hessian block diagonal.

As $H_{\hat{k},\hat{l}}$ depends on $\hat{k}^2$, $\hat{l}^2$, and $\hat{k}\cdot\hat{l}$, one might expect to find a symmetry under arbitrary rotations in $(n+1)d$ dimensions, which would simplify the diagonalization of the Hessian still further. However, the factor $\delta_{\tilde{\mathbf{k}},\tilde{\mathbf{l}}}$ is not invariant under some of those rotations. Instead, H only displays a rotational symmetry in nd dimensions, but this will enable us to simplify the task in much the same way as is commonly done for central potentials in quantum mechanics.

In order to make this symmetry explicit, we choose a *fixed* matrix $T\in SO[(1+n)d]$ such that for any vector $\hat{v}$ in replicated space we explicitly isolate $\tilde{\mathbf{v}}$ from the other nd independent coordinates, which we call $\check{v}$:

$$T\hat{v}=\begin{pmatrix}\dfrac{\tilde{\mathbf{v}}}{\sqrt{1+n}}\\ \check{v}\end{pmatrix}. \tag{2.18}$$

Due to T being orthogonal, scalar products remain simple in the new coordinates:

$$\hat{v}\cdot\hat{w}=\frac{\tilde{\mathbf{v}}\cdot\tilde{\mathbf{w}}}{1+n}+\check{v}\cdot\check{w}. \tag{2.19}$$

In the new coordinates, we have

$$H_{\tilde{\mathbf{k}}\check{k},\,\tilde{\mathbf{l}}\check{l}}=\delta_{\tilde{\mathbf{k}},\tilde{\mathbf{l}}}\left\{\delta_{\check{k},\check{l}}\left[\epsilon+\frac{1}{2}\left(\check{k}^2+\frac{\tilde{\mathbf{k}}^2}{1+n}\right)\right]-2\epsilon\int_0^\infty d\theta\,\pi(\theta)e^{-(\check{k}-\check{l})^2/\epsilon\theta}\right\}. \tag{2.20}$$

This expression, taken naively, would immediately tell us that the Hessian is invariant under rotations in nd dimensions:

$$\forall\check{R}\in SO(nd):\quad H_{\tilde{\mathbf{k}}\check{R}\check{k},\,\tilde{\mathbf{l}}\check{R}\check{l}}=H_{\tilde{\mathbf{k}}\check{k},\,\tilde{\mathbf{l}}\check{l}}. \tag{2.21}$$

However, there is an important caveat. Our Hessian is only defined for wave vectors in the higher replica sector, but the proposed rotations can take a vector in the higher replica sector and transform it into a vector in the one-replica sector. For the moment we are going to ignore this difficulty, and simply diagonalize the matrix obtained by using Eq. (2.17) as its definition, with $\hat{k}$ and $\hat{l}$ taking *any* nonzero values, both in the higher and in the one-replica sector. (This enlarged Hessian matrix will be termed the ''extended Hessian'' to distinguish it from the ''original Hessian'' which does not have those additional matrix elements; see Fig. 1.) After having diagonalized the extended Hessian, we will return to the issue of the one-replica sector. For the moment, let us just

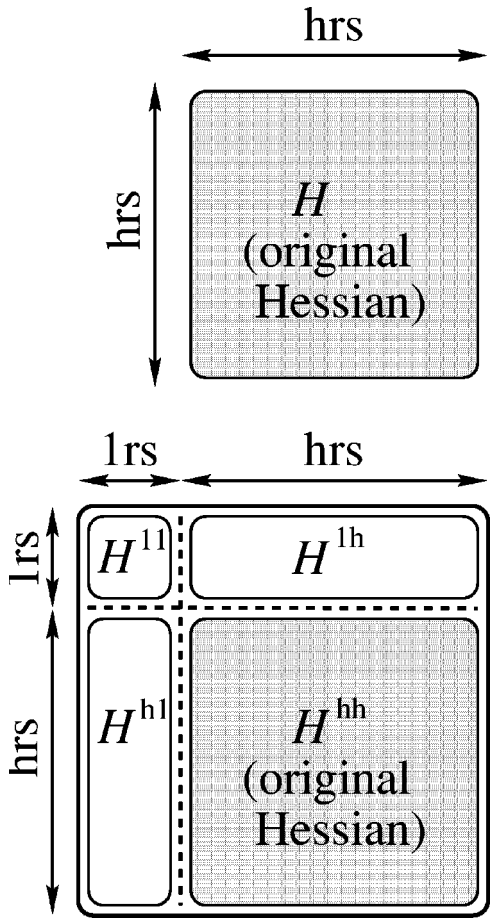

FIG. 1. Comparison of the original Hessian matrix (upper figure) and the extended Hessian matrix (lower figure). The extended Hessian matrix is depicted as being formed by four blocks, respectively connecting: the 1rs with itself (labeled H^{11}), the 1rs with the hrs (labeled H^{1h}), the hrs with the 1rs (labeled H^{h1}), and the hrs with the hrs (labeled H^{hh}). The block H^{hh} corresponds exactly to the original Hessian.

anticipate that, in the replica limit $n\to 0$, the only effect of this extension of the Hessian on its spectrum of eigenvalues will be the addition of one spurious eigenvalue, corresponding to a fluctuation localized in the one-replica sector.

For the modified problem of diagonalizing the extended Hessian, the $SO(nd)$ symmetry holds, and Eq. (2.21) is correct without caveat. In what follows, we will use the same strategies as in the diagonalization of a quantum-mechanical Hamiltonian for a particle in a central potential. The role of the Hamiltonian will be played by $H_{\hat{k},\hat{l}}$. We will also exploit the symmetries of the problem: the rotational symmetry in nd-dimensional space will allow us to write each eigenfunction as a product of a radial part, which will be obtained by solving a one-dimensional eigenvalue equation, and an angular part, which will simply be a surface harmonic function[19] in nd dimensions. The quantity $\tilde{\mathbf{k}}$, which is exactly conserved by $H_{\hat{k},\hat{l}}$, will play the role of a conserved quantum number. We will obtain distinct sets of eigenfunctions for each fixed value of $\tilde{\mathbf{k}}$.

We are going to work in the Hilbert space of complex functions of the variable $\hat{k}(\neq\hat{0})$. We exclude the origin because we are interested in fluctuations of the order parameter, and $\Omega_{\hat{0}}$ cannot fluctuate. We define the scalar product in this space as follows:

$$\langle f|g\rangle \equiv \frac{1}{V^n}\sum_{\hat{k}\neq\hat{0}} f^*(\hat{k})g(\hat{k}), \tag{2.22}$$

which simplifies, in the thermodynamic limit, to[21]

$$\begin{aligned}\langle f|g\rangle &\simeq V\int \frac{d\hat{k}}{(2\pi)^{(1+n)d}} f^*(\hat{k})g(\hat{k})\\ &= V\int \frac{d\tilde{\mathbf{k}}\,d\check{k}}{(1+n)^{d/2}(2\pi)^{(1+n)d}} f^*(\tilde{\mathbf{k}},\check{k})g(\tilde{\mathbf{k}},\check{k}).\end{aligned} \tag{2.23}$$

We define a basis set for this Hilbert space by

$$\begin{aligned}\varphi_{p\tilde{\mathbf{p}}\sigma}(\tilde{\mathbf{k}},\check{k}) \equiv (1+n)^{d/4}(2\pi)^{nd/2}\delta_{\tilde{\mathbf{p}},\tilde{\mathbf{k}}}\delta(|\check{k}|-p)\\ \times p^{(1-nd)/2}S_\sigma(\phi_{\check{k}}),\end{aligned} \tag{2.24}$$

Here $\{S_\sigma(\phi)\}$ are the normalized surface harmonic functions defined on the unit sphere in nd-dimensional space,[19] $\tilde{\mathbf{p}}$ is any wave vector in d dimensions, and p is any positive number. [Surface harmonics are homogeneous trigonometric polynomials, they are generalizations of spherical harmonics to any space dimension $d\geqslant 3$. The label σ is a set of integers that characterize the appropriate trigonometric polynomial: for example, for $d=3$, the surface harmonics are the usual spherical harmonics, and $\sigma\equiv(l,m)$, with l the degree of the trigonometric polynomial and m a label that distinguishes between polynomials of the same degree.] The notation $\phi_{\check{k}} \equiv \check{k}/|\check{k}|$ denotes the unit nd-dimensional vector along the direction of $\check{k}$. The elements of the basis set $\{\varphi_{p\tilde{\mathbf{p}}\sigma}\}$ are orthogonal and normalized under the scalar product Eq. (2.22):

$$\langle \varphi_{p'\tilde{\mathbf{p}}'\sigma'}|\varphi_{p\tilde{\mathbf{p}}\sigma}\rangle = \delta(p'-p)\,\delta_{\tilde{\mathbf{p}}',\tilde{\mathbf{p}}}\,\delta_{\sigma',\sigma}. \tag{2.25}$$

As suggested above, we propose to express each eigenfunction for the problem in the form

$$\begin{aligned}\psi_{r\tilde{\mathbf{p}}\sigma}(\tilde{\mathbf{k}},\check{k}) &= (1+n)^{d/4}(2\pi)^{nd/2}\\ &\quad\times\delta_{\tilde{\mathbf{p}},\tilde{\mathbf{k}}}|\check{k}|^{(1-nd)/2}R_r(|\check{k}|)\,S_\sigma(\phi_{\check{k}}),\\ &= \int_0^\infty dp\,R_r(p)\,\varphi_{p\tilde{\mathbf{p}}\sigma}(\tilde{\mathbf{k}},\check{k}),\end{aligned} \tag{2.26}$$

where the discrete δ function ensures that the eigenfunction is localized on points with a fixed value of $\tilde{\mathbf{k}}$, the surface harmonic S_σ gives the angular dependence on $\check{k}$, and the radial function R_r gives the radial dependence on $\check{k}$. By using the normalization condition for the basis set, we obtain the normalization condition for the radial part:

$$\int_0^\infty dk|R_r(k)|^2 = 1. \tag{2.27}$$

We now compute the matrix elements of the Hessian between the elements of the basis set $\{\varphi_{p\tilde{\mathbf{p}}\sigma}\}$.

