



The transverse nature of the Boson peak: A rigidity theory approach

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ABSTRACT

The transversal nature of the Boson peak in crystals and glasses is investigated by using a model inspired from rigidity theory of glasses. By tuning the rigidity of the network using second-neighbor interactions, we show that the transversal van Hove singularity – associated with the Boson peak – arises when the transverse dispersion branch touches for the first time the boundary of the first Brillouin zone, leading to an anomaly in the low frequency region. The frequency of the singularity is determined by the rigidity of the network. For the disordered version of the model, the singularity arises when the transversal dispersion branch touches the limit of a pseudo-Brillouin zone, suggesting that the Boson peak in glasses has a similar origin. Increasing rigidity shifts the position of the Boson peak towards high frequencies while its intensity decreases. This provides an important clue to understand pressure effects on the Boson peak in glasses and crystals.

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1. Introduction

Thermodynamics as well as dynamical properties of glasses have been subjects of intense studies, since they are significantly different from those of crystals, specially at low temperatures [1,2]. Glasses also present an excess of low frequency vibrational modes (LVFMs) relative to the Debye crystal model, known as the Boson peak (BP). It appears in the THz range of frequencies, as confirmed for example by Raman and neutron scattering experiments [1–4]. However, it is not so well known that crystals can also present a Boson peak, like in SiO₂ [5–8]. Furthermore, very recently it has been given experimental evidence [9] that the Boson peak in glasses is equivalent to the transverse acoustic van Hove singularity in crystals, supporting some analytical and computer models [10–15]. This suggests that theoretical models based on features beyond acoustic dynamics or driven by the distinction between disorder and order [3,16–19] are not totally valid. Almost at the same time, in a previous work we obtained that the Boson peak can be explained in a unified way in glasses and crystals if Phillips and Thorpe Rigidity Theory [20,21] is used to understand the changes in the elastic properties due to a reduction in the number or strength of atomic bonds [21]. In fact, very recently it has been found that rigidity is a very powerful tool to design glasses, as those used in tablet screens [22–24]. Using these kinds of rigidity ideas, we were able to prove that in the case of small disorder in periodic systems, the modes that contribute to the Boson peak arise either from a reduction or a weakening of the bonds in an otherwise overconstrained atomic

network [25]. We also showed that the position of the Boson peak, Ω , can appear at most at one-third of the Debye frequency ω_D [25]. In almost all glasses $\Omega = 0.1\omega_D$ [26]. In addition, we found [25] that the position of the peak scales as $(Z-Z_c)^{1/2}$, where Z is the coordination of the network and Z_c a critical coordination. A similar result has also been found for strong disorder using the coherent potential approximation [27].

However, in our previous works [25,28–32] we did not consider a well-established fact: the transverse nature of modes at or near the Boson peak [9]. Here we extend our work [25] to show that rigidity allows us to obtain the transverse nature in a simple way. To do this, here we will consider a model in which we can tune the rigidity, and in which elastic order or disorder can be included at will [33]. The model consists in a square lattice, with boundary periodic conditions, where nearest neighbors (NN) atoms are joined by harmonic springs. In principle, this lattice is isostatic. To modulate rigidity, we introduce next nearest neighbors (NNN) interactions. The stiffness of the NNN bonds will be a fraction of the NN elastic constant joins. It is worthwhile mentioning that our model is also able to explain in a qualitative way the experimental results by Chumakov et al. [9] and other groups [34], concerning the movement of the Boson peak as pressure is applied. The outline of the paper is the following. In Section 2 we develop the crystalline version of the model, while in Section 3 we present the disordered version. Finally, the conclusions are given in Section 4.

2. Crystalline model

Explicitly, our crystalline model to study rigidity consists in a square lattice of N masses (m) joined by harmonic springs k_0 for

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first neighbor interactions, as seen in Fig. 1. In order to tune the rigidity of the network and the Boson peak position, we introduce the second nearest neighbor interactions by harmonic springs $k_1 = \gamma k_0$, as shown with dash diagonal lines in Fig. 1. γ is a rigidity tuning dimensionless parameter between 0 and 1. When $\gamma = 0$, we have an isostatic lattice, since it has $2N$ constrictions and $2N$ degrees of freedom. When $\gamma \in (0,1]$ we increase the average coordination of the lattice and as a consequence, the network is more rigid [25,33].

The dynamical matrix of this model can be written down in the wave vector space $\mathbf{q}$ as

$$\mathbb{D}(\mathbf{q}) = \begin{pmatrix} \omega_{xx}^2(\mathbf{q}) + \frac{\gamma}{2} \omega_{xy}^2(\mathbf{q}) & \frac{\gamma}{2} \omega_{xy}^2(\mathbf{q}) \\ \frac{\gamma}{2} \omega_{xy}^2(\mathbf{q}) & \omega_{yy}^2(\mathbf{q}) + \frac{\gamma}{2} \omega_{yx}^2(\mathbf{q}) \end{pmatrix}, \quad (1)$$

where $\omega_{xx}^2(\mathbf{q}) = (4v_s^2/a^2) \sin^2(q_x a/2)$, $\omega_{yy}^2(\mathbf{q}) = (4v_s^2/a^2) \sin^2(q_y a/2)$ and $\omega_{xy}^2(\mathbf{q}) = \omega_{yx}^2(\mathbf{q}) = (4v_s^2/a^2) \sin^2[(q_x + q_y)a/2]$, where a is the lattice constant and v_s the speed of sound, given by $v_s = a\sqrt{k_0/m}$.

