Quantum structure of glasses and the boson peak: a theory of vibrations

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We present a novel analytical model for glasses, starting from the first principle that the disorder in a glass mimics the disorder in a fluid. The origin of the boson peak is attributed to the intrinsically noncommutative geometry of the fluid disorder, which induces a van Hove singularity in the vibrational density of states. The universality of the model is exhibited by applying it to amorphous silicon, vitreous GeO$_2$ and Ba$_8$Ga$_{16}$Sn$_{30}$ clathrate, which show a remarkable agreement between the theoretical predictions for specific heat and the experimental data.

I. INTRODUCTION

Glasses are a peculiar state of matter whose mechanical rigidity is similar to that of crystalline solids, while the molecular disorder makes them akin to liquids [1]. The significant differences in the thermodynamical and transport properties of glasses as compared to crystalline solids are generally attributed to a universal anomaly in the frequency spectra of atomic vibrations known as the boson peak. This appears at low energies as an excess in the vibrational density of states (VDOS) compared to the one predicted by the standard Debye theory, and manifests itself in measurements of specific heat and thermal conductivity, as well as scattering of electromagnetic radiation and neutrons. The lack of a general theory for disordered solids based on first principles is a standing challenge in condensed matter physics. The theoretical description of the anomalous behavior of disordered solids is a recurrent theme in the literature [1, 2]. Interpretations of experimental studies seem to support various hypotheses: the glass anomaly could be assigned to structural motifs with (quasi-)localized transverse vibrational modes that resonantly couple with transverse phonons and thus govern their dissipation [3], or to a broadening of the transverse acoustic van Hove singularity of the corresponding crystal [4], and still to the presence of additional vibrational modes which can be induced solely by structural disorder [5]. There are mainly two classes in which the theoretical models can be grouped: i) models attributing the boson peak to quasilocalized modes, of non-acoustic nature [6, 7] and ii) models with broadening of the crystalline van Hove singularity, like those based on randomly fluctuating elastic constants inserted in an otherwise crystalline arrangement [8-9]. There is an impressive array of phenomenological models of glass structure and dynamics (for an inevitably incomplete selection, see Refs. [10-20]). However, none of these advances has allowed the derivation of a complete, widely-accepted theory of amorphous solids. Thus, the physical origin of two most outstanding anomalous behaviors displayed by glasses at intermediate temperatures (1 – 40 K), i.e., the excess of heat capacity and the boson peak, is still under debate.

In this work, we present a novel theory for the vibrations in amorphous solids, relying on the fundamental principle that the disorder in a glass is a reminiscence of the disorder in a fluid. The analytical model for glasses based on this hypothesis naturally contains the boson peak as a manifestation of an extended van Hove singularity.

II. FLUIDS IN LAGRANGIAN DESCRIPTION

A fluid can be described in the Lagrangian picture (see, e.g., [21]), in which one follows the motion of each individual fluid particle. The Lagrange coordinates are co-moving with the fluid. Assuming that the fluid is a continuum, it has been shown [22, 23] that the fluid dynamics encoded in the Lagrangian of the system is invariant under a reparametrization of the coordinates. In the discrete description, this is equivalent to invariance under renumbering the arbitrary particle labels. Such transformations are volume-preserving diffeomorphisms:

$$x \rightarrow x' = x + \delta x, \quad \delta x = f(x),$$

(1)
with $\nabla \cdot \mathbf{f}(\mathbf{x}) = 0$. For simplicity, we consider a two-dimensional space. Then the latter condition can be written in terms of a scalar function $f$ as

$$f_i(\mathbf{x}) = \epsilon_{ij} \frac{\partial f}{\partial x_j}. \tag{2}$$

It has been proven (see also [20, 26]) that in this approach, the reparametrization symmetry can be re-cast in the form of noncommuting coordinates, namely by introducing additional Poisson brackets

$$\{x_i, x_j\} = \theta_{ij}, \tag{3}$$

with an arbitrary set of constants $\theta_{ij}$. The isotropy of the fluid is ensured through the arbitrariness of the elements of the matrix $\theta_{ij}$. Rescaling $f$ by $\theta^{-1}$, we can re-write $\delta x_i$ as

$$\delta x_i = \theta_{ij} \partial_j f = \{x_i, f\}. \tag{4}$$

The Poisson brackets (3) are invariant under the transformations (1), the elements $\theta_{ij}$ remaining invariant under the reparametrization of coordinates [23]. The generalization to three- and higher-dimensional spaces is straightforward.

In the quantum treatment of the fluid, the Poisson bracket of coordinates (3) becomes the commutator

$$[\hat{x}_i, \hat{x}_j] = i\theta_{ij}, \quad i,j = x,y,z, \tag{5}$$

(with an antisymmetric matrix $\theta_{ij}$), which has to be added to the usual canonical commutation relations

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}, \quad [\hat{p}_i, \hat{p}_j] = 0. \tag{6}$$

The theory based on the commutators (5) and (6) is customarily called noncommutative quantum mechanics.

To the matrix $\theta_{ij}$ we can associate a vector $\hat{\theta}$, whose components are given by $\theta_{ij} = \epsilon_{ijk} \theta_{jk}$. We note that there are volume-preserving diffeomorphisms which leave invariant simultaneously $\hat{\theta}$ and the surface density of particles $\sigma_0$ in any plane of the fluid. We expect a relation between these two invariants, which can be derived by analogy with usual quantum mechanics. In the latter case, the commutation relation $[\hat{x}, \hat{p}] = i\hbar$ leads to a quantization of the two-dimensional phase space in cells of area $2\pi \hbar$. In the case of noncommuting coordinates, the commutator (4) leads to a quantization of the reference configuration space in cells of area $2\pi \theta$. We attribute to this basic quantum of area the meaning of surface “occupied” by a single particle [23]. But the inverse density of particles has the same significance, leading to the relation

$$\theta = \frac{1}{2\pi \sigma_0}. \tag{7}$$

Incidentally, this approach has been applied to the quantum Hall fluid, providing an alternative description to Laughlin’s theory by a noncommutative Chern–Simons quantum field theory [23].