Consider first the part H^D of the Hessian that is diagonal in $\check{k}$, i.e., the first term on the right-hand side (rhs) of Eq. (2.20). This part is also diagonal in the basis $\{\varphi_{p\tilde{\mathbf{p}}\sigma}\}$, with the matrix elements

$$\langle \varphi_{p'\tilde{\mathbf{p}}'\sigma'}|H^D|\varphi_{p\tilde{\mathbf{p}}\sigma}\rangle = \delta(p'-p)\,\delta_{\tilde{\mathbf{p}}',\tilde{\mathbf{p}}}\delta_{\sigma',\sigma} \times\left[\epsilon+\frac{1}{2}\left(\check{p}^2+\frac{\tilde{\mathbf{p}}^2}{1+n}\right)\right]. \quad (2.28)$$

The nondiagonal part H^O of the Hessian, given by the second term on the rhs of Eq. (2.20), has, in the new basis, matrix elements that only connect different values of the radial coordinate p but are still diagonal in $\tilde{\mathbf{p}}$ and σ. It is shown in Appendix A that the matrix elements of H^O have the form

$$\langle \varphi_{p'\tilde{\mathbf{p}}'\sigma'}|H^O|\varphi_{p\tilde{\mathbf{p}}\sigma}\rangle = \delta_{\tilde{\mathbf{p}}',\tilde{\mathbf{p}}}\delta_{\sigma',\sigma}(-2\epsilon)\,\epsilon^{-1/2}C_n \times \eta^{(n)}_{|\sigma|}(p'/\sqrt{\epsilon},p/\sqrt{\epsilon}), \quad (2.29)$$

with

$$C_n \equiv (\epsilon/4\pi)^{nd/2}(1+n)^{-d/2} \quad (2.30)$$

and

$$\eta^{(n)}_l(x',x) \equiv 2\sqrt{x'x} \times\int_0^\infty \frac{d\theta\,\pi(\theta)}{\theta^{1-nd/2}} e^{-(x'^2+x^2)/\theta} I_{l-1+nd/2}\left(\frac{2x'x}{\theta}\right), \quad (2.31)$$

where $I_\nu(x)$ is the modified Bessel function of order ν. The label $l(\equiv|\sigma|)$ indicates the degree of the surface harmonic S_σ as a trigonometric polynomial. The constant C_n satisfies the condition

$$\lim_{n\to 0} C_n = 1, \quad (2.32)$$

via which it disappears from the eigenvalue equation in the replica limit. The kernel $\eta^{(n)}_l(x',x)$ is real and symmetric, and controls the nondiagonal nature of the matrix elements. Due to the positivity of $I_\nu(y)$ for $\nu \geqslant -1$ and $y>0$, the kernel $\eta^{(n)}_l(x',x)$ is positive for $xx'>0$. For $xx'\to 0^+$, $\eta^{(n)}_l(x',x)$ vanishes, except if $l=0$ and $nd>0$, in which case it is divergent.

As both H^D and H^O are diagonal on the $\tilde{\mathbf{p}}$ and σ labels, the eigenvalue equation for the Hessian,

$$H|\psi\rangle = \kappa|\psi\rangle, \quad (2.33)$$

can now be simplified to a radial equation:

$$\kappa R(p) = \int_0^\infty dp'\,\langle \varphi_{p\tilde{\mathbf{p}}\sigma}|H|\varphi_{p'\tilde{\mathbf{p}}\sigma}\rangle R(p'),$$

$$= \left[\epsilon+\frac{1}{2}\left(p^2+\frac{\tilde{\mathbf{p}}^2}{1+n}\right)\right]R(p) - 2\,\epsilon\,C_n\int_0^\infty \frac{dp'}{\sqrt{\epsilon}}\,\eta^{(n)}_{|\sigma|}(p/\sqrt{\epsilon},p'/\sqrt{\epsilon})R(p'). \quad (2.34)$$

This radial equation can be simplified further by the rescaling

$$\zeta = \frac{1}{\epsilon}\left[\kappa-\left(\epsilon+\frac{\tilde{\mathbf{p}}^2}{2(1+n)}\right)\right], \quad (2.35a)$$

$$x = p/\sqrt{\epsilon},\quad u(x) = \epsilon^{1/4}R(\sqrt{\epsilon}x), \quad (2.35b)$$

which removes the ϵ dependence from the eigenvalue equation, thus making both the eigenvalue ζ and the eigenfunction $u(x)$ ϵ-independent and obeying

$$\zeta u(x) = \frac{x^2}{2}u(x) - 2\,C_n\int_0^\infty dx'\,\eta^{(n)}_{|\sigma|}(x,x')u(x'). \quad (2.36)$$

In the replica limit, $n\to 0$, this radial equation reduces to

$$\zeta u(x) = \frac{x^2}{2}u(x) - 2\int_0^\infty dx'\,\eta^{(0)}_{|\sigma|}(x,x')u(x'). \quad (2.37)$$

For all cases except $|\sigma|=0$ this limit is straightforward, because $\eta^{(n)}_{|\sigma|}(x,x')$ smoothly converges to $\eta^{(0)}_{|\sigma|}(x,x')$. For the special case of $|\sigma|=0$, the limit $n\to 0$ for $\eta^{(n)}_{|\sigma|}(x,x')$ is singular near the origin. Let us mention here a property of Eq. (2.37) that does *not* apply to Eq. (2.36). As $I_{-1}(z) = I_1(z)$ for all values of the variable z, we have the equality

$$\eta^{(0)}_0(x,x') = \eta^{(0)}_2(x,x'), \quad (2.38)$$

which means that the radial Eq. (2.37) is the same for $|\sigma|=0$ and for $|\sigma|=2$. In Sec. III C we discuss in more detail the relations between the solutions to Eqs. (2.36) and (2.37).

Both radial equations, Eqs. (2.36) and (2.37), are eigenvalue equations for Hermitian operators. This guarantees the existence of a complete orthonormal basis of eigenfunctions, all of them having real eigenvalues. Notice also the nontrivial fact that the radial equation is well defined in the replica limit $n\to 0$.

The form of the radial eigenvalue equation tells us that the radial eigenfunction and the eigenvalue depend on the degree $l=|\sigma|$ of the surface harmonic considered (which plays a role analogous to that of the total angular momentum quantum number l in the central potential problem for a quantum-mechanical particle), and on an additional label r, playing a role analogous to the radial quantum number in quantum mechanics. Therefore the eigenvalues of the extended Hessian are given by the relation

$$\kappa_{lr}(\tilde{\mathbf{k}}) = (1+\zeta_{lr})\epsilon + \frac{\tilde{\mathbf{k}}^2}{2}. \quad (2.39)$$

As it is easier to work with scaled variables, let us express the condition that there be no unstable fluctuation directions (i.e., $\kappa \geqslant 0$) in terms of ζ:

$$\kappa_{lr}(\tilde{\mathbf{k}})>0 \quad \forall\tilde{\mathbf{k}} \Leftrightarrow \zeta_{lr}+1>0. \quad (2.40)$$

The right-hand side of the equivalence sign is the condition that we are going to establish in what follows.

III. LANDAU THEORY: EIGENVALUES OF THE HESSIAN

In this section we are going to establish positive lower bounds for all the eigenvalues of the Hessian of the Landau

theory, except for the zero mode associated with the spontaneously broken translational symmetry. In other words, we study the set $\mathcal{S}_o$ containing the limits, when $n\to 0$, of the eigenvalues of the *original* Hessian. However, for technical reasons, it is convenient to first study two other sets of numbers, denoted by $\mathcal{S}_e$ and $\mathcal{S}_r$. $\mathcal{S}_e$ is the set containing the $n\to 0$ limits of the eigenvalues of the *extended* Hessian; each element in $\mathcal{S}_e$ can be written in the form given by Eq. (2.39), where ζ_{lr} is taken to be the $n\to 0$ limit of an eigenvalue in Eq. (2.36). $\mathcal{S}_r$ is the set containing all numbers $\kappa_{lr}(\tilde{\mathbf{k}})$ computed according to Eq. (2.39), with ζ_{lr} chosen to be an eigenvalue in the *radial* Eq. (2.37).

In Sec. III A we show that $\mathcal{S}_r$ contains a zero element corresponding to the zero mode associated with the spontaneously broken translational symmetry. In Sec. III B we compute positive lower bounds for all other elements of $\mathcal{S}_r$. In Sec. III C, we show that the only difference between the limit for $n\to 0$ of the eigenvalue spectrum of Eq. (2.36) and the eigenvalue spectrum of Eq. (2.37) is that in the former a spurious eigenvalue corresponding to fluctuations in the 1rs appears, which is not present in the latter. Therefore the spectrum $\mathcal{S}_e$ of the extended Hessian contains a spurious eigenvalue not present in $\mathcal{S}_r$. We also show, in Sec. III C, that the eigenvectors of the original Hessian correspond to all the eigenvectors of the extended Hessian, except the spurious one, i.e., that $\mathcal{S}_o$ and $\mathcal{S}_r$ are identical. Using the results obtained in Secs. III A and III B, this will allow us to conclude that the amorphous solid state is locally stable.

A. Obtaining the zero mode

We first consider a generic eigenfluctuation associated with the translational symmetry, and show that it is a zero mode. From Eq. (2.9), we see that this fluctuation can be written as

$$\delta\Omega_{\hat{k}} = i\hat{k}\cdot\hat{a}\,(2\epsilon/3)\,\delta_{\tilde{\mathbf{k}},\mathbf{0}}\int_0^\infty d\theta\,\pi(\theta)e^{-\hat{k}^2/\epsilon\theta}$$

$$= i\check{k}\cdot\check{a}\,(2\epsilon/3)\,\delta_{\tilde{\mathbf{k}},\mathbf{0}}\int_0^\infty d\theta\,\pi(\theta)e^{-\check{k}^2/\epsilon\theta}. \qquad (3.1)$$

The only angular dependence of $\delta\Omega_{\hat{k}}$ is given by the prefactor $\check{k}\cdot\check{a}$, which is a degree-one polynomial in $\check{k}$. This guarantees that this fluctuation resides in the $|\sigma|=1$ sector. By taking the scalar product with the appropriate element in the basis $\{\varphi_{p\tilde{\mathbf{p}}\sigma}\}$ [which we label by $\sigma=(1,0)$ by analogy to the spherical harmonic $Y_{10}\propto z/r$], we obtain the radial function associated with $\delta\Omega_{\hat{k}}$:

$$R(k) = \langle\varphi_{p,\tilde{\mathbf{p}}=\mathbf{0},\sigma=(1,0)}|\,\delta\Omega\rangle,$$

$$= iA_n\epsilon\,k^{(1+nd)/2}\int_0^\infty d\theta\,\pi(\theta)e^{-k^2/\epsilon\theta}, \qquad (3.2)$$

where A_n is a numerical prefactor, which we can ignore in what follows. Taking the replica limit, and transforming to scaled variables, we obtain the scaled radial function

$$u(x) = \sqrt{x}\int_0^\infty d\theta\,\pi(\theta)e^{-x^2/\theta}. \qquad (3.3)$$

In Appendix (B) we show by explicit computation that this form for $u(x)$ satisfies Eq. (2.37) with $\zeta=-1$. By Eq. (2.39), this means that the corresponding $\delta\Omega_{\hat{k}}$ given by Eq. (3.1) is an eigenvector of the Hessian with zero eigenvalue. [As $\delta\Omega_{\hat{k}}$ given by Eq. (3.1) is only nonzero for $\hat{k}$ in the hrs because otherwise $\check{k}=\check{0}$, it is simultaneously an eigenvector of the extended Hessian and of the original Hessian.]

