

Normal modes and acoustic properties of an elastic solid with line defects

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The normal modes of a continuum solid endowed with a random distribution of line defects that behave like elastic strings are described. These strings interact with elastic waves in the bulk, generating wave dispersion and attenuation. Explicit formulas are provided that relate these properties to the density of string states. For a density of states that mimics the boson peak (BP) in amorphous materials, the attenuation as a function of frequency ω behaves as ω^4 for low frequencies, and, as frequency increases, crosses over to ω^2 near the BP, and then to linear in ω . An Ioffe-Regel criterion is satisfied at the BP. Dispersion is negative in the frequency range where attenuation is quartic and quadratic in frequency, with effective velocity reaching a minimum near the BP. Continuum mechanics can thus be applied to both crystalline materials and their amorphous counterparts at similar length scales. The possibility of linking this model with the microstructure of amorphous materials is discussed.

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I. INTRODUCTION

The normal modes of a continuum elastic solid can be easily counted using the classical theory of elasticity. However, since there is no intrinsic length scale, an artificial short distance cutoff must be introduced in order to obtain a finite result for the total number of modes of a given material. The Debye model does that, imposing a high frequency cutoff, the Debye frequency ω_D , so that the resulting total number of degrees of freedom equals the number of degrees of freedom inferred from the number of atoms in the solid. This provides a firm underpinning, at wavelengths long compared to interatomic spacing, for all properties of solids that depend on the counting on such modes. If the solid is crystalline, a similar counting can also be performed, exploiting the invariance of the system under discrete translations. This counting reduces to that provided by the Debye model at long wavelengths and provides, as well, a firm underpinning for properties at shorter wavelengths, down to the size of the unit cell.

The situation for amorphous solids, without a discrete translation invariance, has long been unsatisfactory. While at long wavelengths the situation is well described, as expected, by the Debye model, at wavelengths on the order of tens of mean interatomic distances, abundant evidence, from specific heat [1], thermal conductivity [2], Raman scattering [3], neutron scattering [4], and inelastic x-ray scattering measurements [5], points to the existence of normal modes with a frequency distribution that is peaked around $0.1\omega_D$ – $0.2\omega_D$. This distribution is qualitatively similar for many such materials, and the details, but not the broad features, depend on external parameters such as temperature, density, and pressure, as well as chemical and thermal history [6–15]. This distribution, dubbed the “boson peak” (BP), cannot be blamed on a (nonexistent) crystalline structure and deviates without ambiguity from the distribution for a continuum, at frequencies where the continuum approximation works reasonably well in the case of crystals. Much research has been performed in order to provide some rationale for this

state of affairs [16–23]. Nevertheless, it does not seem unfair to say that no satisfactory understanding exists yet, although significant insights have been obtained through large-scale ($\sim 10^7$ particles) simulations with Lennard-Jones [24] and soft sphere [25] potentials and through inelastic x-ray scattering experimental studies of SiO₂ glasses and crystals [26].

In addition to the above, Rufflé *et al.* discovered that, at low frequencies, acoustic attenuation as a function of frequency ω behaves like ω^4 in densified silica [27] and in lithium diborate [28], and more recent experiments [29–34] have provided a detailed measurement of the properties of acoustic waves in amorphous materials at wavelengths that probe length scales around the BP. Unexpected behavior for dispersion and attenuation has been uncovered, and the thought naturally comes to mind that whatever the physical mechanism is that gives rise to the BP, it should also explain the acoustic behavior at THz frequencies. This paper provides one such possible explanation, together with an answer to the following question: How can continuum mechanics, at similar length scales, be made to work similarly well for crystals and for their amorphous counterparts?

II. THE MODEL AND ITS DENSITY OF STATES

At THz frequencies, continuum mechanics provides an adequate description for the vibrational degrees of freedom of crystals. It is proposed that it should also provide an adequate explanation for amorphous materials: Consider then an elastic isotropic solid, as in the Debye model, with c_L and c_T the speed of propagation of longitudinal and transverse waves, respectively. In addition, this solid may have line defects that can be thought of as elastic strings endowed with mass per unit length $m \sim \rho b^2$ and line tension $T \sim \mu b^2$, where ρ is the mass density of the bulk, μ is its shear modulus, and b is a distance on the order of a typical interatomic spacing. These line defects can be pinned segments of length L that can vibrate around a straight equilibrium position, or circular loops that can oscillate, moving along the mantle of a cylinder around a circular equilibrium position (Fig. 1). The precise physical nature of these line defects is delayed for later discussion. The fact that they are defects is used to relate m with ρ and T with