Let us dwell for a while on the physical significance of the commutator (5): its presence in the quantum algebra introduces an additional uncertainty relation, which manifests itself as a “blurriness” of space points. Precise localization, even theoretical, of the particles becomes impossible. This suggests an intrinsic “disorder”. As we shall see further, the dynamics is profoundly affected, by the coupling of vibrational modes specific to noncommutative quantum mechanics.

The dynamics in noncommutative quantum mechanics is described by the Schrödinger equation for $N$ degrees of freedom, with the Hamiltonian

$$\hat{H} \equiv \sum_i \frac{\hat{p}_i \hat{p}_i}{2M} + V(\hat{x}_1, \ldots, \hat{x}_N), \tag{8}$$

where the canonical coordinates $\hat{x}_i, \hat{p}_i, i = 1, \ldots, N$ satisfy the extended Heisenberg algebra [5]. The mathematical manipulations are considerably simplified by noting (see, e.g., [27, 28]) that the shifted coordinates

$$\hat{X}_i = \hat{x}_i + \frac{1}{2\hbar} \theta_{ij} \hat{p}_j, \quad \hat{P}_i = \hat{p}_i \tag{9}$$

satisfy the usual Heisenberg algebra $[\hat{X}_i, \hat{P}_j] = i\hbar \delta_{ij}$, $[\hat{X}_i, \hat{X}_j] = 0$, $[\hat{P}_i, \hat{P}_j] = 0$ (summation over the repeated index is assumed in (9)). This allows a physical interpretation of the $\theta$-term in (9) as a quantum shift operator [29], namely, a translation in space by $\frac{1}{2\hbar} \theta_{ij} \hat{p}_j$, while $X_i$ is the classical geometrical coordinate. This technique has been used for deriving noncommutative space corrections to various quantum mechanical phenomena, for example, the Lamb shift [30]. If the potential energy in (5) is of the harmonic oscillator type, then, when the shift (9) is applied to $H(\hat{x}, \hat{p})$, one obtains a Hamiltonian $H(X, P)$ consisting of a sum of usual quantum mechanical harmonic oscillators plus an additional interaction term proportional to the noncommutativity parameter.
III. MODEL FOR GLASSY MATERIALS: REDUCED SPECIFIC HEAT AND THE BOSON PEAK

The glass structure model we propose avails itself of the noncommutative fluid picture. Glasses are not normal liquids due to their rigidity, nor regular solids, due to their disorder. The rigidity is introduced by means of a simple cubic lattice. The disorder reminiscent of the fluid which was quenched into the glass will be implemented through the noncommutative quantum algebra [3]-[6].

We assume the glass composed of a simple cubic lattice of neutral atoms of mass \( M \), with the unit cell vector \( a \). The dynamics of the disordered lattice is described by a noncommutative harmonic oscillator potential function and we consider harmonic interactions only between the first neighbors of the atoms in a lattice. We take the vector \( \theta \) with equal projections denoted by \( \theta \) on the coordinate axes, i.e. on the directions of the edges of the unit cells.

Let us analyze the atom indexed by the integer labels \( lmn \). The quantum coordinate operators which define it are \( \hat{x}_{lmn} = l a + \hat{a}_{lmn}^x \), \( \hat{y}_{lmn} = m a + \hat{a}_{lmn}^y \), \( \hat{z}_{lmn} = n a + \hat{a}_{lmn}^z \), where \( \hat{a}_i \), with \( i = x, y, z \), denote generically the displacement operators from the lattice site in the corresponding direction. The Hamiltonian governing the time evolution of the atom \( (lmn) \) is then

\[
\hat{H}_{lmn} = \sum_{i=x,y,z} \frac{1}{2M} (\hat{p}_{lmn}^i)^2 + M\omega_0^2 \left[ (\hat{a}_{lmn}^i - \hat{a}_{lmn+1}^i)^2 + (\hat{a}_{lmn}^i - \hat{a}_{lmn-1}^i)^2 \right] + \frac{M\omega^2}{2} \left[ (\hat{a}_{lmn}^y - \hat{a}_{lmn-1}^y)^2 + (\hat{a}_{lmn}^y - \hat{a}_{lmn+1}^y)^2 \right] + \frac{M\omega^2}{2} \left[ (\hat{a}_{lmn}^z - \hat{a}_{lmn+1}^z)^2 + (\hat{a}_{lmn}^z - \hat{a}_{lmn-1}^z)^2 \right],
\]

where \( \hat{p}_{lmn}^i \) is the momentum canonically conjugated to the displacement \( \hat{a}_{lmn}^i \) and \( \omega_0 \) is the usual harmonic oscillator frequency.

In order to make sure that the disorder effects are not doubly-counted, nor washed out, we make an additional assumption about the dynamics of the atoms on the lattice. Namely, we consider an alternation of ordered and disordered atoms. By ordered atoms, we mean atoms whose quantum coordinates and momenta satisfy the usual Heisenberg algebra, i.e. whose coordinate operators commute. By disordered atoms, we mean atoms whose coordinates and momenta satisfy the noncommutative space algebra [3]-[6]. The arrangement of the lattice is such that one ordered atom is surrounded by disordered first neighbors and vice-versa. Due to the elastic couplings, the equations of motion of the so-called ordered atoms will be also influenced by the disorder of their neighbors, such that the lattice as a whole will be disordered.

Let us specify the Hamiltonian [A1] for the two types of atoms. Considering that the atom \( lmn \) is a disordered one, which suffers itself the effects of the noncommutativity of coordinates, we perform the shift [9] by replacing in [A1]

\[
\hat{u}_{lmn}^i = \hat{U}_{lmn}^i - \frac{1}{2\theta} \theta_{ij} \hat{P}_{lmn}^j,
\]

while for all the displacements of the nearest neighbors we have \( \hat{u}_{lmn+1}^y = \hat{U}_{lmn+1}^y \) etc.

If the generic atom \( lmn \) is an ordered one, the shifts [9] in the Hamiltonian [A1] have to be performed for the coordinates of the neighbors, i.e.

\[
\hat{u}_{lmn}^y = \hat{U}_{lmn}^y - \frac{1}{2\theta} \theta_{xy} \hat{P}_{lmn}^x, \quad j = y, z,
\]

while \( \hat{u}_{lmn}^i = \hat{U}_{lmn}^i \), for \( i = x, y, z \). In both cases, \( \hat{p}_{lmn}^i = \hat{P}_{lmn}^i \).