It will be shown in the next section that the radial eigenfunction of Eq. (3.3) is the *only* one that gives rise to zero modes. Since any of the *nd* linearly independent surface harmonics of degree 1 can be chosen as the angular part of the eigenvector, there are exactly *nd* independent zero modes. (However, since we will be mostly discussing the radial equation, we will talk about the ''zero mode'' and not the ''zero modes.'')

B. Positive lower bounds for the eigenvalues

Having obtained the zero mode for a specific form of fluctuation, we now discuss generic fluctuations in the order-parameter field, and show that all the other eigenvalues are positive-definite. For the case $l\neq 1$, we will obtain positive lower bounds for the eigenvalues by analytical manipulation of Eq. (2.37). For the case $l=1$, we will solve Eq. (2.37) numerically and show explicitly that the lowest eigenvalue corresponds to the zero mode already obtained, and that all other eigenvalues correspond to positive values of $\kappa(\tilde{\mathbf{k}})$.

Consider one particular scaled radial eigenfunction $u(x)$ in Eq. (2.37), with eigenvalue ζ. To simplify the argument we temporarily switch to the normalization

$$\int_0^\infty dx|u(x)| = 1, \qquad (3.4)$$

and we define the quantity

$$s(x) \equiv \mathrm{sgn}(u(x)). \qquad (3.5)$$

In what follows, we express the eigenvalue ζ in an unusual but convenient form that allows a lower bound to be derived from it. By combining the eigenvalue Eq. (2.37), with the normalization condition (3.4) and the definition (3.5), we obtain

$$\zeta = \zeta\int_0^\infty dx|u(x)|$$

$$= \int_0^\infty dx\,s(x)\zeta\,u(x)$$

$$= \int_0^\infty dx\,s(x)\left[\frac{x^2}{2}u(x) - 2\int_0^\infty dx'\,\eta^{(0)}_{|\sigma|}(x,x')u(x')\right]$$

$$= \int_0^\infty dx\,\frac{x^2}{2}|u(x)| - 2\int_0^\infty dx\,dx'$$

$$\times\,\eta^{(0)}_{|\sigma|}(x',x)|u(x)|s(x)s(x'). \qquad (3.6)$$

(In the last line we have interchanged the dummy variables x and x'.) From the expression just derived for the eigenvalue ζ, it follows from the non-negativity of $\eta^{(0)}_{|\sigma|}(x',x)$ that

$$\zeta \geqslant \int_0^\infty dx\ \gamma_{|\sigma|}(x)|u(x)| \geqslant \overline{\gamma}_{|\sigma|}, \tag{3.7a}$$

$$\gamma_l(x) \equiv \frac{x^2}{2} - 2\int_0^\infty dx'\ \eta^{(0)}_l(x',x), \tag{3.7b}$$

$$\overline{\gamma}_l \equiv \inf_x \gamma_l(x). \tag{3.7c}$$

Here, the symbol inf indicates the greatest lower bound[22] for a set of real numbers.

It is convenient to write $\gamma_l(x)$ in terms of another function $\beta_l(v)$, as follows:

$$\gamma_l(x) = \int_0^\infty d\theta\ \pi(\theta)\beta_l(x/\sqrt{\theta}), \tag{3.8a}$$

$$\beta_l(v) \equiv \frac{v^2}{2\langle\theta^{-1}\rangle_\pi} - 4\int_0^\infty du\ \sqrt{uv}e^{-(u^2+v^2)}I_{l-1}(2uv). \tag{3.8b}$$

Here, we have used the definition of an average with respect to the distribution π,

$$\langle f(\theta)\rangle_\pi \equiv \int_0^\infty d\theta\ \pi(\theta)f(\theta), \tag{3.9}$$

and we need, in particular, the numerical value

$$\langle\theta^{-1}\rangle_\pi \approx 0.881\,768, \tag{3.10}$$

which can be obtained by using the function $\pi(\theta)$ of Ref. 3. As $\pi(\theta)$ is non-negative and normalized to unity, Eq. (3.8a) implies that

$$\zeta \geqslant \overline{\gamma}_{|\sigma|} \geqslant \overline{\beta}_{|\sigma|}, \tag{3.11}$$

where

$$\overline{\beta}_l \equiv \inf_v \beta_l(v). \tag{3.12}$$

The bounds for different values of the index l are not independent. In fact, because $I_l(x) < I_{l-1}(x)$ for $x > 0$ and $l \geqslant 1$, we have the inequality $\eta^{(0)}_{l+1}(x,x') < \eta^{(0)}_l(x,x')$ for $xx' > 0$ and $l \geqslant 1$, and from this inequality it follows that all the bounds defined so far [$\gamma_l(x)$, $\overline{\gamma}_l$, $\beta_l(v)$, and $\overline{\beta}_l$] are *increasing* functions of l for $l \geqslant 1$. Thus if we obtain a positive lower bound for one value of $l \geqslant 1$, the same bound applies for all larger values of l.

In order to obtain more concrete results, we need an explicit expression for $\beta_l(v)$. In Appendix (C) we obtain the exact expression

$$\beta_l(v) = \frac{v^2}{2\langle\theta^{-1}\rangle_\pi} - 2\frac{\Gamma(l/2+1/4)}{\Gamma(l)}v^{l-1/2}M\left(\frac{l}{2}-\frac{1}{4}, l, -v^2\right), \tag{3.13a}$$

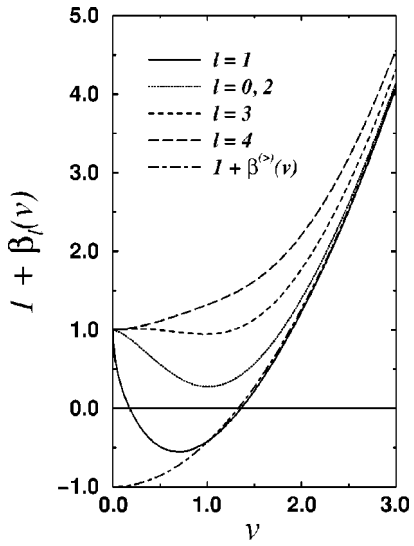

FIG. 2. Plot of $1+\beta_l(v)$ (for $0 \leqslant l \leqslant 4$) and $1+\beta^{(>)}(v)$ as functions of v.

along with the asymptotic forms $\beta^{(>)}(v)$ and $\beta^{(<)}(v)$, given by

$$\beta_l(v) \sim \beta^{(>)}(v) \equiv \frac{v^2}{2\langle\theta^{-1}\rangle_\pi} - 2 \quad \text{for} \quad v \gg 1, \tag{3.13b}$$

$$\beta_l(v) \sim \beta^{(<)}(v) \equiv \frac{v^2}{2\langle\theta^{-1}\rangle_\pi} - 2\frac{\Gamma(l/2+1/4)}{\Gamma(l)}v^{l-1/2} \quad \text{for} \quad v \ll 1, \tag{3.13c}$$

as well as the lower bounds

$$\beta_l(v) > \beta^{(>)}(v) \quad \text{for} \quad l > 1, \tag{3.14a}$$

$$\beta_l(v) \geqslant \beta^{(<)}(v) \quad \forall l. \tag{3.14b}$$

Here $\Gamma(z)$ is the gamma function, and $M(a,b,z)$ is a confluent hypergeometric function (Ref. 23, Chap. 13).

As mentioned above, we need to show that $1+\zeta$ is positive. Thus the quantity of interest is really $1+\beta_l(v)$, as opposed to $\beta_l(v)$. In Fig. 2 we plot $1+\beta_l(v)$ as a function of v for $0 \leqslant l \leqslant 4$, together with its asymptotic form $1+\beta^{(>)}(v)$ valid for large values of the argument v.

Let us now obtain the lower bounds $1+\overline{\beta}_l$ for $1+\zeta$, and show that they are positive for $l \neq 1$. For $l=4$ [and, as $\beta_l(v)$ grows with l, for all $l \geqslant 4$], $\beta_l(v)$ is positive for all nonzero v, and thus $\overline{\beta}_l = \beta_l(0) = 0$. For $0 \leqslant l \leqslant 3$, $\overline{\beta}_l$ is obtained by numerically minimizing Eq. (3.13a). In Table I, we give the numerical values for these bounds. These lower bounds establish that all of the $\kappa_{lr}(\tilde{\mathbf{k}})$ are positive for $l \neq 1$.

TABLE I. Lower bounds for eigenvalues of the Hessian.

l	$1+\overline{\beta}_l$
1	−0.55571
0, 2	0.27376
3	0.94274
$\geqslant 4$	1

Let us now focus on the remaining sector, namely $l=1$. As, for this case, our lower bound is negative, we cannot draw any conclusion from it. We have already shown that there is a zero mode, but there could still be one or more negative eigenvalues, which would render the proposed amorphous solid state unstable. The numerical solution of the radial Eq. (2.37) for this case yields, within numerical error,[24] the following two lowest eigenvalues (both nondegenerate):

$$1+\zeta_{10}=-0.000\,02\pm 0.000\,05,$$

$$1+\zeta_{11}=0.984\,12\pm 0.000\,09. \tag{3.15}$$

Evidently, $1+\zeta_{10}$ corresponds to the expected zero mode, and we can conclude that there are no further zero modes and that all other eigenvalues are positive definite.

To summarize, we have shown that $1+\zeta\geqslant 0$ for any eigenvalue ζ of Eq. (2.37), i.e., that all elements of $\mathcal{S}_r$ are positive or zero. In the next subsection we will show that $\mathcal{S}_r$ and $\mathcal{S}_o$ are identical, and therefore that all of the eigenvalues of the original Hessian are either positive or zero.

C. The one-replica sector and the spurious eigenvalue

We now need to return to the issues that we postponed earlier, namely our extending of the Hessian matrix defined by Eq. (2.17) so that it can also be defined in the one-replica sector, and the differences between the spectra of the radial Eqs. (2.36) and (2.37).