The dispersion relation is obtained by diagonalizing Eq. (1)

$$\omega_{\pm}^2(\mathbf{q}) = \frac{1}{2} [1 \pm \eta(\mathbf{q})] \omega_{xx}^2(\mathbf{q}) + \frac{1}{2} [1 \mp \eta(\mathbf{q})] \omega_{yy}^2(\mathbf{q}) + \frac{\gamma}{2} \omega_{xy}^2(\mathbf{q}), \quad (2)$$

with

$$\eta(\mathbf{q}) = \sqrt{1 + \gamma^2 \left[\frac{\omega_{xy}^2(\mathbf{q})}{\omega_{xx}^2(\mathbf{q}) - \omega_{yy}^2(\mathbf{q})} \right]^2}. \quad (3)$$

The signs in $\omega_{\pm}^2(\mathbf{q})$ are used to denote two branches. The branch with plus (minus) sign is labeled as the longitudinal (transverse) branch. Such identification is obtained by looking at the acoustic limit $qa \ll 1$ in Eq. (2),

$$\omega_{\pm}(\mathbf{q}) \approx f_{\pm}(\theta)(v_s q), \quad (4)$$

where $f_{\pm}(\theta)$ is a directional modulation of the speed of sound, depending on the polar angle θ as,

$$f_{\pm}^2(\theta) = \frac{(1 + \gamma(1 + \sin 2\theta) \pm \sqrt{\cos^2 2\theta + \gamma^2(1 + \sin 2\theta)^2})}{2}. \quad (5)$$

The minus sign leads to a lower phase velocity when compared with the plus. Usually, this implies transversal modes. In the present model, this point can be confirmed by comparing the directions of the atomic vibrations relative to the wave vector of the phonon propagation. To do such comparison, we write the

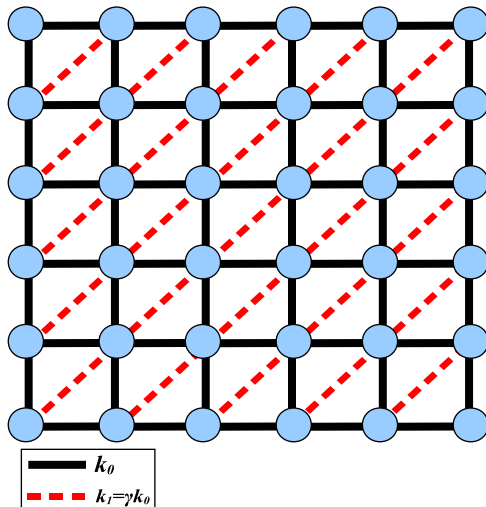


Fig. 1. Square lattice with nearest-neighbors and second nearest-neighbors harmonic springs of constant k_0 and $k_1 = \gamma k_0$ respectively. Periodic boundary conditions are used. γ is a rigidity dimensionless parameter.

dynamical matrix for $qa \ll 1$ in polar coordinates,

$$\mathbb{D}(\mathbf{q}) = v_s^2 q^2 \begin{pmatrix} \cos^2 \theta + \frac{\gamma}{2}(1 + \sin 2\theta) & \frac{\gamma}{2}(1 + \sin 2\theta) \\ \frac{\gamma}{2}(1 + \sin 2\theta) & \sin^2 \theta + \frac{\gamma}{2}(1 + \sin 2\theta) \end{pmatrix}. \quad (6)$$

The atomic displacements are given by the corresponding eigenvectors $\mathbf{u}_{\pm}$ of the previous matrix. For γ different from zero, these eigenvectors can be written as $\mathbf{u}_{\pm} = (\sin \alpha_{\pm}(\theta), \cos \alpha_{\pm}(\theta))$, where $\alpha_{\pm}(\theta)$ is an angle defined by

$$\tan \alpha_{\pm}(\theta) = \frac{\gamma(1 + \sin 2\theta)}{1 - 2 \cos^2 \theta \pm \sqrt{\cos^2 2\theta + \gamma^2(1 + \sin 2\theta)^2}}. \quad (7)$$

To determine the transversal or longitudinal nature of the modes, we perform the dot product of $\mathbf{u}_{\pm}$ with the vector $\hat{\mathbf{q}} = (\cos \theta, \sin \theta)$ to obtain

$$\hat{\mathbf{q}} \cdot \mathbf{u}_{\pm} = \sin(\theta + \alpha_{\pm}(\theta)). \quad (8)$$

For $\theta = \pi/4$, it is easy to see that $\hat{\mathbf{q}} \cdot \mathbf{u}_{+} = 1$, while $\hat{\mathbf{q}} \cdot \mathbf{u}_{-} = 0$. This implies that for this direction, the branch with the minus sign corresponds to pure transversal modes since the propagation vector is perpendicular to the vibrations for any value of γ (except of course, for $\gamma = 0$, in which modes are always longitudinal, see below). As θ is varied, there is a certain amount of mixing between transversal and longitudinal modes, although the lower branch has always a predominant transversal character. This mixing can be further reduced by using another set of perpendicular diagonals in the direction $\theta = -\pi/4$ to increase rigidity, leading to an overconstrained lattice. Here we study the transition from isostatic, which is more interesting because transversal modes appear gradually, and the transition can be followed in a more detailed way.

The evolution of the longitudinal and transverse branches in the first Brillouin zone is shown in Fig. 2 for $\gamma = 0$ and $\gamma = 1$. Both represent the extremal rigidity cases of the model.

Let us first study the limiting case $\gamma = 0$ corresponding to the isostatic lattice. Immediately we observe that Eq. (1) is already diagonal and the dispersion relation corresponds to two uncoupled linear chains in the x - and y -directions

$$\omega_x(\mathbf{q}) = \frac{2v_s}{a} \left| \sin\left(\frac{q_x a}{2}\right) \right|, \quad \omega_y(\mathbf{q}) = \frac{2v_s}{a} \left| \sin\left(\frac{q_y a}{2}\right) \right|. \quad (9)$$