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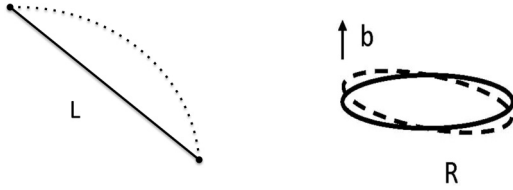


FIG. 1. Line defects in a continuum elastic solid. (Left) An elastic string of length L with pinned ends that can oscillate around a straight-line equilibrium position. (Right) An elastic circular string of radius R that can oscillate around a circular equilibrium position, along the mantle of a circular cylinder with generator b . Only the case of a straight line is considered in the present paper; results for the circle are qualitatively similar.

μ . As a result, the speed of propagation of elastic waves *along* the strings, c_S , is of the same order of magnitude as c_L and c_T .

To start with a simple description, assume that only the fundamental mode of vibration of the strings is relevant, ignoring higher harmonics. The strings have a length L with a distribution of such lengths: Let $p(L)dL$ be the number of strings per unit volume with length between L and $L + dL$. The assumption that only the fundamental mode, with frequency ω_1 , counts means there is a one-to-one correspondence between ω_1 and L and leads to a string density of states $g_S(\omega_1)$ (number of states per unit frequency per unit volume) given by $g_S(\omega_1)d\omega_1 \equiv p(L)dL$. The total density of states $g(\omega)$ of this model solid is

$$g(\omega) = g_D(\omega) + g_S(\omega), \quad (1)$$

where $g_D(\omega) = 3\omega^2/2c^3\pi^2$ is the Debye distribution, with $3c^{-3} \equiv c_L^{-3} + 2c_T^{-3}$. For later convenience, we normalize the distribution g_S to g_D and frequencies to the Debye frequency,

$$g_S(\omega) \equiv \tilde{g}(\tilde{\omega})g_D(\omega), \quad (2)$$

where $\tilde{\omega} \equiv \omega/\omega_D$, so $g(\omega) = g_D[1 + \tilde{g}(\tilde{\omega})]$.

III. ACOUSTIC PROPERTIES

An elastic string will oscillate in response to loading by an elastic wave. These oscillations will, in turn, generate secondary, scattered waves, a process that has been studied in great detail by Maurel *et al.* [35–37]. The dynamics is described by the string displacements $X(s, t)$ away from its equilibrium position X_0 , where s is a Lagrangian parameter to label string points and t is time. The displacement X satisfies an elastic string equation [38],

$$m\ddot{X}(s, t) + B\dot{X}(s, t) - TX''(s, t) = \mu b \mathbf{M}_{lk} \nabla_l u_k(\vec{X}_0, t), \quad (3)$$

with B a phenomenological viscous damping coefficient and $\nabla_l u_k(\vec{X}_0, t)$ the gradient of the displacement $\vec{u}(\vec{x}, t)$ associated with the incoming wave, evaluated at the string equilibrium position $\vec{x} = \vec{X}_0$. An overdot denotes differentiation with respect to time t , and a prime denotes differentiation with respect to s . The motion $X \equiv \vec{X} \cdot \hat{t}$ is along a plane spanned by the tangent \hat{t} to the string and a normal \hat{f} . Until further notice, B is an adjustable parameter of the model. However, we take it to be small, in a sense made more precise later, so that we have underdamped string oscillations and it makes

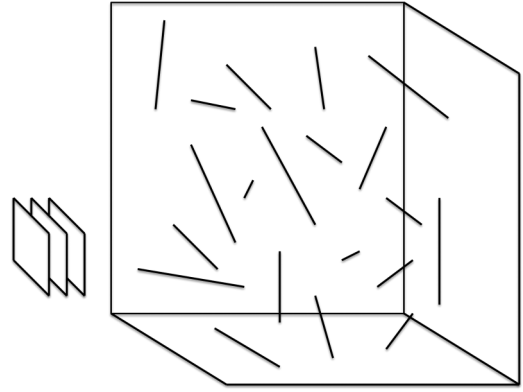


FIG. 2. Line defects, randomly distributed and oriented, have an effect on the properties of an acoustic wave, here depicted as a set of planes incident from the left. Attenuation is given by Eq. (14), and velocity dispersion is given by Eq. (17). Their lengths have a distribution that, through the frequency of their fundamental mode of oscillation, translates to a frequency distribution.

sense to speak of its modes of vibration. The binormal is $\hat{n} \equiv \hat{t} \times \hat{f}$ and $\mathbf{M}_{lk} \equiv t_l n_k + t_k n_l$. The right-hand side of (3) is the Peach-Koehler force for line dislocations in elastic continua. This coupling ensures that only the shear modulus, and not the bulk modulus, will become frequency dependent, a fact that has been observed in the numerical simulations of Maruzzo *et al.* [25].

