

Further testing the validity of generalized heterogeneous-elasticity theory for low-frequency excitations in structural glasses

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We summarize the salient features of our theory of nonphononic vibrational excitations in glasses [W. Schirmacher *et al.*, *Nat. Commun.* **15**, 3107 (2024)]. Next, we provide further evidence of the nonuniversality of the ω^4 scaling of the nonphononic vibrational density of states (DoS), and the existence of an important class of nonphononic excitations in glasses, which we call defect states. These modes are induced by frozen-in stresses and can be classified as quasilocalized. Our results suggest that the commonly observed low-frequency ω^4 scaling of the nonphononic vibrational density of states is highly dependent on the technical aspects of the molecular dynamics simulations employed to compute the DoS.

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I. INTRODUCTION

The vibrational properties of glasses are until now subject to extensive experimental, theoretical, and simulational investigations due to their anomalous features—as compared to crystals—and the difficulty in treating a noncrystalline solid theoretically [1,2]. The low-frequency vibrational properties of glasses and their associated low-temperature thermal properties differ appreciably from those of their crystalline counterparts [3]. Experimental information relies on inelastic light scattering (Raman and Brillouin [4]), inelastic neutron [5] and X-ray scattering [6], and indirectly via the specific heat and thermal conductivity [3]. The most striking difference between the vibrational density of states (DoS) $g(\omega)$ and that of a crystal is an enhancement with respect to Debye’s $g(\omega) \propto \omega^2$ law (“boson peak” [7]). This anomalous feature appears as a shoulder in the DoS and a peak in $g(\omega)/\omega^2$.

Macroscopic glasses, and, more generally, disordered solids support acoustic waves like crystals, which therefore are generic low-frequency excitations, which phenomenologically may be described in both crystals and glasses by elasticity theory. It has been demonstrated in a series of scientific works [8–12] that *spatially fluctuating elastic constants* give rise to a deviation from Debye’s ω^2 law due to the phonons. This has been verified by calculations

based on the self-consistent Born approximation (SCBA) [8], the coherent-potential approximation [11], as well by numerical simulations [10]. This approach is known as the heterogeneous-elasticity theory (HET).

Subsequently, several groups published results of numerical simulations of systems, which are so small that they are not able to support elastic waves [13–18]. A class of anomalous modes was identified, whose DoS scales as a power law of the frequency. However, some disagreement was found concerning the precise value of the scaling exponent. More specifically, in a representation $g(\omega) \propto \omega^s$, one group of authors universally obtained $s = 4$, independently on the sample preparation [13,14,17], whereas the authors of [16,18] found $2 \leq s \leq 4$, depending on the parental temperature T^* in the liquid state, from which the glassy sample was obtained by quenching. For high T^* they found $s \approx 2$, and for low T^* $s \approx 4$.

In order to make further progress, we developed a generalized elasticity theory (GHET), in which, in addition to spatial fluctuations of elastic constants, spatially fluctuating frozen-in stresses were taken into account [19]. These stresses were found to couple to vortexlike displacement fields. These nonphononic vibrational excitations were termed *type-II*, whereas those due to spatially fluctuating elastic constants were termed *type-I*. With the help of a GHET the parental-temperature scenario was explained in the following way: For rather high T^* the system is in a state of marginal stability, for which HET predicts a DoS with $s = 2$, which is not a Debye exponent but a critical one. For stable systems, HET (without the type-II modes) predicts—for small samples without phonons—a low-frequency gap in the spectrum. Within GHET this gap is filled with the type-II excitations. The DoS of these type-II

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excitations depends on the distribution of the internal stresses. This distribution of internal stresses, and hence the DoS, was found to be sensitive to the way the potential is smoothed around its cutoff (tapering procedure).

Recently, in a letter to the Editor of Phys. Rev. E [20], Lerner and Bouchbinder raised concerns about the results of Ref. [19]. Specifically, they insist on the universality of a $g(\omega) \propto \omega^4$ scaling of the low-frequency nonphononic density of states for glasses, and suggest that our theoretical treatment would be “inherently deficient in capturing the ... nature of quasilocalized, nonphononic excitations in structural glasses.”

In this paper we first briefly present the derivation and the main results of GHET, in particular focusing on the role of frozen-in stresses. We then present further evidence of our findings and discuss them in the context of concerns raised by Lerner and Bouchbinder.