Eq. (9) is shown in Fig. 2(a) and (b). As it is easy to see that there are no transverse modes since there is no coupling between vibrations in the x - and y -directions. Thus, the branches of the dispersion relation degenerate and the nature of the vibrational DOS is purely longitudinal. As we will see next, there is a finite vibrational DOS at $\omega \rightarrow 0$ for the isostatic case. This can be proved by taking the acoustic limit in Eq. (9) or in Eq. (4). Since the dispersion goes as $\omega_x(\mathbf{q}) = v_s q_x$ and $\omega_y(\mathbf{q}) = v_s q_y$, it follows that the vibrational density of states is $\rho(\omega) = 1/(\pi v_s)$, i.e., is constant at low frequencies. This is anomalous for a two-dimensional system, and is basically due to the fact that ω does not scale as q^d , where d is the dimensionality. This unusual behavior can be traced back to the accumulation of zero frequency modes due to the lack of mechanical constraints [25]. The addition of constraints by putting diagonals pushes these states to non-zero frequency [25], as can be seen from Eq. (4) for $\gamma \neq 0$. This restores the usual relationship $\omega \approx q^d$ and thus $\rho(\omega) \rightarrow 0$ as $q \rightarrow 0$. From the reduced DOS $\rho(\omega)/\omega$, it is clear that for $\gamma = 0$ we expect $\rho(\omega)/\omega = 1/(\pi v_s \omega) \rightarrow \infty$ as $\omega \rightarrow 0$, while for $\gamma \neq 0$, we expect $\lim_{\omega \rightarrow 0} \rho(\omega)/\omega = C$, where C is a constant. This suggests that the Boson peak modes are transformed into floppy modes at zero frequency, as has been obtained using perturbation theory [25,35,36], or can be observed in Fig. 3, where $\rho(\omega)/\omega \rightarrow \infty$ as γ goes to zero, indicating an excess of modes.

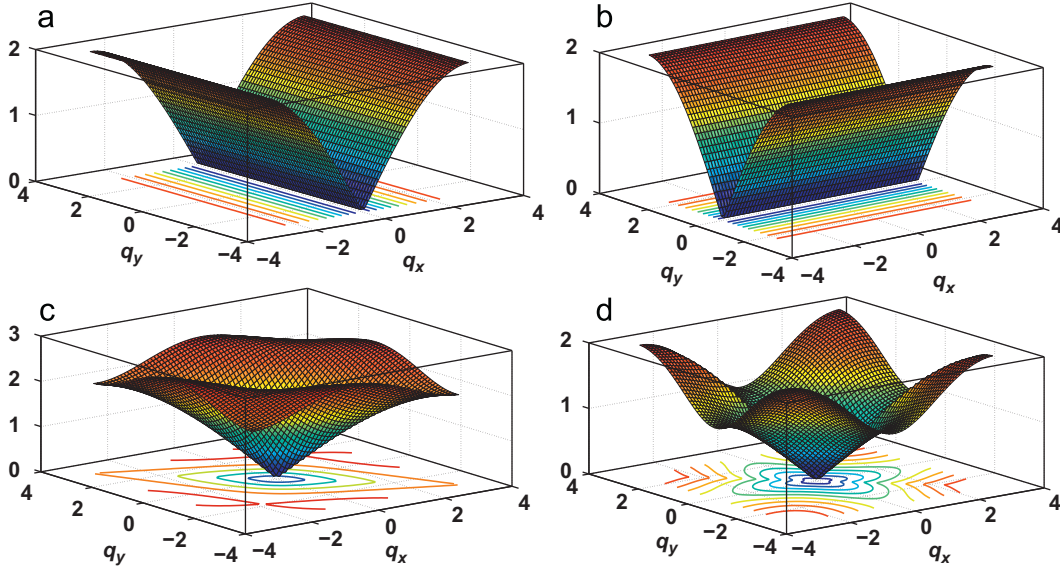


Fig. 2. Dispersion relation for a square lattice with first neighbor interactions, $\gamma = 0$, and second neighbor interactions, $\gamma = 1$. Contour plots are shown below each surface. In the first case, $\gamma = 0$, two branches are found in Eq. (2), however they are uncoupled in the x and y directions, and they behave as one-dimensional vibrational longitudinal branches in x (a) and y (b). In the second case, $\gamma = 1$, two newly branches are found in Eq. (2), (c) corresponds to the longitudinal branch (labeled with a plus sign), and (d) the transverse branch (labeled with a minus sign).

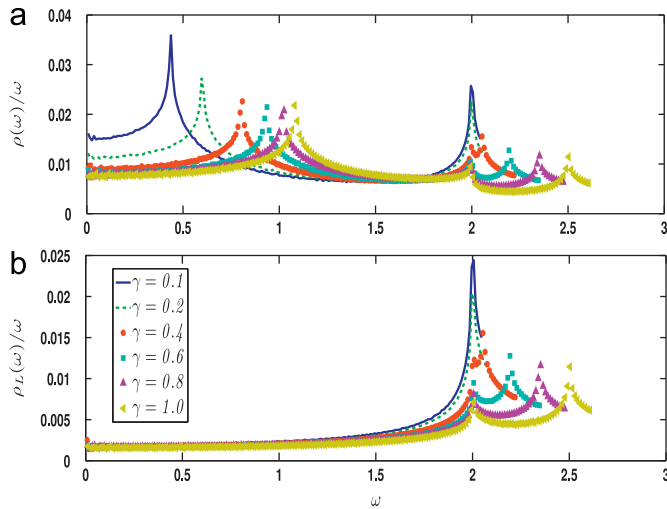


Fig. 3. Reduced vibrational density of states ($\rho(\omega)/\omega$) as a function of the frequency for a square lattice at various values of γ . (a) Total reduced vibrational DOS $\rho(\omega)/\omega$, and (b) the partial contribution from the longitudinal modes to $\rho(\omega)/\omega$, labeled by $\rho_L(\omega)/\omega$. Notice that in the frequencies range 0–1.085 (a) shows a Boson peak which changes with the tuning rigidity parameter γ . In the same range of frequencies one does not observe any peak in (b).