We now wish to consider the interaction of acoustic waves with many such strings, randomly distributed and randomly oriented (Fig. 2). We assume all positions to be equally likely, as well as all orientations. Lengths, however, have a distribution $p(L)$. An elastic wave progressing through this medium will attenuate, and will propagate with a frequency-dependent velocity, both for longitudinal as well as transverse polarizations. In the following we treat the transverse case, for which the effect is stronger [35]. This is also in agreement with the measurements of Chumakov *et al.* [39] that link the BP of a glass with the transverse acoustic van Hove singularity of its crystalline counterpart.

A. A toy model: All strings have the same length

In order to get physical insight we consider first the idealized case of all strings having the same length. This is the same as bunching all excess modes within the BP under a δ function,

$$g_S(\omega) = n\delta(\omega - \omega_1), \quad (4)$$

where n is the total number of strings of length L per unit volume and $\omega_1 = \sqrt{(\pi c_S/L)^2 - (B/2m)^2}$.

1. Attenuation and the Ioffe-Regel limit

(a) *Attenuation.* The attenuation coefficient Γ_T is given by (in units of frequency)

$$\Gamma_T = n c_T \sigma_T(L), \quad (5)$$

where σ_T is the total scattering cross section for a transverse wave by a single defect. It will, in general, depend on the relative orientation of the string and the incident wave, so we

take the average value. The resulting average cross section is [35]

$$\sigma_T(L) = \frac{16L^2}{25\pi^5} \left(\frac{\rho b^2}{m} \right)^2 \frac{\omega^4}{[\omega^2 - (\pi c_S/L)^2]^2 + \omega^2 B^2/m^2}. \quad (6)$$

Taking $m = \rho b^2/\pi$ and $c_T = c_S \equiv c$, we have that (5) and (6) lead to

$$\Gamma_T = \frac{16}{25\pi^4} n L^3 \left(\frac{c\pi}{L} \right) \frac{\omega^4}{[\omega^2 - (c\pi/L)^2]^2 + \omega^2 B^2/m^2}. \quad (7)$$

It is apparent that the attenuation Γ_T as a function of frequency ω behaves as ω^4 for low frequencies, that is, when $\omega \ll c\pi/L$. When $\omega \sim c\pi/L$, that is, when $\omega^2 \sim \omega_1^2 + (B/2m)^2$, which is near, and slightly above the BP for small $B/2m\omega_1$, the attenuation behaves like frequency squared: $\Gamma_T \sim \omega^2$. This is in agreement with measurements on densified silica [27], lithium diborite [28], glycerol [29], sorbitol [30,34], and silica [31–33]. At higher frequencies the attenuation reaches a maximum, decreases, and flattens out at a constant asymptotic value when $\omega \gg c\pi/L$ and $\omega \gg B/m$.

Note that expression (7) depends on three independent string parameters: density n , length L , and attenuation frequency B/m . The qualitative behavior discussed in the previous paragraph is independent of their numerical values, as long as the attenuation parameter B is small.

(b) *Ioffe-Regel limit.* Thermal conductivity measurements indicate that the BP is also a frequency at which phonons lose their propagating character due to the condition, the Ioffe-Regel (IR) limit, that mean free path ℓ becomes smaller than wavelength [23,40,41]. More precisely, if k is wave number, the IR condition is $k\ell \sim 1$. In our notation, $\ell^{-1} = n\sigma_T(L)$, so that the IR criterion means $\Gamma_T = \omega$. Using (6) this translates into

$$\frac{16}{25\pi^4} n' \frac{\omega^3}{(\omega^2 - 1)^2 + \omega^2 b^2} = 1, \quad (8)$$

where $b' \equiv (B/m)/(\pi c/L)$, $\omega' \equiv \omega/(\pi c/L)$, and $n' \equiv nL^3$. How does this condition constrain the model?