As the Hessian matrix (both in its ''original'' and its ''extended'' versions) leaves exactly uncoupled fluctuations with different values of $\tilde{\mathbf{k}}$, it is consistent to consider separately the MTI fluctuations (those with $\tilde{\mathbf{k}}=\mathbf{0}$) and the non-MTI fluctuations (those with $\tilde{\mathbf{k}}\neq\mathbf{0}$).

For the case of non-MTI fluctuations we will show that, in the limit $n\to 0$, the hrs and 1rs are not coupled by the extended Hessian matrix. Furthermore, each one of the eigenvectors belongs to one of the sectors, inasmuch as it has a vanishing overlap (as $n\to 0$) with vectors in the other sector.

To understand this issue, we need to look at the form that the 1rs and hrs take, in the replica limit. For a wave vector

$$\hat{p}=(\mathbf{0},\ldots,\mathbf{0},\mathbf{p},\mathbf{0},\ldots,\mathbf{0}) \tag{3.16}$$

in the one-replica sector, we have

$$\tilde{\mathbf{p}}=\mathbf{p} \quad \text{and} \quad \hat{p}^2=\mathbf{p}^2, \tag{3.17}$$

and, by using Eq. (2.19) with $\hat{v}=\hat{w}=\hat{p}$, we have

$$|\breve{p}|=\sqrt{\hat{p}^2-\frac{\tilde{\mathbf{p}}^2}{1+n}}=\sqrt{\mathbf{p}^2-\frac{\mathbf{p}^2}{1+n}}=\sqrt{\frac{n}{1+n}}|\mathbf{p}|. \tag{3.18}$$

This means that the radial coordinate $|\breve{p}|$ goes to zero like $n^{1/2}$ in the replica limit, $n\to 0$. Moreover, for each fixed value of $\tilde{\mathbf{p}}$ $(=\mathbf{p})$, the $n+1$ wave vectors defined by

$$\hat{e}_\alpha(\mathbf{p})\equiv(\mathbf{e}^0,\mathbf{e}^1,\ldots,\mathbf{e}^n), \tag{3.19a}$$

$$\mathbf{e}^\beta\equiv\begin{cases}\mathbf{0} & \text{for } \beta\neq\alpha,\\ \mathbf{p} & \text{for } \beta=\alpha,\end{cases} \tag{3.19b}$$

with $\alpha=0,\ldots,n$, are the only vectors in the one-replica sector that satisfy the condition that the sum of their $(n+1)$ component d-dimensional wave vectors is equal to $\mathbf{p}$. These two results tell us that the one-replica sector corresponds, for fixed $\tilde{\mathbf{p}}$, to a set of $n+1$ points that, in the replica limit, converge to the origin of $\breve{p}$ space. Consequently, to see whether or not a given eigenvector has any overlap with the 1rs, one needs to look at the properties of the corresponding radial eigenfunction near the origin.

Let us then consider the scaled radial Eq. (2.36) for the region close to the origin, and let us keep $n>0$ for the moment. By using the small-argument behavior of the modified Bessel function (valid for $\nu\neq -1,-2,\ldots$),

$$I_\nu(z)\approx\frac{(z/2)^\nu}{\Gamma(\nu+1)}, \tag{3.20}$$

we obtain the asymptotic form of the kernel η for $x\ll 1$ and $x'\lesssim 1$:

$$\eta_l^{(n)}(x,x')\approx 2\frac{x^{l+(nd-1)/2}}{\Gamma(l+nd/2)}m_l(x'), \tag{3.21a}$$

$$m_l(y)\equiv\int_0^\infty d\theta\,\pi(\theta)\,\theta^{-l}e^{-y^2/\theta}y^{l+(nd-1)/2}. \tag{3.21b}$$

By inserting this asymptotic form into Eq. (2.36), we obtain

$$\left(\zeta-\frac{x^2}{2}\right)u(x)\approx\frac{-4x^{l+(nd-1)/2}}{\Gamma(l+nd/2)}U_l, \tag{3.22a}$$

$$U_l\equiv\int_0^\infty dy\,m_l(y)u(y). \tag{3.22b}$$

For n positive and small, Eq. (3.22a) can only be satisfied for $\zeta\neq 0$.[25] The term proportional to x^2 is thus negligible, and we obtain, for $x\ll 1$,

$$u(x)\approx\frac{-4U_l}{\Gamma(l+nd/2)}\frac{x^{l+(nd-1)/2}}{\zeta}. \tag{3.23}$$

The leading behavior of this radial eigenfunction for nd small and positive depends on the value of the degree $l=|\sigma|$ of the surface harmonic function. For $l=0$ there is one eigenfunction that diverges at the origin like $x^{(nd-1)/2}$. Its eigenvalue ζ_- is given by the expression

$$\zeta_-\approx-\frac{4\int_0^\infty dy\int_0^\infty d\theta\,\pi(\theta)e^{-y^2/\theta}y^{nd-1}}{\Gamma(nd/2)}, \tag{3.24}$$

which, in the replica limit, becomes

$$\lim_{n\to 0}\zeta_-=-2. \tag{3.25}$$

The presence of this divergent eigenfunction as a solution of Eq. (2.36) depends crucially on the singularity of $\eta_0^{(n)}(x,x')$ at the origin for n small but positive. It is *not* a solution of Eq. (2.37), which only has solutions that go to zero at the

origin: by Eq. (2.38), the radial equation for $n=0$ and $l=0$, is identical to the radial equation for $n=0$ and $l=2$, which means, by Eq. (3.23), that the radial eigenfunction satisfies the condition

$$|u(x)| \lesssim x^{3/2}. \tag{3.26}$$

We will show below that the divergent eigenfunction present for $n>0$ corresponds, in the replica limit, to an unphysical fluctuation, i.e., a fluctuation in the one-replica sector. In fact, from Eqs. (2.39) and (3.25), we see that its eigenvalue $\kappa_-(\tilde{\mathbf{k}})$ is negative for small $\tilde{\mathbf{k}}$:

$$\kappa_-(\tilde{\mathbf{k}}) = -\epsilon + \frac{\tilde{\mathbf{k}}^2}{2}. \tag{3.27}$$

However, for $l=0$, all other radial eigenfunctions are orthogonal to the one just found, and thus make the integral U_l vanish. Their behavior is controlled by the next power in the expansion of $\eta_0^{(n)}(x,x')$, and consequently they vanish for $x \to 0$ at least as fast as $x^{(nd+3)/2}$. Moreover, for $l>0$, by Eq. (3.23) we see that all the radial eigenfunctions vanish for $x \to 0$ as $x^{l+(nd-1)/2}$ or faster.

These results can be summarized as follows: for $n \to 0^+$ all but one of the radial eigenfunctions are regular at the origin. The one singular eigenfunction corresponds to $l=0$ and scales like $x^{(nd-1)/2}$ for $x \ll 1$. The regular eigenfunctions can have any value of l and vanish for $x \to 0$ as $x^{(|l-1|+1/2)}$ or faster.

In all cases in which the eigenfunction is regular at the origin, it is permissible to take the limit $n \to 0$ in Eq. (2.36). This is because these eigenfunctions vanish at the origin fast enough that the integral term in Eq. (2.36) does not pick up any extra contribution from the singularity of $\eta_l^{(n)}(x,x')$ [which, by Eqs. (3.21a) and (3.21b), is at most of order $nd(xx')^{(nd-1)/2}$]. Thus the spectrum of eigenvalues of Eq. (2.37) is the same as the limit of the spectrum of Eq. (2.36) when $n \to 0$, except that the spurious eigenvalue ζ_- is absent in the former and present in the latter.

We now show that the one-replica sector fluctuations decouple from the higher replica sector fluctuations in the replica limit. Consider the following complete orthonormal basis set for the fluctuations in the one-replica sector with fixed $\tilde{\mathbf{p}}=\mathbf{p}$:

$$w_j(\hat{k}) \equiv \sum_{\alpha=0}^{n} w_{j,\alpha} \delta_{\hat{k},\hat{e}_\alpha(\mathbf{p})},$$

$$w_{j,\alpha} \equiv \frac{V^{n/2}}{\sqrt{n+1}} e^{i2\pi j\alpha/(n+1)}, \tag{3.28}$$

where $j=0,\ldots,n$.

Let us compute the scalar product $\langle w_j|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle$ of one of these basis functions for the one-replica sector with one of the eigenfunctions of the extended Hessian, which has the general form given in Eq. (2.26):

$$\begin{aligned}\langle w_j|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle &= \frac{1}{V^n}\sum_{\hat{k}\neq\hat{0}} w_j^*(\hat{k})\psi_{r\tilde{\mathbf{p}}\sigma}(\hat{k}) \\ &= \frac{1}{V^n}\sum_{\alpha=0}^{n} w_{j,\alpha}^*[(1+n)^{d/4}(2\pi)^{nd/2} \\ &\quad \times S_\sigma(\phi_{\tilde{e}_\alpha(\mathbf{p})})(\sqrt{n/(1+n)}|\mathbf{p}|)^{(1-nd)/2} \\ &\quad \times R_r(\sqrt{n/(1+n)}|\mathbf{p}|)].\end{aligned} \tag{3.29}$$

Here, we have made use of the relation Eq. (3.18). There are two possible cases to consider, depending on whether or not R_r is singular at the origin. If it is singular, we have $l=0$ and, for small k,

$$R(k) = \epsilon^{-1/4} u(k/\sqrt{\epsilon}) \approx \mathcal{N}\epsilon^{-nd/4} k^{(nd-1)/2}, \tag{3.30}$$

where $\mathcal{N}$ is a normalization constant determined by Eq. (2.27). Its value is given by

$$\mathcal{N} = \sqrt{nd}[1+\mathcal{O}(nd)]. \tag{3.31}$$

As $l=0$, the angular part of $\psi_{r\tilde{\mathbf{p}}\sigma}$ is isotropic, and is given by

$$S_0(\phi) = \sqrt{\frac{1}{\tau_{nd}}} = \sqrt{\frac{\Gamma(nd/2)}{2\pi^{nd/2}}} = (nd)^{-1/2}[1+\mathcal{O}(nd)], \tag{3.32}$$

where $\tau_{nd} = 2\pi^{nd/2}/\Gamma(nd/2)$ is the surface area of a unit sphere in nd dimensions. By combining Eqs. (3.29)–(3.32), we obtain

$$\begin{aligned}\langle w_j|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle &= \sum_{\alpha=0}^{n} w_{j,\alpha}^*[1+\mathcal{O}(n)] = \langle w_j|w_0\rangle[1+\mathcal{O}(n)] \\ &= \delta_{j,0}[1+\mathcal{O}(n)].\end{aligned} \tag{3.33}$$

This result implies that, in the limit $n \to 0$, the eigenfunction that is singular at the origin lies entirely in the one-replica sector.

