Extended and localized vibration models in disordered systems

Barak Galanti and Zeev Olami
Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel

We discuss vibrational localization problems in glasses and disordered media in this paper. It is claimed that the essence of the localization problem is already observed in disordered lattice models. These kinds of vibrations belong to a different universality class than bonded electrons. Specifically, the eigenvectors are extended even in two dimensions. Moreover, the correlation exponent does not diverge in the transition from localized to delocalized states. Furthermore, the volume of the universality class than bonded electrons. Specifically, the eigenvectors are extended even in two dimensions. Moreover, the correlation exponent does not diverge in the transition from localized to delocalized states. Furthermore, the volume of the extended states is scaled according to the distance from the transition as \( V \sim |\omega - \omega_c| L^d \). Interestingly, boson peaks can be observed in the density of states in both two and three dimensions. We studied the eigenstates of this problem and analyzed the scattering effects in these lattices. Importantly, we found that in two dimensions the boson peak, the localization edge, and the beginning of anomalous scattering are at the same frequency. In three dimensions, however, there are three separate regions: (1) localized, (2) weakly scattered, and (3) anomalously scattered. Finally, we discuss the relevance of this study to actual experiments and glasses.

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I. INTRODUCTION

It is well-known that a disorder in the properties of a physical system can in turn induce localization and scattering effects. For the past three decades, disordered electronic systems have been the main focus of much research, having received enormous attention as manifested by the numerous books and reviews on the subject [1-10]. In contrast, though the disordered vibration problem is as important as the electronic one, we have found almost no discussion on the analogous problem of phonon localization. Though the vibrational properties of disordered solids were reviewed in several papers [1], subjects like localization, scattering, and properties of the eigenstates were not analyzed. There are various reasons for this. The main one is that localization effects for electrons are more pronounced physically for statistical reasons. They occur at a well-defined Fermi energy state, so it is much easier to observe them under experimental conditions. In contrast, the localization effects of phonons are often obscured behind the calculations and the statistics; therefore, their role in influencing properties like heat conductivity or scattering is much less clear. We believe therefore that the theoretical understanding of these localization effects is crucial to the understanding of glasses.

Unfortunately, we found almost no systematic treatment of vibration in disordered media above one-dimension in the literature. However, there is some literature relating to two main issues. The first is a bonded network with cuts in the connections, which is the percolation problem. In such a problem anomalous fractal excitations called fractons may appear instead of the usual long-range phonons. This phenomenon was first mentioned in [12] and has been repeatedly observed in experiments and simulations. The second type of problem comprises simulations of ‘real’ glasses [13]. Though such simulations do yield some information about the relevant systems, it is rather difficult to obtain any concrete ideas because of various reasons. For example, simulations of glasses are completely uncontrolled in as much as the source of the disorder and its size are unknown, since the glass is defined by a dynamical relaxation algorithm. It is indeed possible to study these glasses and probe the degree of elastic and structural disorder; however, the disorder is still uncontrollable. Clearly, the effects of the disorder are manifested in many experimental measurements in glasses, but it is difficult to make a reasonable and rational interpretation of the data.

Disorder in glasses and other materials can originate from various physical sources. Structural characteristics can change the topology of the material and thus affect the vibrations. Another major source of disorder is elastic variability in the local elastic constants. In simple glasses this is the main source of disorder, which is caused by the quenched pressure that remains in the glass after the quench from the liquid. Such quenched pressures are correlated with the existence of second-order gradients that generate large variations in the local elastic constants [16]. Another important component for disorder is the mass disorder that occurs when two or more kinds of atoms exist in the lattice.