Equation (8) can be thought of as an equation for ω' that depends on string length and density, through n' , and string attenuation b' . Remember that $b' < 1$ for the underdamped strings we are considering. The left-hand side of (8) has a maximum at $\omega' \sim 1$, the same frequency where the attenuation behaves as ω^2 . If n' is very small or b' not small enough, the equality (8) will not be satisfied. Introducing $\omega' = 1$ into (8) provides a threshold for these two parameters:

$$b^2 = \frac{16}{25\pi^4} n'. \quad (9)$$

If we take $n' = nL^3 \sim 1$, that is, an ensemble of strings separated by a mean distance comparable to their length, this condition is satisfied by $b' \sim 0.1$, a reasonable value. Lower (higher) densities imply also lower (higher) attenuations. At these values of the parameters, the attenuation at the BP becomes

$$\Gamma|_{\omega \sim \omega_1} \sim \frac{\pi c}{L} \quad (10)$$

up to corrections of order b'^2 . For a BP located at one-tenth of the Debye frequency, this translates into an attenuation at that level as well, in rough agreement with experimental measurements.

To conclude this section, the BP frequency coincides with the IR frequency for reasonable values of the model parameters.

2. Dispersion relation for transverse acoustic waves

The scattering by strings also modifies the coherent behavior of acoustic waves, a phenomenon that has been studied by Maurel *et al.* [42]. Their result, obtained through a multiple scattering formalism, is that the velocity of propagation c_T is renormalized to an effective, frequency-dependent velocity v_T given by

$$\begin{aligned} v_T &= c_T \left(1 + \frac{4nL}{5\pi^2} \frac{\rho b^2}{m} c_T^2 \frac{(\omega^2 - (\pi c_S/L)^2)}{[\omega^2 - (\pi c_S/L)^2]^2 + \omega^2 B^2/m^2} \right) \\ &= c_T \left(1 + \frac{4n'}{5\pi^3} \frac{(\omega^2 - 1)}{(\omega^2 - 1)^2 + \omega^2 b^2} \right), \end{aligned} \quad (11)$$

where the second line uses the same notation as in (8).

In the limit of very low frequencies, $\omega' \rightarrow 0$,

$$v_T \rightarrow c_T \left(1 - \frac{4n'}{5\pi^3} \right).$$

That is, the strings have an effect on the speed of transverse acoustic waves even at very low frequencies.

As the frequency increases, v_T decreases until it reaches a minimum,

$$v_{T\min} \approx c_T \left(1 - \frac{4n'}{5\pi^3} \frac{1}{2b'} \right), \quad (12)$$

when $\omega'^2 = 1 - b'$, that is, for the small string dampings we are hypothesizing, near and slightly below the BP. Negative velocity dispersion of this kind, up to frequencies comparable to the BP, has been observed in glycerol [29], silica [33], and sorbitol [34].

B. A distribution of lengths

The BP is not a δ function, but a set of modes distributed over a frequency interval. Within the present model, as discussed in Sec. II, this corresponds to an ensemble of strings with a distribution of lengths $p(L)$. The attenuation coefficient Γ_T will now be given by (in units of frequency) [42]

$$\Gamma_T = c_T \int \sigma_T(L) p(L) dL, \quad (13)$$

where σ_T is the total scattering cross section for a transverse wave by a single defect. Using (2), (6), $\omega_1^2 = (\pi c_S/L)^2 - (B/2m)^2$, and $m = \rho b^2/\pi$, Eq. (13) becomes

$$\tilde{\Gamma}_T(\tilde{\omega}) = \frac{24\tilde{\omega}^4}{25\pi^3} \int \frac{\tilde{g}(\tilde{\omega}_1) \tilde{\omega}_1^2 d\tilde{\omega}_1}{\mathcal{A}(\tilde{\omega}_1) \mathcal{B}(\tilde{\omega}, \tilde{\omega}_1)}, \quad (14)$$

with $\tilde{b} \equiv B/m\omega_D$, $\tilde{\Gamma}_T \equiv \Gamma_T/\omega_D$, and

$$\mathcal{A}(\tilde{\omega}_1) \equiv \tilde{\omega}_1^2 + \tilde{b}^2/4, \quad (15)$$

$$\mathcal{B}(\tilde{\omega}, \tilde{\omega}_1) \equiv (\tilde{\omega}^2 - \tilde{\omega}_1^2 - \tilde{b}^2/4)^2 + \tilde{\omega}^2 \tilde{b}^2. \quad (16)$$