II. GENERALIZED HETEROGENEOUS-ELASTICITY THEORY

A. Derivation

In our derivation of GHET [19], we started from the expression for the harmonic potential energy of a system interacting via a pairwise potential $\phi(r)$:

$$E_{\text{harm}}\{\mathbf{r}_i\} = \sum_{(i,j)} \mathbf{u}_i \cdot \vec{H}_{ij} \cdot \mathbf{u}_j \doteq \sum_{(i,j)} V_{ij}. \quad (1)$$

Here $\sum_{(i,j)}$ denotes a sum over pairs (i, j) , $\mathbf{u}_i$ are infinitesimal displacements from the disordered locations $\mathbf{r}_i$ of the atoms in the glass, and $\vec{H}_{ij}$ is the dynamical (Hessian) matrix given in terms of force constants $K_{ij}^{\alpha\beta}$:

$$\begin{aligned} H_{ij}^{\alpha\beta} &= \frac{\partial}{\partial r_i^\alpha} \frac{\partial}{\partial r_j^\beta} E_{\text{harm}}\{\mathbf{r}_i\} \\ &= -K_{ij}^{\alpha\beta} (1 - \delta_{ij}) + \left(\sum_{\ell \neq i} K_{i\ell}^{\alpha\beta} \right) \delta_{ij}. \end{aligned} \quad (2)$$

The force constants are given by

$$\begin{aligned} K_{ij}^{\alpha\beta} &= \left[\phi''(r_{ij}) - \frac{1}{r_{ij}} \phi'(r_{ij}) \right] \frac{r_{ij}^\alpha r_{ij}^\beta}{r_{ij}^2} + \frac{1}{r_{ij}} \phi'(r_{ij}) \delta_{\alpha\beta} \\ &\doteq \phi^{(1)}(r_{ij}) \frac{r_{ij}^\alpha r_{ij}^\beta}{r_{ij}^2} + \phi^{(2)}(r_{ij}) \delta_{\alpha\beta} \end{aligned} \quad (3)$$

with implicit definition of the functions $\phi^{(1)}(r_{ij})$ and $\phi^{(2)}(r_{ij})$.

In order to derive the disordered version of elasticity theory from the microscopic Hamiltonian, we cannot use the standard procedure of lattice dynamics [21], which is based on the translational symmetry of crystals. Instead we follow the ideas of Lutsko [22,23] and Alexander [24], using the fact that E_{harm} only depends on the distances between the atoms. We therefore introduce difference and center-of-mass variables $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{R}_{ij} = \frac{1}{2}[\mathbf{r}_i + \mathbf{r}_j]$. We interpret $\mathbf{R}_{ij} \doteq \mathbf{R}$ as the local vector of the continuum theory and define the

potential-energy density $\mathcal{V}$ as

$$\begin{aligned} \mathcal{V}(\mathbf{R}) &= \frac{V_{ij}}{\Omega_Z} \\ &= \frac{1}{2\Omega_Z} \left(\phi^{(1)}(r_{ij}) \sum_{\alpha\beta} r_{ij}^\alpha r_{ij}^\beta u_{ij}^\alpha u_{ij}^\beta + \phi^{(2)}(r_{ij}) u_{ij}^2 \right) \\ &\doteq \mathcal{V}^{(1)}(\mathbf{R}) + \mathcal{V}^{(2)}(\mathbf{R}), \end{aligned} \quad (4)$$

where $\mathbf{u}_{ij} = \mathbf{u}_i - \mathbf{u}_j$ and Ω_Z is the inverse of the average number of bonds (i, j) per volume, given by $\frac{1}{\Omega_Z} = \frac{1}{2\Omega} N(Z-1)$. Here Ω is the total volume, N the number of atoms, and Z the average coordination number. It is important to note that $\sqrt[3]{\Omega_Z}$ is the minimal possible length scale to formulate a continuum theory. We make a Taylor expansion of $\mathbf{u}(\mathbf{r}_i)$ around $\mathbf{R}$:

$$\begin{aligned} \mathbf{u}(\mathbf{r}_i) &= \mathbf{u}(\mathbf{R}) + (\mathbf{r}_i - \mathbf{R}) \cdot \nabla \mathbf{u}(\mathbf{R}) \\ &= \mathbf{u}(\mathbf{R}) + \frac{1}{2} (\mathbf{r}_{ij} \cdot \nabla) \mathbf{u}(\mathbf{R}). \end{aligned} \quad (5)$$