The equations of motion are obtained by applying the Heisenberg equations \( i\hbar \frac{d\hat{O}(t)}{dt} = \left[ \hat{O}(t), H \right] \), taking into account the canonical commutation relations

\[
\left[ \hat{U}_{lmn}^i, \hat{P}_{lmn'}^i \right] = i\hbar \delta_{ii'} \delta_{ll'} \delta_{mm'}, \quad \delta_{ii'} = 0.
\]

The equations of motion (see Appendices) are differential equations which couple displacements in all three directions. We introduce the notation \( \omega_\theta = \frac{\hbar}{M\theta} \) and \( R = \omega_0/\omega_\theta \). The latter is a dimensionless expansion parameter,
proportional to \( \theta \). We have retained only terms up to the second order in \( R \), as this parameter is expected to be very small. This expectation will be fully justified later, in the comparison with the experimental data.

Further, we use Born’s approach to the vibrations of a lattice, expanding in Fourier series the operators

\[
\hat{U}^i_{lmn} = \sum_k \hat{u}^i_k \exp \left[ i \left( \omega_k t + a(k_x + mk_y + nk_z) \right) \right],
\]

and applying the Born–von Kármán boundary conditions (see, e.g., [31]). In the above expression, \( k_i \) represent the wave vector projections and \( \omega_k \) the mode vibration frequencies. We obtain the dispersion relations by inserting the expansion (14) into the equations of motion.

So far, the model has two sources of anisotropy: the crystal lattice and the vector \( \theta \). As far as the noncommutativity is concerned, the disorder effect is manifest only in the plane orthogonal to \( \theta \), and not in the direction of \( \theta \). In order to render the model isotropic, we choose as representative axis one of the coordinate axes (e.g. \( Oz \)), and determine the dispersion relations for it, \( \omega_{k_z}(k_z) \). With our choice of \( \theta \) having equal projections on the coordinate axes, we insure that the disorder induced by noncommutativity is similar along \( Oz \) and in the plane orthogonal to it. Subsequently, we replicate the \( Oz \) axis by rotational symmetry to all the directions of the Cartesian frame, i.e. \( \omega_{k_z}(k_z) \rightarrow \omega_k(|k|) \), by replacing in \( \omega_{k_z}(k_z) \) everywhere \( k_z \) by \( |k| \).

The isotropised model gives the following dispersion relations:

\[
k_z^2 + k_y^2 + k_z^2 = \frac{1}{a^2} \left( \frac{\omega_k^2}{\omega_0^2} - \frac{3R^2}{1 + R^2} \right),
\]

for disordered atoms, and

\[
k_x^2 + k_y^2 + k_z^2 = \frac{1}{a^2} \left( \frac{\omega_k^2}{\omega_0^2} - \frac{3R^2}{\omega_0^2} \right),
\]

for ordered atoms. These expressions are obtained in the small-angle approximation (i.e. \( \sin(ak_i) \approx ak_i \)), but they are valid with excellent accuracy over the whole Brillouin zone, due to the smallness of the \( R \)-parameter (for \( R = 0.1 \), the ratio between the approximate and the exact values of the frequency at the border of the Brillouin zone, where the discrepancy is maximal, is about 1.5 %). We obtain three degenerated acoustic and three optical branches, the latter being a pure noncommutativity effect.

Due to the rotational symmetry, the VDOS is easily derived from (15) and (16) using standard methods, with the result:

\[
g_{\text{glass}}(\omega) = g_0(\omega) \left[ 1 + \frac{\omega^2}{\omega_0^2R^2} \left( \frac{3 - \frac{\omega^2}{\omega_0^2 R^2}}{1 - \frac{\omega^2}{\omega_0^2 R^2}} \right)^2 \right],
\]

where

\[
g_0(\omega) = \frac{3V}{(2\pi)^2} \frac{1}{a^3} \frac{1}{\omega_0^3} \sqrt{\frac{3 - \frac{\omega^2}{\omega_0^2 R^2}}{1 - \frac{\omega^2}{\omega_0^2 R^2}}}
\]

is the contribution to VDOS from the ordered atoms. We note the divergence in VDOS, i.e. a van Hove singularity, which occurs for \( \omega_{\text{div}} = \omega_0R \). In the limit \( \theta \rightarrow 0 \), we recover the VDOS of a usual simple cubic lattice with one atom per cell.

The reduced specific heat is determined from the following expression (see, e.g., [31])

\[
\frac{C}{T^3} = \int_0^{\omega_{\text{max}}} g_{\text{glass}}(\omega) d\omega,
\]

in which \( Z \) is the number of formula units per unit cell (in our model, \( Z = 1 \)) and \( k_B \) is the Boltzmann constant. We take \( \omega_{\text{max}} = 3\omega_0R \) as the frequency of the optical branches at \( k = 0 \).

The motif of the disordered lattice can be a single atom, a small molecule, a protein or any combination thereof. Hereafter, three distinct disordered materials, amorphous silicon (a-Si) [32], vitreous GeO\(_2\) [33] and \( \alpha-n-\text{Ba}_8\text{Ga}_1\text{Si}_3\text{O}_{12} \) clathrate [34], are considered. The model has two free parameters: the characteristic frequency \( \omega_0 \) and the noncommutativity parameter \( \theta \). They are determined by fitting the theoretical curve (19) to the
TABLE I: Characteristic parameters for various glasses. All frequencies in rad s\(^{-1}\). The value of \(\theta\) (in m\(^{-2}\)) is determined from the relation \(\omega_{\text{div}} = \omega_0 R\), using the experimental curves. \(N\) is the number density in m\(^{-3}\), whereas \(a\) is the lattice spacing for our model in m\(^2\). \(T_{\text{peak}}\) is the temperature at the peak of the reduced specific heat in K.

| Glassy material     | \(R\)   | \(\omega_0 \times 10^{13}\) | \(\omega_g \times 10^{13}\) | \(\omega_{\text{div}} \times 10^{14}\) | \(2\pi \theta \times 10^{-24}\) | \(N \times 10^{25}\) | \(a^2 \times 10^{-24}\) | \(T_{\text{peak}}\) |
|---------------------|----------|-----------------------------|-----------------------------|-----------------------------------|---------------------------------|----------------|----------------|-------------|
| \(a\text{-Si}\)     | 0.0478   | 4.916                       | 10.285                      | 23.500                            | 1.382                           | 4.710          | 5.523          | 35          |
| \(a\text{-GeO}_2\)  | 0.0668   | 1.003                       | 1.501                       | 6.700                             | 2.518                           | 2.655          | 8.066          | 10          |
| \(\alpha\text{nBGS clathrate}\) | 0.290    | 0.241                       | 0.083                       | 7.000                             | 31.504                          | 0.392          | 34.106         | 10.32       |

Experimental data, such that the frequency and reduced specific heat at the peak match (see table I). In Fig. 1 is shown the remarkable agreement around the peak between the experimental curves and the theoretical predictions of our model based on liquid-type disorder effects.