Let us now consider the case in which R_r is not singular at the origin. In this case, for small k, the radial eigenfunction has the form

$$R(k) = \epsilon^{-1/4} u(k/\sqrt{\epsilon}) \lesssim \mathcal{N}\epsilon^{-(|l-1|+1)/2} k^{(|l-1|+1/2)}, \tag{3.34}$$

where the normalization constant $\mathcal{N}$ does not vanish in the replica limit. As, in this regular case, l need not be zero, we have to obtain an estimate for the normalization constant of the surface harmonic for all values of l. Consider a monomial $M_m(\phi)$ defined on the D-dimensional unit sphere

$$M_m(\phi) \equiv \phi_1^{m_1}\cdots\phi_D^{m_D} = \frac{x_1^{m_1}\cdots x_D^{m_D}}{r^{m_1+\cdots+m_D}}. \tag{3.35}$$

Here $(x_1,\ldots,x_D)$ are the Cartesian coordinates of a point x,

$r \equiv (x_1^2 + \cdots + x_D^2)^{1/2}$ is the radial coordinate for the same point, and $\phi \equiv (\phi_1, \ldots, \phi_D) \equiv x/r$ is the unit vector pointing in the direction of x. The integral of the monomial over the unit sphere is

$$\int d\phi M_m(\phi) = \frac{\int d^D x x_1^{m_1} \cdots x_D^{m_D} e^{-(x_1^2 + \cdots + x_D^2)}}{\int_0^\infty dr\, r^{D-1}\ r^{m_1 + \cdots + m_D} e^{-r^2}} = \begin{cases} \dfrac{2\prod_{j=1}^{D} \Gamma\left(\dfrac{1+m_j}{2}\right)}{\Gamma\left(\dfrac{D+\Sigma_{j=1}^{D} m_j}{2}\right)} & \text{if } m_j \text{ even } \forall j, \\ 0 & \text{otherwise.} \end{cases} \tag{3.36}$$

In the case of interest to us $D = nd$ and $\Sigma_{j=1}^{D} m_j = 2|\sigma|$. From Eq. (3.36) we conclude that the normalization factor N_σ for the surface harmonic S_σ has, in the $n \to 0$ limit, the asymptotic form

$$N_\sigma \sim \sqrt{\Gamma\left(\frac{nd}{2} + |\sigma|\right)} \sim \begin{cases} n^{-1/2} & \text{for } |\sigma| = 0, \\ n^0 & \text{for } |\sigma| \neq 0. \end{cases} \tag{3.37}$$

Here, we have ignored factors that have finite limits when $n \to 0$. This result can be summarized as follows

$$S_\sigma(\phi) \sim n^{\nu(\sigma)},$$

$$\nu(\sigma) = \begin{cases} -1/2 & \text{for } |\sigma| = 0, \\ 0 & \text{for } |\sigma| \neq 0. \end{cases} \tag{3.38}$$

By inserting Eqs. (3.34) and (3.38) into Eq. (3.29), we obtain the following scaling with n for the sought scalar product:

$$|\langle w_j | \psi_{r\tilde{\mathbf{p}}\sigma} \rangle| \lesssim (\sqrt{n}|\tilde{\mathbf{k}}|)^{1/2} (\sqrt{n}|\tilde{\mathbf{k}}|)^{1/2+|l-1|} n^{\nu(\sigma)}, \lesssim \begin{cases} n^{1/2} & \text{for } l = 0, \\ n^{(|l-1|+1)/2} & \text{for } l \neq 0. \end{cases} \tag{3.39}$$

This relation shows that in the limit $n \to 0$ those radial eigenfunctions that are regular at the origin give rise to eigenvectors that lie entirely in the higher replica sector.

For completeness, we now also compute explicitly the matrix elements of the extended Hessian between members of the basis set $\{w_j\}_{j=0}^{n}$ for the one-replica sector fluctuations with $\tilde{\mathbf{k}} = \mathbf{p}$,

$$\begin{aligned} \langle w_m | H | w_j \rangle &= \frac{1}{V^{2n}} \sum_{\hat{k},\hat{l} \neq \hat{0}} w_m^*(\hat{k}) H_{\hat{k},\hat{l}} w_j(\hat{l}) \\ &= \frac{1}{V^n (1+n)} \Bigg[\sum_{\alpha=0}^{n} \left(\epsilon + \frac{\mathbf{p}^2}{2} \right) w_{m,\alpha}^* w_{j,\alpha} \\ &\quad - 2\epsilon \int_0^\infty d\theta\, \pi(\theta) \\ &\quad \times \sum_{\alpha,\beta=0}^{n} e^{-[\hat{e}_\alpha(\mathbf{p}) - \hat{e}_\beta(\mathbf{p})]^2/\epsilon\theta} w_{m,\alpha}^* w_{j,\beta} \Bigg] \\ &= \delta_{m,j} \left(-\epsilon + \frac{\mathbf{p}^2}{2} \right) + \mathcal{O}(n). \end{aligned} \tag{3.40}$$

Thus we see that, as expected, the eigenvalue obtained here is the same as the one obtained in Eq. (3.27) for the singular eigenfunction of the extended Hessian.

In summary, for non-MTI fluctuations, in the replica limit all regular eigenfunctions of the extended Hessian are orthogonal to all of the 1rs vectors, and the singular eigenfunction of the extended Hessian coincides with the isotropic ($j = 0$) fluctuation in the 1rs. Consequently, in the replica limit, the higher replica sector is an invariant subspace for the extended Hessian, and therefore the regular eigenfunctions of the extended Hessian are the eigenfunctions of the original Hessian. More significantly, the eigenvalues of the original Hessian are the eigenvalues of the extended Hessian for its regular eigenfunctions.

For the case of MTI fluctuations, their components in the one-replica sector are exactly zero, because the conditions $\hat{k} \in$ 1rs and $\tilde{\mathbf{k}} = \mathbf{0}$ are incompatible. However, all of the argument presented above still holds, except that now the radial eigenfunction that is singular at the origin coincides with a spurious fluctuation in the zero-replica sector (i.e., a fluctuation of $\Omega_{\hat{0}}$).[26] The spectrum of the original Hessian is, also in this case, given by the eigenvalues corresponding to radial eigenfunctions regular at the origin. Thus we have shown that the sets $\mathcal{S}_r$ and $\mathcal{S}_o$ are identical, and we can use the results of Secs. III A and III B to characterize the spectrum of the original Hessian.

The eigenvalues of the original Hessian have the general form

$$\kappa_{lr}(\tilde{\mathbf{k}}) = (1 + \zeta_{lr})\epsilon + \frac{\tilde{\mathbf{k}}^2}{2}, \tag{3.41}$$

with

$$1 + \zeta_{10} = 0 \tag{3.42}$$

and

$$1 + \zeta_{lr} > 0 \quad \text{for} \quad (l,r) \neq (1,0). \tag{3.43}$$

Therefore there is a *nd* degenerate zero mode corresponding to $(l,r) = (1,0)$ and $\tilde{\mathbf{k}} = \mathbf{0}$, which is continued by a branch of soft modes with eigenvalues

$$\kappa_{10}(\tilde{\mathbf{k}})=\frac{\tilde{\mathbf{k}}^2}{2}\ (>0 \text{ for } \tilde{\mathbf{k}}\neq\mathbf{0}). \tag{3.44}$$

All other eigenvalues are positive, with one continuous branch of modes labeled by $\tilde{\mathbf{k}}$ for each value of (l,r). The minimum eigenvalue for each branch is given by

$$\kappa_{lr}(\mathbf{0})=(1+\zeta_{lr})\epsilon>0, \tag{3.45}$$

which goes to zero as the transition is approached (i.e., as $\epsilon\to 0$). Consequently, the amorphous solid state of Ref. 3 is locally stable near the transition.

IV. RANDOMLY CROSS LINKED MACROMOLECULES

We now consider one example of a semimicroscopic theory that exhibits the amorphous solidification transition, namely the case of randomly crosslinked linear macromolecules. In this theory there appears a control parameter μ^2 $(\equiv 1+\epsilon/3)$ that determines the crosslink density, and such that the system exhibits the liquid phase for $\mu^2<1$ and the amorphous solid phase for $\mu^2>1$. In this semimicroscopic theory, the field $\Omega_{\hat{p}}$ (with $\hat{p}$ in the one-replica sector) is present and allowed to fluctuate, and there is a coupling parameter $\tilde{\lambda}_n^2\equiv\lambda^2-\mu^2(V/N)(1/V^n)$ associated with its fluctuations. (The parameter λ^2 gives the strength of the excluded-volume interaction between the macromolecules.) The free-energy functional (per macromolecule) has the form[1,4]

$$\begin{aligned} nd\mathcal{F}_n(\{\Omega_{\hat{k}}\})=&\tilde{\lambda}_n^2\frac{N}{V}\sum_{\hat{p}}{}^{\dagger}|\Omega_{\hat{p}}|^2+\frac{\mu^2}{V^n}\sum_{\hat{k}}{}^{\dagger}|\Omega_{\hat{k}}|^2\\ &-\ln\left\langle \exp\left(i\tilde{\lambda}_n^2\frac{2N}{V}\sum_{\hat{p}}{}^{\dagger}\mathrm{Re}\,\Omega_{\hat{p}}\rho_{\hat{p}}^{*}\right.\right.\\ &\left.\left.+\frac{2\mu^2}{V^n}\sum_{\hat{k}}{}^{\dagger}\mathrm{Re}\,\Omega_{\hat{k}}\rho_{\hat{k}}^{*}\right)\right\rangle_{n+1}^{W}, \end{aligned} \tag{4.1}$$

where the symbol $\sum_{\hat{p}}$ denotes a sum over replicated wave vectors in the one-replica sector, and the † symbol additionally restricts any summation to the half space of relevant wave vectors [i.e., d-dimensional or $(n+1)d$-dimensional] such that their scalar product with a fixed unit vector ($\mathbf{n}$ or $\hat{n}$) is positive. Here, we have used the definition of the one-macromolecule Fourier transformed density $\rho_{\hat{k}}$, i.e.,

$$\rho_{\hat{k}}\equiv\int_0^1 ds\,\exp i\hat{k}\cdot\hat{c}(s), \tag{4.2}$$

for a macromolecular configuration $\hat{c}(s)$, and the Wiener replicated average $\langle\cdots\rangle_{n+1}^{W}$ is defined by

$$\langle O\rangle_{n+1}^{W}\equiv\frac{\int\mathcal{D}\hat{c}\,O\exp\left\{-(1/2)\int_0^1 ds|d\hat{c}(s)/ds|^2\right\}}{\int\mathcal{D}\hat{c}\exp\left\{-(1/2)\int_0^1 ds|d\hat{c}(s)/ds|^2\right\}}. \tag{4.3}$$

Let us note here that to leading order in ϵ the amorphous solid stationary point in this theory is the same as in the Landau theory discussed above, i.e., it is also described by Eqs. (2.5)–(2.7).