As our main point, consider now the reduced vibrational density of states for different degrees of rigidity, i.e., for various values of γ . In Fig. 3 we present the corresponding reduced vibrational DOS, $\rho(\omega)/\omega$, and the reduced longitudinal DOS $\rho_L(\omega)/\omega$. In Fig. 3(a) one can see how the Boson peak sits at a maximal frequency $\omega = 1.085$ when $\gamma = 1$, and then it is shifted to the left as the rigidity decreases ($\gamma \rightarrow 0$). At the same time, the height of the peak increases. At $\gamma = 0$, it finally touches zero frequency. As a counterpart, in Fig. 3(b) we observe a constant behavior of $\rho_L(\omega)/\omega$ in the range of frequencies 0–1.085, while a Boson peak appears in the total $\rho(\omega)/\omega$.

Now we will prove the transverse nature of the Boson peak. To do this, in Fig. 4 we present the reduced vibrational transverse DOS $\rho_T(\omega)/\omega$. It is clear that the Boson peak has a transverse nature, since no peak appears in the longitudinal branch

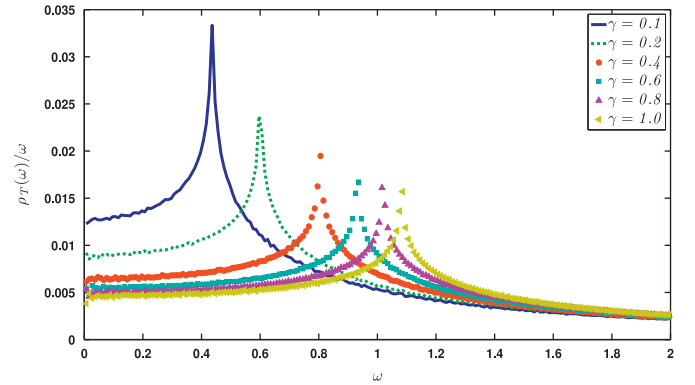


Fig. 4. Reduced transverse vibrational density of states ($\rho_T(\omega)/\omega$) as a function of the frequency, for a square lattice at different values of γ . Notice how the position of the Boson peak moves to high frequencies when the rigidity of the lattice is increased, $\gamma \rightarrow 1$, and at the same time, the height of the Boson peak decreases. This phenomenology is in qualitative agreement with experiments in which pressure is applied [9,34]. We also see the decay of $\rho_T(\omega)/\omega$ away from the Boson peak position, as observed experimentally [37].

(see Fig. 3(b)). Here we can understand its transversal origin just by analyzing the dispersion relation. To do this, in Fig. 5 we present contour plots of Eq. (2) for the transverse branch at three different values of γ , 0.01, 0.5 and 1.0. The Boson peak arises in $\rho_T(\omega)/\omega$ when the transverse dispersion branch touches for first time the boundary of the first Brillouin zone. This leads to the first van Hove singularity since the transverse group velocity vanishes. Thus here we can identify the Boson peak as a consequence of such singularity. This phenomenon can be clearly seen from the integral definition of the vibrational DOS [38]

$$\rho(\omega) = \sum_s \int \frac{d\mathbf{s}}{(2\pi)^d} \frac{1}{|\nabla \omega_s(\mathbf{q})|}, \quad (10)$$

where s labels the branch, $\nabla \omega_s(\mathbf{q})$ the group velocity, d the space dimension and the integral is over that surface in the first zone on which $\omega_s(\mathbf{q}) = \omega$. When $\nabla \omega_s(\mathbf{q})$ vanishes, the critical points of the surface $\omega_s(\mathbf{q}) = \omega$ could be minima, maxima or saddle points. These critical points lead to singularities in $\rho(\omega)$. We are interested in the first singularity, which is related to the transversal

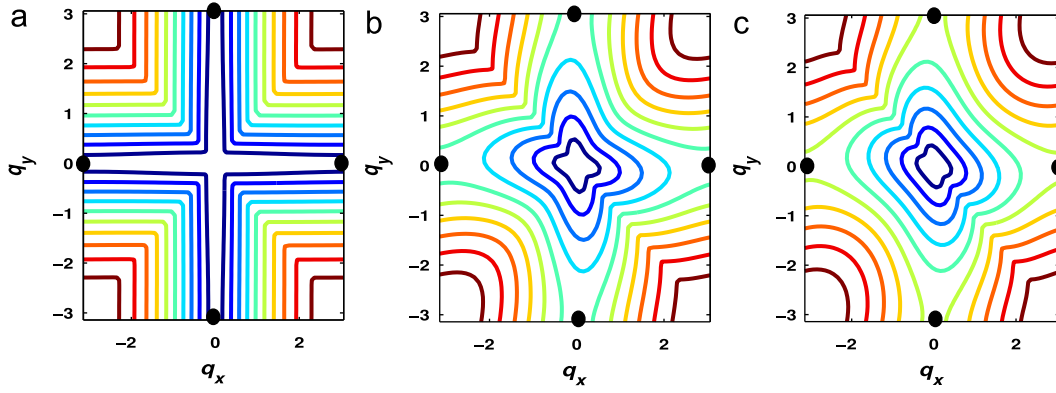


Fig. 5. Contour plot of the transverse branch at three values of γ . (a) $\gamma = 0.01$, (b) $\gamma = 0.5$ and (c) $\gamma = 1.0$. The black circles represent the saddle-points that correspond to singularities in $\rho_T(\omega)/\omega$.