Let us recall the physical meaning of the parameter \(\theta\): according to (7), \(2\pi \theta = \frac{1}{\sigma_0}\) is the area “occupied” by a particle in the quantized configuration space, or the area within which the uncertainty in the position of the particle is significant. On the other hand, the mass density of the glass leads to a value of the average interatomic distance \(a\), which we consider to be the lattice spacing for our model. We note that the ratio \(2\pi \theta/a^2\) is of the same order of magnitude for the analyzed glasses (see table I). It would be interesting to investigate whether this regularity is valid for other glasses as well and find its physical significance.

![Graphs](image)

**FIG. 1: Experimental data versus theoretical prediction.** Experimental data for (a) amorphous silicon (\(a\text{-Si}\)) [32]; (b) amorphous germanium dioxide (\(a\text{-GeO}_2\)) [33]; (c) \(\alpha - n\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}\) clathrate [34], respectively, given by the empty balls. The theoretical prediction according to (19) is represented by the solid line.

### IV. CONCLUSIONS AND OUTLOOK

In summary, an amorphous solid can be interpreted as a system with a frozen-in liquid-type of disorder, implemented mathematically as a noncommutative algebra of coordinate operators. Intuitively, this is equivalent to a blurriness or uncertainty in the positions of the particles that form the glass. However, this is not a simple positional disorder, as the delocalization depends essentially on the moments of the particles – a feature specific to noncommuting coordinates. The quantum mechanical model we propose is developed from first principles and permits the derivation of analytic formulas for the density of states and specific heat of the glass. Other important features of the model are its simplicity and the very small number of free parameters (\(\omega_0\) and \(\theta\), the former connected to the electromagnetic interactions among the glass particles and the latter being a measure of the disorder). This new theory naturally accounts for the excess of heat capacity and the boson peak phenomena (see Fig. 1), which are manifestations of a pronounced divergence in the density of states in the acoustic branches, i.e. a van Hove singularity. The universality of the model is confirmed by the excellent agreement between the theoretical predictions and the experimental specific heat data around the peak for an array of diverse glasses.

Glasses are complex systems, and their quantum behaviour at different temperatures is dominated by different aspects of their structure and dynamics. We remark that the departure of the experimental curves from the analytic curve is natural at temperatures further away from the peak, since formula for VDOS [D1] includes only the contribution of acoustic modes of the noncommutative simple cubic lattice with nearest-neighbor interactions. The model
can be refined by including the next-to-nearest neighbor couplings, in which case we expect to see the peak in the transverse acoustic branch. It is also interesting to study whether adopting in the model the actual lattice type of the crystal counterpart of the analyzed glasses would improve the agreement with experimental data. A more detailed analysis of the structural and dynamical aspects of the model is in progress [35].

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Appendix A: Noncommutative normal modes of vibration

Assuming harmonic interactions among the nearest neighbors of a neutral monatomic simple cubic lattice, the dynamics in noncommutative quantum mechanics for normal modes of vibration of a simple cubic lattice is described by the Schrödinger equation for \( N \) degrees of freedom. Our starting point is the Hamiltonian governing the time evolution of the atom \((l,m,n)\):

\[
\hat{H}_{lmn} = \sum_{i=x,y,z} \frac{1}{2M} \left( \hat{p}_{i}^{lmn} \right)^2 + \frac{M\omega_0^2}{2} \left[ \left( \hat{u}_{i}^{lmn} - \hat{u}_{i-1mn} \right)^2 + \left( \hat{u}_{i+1mn} - \hat{u}_{i}^{lmn} \right)^2 \right] + \frac{M\omega_0^2}{2} \left[ \left( \hat{u}_{i}^{y} - \hat{u}_{i}^{l+1n} \right)^2 + \left( \hat{u}_{i}^{ym+1n} - \hat{u}_{i}^{l} \right)^2 \right] + \frac{M\omega_0^2}{2} \left[ \left( \hat{u}_{i}^{z} - \hat{u}_{i}^{lmn-1} \right)^2 + \left( \hat{u}_{i}^{lmn+1} - \hat{u}_{i}^{z} \right)^2 \right],
\]

where \( \hat{p}_{i}^{lmn} \) is the momentum canonically conjugated to the displacement \( \hat{u}_{i}^{lmn} \) and \( \omega_0 \) is the usual harmonic oscillator frequency. The quantum algebra satisfied by the canonical variables is:

\[
\begin{align*}
\left[ \hat{u}_{i}^{lmn}, \hat{p}_{i}^{lmn'} \right] &= i\hbar \delta_{ii'} \delta_{mm'} \delta_{nn'}, \\
\left[ \hat{u}_{i}^{lmn}, \hat{u}_{i}^{lmn'} \right] &= i\theta_{ii'}, \\
\left[ \hat{p}_{i}^{lmn}, \hat{p}_{i}^{lmn'} \right] &= 0.
\end{align*}
\]

As explained earlier, the model consists of an alternation of ordered and disordered atoms in a simple cubic lattice. \textit{Ordered atoms} mean atoms whose quantum coordinates and momenta satisfy the usual Heisenberg algebra, i.e., whose coordinates commute, while the \textit{disordered atoms} have coordinates and momenta satisfying the noncommutative space algebra. (There are “two species” of atoms in this case, like, for example, in a NaCl lattice, just that the atoms are identical, but half are ordered and half are not.)