It follows

$$\frac{1}{2} [\mathbf{u}(\mathbf{r}_i) + \mathbf{u}(\mathbf{r}_j)] = \mathbf{u}(\mathbf{R}) \quad (6)$$

and

$$u^\alpha(\mathbf{r}_i) - u^\alpha(\mathbf{r}_j) = \sum_\gamma r_{ij}^\gamma u_{\alpha|\gamma}(\mathbf{R}) = u_{ij}^\alpha, \quad (7)$$

with abbreviation $u_{\alpha|\gamma} \doteq \partial_\gamma u^\alpha$. The two terms of the potential-energy density then become

$$\begin{aligned} \mathcal{V}^{(1)}(\mathbf{R}) &\doteq \frac{1}{\Omega_Z} V_{ij}^{(1)} \Big|_{\mathbf{R}=\mathbf{R}_{ij}} \\ &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} B^{\alpha\beta\gamma\delta}(\mathbf{R}) \varepsilon^{\alpha\gamma}(\mathbf{R}) \varepsilon^{\beta\delta}(\mathbf{R}), \end{aligned} \quad (8)$$

$$\begin{aligned} \mathcal{V}^{(2)}(\mathbf{R}) &\doteq \frac{1}{\Omega_Z} V_{ij}^{(2)}(\mathbf{R}) \Big|_{\mathbf{R}=\mathbf{R}_{ij}} \\ &= \frac{1}{2} \sum_{\alpha\gamma\delta} \sigma^{\gamma\delta}(\mathbf{R}) u_{\alpha|\gamma}(\mathbf{R}) u_{\alpha|\delta}(\mathbf{R}) \end{aligned} \quad (9)$$

with the strain tensor

$$\varepsilon^{\alpha\gamma}(\mathbf{R}) = \frac{1}{2} [u_{\gamma|\alpha}(\mathbf{R}) + u_{\alpha|\gamma}(\mathbf{R})], \quad (10)$$

the Born-Cauchy elastic constants

$$B^{\alpha\beta\gamma\delta}(\mathbf{R}) \doteq \frac{1}{\Omega_Z} \phi^{(1)}(r_{ij}) r_{ij}^\alpha r_{ij}^\beta r_{ij}^\gamma r_{ij}^\delta \Big|_{\mathbf{R}=\mathbf{R}_{ij}}, \quad (11)$$

and the local stresses

$$\sigma^{\gamma\delta}(\mathbf{R}) \doteq \frac{1}{\Omega_Z} \phi^{(2)}(r_{ij}) r_{ij}^\gamma r_{ij}^\delta \Big|_{\mathbf{R}=\mathbf{R}_{ij}}. \quad (12)$$

Here, $\mathcal{V}^{(1)}$ is the stress-independent local potential energy density with spatially fluctuating elastic constants, whereas $\mathcal{V}^{(2)}$ is the term due to the frozen-in stresses $\sigma^{\alpha\beta}(\mathbf{R})$.

It has been noted by Lutsko [22,23], that the local stresses affect the local elasticity. More importantly, Alexander [24,25] noted that the stress-related terms violate local rotational invariance. Therefore the stress-related terms not

only involve the strain tensor in Eq. (10), but also the rotation tensor

$$\eta^{\alpha\gamma}(\mathbf{R}) = \frac{1}{2}[u_{\gamma|\alpha}(\mathbf{R}) - u_{\alpha|\gamma}(\mathbf{R})]. \quad (13)$$

The tensor $\eta^{\alpha\gamma}$ has only three entries, and is related to the vorticity vector $\boldsymbol{\eta}$ by

$$\eta_\alpha(\mathbf{R}) = \sum_{\beta\gamma\delta} \lambda_{\alpha\beta\gamma} \eta_{\beta\gamma}(\mathbf{R}), \quad (14)$$

where $\lambda_{\alpha\beta\gamma}$ is the Levi-Civita symbol. Following [22], we incorporate the symmetrized stress terms into the elastic constant tensor as

$$C_{ij}^{\alpha\beta\gamma\delta} = B_{ij}^{\alpha\beta\gamma\delta} + \frac{1}{4}(\sigma^{\gamma\delta}\delta_{\alpha\beta} + \sigma^{\alpha\delta}\delta_{\gamma\beta} + \sigma^{\gamma\beta}\delta_{\alpha\delta} + \sigma^{\alpha\beta}\delta_{\gamma\delta}). \quad (15)$$

This modifies the two terms of the local potential-energy density $\mathcal{V}(\mathbf{R}) \rightarrow \tilde{\mathcal{V}}^{(1)}(\mathbf{R}) + \tilde{\mathcal{V}}^{(2)}(\mathbf{R})$ with

$$\tilde{\mathcal{V}}^{(1)}(\mathbf{R}) = \frac{1}{2}C^{\alpha\beta\gamma\delta}(\mathbf{R})\varepsilon^{\alpha\gamma}(\mathbf{R})\varepsilon^{\beta\delta}(\mathbf{R}) \quad (16)$$

and

$$\tilde{\mathcal{V}}^{(2)}(\mathbf{R}) = \frac{1}{2} \sum_{\alpha\gamma\delta} \sigma^{\gamma\delta}(\mathbf{R}) \eta^{\alpha\gamma}(\mathbf{R}) (\eta^{\alpha\delta}(\mathbf{R}) - \varepsilon^{\alpha\delta}(\mathbf{R})) \quad (17)$$