We now expand the free-energy functional to quadratic order around a stationary point, and obtain its second derivatives with respect to the fields $\{\Omega_{\hat{q}}\}$. In this section we use the notations H and $\overline{H}$ to refer to the exact Hessian for the microscopic theory and the extended Hessian for the Landau theory, respectively. For $\hat{k}$ and $\hat{k}'$ both in the higher replica sector we have

$$\begin{aligned} \frac{\delta^2[nd\mathcal{F}_n]}{\delta\Omega_{\hat{k}}\delta\Omega_{-\hat{k}'}}=H^{\mathrm{hh}}_{\hat{k},\hat{k}'}&=\frac{\mu^2}{V^n}\left(\delta_{\hat{k},\hat{k}'}-\frac{\mu^2}{V^n}\langle\rho_{-\hat{k}}\rho_{\hat{k}'}\rangle_{n+1,c}^{W,\overline{\Omega}}\right)\\ &=\frac{\mu^2}{3}\left[\delta_{\hat{k},\hat{k}'}\left(\epsilon+\frac{\hat{k}^2}{2}\right)-\delta_{\tilde{\mathbf{k}},\tilde{\mathbf{k}}'}2\epsilon\right.\\ &\quad\left.\times\int_0^\infty d\theta\,\pi(\theta)e^{-(\hat{k}-\hat{k}')^2/\epsilon\theta}\right]+\mathcal{O}(\epsilon^2)\\ &=\frac{1}{3}\overline{H}^{\mathrm{hh}}_{\hat{k},\hat{k}'}+\mathcal{O}(\epsilon^2). \end{aligned} \tag{4.4}$$

For $\hat{k}$ in the higher replica sector and $\hat{p}$ in the one-replica sector we have

$$\begin{aligned} \frac{\delta^2[nd\mathcal{F}_n]}{\delta\Omega_{\hat{k}}\delta\Omega_{-\hat{p}}}=H^{\mathrm{h1}}_{\hat{k},\hat{p}}&=-i\tilde{\lambda}_n^2\frac{N\mu^2}{V^{1+n}}\langle\rho_{-\hat{k}}\rho_{\hat{p}}\rangle_{n+1,c}^{W,\overline{\Omega}}\\ &=-i\frac{\tilde{\lambda}_n^2}{V}\frac{N\mu^2}{3}\delta_{\tilde{\mathbf{k}},\tilde{\mathbf{p}}}2\epsilon\int_0^\infty d\theta\,\pi(\theta)e^{-(\hat{k}-\hat{p})^2/\epsilon\theta}\\ &\quad+\mathcal{O}(\epsilon^2)\\ &=\frac{i\tilde{\lambda}_n^2N}{3V}\overline{H}^{\mathrm{h1}}_{\hat{k},\hat{p}}+\mathcal{O}(\epsilon^2). \end{aligned} \tag{4.5}$$

Finally, for both $\hat{p}$ and $\hat{p}'$ in the one-replica sector we have

$$\begin{aligned} \frac{\delta^2[nd\mathcal{F}_n]}{\delta\Omega_{\hat{p}}\delta\Omega_{-\hat{p}'}}=H^{11}_{\hat{p},\hat{p}'}&=\frac{\tilde{\lambda}_n^2N}{V}\left(\delta_{\hat{p},\hat{p}'}+\frac{\tilde{\lambda}_n^2N}{V}\langle\rho_{-\hat{p}}\rho_{\hat{p}'}\rangle_{n+1,c}^{W,\overline{\Omega}}\right)\\ &=\delta_{\hat{p},\hat{p}'}\frac{\tilde{\lambda}_n^2N}{V}\left\{1+\frac{\tilde{\lambda}_n^2N}{V}[1+\mathcal{O}(\epsilon)+\mathcal{O}(\hat{p}^2)]\right\}. \end{aligned} \tag{4.6}$$

In obtaining these formulas we have made use of the definition

$$\langle O\rangle_{n+1}^{W,\bar{\Omega}} \equiv \frac{\left\langle O \exp\left(i\tilde{\lambda}_n^2 \frac{N}{V} \sum\!\!\!\!\!\!\sim_{\hat{p}} \bar{\Omega}_{\hat{p}}\, \rho_{\hat{p}}^* + \frac{\mu^2}{V^n} \sum\!\!\!\!\!\!\sim_{\hat{k}} \bar{\Omega}_{\hat{k}}\, \rho_{\hat{k}}^* \right) \right\rangle_{n+1}^{W}}{\left\langle \exp\left(i\tilde{\lambda}_n^2 \frac{N}{V} \sum\!\!\!\!\!\!\sim_{\hat{p}} \bar{\Omega}_{\hat{p}} \rho_{\hat{p}}^* + \frac{\mu^2}{V^n} \sum\!\!\!\!\!\!\sim_{\hat{k}} \bar{\Omega}_{\hat{k}} \rho_{\hat{k}}^* \right) \right\rangle_{n+1}^{W}}. \tag{4.7}$$

The notations H^{hh}, H^{h1}, and H^{11}, respectively, refer to the higher replica, cross-sector, and one-replica parts of the Hessian matrix. Figure 3 depicts the relation between H and $\bar{H}$.

As MTI (i.e., $\tilde{\mathbf{k}}=\mathbf{0}$) fluctuations do not have any component in the 1rs, the relevant Hessian in this case is just $H^{\mathrm{hh}} = (1/3)\bar{H}^{\mathrm{hh}}$. Consequently, the results obtained for the Landau theory tell us that there is a *nd* degenerate zero eigenvalue corresponding to the anticipated zero mode, and that the remaining eigenvalues are positive.

Let us now consider general fluctuations. We will show that, in the replica limit, the eigenvectors of the Hessian H for this problem are the same as the eigenvectors of the extended Hessian $\bar{H}$ for the Landau theory, and the one-replica and higher replica sectors are again invariant subspaces for this Hessian.

Let us consider a regular eigenvector $|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle$ of $\bar{H}$ and one of the elements of the basis set $\{|w_j\rangle\}_{j=0}^{n}$ of the one-replica sector fluctuations. By Eq. (4.6),

$$H^{11}|w_j\rangle = \kappa_{1\mathrm{rs}}|w_j\rangle,$$

$$\kappa_{1\mathrm{rs}} = \frac{\tilde{\lambda}_n^2 N}{V}\left\{ 1 + \frac{\tilde{\lambda}_n^2 N}{V}[1 + \mathcal{O}(\epsilon) + \mathcal{O}(\hat{p}^2)] \right\}, \tag{4.8}$$

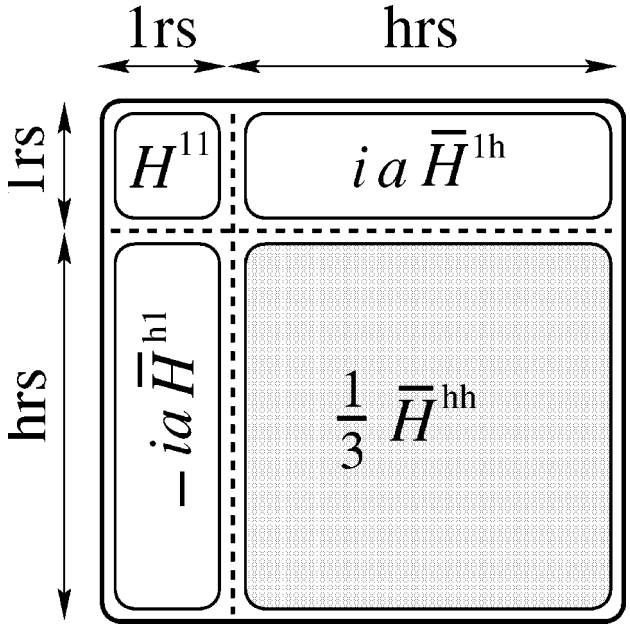

FIG. 3. The Hessian matrix H for the semimicroscopic theory in terms of the extended Hessian matrix $\bar{H}$ for the Landau theory. Each block of H is written in terms of the corresponding block of $\bar{H}$, except for H^{11}. (H^{11} is nonzero when $\epsilon \to 0$, as opposed to $\bar{H}^{11}$, which vanishes linearly with ϵ near the transition.)

and therefore

$$|\langle w_j|H^{11}|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle| = |\kappa_{1\mathrm{rs}}\langle w_j|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle| \lesssim \mathcal{O}(\sqrt{n}). \tag{4.9}$$

Analogously, by Eq. (3.40),

$$\bar{H}^{11}|w_j\rangle = \left(-\epsilon + \frac{\mathbf{p}^2}{2} \right)|w_j\rangle + \mathcal{O}(n), \tag{4.10}$$

and

$$|\langle w_j|\bar{H}^{11}|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle| = \left| \left(-\epsilon + \frac{\mathbf{p}^2}{2} \right)\langle w_j|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle \right| \lesssim \mathcal{O}(\sqrt{n}). \tag{4.11}$$

By combining Eqs. (4.5), (4.9), and (4.11), we can now estimate the matrix element:

$$\begin{aligned} |\langle w_j|H|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle| &= |\langle w_j|H^{11} + H^{1\mathrm{h}}|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle| \\ &= |\langle w_j|H^{1\mathrm{h}}|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle + \mathcal{O}(\sqrt{n})| \\ &= \left| \langle w_j| \frac{i\tilde{\lambda}_n^2 N}{3V} \bar{H}^{1\mathrm{h}}|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle + \mathcal{O}(\sqrt{n}) \right| \\ &= \left| \frac{i\tilde{\lambda}_n^2 N}{3V} \langle w_j|\bar{H}^{1\mathrm{h}} + \bar{H}^{11}|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle + \mathcal{O}(\sqrt{n}) \right| \\ &= \left| \frac{i\tilde{\lambda}_n^2 N}{3V} \langle w_j|\bar{H}|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle + \mathcal{O}(\sqrt{n}) \right| \\ &\lesssim \mathcal{O}(\sqrt{n}). \end{aligned} \tag{4.12}$$

This means that, in the replica limit, $H|\psi_{r\tilde{\mathbf{p}}\sigma}\rangle$ has no projection in the one-replica sector, and also that $H|w_j\rangle$ has no projection in the higher replica sector. Therefore also in this problem the one-replica sector and the higher replica sector are decoupled invariant subspaces of the Hessian in the $n \to 0$ limit. In the one-replica sector, the eigenvalue is $\kappa_{1\mathrm{rs}} > 0$. In the higher replica sector, as $H^{\mathrm{hh}} = (1/3)\bar{H}^{\mathrm{hh}}$, the eigenvectors are the same as for the Landau theory, and the eigenvalues are obtained from those in the Landau theory by multiplying by 1/3. As discussed before, all of these eigenvalues are positive, except for a *nd* degenerate zero mode. Thus also for the semimicroscopic theory of randomly crosslinked macromolecules, the amorphous solid state of Ref. 3 is locally stable near the transition.