We should emphasize that the distinction \textit{ordered/disordered atoms} is a matter of semantics, because \textit{all} atoms suffer the effects of the noncommutativity of coordinates either directly or through the dynamical couplings. The lattice, as a whole, will be disordered.

Appendix B: Equations of motion and dispersion relations for disordered atoms

Considering that the atom \( lmn \) is a disordered one, which suffers itself the effects of the noncommutativity of coordinates, we perform in (A1) the shift

\[
\hat{u}_{i}^{i} = \hat{U}_{i}^{i} - \frac{1}{2\hbar} \theta_{ij} \hat{p}_{i}^{j}.
\]
while for all the displacements of the nearest (ordered) neighbors we have
\begin{align*}
\overline{u}_{l+1mn} &= \tilde{U}_{l+1mn}^x, \\
\overline{u}_{l+1mn}^y &= \tilde{U}_{l+1mn}^y, \\
\overline{u}_{l+1mn}^z &= \tilde{U}_{l+1mn}^z.
\end{align*}
(B2)
For the momenta, \(\tilde{p}_{lmn}^i = \tilde{p}_{lmn}^i\), with \(i = x, y, z\). The shifted displacements obey the canonical commutation relations
\[\left[ \tilde{U}_{lmn}, \tilde{U}_{l'm'n'}^i \right] = i\hbar \delta_{ii'} \delta_{mm'} \delta_{nn'}, \quad \left[ \tilde{U}_{lmn}, \tilde{U}_{l'm'n'}^i \right] = \left[ \tilde{p}_{lmn}, \tilde{p}_{l'm'n'}^i \right] = 0. \quad \text{(B3)}\]
The Hamiltonian (A1) becomes:
\[
\hat{H}_{lmn}^D = \frac{1}{2M} \left[ (\tilde{p}_{lmn}^x)^2 + (\tilde{p}_{lmn}^y)^2 + (\tilde{p}_{lmn}^z)^2 \right] - \frac{R^2}{2M} \left( \tilde{p}_{lmn}^x \tilde{p}_{lmn}^y \right) - \frac{R^2}{2M} \left( \tilde{p}_{lmn}^x \tilde{p}_{lmn}^z \right) - \frac{R^2}{2M} \left( \tilde{p}_{lmn}^y \tilde{p}_{lmn}^z \right) + \frac{\omega_0 R}{2} \left( \tilde{p}_{lmn}^x - \tilde{p}_{lmn}^y \right) \left[ 2\tilde{U}_{lmn}^x - \tilde{U}_{l-1mn}^x - \tilde{U}_{l+1mn}^x + \tilde{U}_{lmn}^x - \tilde{U}_{lmn}^y \right] + \frac{M \omega_0^2}{2} \left[ \left( \tilde{p}_{lmn}^x - \tilde{p}_{lmn}^y \right)^2 + \left( \tilde{U}_{lmn}^x - \tilde{U}_{lmn}^y \right)^2 \right]
\]
\[
+ \left( \tilde{U}_{lmn}^x - \tilde{U}_{lmn}^y \right)^2 + \left( \tilde{U}_{lmn+1}^x - \tilde{U}_{lmn}^x \right)^2 + \left( \tilde{U}_{lmn+1}^y - \tilde{U}_{lmn}^y \right)^2 \right),
\quad \text{(B4)}
\]
where we have defined \(\omega_0 = \frac{\hbar}{M R}\) and \(R = \frac{\omega_0}{\omega_k}\).

The equations of motion are obtained via Heisenberg’s equations
\[
\frac{\hbar}{i} \frac{d\hat{O}(t)}{dt} = \left[ \hat{O}(t), \hat{H} \right],
\quad \text{(B5)}
\]
where the generic operator stands for either the displacements or momenta of the atom \((lmn)\), and \(\hat{H}\) is \(\hat{H}_{lmn}^D\) given by (B4).

The equations of motion for disordered atoms are
\[
\overline{\dot{u}}_{lmn}^x = -\omega_0 \left( 2\tilde{U}_{lmn}^x - \tilde{U}_{l-1mn}^x - \tilde{U}_{l+1mn}^x \right) + \frac{\omega_0 R}{2} \left( \left( \frac{\dot{\lambda}}{4\nu_{lmn}^x} - \dot{\lambda}^y_{lmn} - \dot{\lambda}^y_{l-1mn} - \dot{\lambda}^y_{l+1mn} \right) - \left( \frac{\dot{\lambda}^z_{lmn}}{4\nu_{lmn}^x} - \dot{\lambda}^z_{l-1mn} - \dot{\lambda}^z_{l+1mn} \right) \right),
\]
\[
\overline{\dot{u}}_{lmn}^y = -\omega_0 \left( 2\tilde{U}_{lmn}^y - \tilde{U}_{l-1mn}^y - \tilde{U}_{l+1mn}^y \right) + \frac{\omega_0 R}{2} \left( \left( \frac{\dot{\lambda}}{4\nu_{lmn}^y} - \dot{\lambda}^x_{lmn} - \dot{\lambda}^x_{l-1mn} - \dot{\lambda}^x_{l+1mn} \right) - \left( \frac{\dot{\lambda}^z_{lmn}}{4\nu_{lmn}^y} - \dot{\lambda}^z_{l-1mn} - \dot{\lambda}^z_{l+1mn} \right) \right),
\]
\[
\overline{\dot{u}}_{lmn}^z = -\omega_0 \left( 2\tilde{U}_{lmn}^z - \tilde{U}_{l-1mn}^z - \tilde{U}_{l+1mn}^z \right) + \frac{\omega_0 R}{2} \left( \left( \frac{\dot{\lambda}}{4\nu_{lmn}^z} - \dot{\lambda}^x_{lmn} - \dot{\lambda}^x_{l-1mn} - \dot{\lambda}^x_{l+1mn} \right) - \left( \frac{\dot{\lambda}^z_{lmn}}{4\nu_{lmn}^z} - \dot{\lambda}^z_{l-1mn} - \dot{\lambda}^z_{l+1mn} \right) \right),
\quad \text{(B6)}
\]
where we kept the terms up to the second order in \(R\).