branch. Of course the main question is why the first singularity in the vibrational spectrum arises in the transverse branch and not in the longitudinal. The answer is simple but deep. The transverse group velocity is always smaller than the longitudinal one, thus, the transverse branch will always touch the Brillouin zone at a lower frequency than the longitudinal one. To have such transversal modes, the lattice needs to present a minimal rigidity. A similar argument can be invoked for disordered systems, since the transverse velocity is always lower than the longitudinal one, and it has been pointed out that it is possible to define a pseudo Brillouin zone even in the presence of disorder [39–41]. In the present case, the first van Hove singularity turns out to be a saddle-point for each of the four equivalent points which are marked with a black circle in the three cases of Fig. 5. We label the frequency associate with these saddle-points in the transverse branch by ω_T^* . Now we proceed to determine ω_T^* analytically. To do that, we take the transverse branch which corresponds to the minus sign in Eq. (2). In the limit $q_x \rightarrow 0$ and $\gamma \rightarrow 0$, the dispersion relation of the transverse branch can be written approximately as $\omega_-^2 \approx 2k_0 q_x^2 a^2 / m + \gamma 4k_0 \sin^2(q_y a / 2) / m$. This expression automatically gives

$$\omega_T^* \approx 2\sqrt{k_0 \gamma / m} = 2\sqrt{k_1 / m}. \quad (11)$$

From Eq. (11), it is clear that the frequency position of the first van Hove singularity is a function of the elastic constant k_1 , which gives origin to the transverse branch. Fig. 6 shows a comparison between Eq. (11) and the position of the Boson peak, Ω , directly obtained from the reduced vibrational DOS (see Fig. 4). According to Fig. 6, we can see that $\Omega \lesssim \omega_T^*$. It is important to point out that ω_T^* is not just roughly the Boson peak or first Van Hove singularity frequency; it also gives a crossover frequency which defines a rigidity behavior of the lattice with the frequency [42,43]. For $\omega \leq \omega_T^*$ we have a rigid case (linear evolution of the total vibrational DOS $\rho(\omega)$ with ω), however, for $\omega > \omega_T^*$ we have a kind of isostatic behavior (constant evolution of $\rho(\omega)$ with ω).

3. Disordered model

In order to have a glass model with different degrees of rigidity, we begin with a network similar as the illustrated in Fig. 1 but this time every single site is bonded each other with a spring of elastic constant $k_0 = 1$. In contrast to the previous section, where the rigidity of the network was reduced by means of a dimensionless parameter γ , here we obtain lattices with less rigidity by randomly choosing a concentration (c) of bonds, regardless if they are in the diagonal, vertical or horizontal

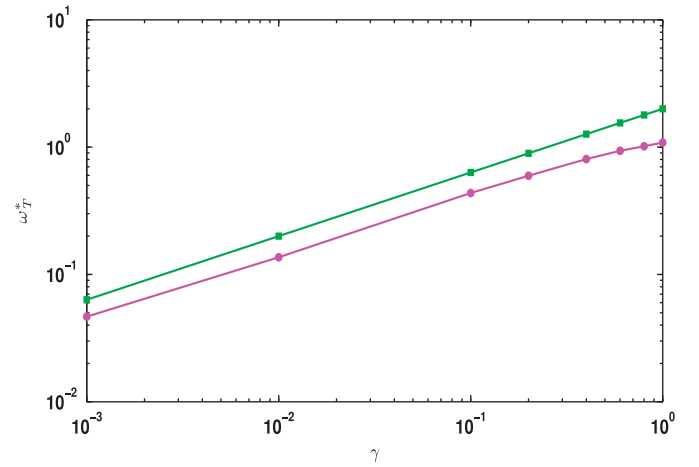


Fig. 6. Log-log plot of the Boson peak position Ω (fuchsia-filled points), and the Van Hove singularity position using the approximation given by Eq. (11) (green squares) as functions of γ . The Ω points were obtained from the numerical results of the reduced vibrational DOS. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

position. Once we have chosen such bonds, its elastic constants k_0 are reduced by a dimensionless factor $\alpha < 1$, namely, $k_1 = \alpha k_0$. In this paper, we will use $\alpha = 0.1$. To obtain the longitudinal and transverse vibrational density of states, first we calculated the longitudinal and transverse dynamical structure factors, $S_L(q, \omega)$ and $S_T(q, \omega)$ [11], defined respectively as

$$S_L(q, \omega) = \frac{k_B T q^2}{m \omega^2} \sum_{\lambda} E_{L,\lambda}(\mathbf{q}) \delta(\omega - \omega_{\lambda}) \quad (12)$$

and

$$S_T(q, \omega) = \frac{k_B T q^2}{m \omega^2} \sum_{\lambda} E_{T,\lambda}(\mathbf{q}) \delta(\omega - \omega_{\lambda}), \quad (13)$$

where

$$E_{L,\lambda}(\mathbf{q}) = \left| \sum_j \hat{\mathbf{q}} \cdot \mathbf{e}_{\lambda}(j) \exp(i\mathbf{q} \cdot \mathbf{R}_j) \right|^2,$$

and

$$E_{T,\lambda}(\mathbf{q}) = \left| \sum_j \hat{\mathbf{q}} \times \mathbf{e}_{\lambda}(j) \exp(i\mathbf{q} \cdot \mathbf{R}_j) \right|^2$$

where $\hat{\mathbf{q}} = \mathbf{q}/q$, $\mathbf{e}_\lambda$ is the eigenvector at the eigenvalue λ and $\{\mathbf{R}\}$ are the particles equilibrium positions. From Eqs. (12) and (13), we obtain the generalized vibrational density of states [44] in the transverse and longitudinal contribution

$$\rho_L(q, \omega) = \frac{m\omega^2}{k_B T q^2} S_L(q, \omega) \quad (14)$$

$$\rho_T(q, \omega) = \frac{m\omega^2}{k_B T q^2} S_T(q, \omega). \quad (15)$$

In order to get either the longitudinal vibrational density of states or the transverse one, an average can be performed over all available q belonging to a particular range, namely