Equation (14) establishes a clear relation between the degrees of freedom responsible for the BP and the degrees of freedom responsible for acoustic attenuation: Indeed, they are one and the same. At low frequencies, there is a $\tilde{\omega}^4$ Rayleigh behavior, as expected for attenuation produced by the scattering from objects much smaller than wavelength and as observed experimentally [27–29,32]. At higher frequencies, there is a crossover to $\tilde{\omega}^2$ behavior, as observed experimentally as well [29,32]. Also, the magnitude of the attenuation is proportional to the magnitude of the BP and its exact functional behavior depends on the parameters of the density of states, as well as the viscous damping \tilde{b} .

The effective velocity becomes, similarly,

$$v_T \approx c_T \left\{ 1 + \frac{1}{\pi^2} \int \frac{[\tilde{\omega}^2 - \mathcal{A}(\tilde{\omega}_1)] \tilde{g}(\tilde{\omega}_1) \tilde{\omega}_1^2 d\tilde{\omega}_1}{\mathcal{A}(\tilde{\omega}_1)^{1/2} \mathcal{B}(\tilde{\omega}, \tilde{\omega}_1)} \right\} \quad (17)$$

in terms of dimensionless, scaled, variables. The string degrees of freedom introduce a dispersion term into the effective velocity of acoustic waves. Equation (17) establishes a clear relation between the dispersion term and the density of states responsible for the BP. At low frequencies dispersion is negative, and it changes sign at about the same frequency that the attenuation (14) behaves as $\tilde{\omega}^2$, as observed experimentally [29,33,34]. The amount of dispersion is proportional to the amplitude of the BP.

In formulas (14) and (17), the distribution $\tilde{g}(\tilde{\omega})$ of the degrees of freedom responsible for the BP appears within an integral sign. Consequently, the resulting attenuation and velocity dispersion will be fairly insensitive to the small-scale details of the BP.

IV. POSSIBLE VALUES FOR MODEL PARAMETERS

In order to get a better understanding of the relation between line defects, density of states and acoustics that is being proposed, consider a BP in which the density of states follows a log-normal distribution:

$$\tilde{g}(\tilde{\omega}_1) = \frac{2\pi^2 nc^3}{3\tilde{\omega}_1^2 \omega_D^3} \frac{1}{\sqrt{2\pi} \sigma \tilde{\omega}_1} e^{-[\ln(\tilde{\omega}_1) - \tilde{\mu}]^2 / 2\sigma^2}. \quad (18)$$

This distribution depends on three parameters— n , $\tilde{\mu}$, and σ —that determine the location, magnitude, and width of the BP. It reduces to (4) when the variance vanishes: $\sigma \rightarrow 0$. The BP will be located at the mode of this distribution, $\tilde{\omega}_1 = e^{\tilde{\mu} - 3\sigma^2}$. The attenuation (14) and the effective velocity (17) become, respectively,

$$\frac{\tilde{\Gamma}_T(\tilde{\omega})}{\tilde{\omega}^2} = \frac{16}{25\pi} \frac{nc^3}{\omega_D^3} \tilde{\omega}^2 \int d\tilde{\omega}_1 \frac{\mathcal{L}(\tilde{\omega}_1)}{\mathcal{A}(\tilde{\omega}_1) \mathcal{B}(\tilde{\omega}, \tilde{\omega}_1)} \quad (19)$$

and

$$\frac{v_T(\tilde{\omega})}{c_T} - 1 = \frac{2}{3} \frac{nc^3}{\omega_D^3} \int \frac{[\tilde{\omega}^2 - \mathcal{A}(\tilde{\omega}_1)] \mathcal{L}(\tilde{\omega}_1) d\tilde{\omega}_1}{\mathcal{A}(\tilde{\omega}_1)^{1/2} \mathcal{B}(\tilde{\omega}, \tilde{\omega}_1)}, \quad (20)$$

with

$$\mathcal{L}(\tilde{\omega}_1) \equiv \frac{1}{\sqrt{2\pi} \sigma \tilde{\omega}_1} e^{-[\ln(\tilde{\omega}_1) - \tilde{\mu}]^2 / 2\sigma^2}. \quad (21)$$