In terms of the vorticity vector $\boldsymbol{\eta}$, Eq. (17) can be written as

$$\begin{aligned} \tilde{\mathcal{V}}^{(2)}(\mathbf{R}) = & \frac{1}{2} \left(\text{Tr}\{\sigma(\mathbf{R})\}\eta^2 - \sum_{\gamma\mu} \sigma^{\gamma\delta}(\mathbf{R})\eta^\gamma(\mathbf{R})\eta^\delta(\mathbf{R}) \right) \\ & - \frac{1}{2} \boldsymbol{\tau} \cdot \boldsymbol{\eta} \end{aligned} \quad (18)$$

with the coupling vector

$$\tau_\alpha = \sum_{\beta\gamma\delta} \lambda_{\alpha\beta\gamma} \sigma^{\beta\delta} \varepsilon^{\delta\gamma}. \quad (19)$$

B. Type-I spectrum: Boson peak and marginal stability

Neglecting the $\mathcal{V}^{(2)}$ term, we have obtained a microscopic derivation of heterogeneous-elasticity theory [8], which, as mentioned above, predicts a boson peak as a consequence of disorder. The associated vibrational modes feature a spectrum according to the Gaussian Orthogonal random-matrix ensemble (GOE) [26]. They are random-matrix modes (eigenfunction of random matrices), and have been called “type-I” nonphononic modes in Ref. [19]. In this paper the type-I modes have been shown numerically to feature a level-distance spectrum according to the GOE [26], and are therefore delocalized. Only at very high frequencies are the states localized. It is known from earlier work, that at very high frequencies, near the Debye frequency, the eigenstates of a disordered harmonic system are localized [27,28].

In the SCBA version of HET the underlying Gaussian distribution of elastic constants leads to an instability at a critical value of the disorder, characterized by the relative variance of the fluctuations. At marginal criticality the boson peak extends to zero frequency, and the DoS is quadratic in ω like in the case of the Debye phonons, albeit with a higher prefactor. In the discussion of nonphononic modes of very small systems, which do not allow for standing waves, we

have argued [19] that the observed $g(\omega) \propto \omega^2$ behavior of samples quenched from very high parental temperatures is due to marginal stability. In a more stable system SCBA-HET predicts a gap below the boson peak. This gap is then filled, in the presence of local frozen-in stresses, by type-II modes, which are governed by the second term $\tilde{\mathcal{V}}^{(2)}$ of the potential energy density.

C. Type-II spectrum: The role of frozen-in stresses

As in Ref. [19] we specify our model now in assuming that the local stresses are confined to a certain volume Ω_ℓ with the center at $\mathbf{R}_\ell$, and we give the label ℓ to these stresses and the corresponding vorticities.

The total Lagrangian density of GHET is given by

$$\mathcal{L}_{\text{GHET}}(\mathbf{R}, t) = \mathcal{L}_{\text{HET}}(\mathbf{R}, t) + \frac{1}{2}\zeta \sum_\ell \dot{\boldsymbol{\eta}}_\ell^2(\mathbf{R}, t) - \mathcal{V}^{(2)}(\mathbf{R}, t), \quad (20)$$

where ζ is an average moment-of-inertia density, and the HET Lagrangian is

$$\mathcal{L}_{\text{HET}}(\mathbf{R}, t) = \frac{\rho}{2} [\dot{\mathbf{u}}(\mathbf{R}, t)]^2 - \tilde{\mathcal{V}}^{(1)}(\mathbf{R}, t). \quad (21)$$