Any function in a space formed by a periodic arrangement of atoms must satisfy periodic boundary conditions, the Born–von Kármán boundary conditions. It is important to highlight that upon the shift of coordinates applied to the quantum Hamiltonian, the disorder effects emerge as a new interaction terms added to the ordinary Hamiltonian of the simple cubic lattice. Therefore, the periodicity of the lattice is maintained, and the Born–von Kármán boundary conditions can be freely applied.

Since the reciprocal lattice of a simple cubic lattice is another simple cubic lattice, one can expand in Fourier series the operators
\[
\tilde{U}_{lmn}^i = \sum_k \tilde{U}_k^i \exp \{i (\omega_k t + a(lk_x + mk_y + nk_z))\},
\quad \text{(B7)}
\]
in the above expression, \(k_i\) represent the wave vectors and \(\omega_k\) the vibrational frequencies.

Replacing the Ansatz (B7) into the equations of motion (B6), we find the saecular equation for the disordered atoms:
\[
\begin{vmatrix}
\omega_k^2 - 4\omega_0^2 \sin^2 \left( \frac{ak}{2} \right) & i\omega_k \omega_0 R \left[ 1 + 2\sin^2 \left( \frac{ak}{2} \right) \right] & -i\omega_k \omega_0 R \left[ 1 + 2\sin^2 \left( \frac{ak}{2} \right) \right] \\
-i\omega_k \omega_0 R \left[ 1 + 2\sin^2 \left( \frac{ak}{2} \right) \right] & \omega_k^2 - 4\omega_0^2 \sin^2 \left( \frac{ak}{2} \right) & i\omega_k \omega_0 R \left[ 1 + 2\sin^2 \left( \frac{ak}{2} \right) \right] \\
i\omega_k \omega_0 R \left( 1 + 2\sin^2 \left( \frac{ak}{2} \right) \right) & -i\omega_k \omega_0 R \left[ 1 + 2\sin^2 \left( \frac{ak}{2} \right) \right] & \omega_k^2 - 4\omega_0^2 \sin^2 \left( \frac{ak}{2} \right)
\end{vmatrix} = 0.
\quad \text{(B8)}
\]
As explained Sect. III, the only physically relevant directions for our model are the directions of coordinate axes. The isotropization of the model is performed by taking the dispersion relations in the direction Oz and replicating it by rotational symmetry to all the directions of the Cartesian system, namely by the replacement \( k_z \rightarrow |k| \).

Upon isotropization, the solutions of equation (B8) (for \( k_z = k_y = 0 \) and \( k_z \rightarrow k \)), are:

\[
\omega_{k\pm}^D = \frac{\omega_0}{2} \left[ 6R^2 + 8 (1 + R^2) \sin^2 \left( \frac{a|k|}{2} \right) \pm 2 \left[-7R^4 - 32R^2 - 16 \right. \right.
\]

\[ + \left. (56R^4 + 72R^2 + 32) \sin^2 \left( \frac{a|k|}{2} \right) + (16R^4 + 32R^2 + 16) \left( 1 - 2 \sin^2 \left( \frac{a|k|}{2} \right) + \sin^4 \left( \frac{a|k|}{2} \right) \right) \right]^{\frac{1}{2}}, \]

where the minus (plus) sign is related to the degenerated acoustic (optical) branch. In the small angle approximation (i.e. \( \sin(ak_i) \approx ak_i \)), this expressions becomes

\[
\omega_{k\pm}^{D-\text{approx}} = \frac{\omega_0}{2} \left[ 6R^2 + 2 (1 + R^2) a^2|k|^2 \pm 2 \sqrt{9R^4 + 2R^2 (3R^2 + 1) a^2|k|^2 + (R^2 + 1)^2 a^4|k|^4} \right] \]

preserving the relation of the minus (plus) sign for the acoustic (optical) branch.

Both functions (B9) and (B10) are monotonically increasing within the Brillouin zone, with the maximum at \( ak_i = \pi \). In Fig. 2 are depicted the dispersion relations for \( R = 0.15 \). We note the characteristic plateau in \( \omega_k \), which leads to the broadened van Hove singularity in the VDOS. The small angle approximation gives a very good estimate of the full solution for small \( R \), therefore we work further with the approximate dispersion relation (B10), which is the solution of the equation

\[
\omega_k^4 + \omega_k^2 \left[ \omega_0^2 R^2 - \omega_k^2 (1 + R^2) \right] a^2|k|^2 - 3\omega_k^2 \omega_0^2 R^2 = 0. \tag{B11}
\]

We may put equation (B11) in the form

\[
k_x^2 + k_y^2 + k_z^2 = \frac{1}{a^2} \frac{3\omega_k^2 R^2 - \omega_k^4}{\omega_k^2 (1 + R^2)} \tag{B12}
\]

and identify the isofrequency surfaces \( \omega_k = \omega = \text{const.} \) in the \( k \)-space as spheres of radius \( \frac{1}{a^2} \frac{3\omega_k^2 R^2 - \omega_k^4}{\omega_k^2 (1 + R^2)} \). The density of states is obtained by taking the derivative of the volume of the sphere with respect to \( \omega \) and subsequently dividing by the volume of one cell in the \( k \)-space, \( (2\pi)^3/V \), where \( V \) is the volume of the system in the direct space. The result is

\[
g_D(\omega) = \frac{3}{2} \frac{V}{(2\pi)^3} \frac{4\pi \omega^2}{\omega_0^2 a^3} \sqrt{\left| \frac{3 - \frac{\omega^2}{\omega_k^2 R^2}}{1 - \frac{\omega^2}{\omega_k^2 R^2}} \right| \left| \frac{\omega_k^2 R^2}{\omega_0^2 R^2} \right|} \left| \frac{\omega_k^2 R^2}{\omega_0^2 R^2} - 2 - \frac{3}{2} \frac{\omega_k^2}{\omega_0^2 R^2} \right| \left( 1 - \frac{\omega^2}{\omega_k^2 R^2} \right)^2, \tag{B13}
\]

where the prefactor \( 3/2 \) accounts for the three acoustic branches and the fact that only half of the atoms are disordered.