It is easy to see that the parameter n satisfies

$$\int g_S(\omega) d\omega = \int p(L) dL = n,$$

so it is the total number of line defects per unit volume, and the average length of the line defects is

$$\begin{aligned} \langle L \rangle &\equiv \frac{\int L p(L) dL}{\int p(L) dL} \\ &= \frac{\pi c}{\omega_D} \int \frac{\mathcal{L}(\tilde{\omega}_1) d\tilde{\omega}_1}{\mathcal{A}(\tilde{\omega}_1)^{1/2}}. \end{aligned} \quad (22)$$

The coefficient in front of the integral sign is of the order of the interatomic spacing—call it $a \equiv \pi c / \omega_D$ —so the mean defect length will be around ten interatomic spacings.

We have four parameters— n , $\tilde{\mu}$, σ , and \tilde{b} —and the following experimental facts need to be explained. (i) Typically,

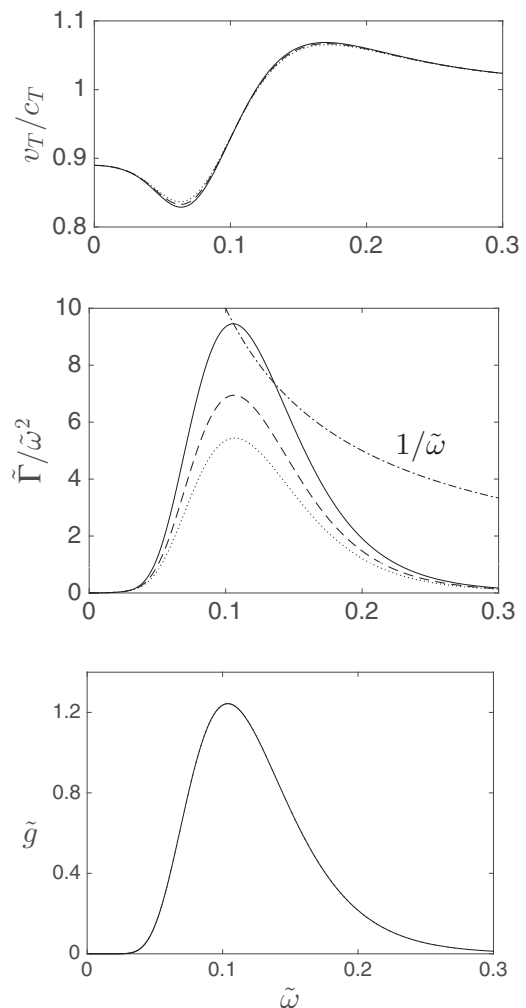


FIG. 3. Density of states (bottom panel) associated with a distribution of strings of varying lengths, given by (18) with $\tilde{\mu} = -1.8971 = \ln(0.15)$, $\sigma = 0.35$, and $na^3 = 0.01$. Attenuation $\tilde{\Gamma}$ (middle panel) given by Eq. (19) and effective velocity v_T (top panel) given by Eq. (20), for $\tilde{b} = 0.01$ (dotted lines), 0.008 (dashed lines), and 0.006 (solid lines). The IR criterion, $\tilde{\Gamma} = \tilde{\omega}$ at the BP, is satisfied for $\tilde{b} = 0.006$. These different values of \tilde{b} have almost no influence on the effective velocity. All frequencies are in units of ω_D .

the magnitude of the BP is a factor of about 2 over the Debye density of states (DOS), it is located at about $0.1 \omega_D$, and has a width of about $0.05 \omega_D$. (ii) Attenuation starts out as $\sim \omega^4$ at low frequencies and crosses over to $\sim \omega^2$ near the BP. (iii) Around the BP, attenuation (in units of frequency) is at the level of a few percent of ω_D . (iv) Also around the BP, the IR criterion, attenuation of the same order of frequency $\tilde{\Gamma} \sim \tilde{\omega}$, is satisfied. (v) There is a velocity dip, due to negative dispersion, at the level of 10% of the low-frequency value, again near the BP. In other words, the acoustic velocity as a function of frequency starts at a constant value, then has a negative dispersion (the velocity decreases as the frequency increases) as the BP frequencies are approached, and then acoustic velocity increases with frequency.