$$\rho_L(\omega) = \frac{1}{N_q} \sum_q \rho_L(q, \omega) \quad (16)$$

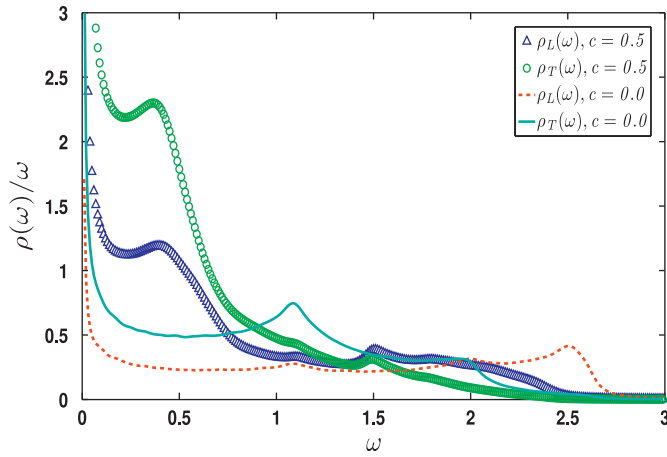


Fig. 7. Evolution of the reduced vibrational DOS $\rho(\omega)/\omega$, at a concentration $c=0.5$ of randomly diluted bonds, for longitudinal (open triangles) and transverse (open circles) modes. The dashed and continuous lines correspond to the longitudinal and transverse reduced vibrational DOS in the crystalline case. At $c=0.5$, we notice at $\Omega_T \approx 0.4$ and $\Omega_L \approx 0.45$ a Boson peak in $\rho_T(\omega)/\omega$ and $\rho_L(\omega)/\omega$ respectively, however the contribution of the transverse modes is bigger than the longitudinal ones.

and

$$\rho_T(\omega) = \frac{1}{N_q} \sum_q \rho_T(q, \omega), \quad (17)$$

where N_q represents the number of terms in the sum.

In order to get the numerical values of the eigenvectors and eigenvalues needed to feed Eqs. (12)–(17), we used square lattices of 80×80 sites at concentrations in the range that spans from $c=0.0$ to $c=0.5$. Due to the size of these networks, we diagonalized the dynamical matrices of $12,800 \times 12,800$ sites using the LAPACK [45] routines, where each result was averaged over 10 disorder realizations. Fig. 7 shows the reduced vibrational density of states for $c=0.0$ and $c=0.5$. A Boson peak is observed (for $c=0.5$) at $\Omega_L \approx 0.45$ in $\rho_L(\omega)/\omega$ and at $\Omega_T \approx 0.40$ in $\rho_T(\omega)/\omega$, however, the amount of modes in $\rho_T(\omega)/\omega$ at either Ω_L or Ω_T is bigger than in $\rho_L(\omega)/\omega$. It is interesting to observe that the values of Ω_L and Ω_T in this disordered model are closer to the value $\Omega \approx 0.41$ at $\gamma = 0.1$ in the ordered model (see Fig. 4). In this last case, we observe a well-defined peak in comparison to the disordered case, where the peak is wider. Also, in Fig. 7 we can notice an accumulation of modes at $\omega \approx 0$, due to a proliferation of soft modes in the network.

A detailed analysis of the generalized vibrational DOS allows us to show that in fact, the same mechanism that works for crystals is behind the singularities in the disordered model, i.e., a well-defined dispersion relationship can be defined till the transversal branch touches the limit of a pseudo-Brillouin zone, which is basically of the same size of its crystalline counterpart. To support this observation, in Fig. 8 we present a contour plot of the generalized vibrational DOS (14) and (15) averaged over all directions in $\mathbf{q}$ for $c=0.5$. In Fig. 8(a) we can see a well-defined average acoustic longitudinal branch in the range $q \approx 0.0$ – 2.0 and $\omega_L \approx 0.0$ – 0.5 . On the other hand, in Fig. 8(b) we show the evolution of ω_T versus q . We can clearly see an average acoustic transverse branch in the range of $q \approx 0.0$ – 3.0 and $\omega_T \approx 0.0$ – 0.5 . On the same plot, we have marked with a fuchsia horizontal line the frequency of the transverse Boson peak, $\Omega_T \approx 0.41$, and with a vertical one the boundary of the pseudo-Brillouin zone. This boundary is defined as the q in which the transversal acoustic branch ends in Fig. 8, at $q \approx 3.1$. The Boson peak in $\rho_L(\omega)/\omega$ (see Fig. 7) is due to the contribution of modes around a plateau that appears in the region that spans from $q \approx 1.5$ to $q \approx 2.0$.

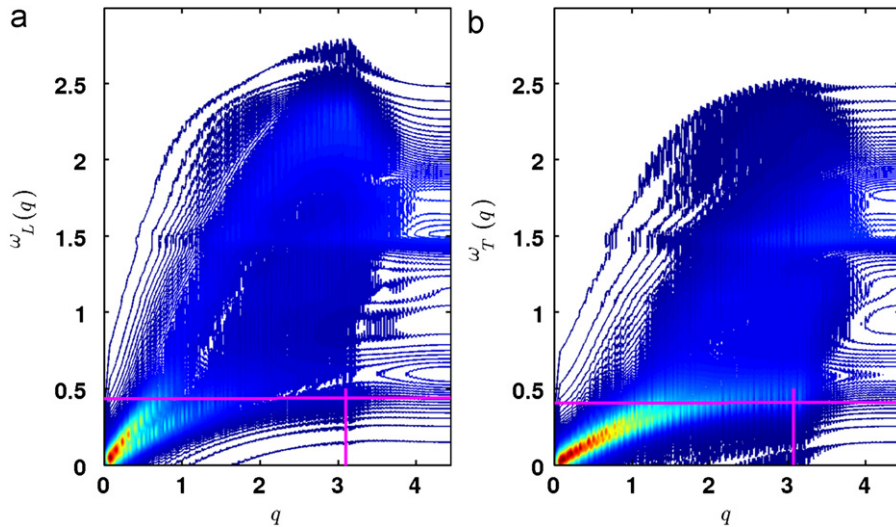


Fig. 8. Contour plot of the generalized vibrational DOS, $\rho(\omega, q)$, averaged over all directions in $\mathbf{q}$ at $c=0.5$. We see in (a) the longitudinal contribution and in (b) the transverse one. We notice in (a) an average longitudinal branch in the range $q \approx 0.0$ – 2.0 and $\omega_L \approx 0.0$ – 0.5 , meanwhile in (b) an average transverse branch around $q \approx 0.0$ – 3.1 and $\omega_T \approx 0.0$ – 0.5 . We have marked with a fuchsia horizontal line in (a) and (b) the frequency position of the longitudinal and transverse Boson peak $\Omega_L \approx 0.45$ and $\Omega_T \approx 0.4$ respectively, meanwhile with a vertical line we represent the border of the pseudo-Brillouin zone.