Now we treat $\mathbf{u}(\mathbf{R}, t)$ and $\boldsymbol{\eta}(\mathbf{R}, t)$ as independent variables and obtain the following Lagrangian equations of motion in frequency space ($z = \omega^2 + i\epsilon$):

$$\begin{aligned} -\zeta z \eta_\ell^\nu(\mathbf{R}, z) = & -\text{Tr}\{\sigma\} \eta_\ell^\nu(\mathbf{R}, z) + \sum_\mu \sigma_\ell^{\nu\mu}(\mathbf{R}) \eta_\ell^\mu(\mathbf{R}, z) \\ & - \tau_\ell^\nu(\mathbf{R}, z), \end{aligned} \quad (22)$$

$$\begin{aligned} -\rho_m z u^\alpha(\mathbf{R}, z) = & \sum_\beta \frac{\partial}{\partial x_\beta} \left(\sum_{\gamma\delta} C^{\alpha\gamma\delta\beta}(\mathbf{R}) \varepsilon^{\gamma\delta}(\mathbf{R}, z) \right. \\ & \left. + \sum_\nu \sum_\ell s_\ell^{(\nu),\alpha\beta}(\mathbf{R}) \eta_\ell^\nu(\mathbf{R}, z) \right), \end{aligned} \quad (23)$$

with

$$\tau_\ell^\mu(\mathbf{R}, z) = \sum_{\beta\gamma\delta} \lambda_{\mu\beta\gamma} \sigma^{\beta\delta}(\mathbf{R}) \varepsilon^{\delta\gamma}(\mathbf{R}, z), \quad (24)$$

$$s_\ell^{(\nu),\alpha\beta}(\mathbf{R}) = \frac{1}{2} \begin{cases} t_\ell^{(\nu),\alpha\alpha}(\mathbf{R}), & \alpha = \beta \\ \frac{1}{2} t_\ell^{(\nu),\alpha\beta}(\mathbf{R}), & \alpha \neq \beta \end{cases} \quad (25)$$

and

$$t_\ell^{(\nu),\alpha\beta}(\mathbf{R}) = \frac{\partial}{\partial \varepsilon^{\alpha\beta}} \tau_\ell^\nu = \sum_\gamma \lambda_{\nu\gamma\alpha} \sigma_\ell^{\beta\gamma}(\mathbf{R}). \quad (26)$$

Equations (22) and (23) comprise the GHET equations of motion. In order to gain qualitative insight into the influence of the stresses on the type-II nonphononic spectrum, we make the following simplifications:

- (1) We disregard the $\mathbf{R}$ dependence of the elastic constants, i.e., disregard the type-I nonphononic vibrations.
- (2) We treat the $\boldsymbol{\eta}$ and $\sigma^{\alpha\beta}$ as scalars η_ℓ and σ_ℓ [29].
- (3) We assume that inside of the vorticity range Ω_ℓ , the stresses σ_ℓ do not depend on $\mathbf{R}$;

(4) We assume that the type-II modes couple only to the transverse elastic waves $\mathbf{u}_T(\mathbf{k}, z)$, which are supposed to propagate in direction of the z coordinate, and polarized in x direction.

Equations (22) and (23), transformed into $\mathbf{k}$ space, then simplify as follows:

$$(-\zeta z + \sigma_\ell)\eta_\ell(\mathbf{k}, z) = -\frac{1}{2}ik\sigma_\ell u_T(\mathbf{k}, z), \quad (27)$$

$$(-\rho z + k^2\mu)u_T(\mathbf{k}, z) = ik\sum_\ell \frac{1}{4}\sigma_\ell\eta_\ell(\mathbf{k}, z). \quad (28)$$

Here μ is the shear modulus. Solving Eq. (27) for $\eta_\ell(\mathbf{k}, z)$ and inserting this into Eq. (27) we get

$$(-\rho z + k^2[\mu - \Sigma(z)])u_T(\mathbf{k}, z) = 0 \quad (29)$$

with

$$\Sigma(z) = \frac{1}{8}\sum_\ell \frac{\sigma_\ell^2}{-\zeta z + \sigma_\ell}. \quad (30)$$

This self-energy gives a frequency-dependent contribution to the shear modulus. The modified density of states of the transverse modes is given by

$$g(\omega) = \frac{2\omega}{\pi} \text{Im} \left\{ \overline{\sum_k \frac{1}{-\rho z + k^2[\mu - \Sigma(z)]}} \right\}, \quad (31)$$

where the overline denotes an average over the stresses σ_ℓ with distribution density $P(\sigma)$. In addition to the contribution of the transverse waves, which is absent in small enough samples, there is a contribution to the DoS from the frozen-in stresses:

$$\Delta g(\omega) \propto \omega \text{Im}\{\Sigma(z)\} \propto \omega \sigma^2 P(\sigma)|_{\sigma=\zeta\omega^2}. \quad (32)$$

Equation (32) implies that according to GHET the low-frequency part of the DoS reflects the distribution of small frozen-in stresses in the glass. It follows that the frequency dependence of the DoS, determined from molecular dynamics (MD) simulations, may depend on technical details of the simulation procedure. We have shown in [19] by our numerical simulations, that the low-frequency DoS, in stable systems far from marginality, in fact, depends on the distribution of small stress values. In MD simulations, however, many low stress values are introduced by the tapering (smoothing) function. This function is used to ensure smooth vanishing of the potential at the cutoff distance. This cutoff is in turn introduced to reduce the number of interacting particles and thus the computational cost. The standard choice is a polynomial tapering function, which ensures that the second derivative of the potential is continuous at the cutoff. According to the theory, this generates a stress distribution density $P(\sigma)$ near the cutoff that scales as $\sigma^{-1/2}$, and this in turn produces a DoS scaling as ω^4 . However, the theory predicts that other choices of tapering function gives rise to an ω^s scaling with an exponent $s \neq 4$.