Figure 3 shows a DOS given by (18) with $\tilde{\mu} = -1.8971 = \ln(0.15)$, $\sigma = 0.35$, and $na^3 = 0.01$, or about one string per 100 atoms. This satisfies the requirements (i) and (ii) above. Now, in principle, \tilde{b} could be different for different string lengths, i.e., a function of $\tilde{\omega}$. To start with the simplest possibility, we assume that it is the same for all strings, $\tilde{b} \lesssim 0.01$. The resulting acoustic attenuation, given by (19), and velocity dispersion, given by (20), for these values of the parameters are shown in Fig. 3 as well. The magnitude of the effects appears to be in order-of-magnitude agreement with experimental observations, as required by (iii) and (v), and the IR criterion is met with $\tilde{b} = 0.006$, satisfying (iv).

V. POSSIBILITY OF A RELATION TO THE MICROSTRUCTURE OF AMORPHOUS MATERIALS

The analysis that has been carried out here is wholly within a continuum mechanics approximation. How could the results be linked with the structure of amorphous materials at the atomic scale? In the case of crystals, Volterra dislocations in a continuum seamlessly blend to dislocations in a crystalline structure, the latter providing a specific value for their Burgers vector. These line defects, at least in small-enough numbers, break the short-range order but not the long-range order. The existence of crystallographic slip planes allows for the large-scale motion of these defects, which explains crystal plasticity. Could line defects, microscopically well defined, exist in amorphous materials, without slip planes? Point defects are well known and are responsible for important technological properties [43]. Indeed, the possibility of specific vitreous state defects as a source of BP vibrations has been explored [44–46]. Could such point defects be arranged in a necklace to give rise to a line defect? At least there does not appear to be an argument of a general nature (say, energetic, entropic, or topologic) to rule out their existence. Alternatively, line defects arranged in knots would also destroy the slip planes.

The connection of the BP to one-dimensional elastic objects has been considered before: Karpov [47] studied the possibility that acoustic waves propagate along closed looplike trajectories, as a consequence of the randomness of the sound velocity, leading to a DOS that competes with that of phonons, and Novikov and Surotsev [48] have shown that Raman scattering in glasses is consistent with BP vibrations belonging to a one-dimensional spatial structure.

From a different point of view, it has been well established, through numerical simulation, that atomic displacements in amorphous Lennard-Jones, silica, and silicon are split into affine and nonaffine modes [49–54]. The possibility arises that the line defects envisaged here are responsible for the nonaffine modes. In addition, Vural and Legget [55] have developed a formalism that blames the low-temperature properties of amorphous materials on a splitting of acoustic properties into phonon and nonphonon modes, a distinction that is similar in spirit to what is carried out here. Finally, signatures of collective stringlike motion in supercooled liquids in computer simulations have also been found [56,57]. A microscopic link to the line defects envisaged in this paper could provide a useful tool to understand the behavior of the BP as a function of external control parameters such as temperature and pressure.

VI. DISCUSSION AND OUTLOOK

A model has been proposed, within the framework of continuum mechanics, that links the BP in amorphous materials to the properties of acoustic waves in interaction with line defects. This approach bears some similarity to the classic treatment of the quantum hydrodynamics of superfluid helium and atomic Bose-Einstein condensates through (quantized) vortex lines [58–60]. It also provides an answer to the long-standing question of how to apply continuum mechanics, at similar length scales, both to crystals and to their amorphous counterparts. In the present work, the degrees of freedom responsible for the BP are taken to be the vibrations of line defects around an equilibrium position; they are also responsible for acoustic attenuation and dispersion. Figure 3 shows an example of the effect of a given DOS on attenuation and dispersion. As expected, a larger number of defects provides a higher effect. Dispersion behaves as ω^4 at low frequencies, then crosses over to ω^2 at frequencies ω_{BP} comparable to the BP, and then, at even higher frequencies, to linear in ω . The IR criterion is satisfied at the BP. The velocity of acoustic waves has a negative dispersion at low frequencies and then increases as a function of frequency around ω_{BP} . Notice that the defects have an effect even at low frequencies, suggesting the model can be tested, say, using resonant ultrasound spectroscopy (RUS), a tool that has been used to measure dislocation densities in polycrystalline materials [61,62], or hyper sound damping in the subterahertz range, as measured in vitreous silica [63,64]. Additional possible topics for further research include a numerical, atomistic study of the hypothesized linear defects; the effect they would have on thermal and electrical conductivity properties, particularly at very low temperatures, where quantum effects would be dominant; and the role they may or may not have in plasticity properties and in the glass transition.

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