4. Conclusions

In conclusion, we have extended our previous work concerning the rigidity origin of the Boson peak to support the idea of its transverse nature. We can summarize the analytical and numerical results as follows: (i) The Boson peak in crystals arises when the transverse branch touches for first time the boundary of the first Brillouin zone. (ii) The transverse Boson peak in our disordered model arises when the averaged transverse branch touches the boundary of a pseudo-Brillouin zone. (iii) The position (Ω_T) and intensity of the Boson peak are functions of the rigidity. Increasing rigidity pushes Ω_T to higher frequencies, meanwhile the intensity decreases. (iv) Finally, these results allows us to understand qualitatively pressure effects on the Boson peak. Experimentally, when a pressure is applied, the frequency of the Boson peak moves to high frequencies and at the same time, its intensity decreases [9,34]. This tendency is similar to the evolution of the Boson peak in our model as rigidity is increased, $\gamma \rightarrow 1$ (see Figs. 3(a) and 4). The pressure effects on the Boson peak can be explained qualitatively by rigidity arguments, since when pressure is applied, the second neighbor interaction increases due to a reduction in the distances between atoms. The same effect happens for the first neighbors, however, the non-linear character of the potential does not preserve the ratio γ between elastic constants of NN and NNN. This leads to a pressure dependent γ , and as a consequence, the system is more rigid as experiments confirm [46,47].