The numerical simulation reported in [19], despite the usual limitation on the range of accessible frequencies, is consistent with this theoretical prediction.

III. ADDITIONAL EVIDENCE OF GHET PREDICTIONS

In their letter [20], Lerner and Bouchbinder raise five distinct concerns about our study [19]. In the following we will comment on these concerns and bring further evidence of the results of [19]. We start with a brief summary of the five main results of Ref. [19] on which concerns have been raised in [20]:

(i) In earlier simulations [16,18] it was shown that the DoS in systems quenched from high parental temperatures scales with an exponent $s=2$, while higher values of s up to $s=4$ are observed when the system is quenched from lower parental temperatures. We have explained this finding by the observation that in these studies the samples with high parental temperature were marginally stable, whereas the low-parental- T samples were more stable.

(ii) In all our simulations the spectral statistics of the non-phononic eigenvalues obey the GOE statistics, from which follows that both the type-I and the type-II modes are delocalized.

(iii) In our simulations, for samples quenched from low parental temperatures, we find a sensitive dependence of the low-frequency DoS on tapering, in agreement with our theoretical prediction.

(iv) In our theory we predict that in systems whose potential displays a minimum (such as Lennard-Jones systems), an exponent $s = 5$ of the DoS scaling is predicted, which, however, is modified by the tapering.

(v) We deduce from our analytic work that the type-II eigenfunctions feature vortexlike patterns, which we observe in the simulations.

We now comment point by point on the concerns expressed in Ref. [20] on these issues:

(i) The authors of [20] do not find the ω^2 ($s = 2$) law in their simulations of samples quenched from high parental temperatures, which is expected for a marginally stable system [30]. On the other hand, in all our simulations in Refs. [16,18,19] we have clear evidence for $s = 2$ in the case of quenching from high enough parental temperatures. In order to show the absence of $s = 2$, and the universality of $s = 4$, the authors of [20] report the integrated DoS $F(\omega) = \int_0^\omega g(\tilde{\omega})d\tilde{\omega}$, divided by ω^{s+1} with $s = 4$ (see [20, Fig. 1]).

First, we note that the data in [20, Fig. 1] never become really flat except, perhaps, in the small frequency region between 0.1 and 0.3, which is a rather small range to fit a powerlaw with reasonable precision. From the small slope observed in [20, Fig. 1], one can deduce that the exponent s ranges from $s = 3$ (small systems) to $s = 3.5$ (larger systems). Furthermore, the data for $N = 32\,768$ and $N = 131\,072$ seem to be very close, indicating that one has reached convergence. We can then conclude that the simulations of Ref. [20], consistently with other studies (see, e.g., [31]), find neither the claimed $s = 4$ nor the marginally stable value $s = 2$.

Second, to obtain a marginally stable system, one needs to (1) start from a very high temperature, and (2) quench it with algorithms that do not allow the system to relax towards “comfortable” (i.e., far from marginality) situations. We cannot comment on the algorithm used to quench in [20], nor on the fact that their parental temperature