**Appendix C: Equations of motion and dispersion relations for ordered atoms**

In a similar manner as described in the preceding section, we proceed with the ordered atoms. If the atom \( (lmn) \) is a ordered one, we have

\[
\bar{u}^i_{lmn} = \frac{\bar{U}^i_{lmn}}{} \tag{C1}, \quad i = x, y, z,
\]

while its nearest neighbors are disordered and the shift of noncommutative coordinates has to be applied to them, as follows:

\[
\begin{align*}
\bar{u}^x_{\pm 1mn} &= \frac{\bar{U}^x_{l \pm 1mn}}{} - \frac{1}{2\hbar} \theta_{xj} \frac{\bar{P}^j_{l \pm 1mn}}{}, & j &= y, z, \\
\bar{u}^y_{lm \pm 1n} &= \frac{\bar{U}^y_{lm \pm 1n}}{} - \frac{1}{2\hbar} \theta_{yj} \frac{\bar{P}^j_{lm \pm 1n}}{}, & j &= z, x, \\
\bar{u}^z_{lmn \pm 1} &= \frac{\bar{U}^z_{lmn \pm 1}}{} - \frac{1}{2\hbar} \theta_{zj} \frac{\bar{P}^j_{lmn \pm 1}}{}, & j &= x, y.
\end{align*} \tag{C2}
\]
As for the momenta, $\hat{\pi}_{lmn} = \hat{P}_{lmn}$. The Hamiltonian \( A1 \) becomes:

\[
\hat{H}^O_{lmn} = \frac{1}{2M} \left[ (\hat{P}_{lmn}^x)^2 + (\hat{P}_{lmn}^y)^2 + (\hat{P}_{lmn}^z)^2 \right] + \frac{M\omega_0^2}{2} \left[ (\hat{\chi}_{lmn}^x - \hat{\chi}_{l-1mn}^x - \frac{\theta}{2} (\hat{P}_{l-1mn}^y - \hat{P}_{l-1mn}^y))^2 + (\hat{\chi}_{l+1mn}^x + \frac{\theta}{2} (\hat{P}_{l+1mn}^y - \hat{P}_{l+1mn}^y) - \hat{P}_{lmn}^x)^2 \right] \]

\[
+ \frac{M\omega_0^2}{2} \left[ (\hat{\chi}_{lmn}^y - \hat{\chi}_{l-1mn}^y - \frac{\theta}{2} (\hat{P}_{l-1mn}^x - \hat{P}_{l-1mn}^x))^2 + (\hat{\chi}_{l+1mn}^y + \frac{\theta}{2} (\hat{P}_{l+1mn}^x - \hat{P}_{l+1mn}^x) - \hat{P}_{lmn}^y)^2 \right] 
+ \frac{M\omega_0^2}{2} \left[ (\hat{\chi}_{lmn}^z - \hat{\chi}_{l-1mn}^z - \frac{\theta}{2} (\hat{P}_{l-1mn}^y - \hat{P}_{l-1mn}^y))^2 + (\hat{\chi}_{l+1mn}^z + \frac{\theta}{2} (\hat{P}_{l+1mn}^x - \hat{P}_{l+1mn}^x) - \hat{P}_{lmn}^z)^2 \right].
\]

Proceeding as in the case of disordered atoms, we find the equations of motion up to the second order in $R$:

\[
\frac{\dot{\mathbf{u}}_{lmn}}{R} = -\omega_0^2 \left( 2\hat{\chi}_{lmn}^x - \hat{\chi}_{l-1mn}^x - \hat{\chi}_{l+1mn}^x \right) + \omega_0 \frac{R}{2} \left\{ \frac{2}{2} \right\} \left[ 2\hat{\chi}_{l+1mn}^x + \hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x \right] 
+ \frac{\omega_0^2 \frac{R}{2}}{4} \left\{ -2 \right\} \left[ 2\hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x \right] 
+ \frac{\omega_0^2 \frac{R}{2}}{4} \left\{ -2 \right\} \left[ 2\hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x - \hat{\chi}_{l+1mn}^x \right].
\]

The saecular equation for the ordered atoms is given by

\[
\det |A_{ij}| = 0,
\]

where the elements of the matrix $A_{ij}$ are

\[
A_{11} = \omega_k^2 - 4\omega_0^2 \sin^2 \left( \frac{ak_x}{2} \right) + 2\omega_0^2 R^2 \left[ 2 \sin^2 \left( \frac{ak_x}{2} \right) - \sin^2 \left( \frac{ak_x}{2} \right) \right],
\]

\[
A_{12} = -i\omega_0 \omega_k R \left[ 1 - 2 \sin^2 \left( \frac{ak_y}{2} \right) \right] + 2\omega_0^2 R^2 \left[ \sin^2 \left( \frac{ak_y}{2} \right) - 2 \sin^2 \left( \frac{ak_y}{2} \right) \sin^2 \left( \frac{ak_z}{2} \right) \right],
\]

\[
A_{13} = i\omega_0 \omega_k R \left[ 1 - 2 \sin^2 \left( \frac{ak_y}{2} \right) \right] + 2\omega_0^2 R^2 \left[ \sin^2 \left( \frac{ak_z}{2} \right) - 2 \sin^2 \left( \frac{ak_z}{2} \right) \sin^2 \left( \frac{ak_x}{2} \right) \right],
\]

\[
A_{21} = i\omega_k \omega_0 R \left[ 1 - 2 \sin^2 \left( \frac{ak_y}{2} \right) \right] + 2\omega_0^2 R^2 \left[ \sin^2 \left( \frac{ak_z}{2} \right) - 2 \sin^2 \left( \frac{ak_z}{2} \right) \sin^2 \left( \frac{ak_y}{2} \right) \right],
\]

\[
A_{22} = \omega_k^2 - 4\omega_0^2 \sin^2 \left( \frac{ak_y}{2} \right) + 2\omega_0^2 R^2 \left[ 2 \sin^2 \left( \frac{ak_y}{2} \right) - \sin^2 \left( \frac{ak_y}{2} \right) \right],
\]

\[
A_{23} = -i\omega_k \omega_0 R \left[ 1 - 2 \sin^2 \left( \frac{ak_y}{2} \right) \right] + 2\omega_0^2 R^2 \left[ \sin^2 \left( \frac{ak_z}{2} \right) - 2 \sin^2 \left( \frac{ak_z}{2} \right) \sin^2 \left( \frac{ak_y}{2} \right) \right],
\]