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References

- [1] S.R. Elliot, *Physics of Amorphous Materials*, 2nd ed., Logman Scientific & Technical, London, 1990.
- [2] K. Binder, W. Kob, *Glassy Materials and Disordered Solids*, World Scientific, Singapore, 2005.
- [3] U. Buchenau, N. Nücker, A.J. Dianoux, *Phys. Rev. Lett.* 53 (1984) 2316, <http://dx.doi.org/10.1103/PhysRevLett.53.2316>.
- [4] B. Hehlen, E. Courtens, R. Vacher, A. Yamanaka, M. Kataoka, K. Inoue, *Phys. Rev. Lett.* 84 (2000) 5355, <http://dx.doi.org/10.1103/PhysRevLett.84.5355>.
- [5] Y. Inamura, M. Arai, N. Kitamura, S. Bennington, A. Hannon, *Phys. B: Condens. Matter* 241–243 (1997) 903, [http://dx.doi.org/10.1016/S0921-4526\(97\)00748-5](http://dx.doi.org/10.1016/S0921-4526(97)00748-5).
- [6] Y. Inamura, M. Arai, O. Yamamuro, A. Inaba, N. Kitamura, T. Otomo, T. Matsuo, S. Bennington, A. Hannon, *Phys. B: Condens. Matter* 263–264 (1999) 299, [http://dx.doi.org/10.1016/S0921-4526\(98\)01362-3](http://dx.doi.org/10.1016/S0921-4526(98)01362-3).
- [7] Y. Inamura, M. Arai, T. Otomo, N. Kitamura, U. Buchenau, *Phys. B: Condens. Matter* 284–288 (Pt 2) (2000) 1157, [http://dx.doi.org/10.1016/S0921-4526\(99\)02788-X](http://dx.doi.org/10.1016/S0921-4526(99)02788-X).
- [8] T. Nakayama, *Rep. Prog. Phys.* 65 (8), 2002, 1195. <http://dx.doi.org/10.1088/0034-4885/65/8/203>.
- [9] A.I. Chumakov, G. Monaco, A. Monaco, W.A. Crichton, A. Bosak, R. Rüffer, A. Meyer, F. Kargl, L. Comez, D. Fioretto, H. Giefers, S. Roitsch, G. Wortmann, M.H. Manghnani, A. Hushur, Q. Williams, J. Balogh, K. Parlinski, P. Jochym, P. Piekarz, *Phys. Rev. Lett.* 106 (2011) 225501, <http://dx.doi.org/10.1103/PhysRevLett.106.225501>.
- [10] S.N. Taraskin, Y.L. Loh, G. Natarajan, S.R. Elliott, *Phys. Rev. Lett.* 86 (2001) 1255, <http://dx.doi.org/10.1103/PhysRevLett.86.1255>.
- [11] H. Shintani, H. Tanaka, *Nat. Mater.* 7, 2008, 870–877, <http://dx.doi.org/10.1038/nmat2293>.
- [12] O. Pilla, S. Caponi, A. Fontana, J.R. Gonçalves, M. Montagna, F. Rossi, G. Vilianni, L. Angelani, G. Ruocco, G. Monaco, F. Sette, *J. Phys.: Condens. Matter* 16 (47), 2004, 8519. <http://dx.doi.org/10.1088/0953-8984/16/47/006>.
- [13] F. Léonforte, A. Tanguy, J.P. Wittmer, J.-L. Barrat, *Phys. Rev. Lett.* 97 (2006) 055501, <http://dx.doi.org/10.1103/PhysRevLett.97.055501>.
- [14] G. Monaco, S. Mossa, *Anomalous properties of the acoustic excitations in glasses on the mesoscopic length scale*, *PNAS* 106 (40) (2009) 16907, <http://dx.doi.org/10.1073/pnas.0903922106>.
- [15] G. Baldi, V.M. Giordano, G. Monaco, B. Ruta, *Phys. Rev. Lett.* 104 (2010) 195501, <http://dx.doi.org/10.1103/PhysRevLett.104.195501>.
- [16] T.S. Grigera, V. Martin-Mayor, G. Parisi, P. Verrocchio, *Nature* 422 (2003) 289, <http://dx.doi.org/10.1038/nature01475>.
- [17] E. Duval, A. Boukenter, T. Achibat, *J. Phys.: Condens. Matter* 2 (51), 1990, 10227, <http://dx.doi.org/10.1088/0953-8984/2/51/001>.
- [18] M. Klinger, A. Kosevich, *Phys. Lett. A* 280 (5–6) (2001) 365.
- [19] D.A. Parshin, H.R. Schober, V.L. Gurevich, *Phys. Rev. B* 76 (2007) 064206, <http://dx.doi.org/10.1103/PhysRevB.76.064206>.
- [20] J. Phillips, *J. Non-Cryst. Solids* 34 (2) (1979) 153.
- [21] M. Thorpe, *J. Non-Cryst. Solids* 57 (3) (1983) 355.
- [22] J. Mauro, *Am. Ceram. Soc. Bull.* 90 (4) (2011) 31.
- [23] M. Potuzak, X. Guo, M.M. Smedskjaer, J.C. Mauro, *J. Chem. Phys.* 138 (12) (2013) 12A501.
- [24] J.C. Mauro, *J. Chem. Phys.* 138 (12) (2013) 12A522.
- [25] H.M. Flores-Ruiz, G.G. Naumis, *Phys. Rev. B* 83 (2011) 184204, <http://dx.doi.org/10.1103/PhysRevB.83.184204>.
- [26] B. Rufflé, D.A. Parshin, E. Courtens, R. Vacher, *Phys. Rev. Lett.* 100 (2008) 015501, <http://dx.doi.org/10.1103/PhysRevLett.100.015501>.
- [27] M. Wyart, *Eur. Phys. Lett.* 89 (6) (2010) 64001, <http://dx.doi.org/10.1209/0295-5075/89/64001>.
- [28] G.G. Naumis, H.M. Flores-Ruiz, *Phys. Rev. B* 78 (2008) 094203, <http://dx.doi.org/10.1103/PhysRevB.78.094203>.
- [29] H.M. Flores-Ruiz, G.G. Naumis, *J. Chem. Phys.* 131 (15) (2009) 154501, <http://dx.doi.org/10.1063/1.3246805>.
- [30] H.M. Flores-Ruiz, G.G. Naumis, J.C. Phillips, *Phys. Rev. B* 82 (2010) 214201, <http://dx.doi.org/10.1103/PhysRevB.82.214201>.
- [31] A. Huerta, G.G. Naumis, *Phys. Rev. B* 66 (2002) 184204, <http://dx.doi.org/10.1103/PhysRevB.66.184204>.
- [32] G.G. Naumis, *Phys. Rev. B* 61 (2000) R9205, <http://dx.doi.org/10.1103/PhysRevB.61.R9205>.
- [33] G.G. Naumis, F. Salazar, *Phys. Lett. A* 375 (39) (2011) 3483, <http://dx.doi.org/10.1016/j.physleta.2011.08.008>.
- [34] A. Monaco, A.I. Chumakov, G. Monaco, W.A. Crichton, A. Meyer, L. Comez, D. Fioretto, J. Korecki, R. Rüffer, *Phys. Rev. Lett.* 97 (2006) 135501, <http://dx.doi.org/10.1103/PhysRevLett.97.135501>.
- [35] G.G. Naumis, *J. Non-Cryst. Solids* 352 (42–49) (2006) 4865, <http://dx.doi.org/10.1016/j.jnoncrsol.2006.01.160>.
- [36] G.G. Naumis, *Phys. Rev. E* 71 (2005) 026114, <http://dx.doi.org/10.1103/PhysRevE.71.026114>.
- [37] A.I. Chumakov, I. Sergueev, U. van Bürck, W. Schirmacher, T. Asthalter, R. Rüffer, O. Leupold, W. Petry, *Phys. Rev. Lett.* 92 (2004) 245508, <http://dx.doi.org/10.1103/PhysRevLett.92.245508>.
- [38] N.W. Ashcroft, N.D. Mermin, *Solid State Physics*, Harcourt College, Philadelphia, 1976.
- [39] G.S. Grest, S.R. Nagel, A. Rahman, *Phys. Rev. Lett.* 49 (1982) 1271, <http://dx.doi.org/10.1103/PhysRevLett.49.1271>.
- [40] J. Hafner, M. Krajci, *J. Phys.: Condens. Matter* 6 (25), 1994, 4631.
- [41] A. Matic, C. Masciovecchio, D. Engberg, G. Monaco, L. Börjesson, S.C. Santucci, R. Verbeni, *Phys. Rev. Lett.* 93 (2004) 145502, <http://dx.doi.org/10.1103/PhysRevLett.93.145502>.
- [42] M. Wyart, L.E. Silbert, S.R. Nagel, T.A. Witten, *Phys. Rev. E* 72 (2005) 051306, <http://dx.doi.org/10.1103/PhysRevE.72.051306>.
- [43] A. Souslov, A.J. Liu, T.C. Lubensky, *Phys. Rev. Lett.* 103 (2009) 205503, <http://dx.doi.org/10.1103/PhysRevLett.103.205503>.
- [44] A. Pasquarello, J. Sarnthein, R. Car, *Phys. Rev. B* 57 (1998) 14133, <http://dx.doi.org/10.1103/PhysRevB.57.14133>.
- [45] E. Anderson, S. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, D. Sorensen, *LAPACK Users' Guide*, 3rd ed., Society for Industrial and Applied Mathematics, Philadelphia, PA, 1999.
- [46] K. Trachenko, M.T. Dove, V. Brazhkin, F.S. El'kin, *Phys. Rev. Lett.* 93 (2004) 135502, <http://dx.doi.org/10.1103/PhysRevLett.93.135502>.
- [47] W.A. Kamitakahara, R.L. Cappelletti, P. Boolchand, B. Halpapp, F. Gompf, D.A. Neumann, H. Mutka, *Phys. Rev. B* 44 (1991) 94, <http://dx.doi.org/10.1103/PhysRevB.44.94>.