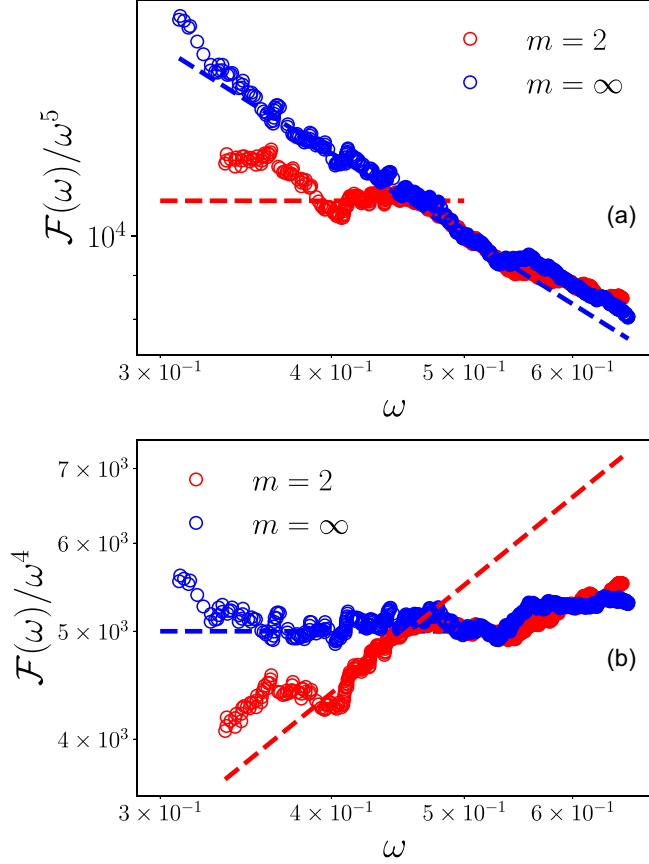


FIG. 1. Panel (a): plot of the function $F(\omega)/\omega^5$ for $m = 2$ (red dots) and $m = \infty$ (blue dots). The horizontal dashed red line emphasizes the expected $s = 4$ for $m = 2$. The blue dashed line has a slope equal to -1 (i.e., $s = 3$). Panel (b): plot of the function $F(\omega)/\omega^4$ for $m = 2$ (red dots) and $m = \infty$ (blue dots). The horizontal dashed blue line emphasizes the expected $s = 3$ for $m = \infty$. The red dashed line has a slope equal to 1 (i.e., $s = 4$).

(“roughly four times larger than the glass transition temperature”) is high enough, as these aspects are strongly system dependent. A detailed study of the procedures to create marginal stable glasses, and of their DoS is underway.

We conclude that at present the origin of the discrepancy between our simulations, where $s = 2$ is found at high parental temperatures, and those reported in [20] remains unclear.

(ii) In their simulations of small glasses, reported in [20], the authors evaluated the participation ratio

$$e = \frac{1}{N} \left[\sum_i (\psi_i \cdot \psi_i)^2 \right]^{-1} \quad (33)$$

(where N is the number of particles and ψ_i is an eigenvector to an eigenvalue ω_i^2) for several system sizes N from $N = 2048$ to $N = 131\,072$. In Ref. [20, Fig. 1(b)] the quantity Ne is reported, showing a dense cloud at low frequencies with values ranging from 20 to 200. As this cloud of data is rather diffuse, showing no trend, the authors conclude that Ne would be constant, and consequently e would scale as $1/N$, from which would follow that the corresponding modes are localized. In their

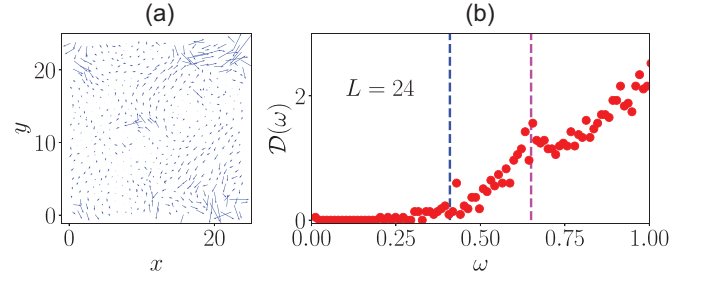


FIG. 2. Panel (a) reports the sketch of a mode at $\omega \approx 0.4$ [blue dashed line in panel (b)], which shows a vortexlike feature. This mode is at lower frequency with respect to the lowest transverse phonons resonance [magenta dashed line in panel (b)] found at $\omega \approx 0.65$.

Ref. [55] the authors of [20] call the corresponding modes quasilocalized.

In our study [19] we evaluated the *spectral statistics* of the eigenvalues both for systems quenched from high and from low parental temperatures. The statistics obeys the GOE in all cases, which means that they exhibit level repulsion and are therefore delocalized. This apparent contradiction can be solved by noting that vibrational modes in disordered systems can have a very nontrivial structure, such that they can be delocalized in a subtle way [32].

We would like to comment more generally on quasilocalized modes in glasses. This term was coined by Schober and Oligschleger [33] who pointed out that local vibrational defect states are inevitably coupled to the elastic degrees of freedom, leading eventually to hybridization with phonons and to delocalization. This point was further investigated by Schober and one of the present authors, in a systematic study of the localization properties of low-frequency vibrational states of small glassy systems upon varying system size [34]. For all system sizes studied ($N = 2048$ – $32\,000$) the participation ratio was reduced at low frequencies ($e = 0.4$) but did not depend on N . The eigenvalue nearest-neighbor statistic, however, showed GOE behavior, even for $N = 2024$. As these findings are in agreement with those in our recent investigation [19], we conclude that, in fact, what we call “type-II” can also be classified as quasilocalized modes and are delocalized. It has, however, been found in Ref. [34] that the energy associated with a quasilocalized mode is concentrated in a certain region in space. This is what we also assume to be the case for the type-II modes [19].