V. SUMMARY AND CONCLUDING REMARKS

In this paper we have shown that in a system with random constraints near the liquid–amorphous-solid transition, the amorphous solid state of Ref. 3 is a locally stable thermodynamic state.[18] In order to do this, we have examined the eigenvalue spectra of the stability matrices, in the contexts of

both the Landau theory for the transition and a semimicroscopic model of randomly crosslinked macromolecular systems. In both cases the spectrum turns out to be nonnegative, with only a *nd* degenerate zero eigenvalue, and all the others positive.

Let us remark that even though we *do* find a zero eigenvalue for the stability matrix, we still declare that the stationary point is locally *stable*, as opposed to locally *marginally stable*. This is because in this system translational invariance is spontaneously broken, and therefore there is a manifold of equivalent states that have exactly the same free energy and are connected to each other by the continuous symmetries of the system. The zero eigenvalue (a.k.a. Goldstone mode) simply indicates that the free energy does not change if one applies an infinitesimal translation to the thermodynamic state.

In close analogy to the phonon spectra of ordinary solids, the fluctuation eigenvalues can be classified into two types: a soft branch of modes associated with ''almost rigid'' displacements of the whole system (analogous to the acoustic-phonon branch), with eigenvalues $\kappa_{10}(\tilde{\mathbf{k}})=\tilde{\mathbf{k}}^2/2$, and a set of stiff modes in which the structure of the system is altered more strongly (analogous to the set of optical-phonon branches), with eigenvalues $\kappa_{lr}(\tilde{\mathbf{k}})=\epsilon(1+\zeta_{lr})+\tilde{\mathbf{k}}^2/2$. In addition, there is in our case a softening of the system, because the eigenvalues of the stiff modes go to zero at the transition.

We have only addressed the issue of the *local* stability of the amorphous solid state. It is much harder to determine whether the amorphous solid state is *globally* stable, as the order parameter space to be explored is enormous. In particular, one could consider the possibility of a replica symmetry breaking saddle point also being present and dominating the physical behavior of the system.[27] However, there are strong indications (although by no means conclusive evidence) that the (replica symmetric) saddle point considered here is indeed *globally* stable. These indications mainly come from molecular-dynamics simulations[28] as the solid state observed in the simulations appears to be identical to the one proposed in Ref. 3.

An intriguing problem, left open for further study, is to establish how the structure of the eigenvalue spectrum of the Hessian matrix, and in particular the softening of the system near the transition, manifest themselves in the dynamics of the system.

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APPENDIX A: NONDIAGONAL MATRIX ELEMENTS FOR THE HESSIAN

In this appendix we collect some useful information concerning surface harmonic functions, and use it to compute the matrix elements of the nondiagonal part H^O of the Hessian in the basis $\{\varphi_{p\tilde{\mathbf{p}}\sigma}\}$.

The Gegenbauer (also called hyperspherical) polynomials play a role in D dimensions and with regard to the surface harmonics S_σ analogous to the role Legendre polynomials play in three dimensions and with regard to the spherical harmonics Y_{lm}. The Gegenbauer polynomial $C_l^\nu(x)$ of degree l is defined by the generating function (see, e.g., Ref. 20, Vol. II, Sec. 11.1.2)

$$(1-2xt+t^2)^{-\nu}=\sum_{l=0}^{\infty} C_l^\nu(x)t^l. \tag{A1}$$

There is a generalization to dimension $D\equiv p+2$ of the addition theorem for spherical harmonics, which relates the Gegenbauer polynomial to a sum of surface harmonics (see, e.g., Ref. 20, Sec. 11.4):

$$C_l^{p/2}(\phi'\cdot\phi)=\frac{C_l^{p/2}(1)\tau_D}{h(l,p)}\sum_{|\sigma|=l} S_\sigma^*(\phi')S_\sigma(\phi)$$
$$=\frac{4\pi^{1+p/2}}{(2l+p)\Gamma(p/2)}\sum_{|\sigma|=l} S_\sigma^*(\phi')S_\sigma(\phi). \tag{A2}$$

Here, ϕ' and ϕ are any unit D-dimensional vectors, $|\sigma|$ is the degree of the surface harmonic S_σ as a trigonometric polynomial, $h(l,p)$ is the number of linearly independent surface harmonics of degree l in dimension $p+2$, and $\tau_D=2\pi^{D/2}/\Gamma(D/2)$ is the surface area of a D-dimensional unit sphere. [As $C_l^{1/2}(x)$ is equal to the Legendre polynomial $P_l(x)$, formula (A2) reduces, for $D=3$, to the usual addition theorem.]

We also make use of the identity (see, e.g., Ref. 20, Vol. II, Sec. 7.15)

$$z^\nu e^{xz}=2^\nu\Gamma(\nu)\sum_{n=0}^{\infty}(n+\nu)C_n^\nu(x)I_{n+\nu}(z), \tag{A3}$$

where $I_\nu(z)$ is the modified Bessel function of order ν.

In the case of dimension $D=nd$, by combining Eqs. (A2) and (A3), the following identity is obtained:

$$\exp(x\phi'\cdot\phi)=2\pi^{nd/2}(x/2)^{1-nd/2}$$
$$\times\sum_{l=0}^{\infty} I_{l-1+nd/2}(x)\sum_{|\sigma|=l} S_\sigma^*(\phi')S_\sigma(\phi). \tag{A4}$$

Here, x is any real number, and ϕ' and ϕ are unit nd-dimensional vectors.

Let us now compute the matrix elements of the nondiagonal part H^O of the Hessian in the basis $\{\varphi_{p\tilde{\mathbf{p}}\sigma}\}$. By using Eqs. (2.24) and (2.20) we obtain

$$\langle\varphi_{p'\tilde{\mathbf{p}}'\sigma'}|H^O|\varphi_{p\tilde{\mathbf{p}}\sigma}\rangle$$
$$=V^2\int\frac{d\tilde{\mathbf{k}}d\tilde{\mathbf{l}}d\check{k}d\check{l}}{(1+n)^d(2\pi)^{(1+n)2d}}(1+n)^{d/2}(2\pi)^{nd}p'^{(1-nd)/2}$$
$$\times\delta_{\tilde{\mathbf{p}}'\tilde{\mathbf{k}}}\delta(|\check{k}|-p')S_{\sigma'}^*(\phi_{\check{k}})p^{(1-nd)/2}\delta_{\tilde{\mathbf{p}},\tilde{\mathbf{l}}}\delta(|\check{l}|-p)$$
$$\times S_\sigma(\phi_{\check{l}})\delta_{\tilde{\mathbf{k}},\tilde{\mathbf{l}}}\ (-2\epsilon)\int_0^\infty d\theta\pi(\theta)e^{-(\check{k}-\check{l})^2/\epsilon\theta}, \tag{A5}$$

$$= \frac{-2\epsilon\ (2\pi)^{-nd}}{(1+n)^{d/2}} \sum_{\tilde{\mathbf{k}},\tilde{\mathbf{l}}} \delta_{\tilde{\mathbf{p}}',\tilde{\mathbf{k}}} \delta_{\tilde{\mathbf{p}},\tilde{\mathbf{l}}} \delta_{\tilde{\mathbf{k}},\tilde{\mathbf{l}}}$$
$$\times \int_0^\infty \delta(|\check{k}|-p')|\check{k}|^{nd-1} d|\check{k}|$$
$$\times \int_0^\infty \delta(|\check{l}|-p)|\check{l}|^{nd-1} d|\check{l}|$$
$$\times \int_0^\infty d\theta \pi(\theta) e^{-(p^2+p'^2)/\epsilon\theta} (pp')^{(1-nd)/2}$$
$$\times \int d\phi_{\check{k}} \int d\phi_{\check{l}}\, S^*_{\sigma'}(\phi_{\check{k}})$$
$$\times \exp(2pp'\phi_{\check{k}} \cdot \phi_{\check{l}}/\epsilon\theta) S_\sigma(\phi_{\check{l}}). \tag{A6}$$

In the second step, we have separated the $\check{k}$ and $\check{l}$ integrals into radial and angular parts. The angular integrals can be performed with the help of the identity (A4) and by using the orthonormality of the surface harmonics to obtain

$$\langle \varphi_{p'\tilde{\mathbf{p}}'\sigma'} | H^O | \varphi_{p\tilde{\mathbf{p}}\sigma} \rangle = \delta_{\tilde{\mathbf{p}}',\tilde{\mathbf{p}}} \delta_{\sigma',\sigma} \frac{(-2\epsilon)\epsilon^{(nd-1)/2}}{2^{nd}\pi^{nd/2}(1+n)^{d/2}}$$
$$\times 2\sqrt{pp'/\epsilon} \int_0^\infty \frac{d\theta \pi(\theta)}{\theta^{1-nd/2}}$$
$$\times e^{-(p'^2+p^2)/\epsilon\theta} I_{|\sigma|-1+nd/2}\left(\frac{2p'p}{\epsilon\theta}\right), \tag{A7}$$

which is equivalent to Eqs. (2.29)–(2.31).