\[
A_{31} = -i\omega_k \omega_0 R \left[ 1 - 2 \sin^2 \left( \frac{ak_z}{2} \right) \right] + 2\omega_0^2 R^2 \left[ \sin^2 \left( \frac{ak_z}{2} \right) - 2 \sin^2 \left( \frac{ak_z}{2} \right) \sin^2 \left( \frac{ak_x}{2} \right) \right],
\]

\[
A_{32} = i\omega_k \omega_0 R \left[ 1 - 2 \sin^2 \left( \frac{ak_z}{2} \right) \right] + 2\omega_0^2 R^2 \left[ \sin^2 \left( \frac{ak_x}{2} \right) - 2 \sin^2 \left( \frac{ak_x}{2} \right) \sin^2 \left( \frac{ak_z}{2} \right) \right],
\]

\[
A_{33} = \omega_k^2 - 4\omega_0^2 \sin^2 \left( \frac{ak_z}{2} \right) + 2\omega_0^2 R^2 \left[ 2 \sin^2 \left( \frac{ak_z}{2} \right) - \sin^2 \left( \frac{ak_z}{2} \right) \right].
\]

Upon isotropization and in the small angle approximation, the saecular equation for ordered atoms becomes

\[
\omega_k^4 - \omega_k^2 \omega_0^2 \left( \omega_0^2 R^2 - \omega_k^2 \right) | \mathbf{k} |^2 + 3\omega_k^2 \omega_0^2 R^2 = 0.
\]
or
\[ k_x^2 + k_y^2 + k_z^2 = \frac{1}{a^2} \frac{3 \omega^2 R^2 - \omega_c^2}{\omega_c^2 - \omega^2}. \]  \hfill (C8)

The solutions for the secular equation coming from (C6) are:
\[ \omega_{k\pm}^O = \frac{\omega_0}{2} \left[ 6R^2 + 8 \sin^2 \left( \frac{a|\mathbf{k}|}{2} \right) \left[ 1 - 2R^2 \sin^2 \left( \frac{a|\mathbf{k}|}{2} \right) \right] \right] \]
\[ \pm 2 \left[ 64R^2 \sin^6 \left( \frac{a|\mathbf{k}|}{2} \right) \left[ R^2 \sin^2 \left( \frac{a|\mathbf{k}|}{2} \right) - 1 \right] + (16 - 48R^4) \sin^4 \left( \frac{a|\mathbf{k}|}{2} \right) + 8R^2 \sin^2 \left( \frac{a|\mathbf{k}|}{2} \right) + 9R^4 \right]^{\frac{1}{2}}. \]  \hfill (C9)

Accordingly, in the small angle approximation, this expression is rewritten as:
\[ \omega_{k\pm}^{O-\text{approx}} = \frac{\omega_0}{2} \left[ 6R^2 + 2a^2|\mathbf{k}|^2 \left( 1 - \frac{R^2}{2a^2|\mathbf{k}|^2} \right) \right] \]
\[ \pm 2 \sqrt{R^2a^6|\mathbf{k}|^6 \left( \frac{R^2}{4}a^2|\mathbf{k}|^2 - 1 \right) + (1 - 3R^4) a^4|\mathbf{k}|^4 + 2R^2a^2|\mathbf{k}|^2 + 9R^4} \right]^{\frac{1}{2}}. \]  \hfill (C10)

Similarly to the case of the disordered atoms, the ordered atoms contribution to the density of states is found to be:
\[ g_O (\omega) = 3 \frac{V}{(2\pi)^3} \frac{1}{a^3 \omega_0^3} \sqrt{3 - \frac{\omega^2}{\omega_0^2 R^2}} \left[ 1 - \frac{\omega^2}{\omega_0^2 R^2} \right]. \]  \hfill (C11)

**Appendix D: Specific heat of the glass**

The complete glass DOS in the small angle approximation is equal to the sum of the disordered and ordered atoms expressions for DOS, namely
\[ g_{\text{glass}} (\omega) = g_O (\omega) \left[ 1 + \frac{\omega^2}{\omega_0^2 R^2} \left[ \frac{\omega^2}{\omega_0^2 R^2} - 2 - \frac{3}{2} \frac{\omega^2}{\omega_0^2} \right] \right], \]  \hfill (D1)

where \( g_O (\omega) \) is the contribution to VDOS from the ordered atoms given by (C11).

The reduced specific heat is determined from the following expression
\[ \frac{C}{T^3} = \int_0^{\omega_{\text{max}}} \frac{h^2 \omega^2}{k_B T^5} N_A \left( e^{\frac{\hbar \omega}{k_B T}} - 1 \right)^2 g_{\text{glass}} (\omega) d\omega, \]  \hfill (D2)

in which \( Z \) is the number of formula units per unit cell (in our model, \( Z = 1 \)) and \( k_B \) is the Boltzmann constant. We take \( \omega_{\text{max}} = \sqrt{3} \omega_0 R \) as the frequency of the optical branches at \( k = 0 \). We adopt this value for the maximum frequency because our small angle approximation makes the acoustic branch frequency at the end of the Brillouin zone slightly larger than the frequency corresponding to the exact solution. In this way we insure that we integrate over the whole acoustic branch.

In order to establish an order of magnitude for the noncommutativity parameter \( \theta \), implicitly a measure of nonlocality, one has to resort to the available experimental data: from the match between the theoretical prediction with the experimental data for the reduced specific heat one can assign that the unique pair of values of \( R \) and \( \omega_0 \) used for the fit gives the value for the frequency of divergence \( \omega_{\text{div}} \). From this set of parameters one can establish the value for \( \theta \) by means of \( \omega_0 = \frac{\hbar}{m \theta} \).

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FIG. 2: Dispersion relations for $R = 0.15$. Panels (a) and (b) present the dispersion relations for disordered and ordered atoms, respectively. The degenerated acoustic branches are represented by the solid lines, while the optical modes are represented by dashed lines. Panels (c) and (d) present a comparison between the approximated (solid line) and exact (dashed line) solutions for the acoustic branch (a zoom in the end of the Brillouin zone, in order to reveal their slight discrepancy).

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