(iii) The authors of Ref. [20] do not agree with our conclusion that the smoothing of the potential near its cutoff $\phi(r) \propto (r_c - r)^{m+1}$ (tapering) strongly influences the DoS of a stable simulated small glass at low frequencies. To show this, they report in Ref. [20, Fig. 2(c)] our $F(\omega)$ data ($m = 2$ and $m = \infty$), taken from [19]. Contrary to our finding ($s \approx 4$ for $m = 2$ and $s \approx 3$ for $m = \infty$) they claim that the data are consistent with $s = 4$ independently of m . We note that this finding is based on an extremely small range of frequencies, $1.2 \leq \omega \leq 1.4$. In order to show that our s values, and the corresponding conclusions concerning the tapering, are correct, we collected new data for $m = 2$ and $m = \infty$. We plot in Fig. 1 the quantities $F(\omega)/\omega^5$, panel (a) and $F(\omega)/\omega^4$, panel

(b) for the two cases $m = 2$ and $m = \infty$. We display the first 5×10^4 eigenfrequencies of a set of order 10^6 eigenmodes. The figure shows that the low-frequency data are closer to a slope $s = 4$ for $m = 2$ and $s = 5$ for $m = \infty$, even if large uncertainties in the determination of s are present. In any case, the DoS are clearly different at low frequencies. We want to emphasize that plotting $F(\omega)$ and passing a straight line on the low-frequency data leads to a much larger uncertainty on s ; testing whether the data agree with a given value of s requires, in our opinion, plotting $F(\omega)/\omega^{s+1}$ as we did in Fig. 1.

(iv) In our paper [19] we point out that the type-II excitations in systems, with pairwise interaction potentials with a minimum, generically should have a contribution to the DoS, scaling as $s = 5$. We quoted simulations [35,36], in which Lennard-Jones potentials are used and in which $s = 5$ is observed. We did not perform any simulations with such potentials ourselves and only want to point out that care must be taken to avoid artifacts associated with the tapering. As the tapering-induced terms in the DoS scale with a lower s , there will be a crossover between the two contributions. We leave the calculations presented in Ref. [20] to refute our statement uncommented, as we cannot retrace the details of these calculations, especially the sample quenching procedure. Of course, we cannot exclude that the theory presented in [19] fails for systems with attractive interactions for some unknown reason.

(v) In our opinion, the most important result of our paper [19] points to the existence of vortexlike modes, being related to local frozen-in stresses. The authors of Ref. [20] state that the vortexlike modes are a superposition of transverse standing waves (phonons). To show this, they report in [20, Fig. 3] the eigenvectors of a couple of transverse modes with “identical wavelength,” and their superposition, which resembles a vortexlike mode. They conclude that *all* the vortexlike modes are of this kind. To support our statements, in Fig. 2 we report a vortexlike mode, together with the DoS of the system from where the mode has been extracted. One can easily see that the frequency of the selected mode (blue dashed line, $\omega \approx 0.4$) is by far lower than that of the lowest transverse phonons (magenta dashed line, $\omega \approx 0.65$). Thus this low-frequency mode is genuine and does not originate from the superposition of

waves. Furthermore, and more importantly, because of level repulsion acting for extended modes in disordered systems, two phonon modes *cannot have* the same frequency, and therefore cannot be combined to generate a superposition. Further clarification on this point would be needed to better understand the procedure used to generate [20, Fig. 3].

IV. DISCUSSION

Our new data provide an example of a system, which clearly shows a sensitive dependence of the DoS exponent s on the tapering procedure, which points to the existence of stress-related vortexlike modes. We have demonstrated that the frequency scaling of the DoS, calculated from molecular dynamics, is sensitive to the cutoff-smoothing (tapering) procedure, and that therefore the ω^4 dependence of the DoS may not be universal. We believe that the arguments presented in the letter of Lerner and Bouchbinder [20] are not in contradiction with the results of [19].

In future simulations care must be taken to investigate the dependence of the data on the employed algorithms, such as the degree of the cutoff smoothing (tapering) of the potential.

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DATA AVAILABILITY

Our numerical data, displayed in the figures, can be downloaded at Ref. [38].

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Correction: The name of the fifth author was misspelled and has been fixed.