APPENDIX B: RADIAL EQUATION FOR THE ZERO MODE

In this appendix we show that the scaled radial function of Eq. (3.3) corresponding to a change in the system due to a rigid displacement is a solution of the scaled radial eigenfunction Eq. (2.37) with $\zeta=-1$. Let us first consider the diagonal term. By inserting the explicit form for $u(x)$, and then performing an integration by parts we obtain

$$\frac{x^2}{2}u(x) = \frac{\sqrt{x}}{2}\int_0^\infty d\theta\, \pi(\theta)\theta^2 \frac{d}{d\theta}(e^{-x^2/\theta})$$
$$= -\frac{\sqrt{x}}{2}\int_0^\infty d\theta\, e^{-x^2/\theta}\frac{d}{d\theta}\{\theta^2\pi(\theta)\}$$
$$= -\sqrt{x}\int_0^\infty d\theta\, e^{-x^2/\theta}\left\{\frac{\theta^2}{2}\frac{d}{d\theta}\pi(\theta)+\theta\pi(\theta)\right\}. \tag{B1}$$

Now the nondiagonal term gives

$$-2\int_0^\infty dx'\, \eta_1^{(0)}(x,x')u(x')$$
$$= -2\int_0^\infty dx'\, d\theta\, d\theta' 2\sqrt{xx'}\,\frac{\pi(\theta)}{\theta} e^{-(x^2+x'^2)/\theta} I_0\left(\frac{2xx'}{\theta}\right)$$
$$\times \sqrt{x'}\pi(\theta') e^{-x'^2/\theta'}. \tag{B2}$$

By making use of the identity[29]

$$2\int_0^\infty dx\, x e^{-ax^2} I_0(bx) = \frac{e^{b^2/4a}}{a}, \tag{B3}$$

we perform the integration over x' in Eq. (B2), thus obtaining

$$-2\int_0^\infty dx'\, \eta_1^{(0)}(x,x')u(x')$$
$$= -2\sqrt{x}\int_0^\infty d\theta\, d\theta' \frac{\theta'\pi(\theta)\pi(\theta')}{\theta+\theta'} e^{-x^2/(\theta+\theta')}$$
$$= -\sqrt{x}\int_0^\infty d\theta\, e^{-x^2/\theta}\int_0^\theta d\theta'\, \pi(\theta)\pi(\theta'). \tag{B4}$$

Finally, we combine Eqs. (B1) and (B4) to obtain

$$u(x)+\frac{x^2}{2}u(x)-2\int_0^\infty dx'\, \eta_{|\sigma|}^{(0)}(x,x')u(x')$$
$$= \sqrt{x}\int_0^\infty d\theta\, e^{-x^2/\theta}\left\{-\frac{\theta^2}{2}\frac{d}{d\theta}\pi(\theta)+(1-\theta)\pi(\theta)\right.$$
$$\left.-\int_0^\theta d\theta'\, \pi(\theta)\pi(\theta')\right\} = 0. \tag{B5}$$

The justification of the last equality comes from the factor in braces being zero by the stationarity condition, Eq. (2.6).

Thus we have shown that Eq. (2.37) is satisfied by $u(x)$ with the eigenvalue $\zeta=-1$.

APPENDIX C: COMPUTATION OF LOWER BOUNDS

In this appendix we study in detail the bound function $\beta_l(v)$. We decompose $\beta_l(v)$ as follows:

$$\beta_l(v) = \frac{v^2}{2\langle\theta^{-1}\rangle_\pi} - 2j_l(v),$$

$$j_l(v) \equiv 2\int_0^\infty du \sqrt{uv} e^{-(u^2+v^2)} I_{l-1}(2uv). \tag{C1}$$

We now compute analytically the integral defining $j_l(v)$:

$$j_l(v)=\sqrt{v}e^{-v^2}\int_0^\infty dy\, y^{-1/4}e^{-y}I_{l-1}(2v\sqrt{y})$$
$$=\frac{\Gamma(l/2+1/4)}{\Gamma(l)}v^{l-1/2}e^{-v^2}M\left(\frac{l}{2}+\frac{1}{4},l,v^2\right)$$
$$=\frac{\Gamma(l/2+1/4)}{\Gamma(l)}v^{l-1/2}M\left(\frac{l}{2}-\frac{1}{4},l,-v^2\right), \quad \text{(C2)}$$

where $M(a,b,z)$ is a confluent hypergeometric function (Ref. 23, Chap. 13). By inserting this expression into Eq. (C1), we obtain Eq. (3.13a).

We can obtain more information by using the following integral formula for the confluent hypergeometric function (Ref. 23, Chap. 13), valid for Re$a>0$ and Re$b>0$:

$$\frac{\Gamma(b-a)\Gamma(a)}{\Gamma(b)}M(a,b,z)=\int_0^1 e^{zt}t^{a-1}(1-t)^{b-a-1}dt. \quad \text{(C3)}$$

This implies that

$$j_l(v)=\frac{(v^2)^{l/2-1/4}}{\Gamma(l/2-1/4)}\int_0^1 e^{-tv^2}t^{(l/2-1/4)-1}(1-t)^{(l/2+1/4)-1}dt. \quad \text{(C4)}$$

By considering the fact that the exponential in the integrand is always less than or equal to 1, this formula can immediately be bounded above, as follows:

$$j_l(v)\leqslant\frac{(v^2)^{l/2-1/4}}{\Gamma(l/2-1/4)}\int_0^1 t^{(l/2-1/4)-1}(1-t)^{(l/2+1/4)-1}dt$$
$$=\frac{(v^2)^{l/2-1/4}}{\Gamma(l/2-1/4)}B\left(\frac{l}{2}-\frac{1}{4},\frac{l}{2}+\frac{1}{4}\right)=\frac{\Gamma(l/2+1/4)}{\Gamma(l)}v^{l-1/2}, \quad \text{(C5)}$$

where $B(x,y)=\Gamma(x)\Gamma(y)/\Gamma(x+y)$ is the Beta function (Ref. 23, Sec. 6.2). By combining this inequality with Eq. (C1) we obtain the bound stated in Eq. (3.14b). Moreover, in the limit $v\ll 1$, it is legitimate to replace the exponential factor in Eq. (C4) by 1 inside the integral, and thus the same expression gives the asymptotic form in the $v\ll 1$ regime, as quoted in Eq. (3.13c).

An additional bound can be obtained for $l>1$ by taking into account the fact that the factor $(1-t)^{(l/2+1/4)-1}$ in the integrand is less than or equal to unity, so that

$$j_l(v)<\frac{(v^2)^{l/2-1/4}}{\Gamma(l/2-1/4)}\int_0^\infty e^{-tv^2}t^{(l/2-1/4)-1}dt=1. \quad \text{(C6)}$$

This gives the lower bound of Eq. (3.14a). When $v\gg 1$, the same expression provides the asymptotic form for all values of l, Eq. (3.13b), as, in that limit, the integral is dominated by the region near the origin, where the factor $(1-t)^{(l/2+1/4)-1}$ is close to unity.

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[15] A similar phenomenon has been observed in the context of supervised learning in neural networks; see H. S. Seung, H. Sompolinsky, and N. Tishby, Phys. Rev. A **45**, 6056 (1992).

[16] A constant is ignored here that has to do with the symmetry under permutations of the macromolecules. See Ref. 4, Secs. 2.4 and 2.6 for a full discussion.

[17] We use the notations $\overline{\Omega}$ for the equilibrium value of the order parameter and Ω for the fluctuating variable (which features in the Landau free energy and of which $\overline{\Omega}$ is the expectation value).

[18] We consider here only the set of ''small fluctuations'' defined as those for which $\delta\Omega_{\hat{k}}$ is small for each individual wave vector $\hat{k}$. As, by Eq. (2.5), the stationary point order parameter is only nonzero in a lower dimensional subspace (defined by the condition $\tilde{\mathbf{k}}=\mathbf{0}$), a more comprehensive definition of small fluctuations would additionally include those in which the support of the order parameter (i.e., the manifold on which it is nonzero) is slightly deformed. In those additional fluctuations, which one might call ''capillary'' or ''interface'' waves, the changes of the order-parameter field would not be small for individual values of the wave vector $\hat{k}$ (a full value of the order parameter would be replaced by zero for some values of $\hat{k}$, while for other values of $\hat{k}$ zero would be replaced by a full value of the order parameter). According to an enlarged definition of this sort, the set of small fluctuations would contain, among others, those fluctuations associated with ''almost rigid'' rotations of the system [notice that, by Eq. (2.10), a set of replica index dependent rigid rotations already produces a change of support for the order parameter].

[19] See, e.g., Ref. 20, Vol. II, Chap. XI, Sec. 11.3.

[20] Bateman Manuscript Project, *Higher Transcendental Functions*

(McGraw-Hill, New York, 1953-55).

[21] We have assumed here that the product $f^*(\hat{k})g(\hat{k})$ goes to zero continuously at the origin of $\hat{k}$ space. This assumption will hold true for the rest of the discussion, except for the problem of the spurious eigenvector in the case of MTI (i.e., $\tilde{\mathbf{k}}=\mathbf{0}$) fluctuations.

[22] The greatest lower bound of a nonempty set $\mathcal{S}$ of real numbers is the real number c such that for any lower bound b of the set $\mathcal{S}$ it is true that $c \geqslant b$. Such a number always exists for any set that has at least a lower bound. See, e.g., H. L. Royden, *Real Analysis* (Macmillan, New York, 1968), Chap. 2.

[23] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (Dover, New York, 1965).

[24] The numerical errors quoted are estimated by using different numerical methods to compute the function $\eta_1^{(0)}(x,x')$ and comparing the highest and lowest estimates for the eigenvalues thus obtained. Other sources of error, not considered in the quoted estimate, include the discretization of the integral equation and the numerical error of the diagonalization algorithm itself.

[25] One could attempt to solve Eq. (3.22a) by assuming that $\zeta=0$, but this leads to the condition

$$4\langle\theta^{-1+nd/2}\rangle_\pi = l-1+nd/2,$$

which can, at most, be satisfied for isolated values of n. In particular, by using Eq. (3.10) we see that for $n=0$ the left-hand side is not an integer, and the equation is not satisfied.

[26] To examine this assertion, let us consider a Hilbert space slightly different from the one defined in Sec. II C, in which the functions $f_{\hat{k}}$ are defined also for $\hat{k}=\hat{0}$. This enlargement of the Hilbert space makes room for spurious fluctuations of the order parameter at the origin to appear. The scalar product in this enlarged space is defined by

$$(f|g) \equiv \frac{1}{V^n}\sum_{\hat{k}} f^*(\hat{k})g(\hat{k}).$$

The scalar product of the eigenvector ψ^s associated with a radial eigenfunction singular at the origin and the normalized function $\psi^z(\hat{k})=V^{n/2}\delta_{\hat{k},\hat{0}}$ concentrated at the zero-replica sector is given by

$$(\psi^z|\psi^s)=\frac{1}{V^{n/2}}\psi^s(\hat{0})=1+\mathcal{O}(n),$$

and thus ψ^s lies entirely in the zero-replica sector for $n\to 0$.

[27] A search for a replica symmetry-breaking stationary point of the free energy functional (2.4) has not yielded any such solution [W. Peng, H. E. Castillo, and P. M. Goldbart, (unpublished); see also P. M. Goldbart and A. Zippelius, J. Phys. A **27**, 6375 (1994)].

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