In glasses there is a set of anomalous thermodynamic properties that do not appear in crystals [18,19]. Examples of such behavior are anomalous heat conductivity and excess vibrations at low frequencies termed ‘boson peak’ in the literature [18,19]. Scattering mechanisms are thought to mainly contribute to the depletion of the thermal transport in glasses. A crossover in the scattering of the glass is expected to be observed on a characteristic scale which is usually identified with the Ioffe-Regel limit, where the scattering length is of the same order.
analyze the one-dimensional case and then proceed to spectra and localization of the scalar models. We first mentioned are satisfied. In section IV we discuss the dynamical matrices of the three previously mentioned systems and in general. In section III we demonstrate that the dynamical systems which, under certain constraints would give is similar when the following constraints are fulfilled: (1) the transmission coefficients are symmetric and positive, (2) the relevant dynamical variables are scalar, and (3) the masses are constant.

Variants from these constraints, i.e. the vectorial case, the negative connectivity, and the variable masses, display different results and will be discussed in other papers. However, the time dependence, the statistics, and physical properties of these systems are very different. If any of the constraints are broken, we can expect to observe a different behavior, as will be described later in detail.

In this paper we extend our discussion of an earlier, shorter paper on the subject. In section II we describe the concepts of localization in electronic theory, and in general. In section III we demonstrate that the dynamical matrices of the three previously mentioned systems are the same, when the parameter constraints that we mentioned are satisfied. In section IV we discuss the spectra and localization of the scalar models. We first analyze the one-dimensional case and then proceed to analyze numerically lattice problems that are analogous to the models studied in the electronic case. By increasing the lattice size we can characterize the eigenstates. The participation ratios of the states are used to measure the degree of localization. A localization transition between extended and localized states is observed both in two and three dimensions. Furthermore, in two dimensions there are three kinds of modes, namely, extended, localized, and multi-fractal separated by mobility edges.

However, the three-dimensional transition is different from the bonded electron transition. Specifically, there is no divergence of the correlation length near the localization edge at \( \omega_c \), and the volume of the extended states (defined by the participation ratio) converges to zero at the mobility edge. It is analogous to the percolation phase transition above its threshold, where the global percolation cluster becomes a finite fraction of the size of the system. Such a transition implies zero electronic conductivity near the mobility edge, which can also have a major effect on the heat conductivity of phonons in glasses, where there are well-known anomalies (for example, a plateau in heat conductivity in medium temperatures), see for example Ref. [19].

We have analyzed the eigenvectors of the two- and three-dimensional systems. Importantly, we found that in the two- and three-dimensional systems studied there are several scattering regimes. The first is at low frequencies in two and three dimensions where there is no interaction between the modes, and they are characterized by well-defined wave vectors. The upper cutoff of this range depends on the system’s scale. Above this cutoff the mapping between the state and the wave vector fails because of scattering. However, an absolute value of the wave vector is still defined for each state. The inverse scattering width is defined by the variance around this mean value. This second range is called a ‘normal’ scattering regime. We believe that it extends to zero frequency when the system is enlarged. Above this range beyond a point \( \omega_b \) we find anomalous scattering. Above these three regimes there are localized states where the wave length is hardly defined at all. For normal scattering we find that the scattering width scales as \( \Gamma \sim \omega^{1.7 \pm 0.1} \) in two dimensions and \( \Gamma \sim \omega^{3.5 \pm 0.5} \) in three dimensions within a relatively small region of \( \omega \). In two dimensions there is an overlap between the appearance of anomalous scattering, the boson peak, and the localization edge i.e. \( \omega_c = \omega_b \). However, in three dimensions there are two distinct scales. The first scale is the localization edge, and the second one is located at the boson peak and at the anomalous scattering edge \( \omega_b \), where a drop-off in the participation is observed.

1. [13,24]. In fact we observe two basic scales in three dimensions as will be discussed later. Both of them do not fit the I-R demand but they are in the same range. In the second part of this paper we focus on scattering effects. Since getting experimental and numerical information is relatively difficult, it is easier to use lattice models to obtain information about the vibrational properties. Indeed, we shall show here that many of the basic phenomena observed in glasses are also observed in lattice models.

In the one-dimensional case, it is known that the vibrations are localized [20,22]. However, the localization length in these systems is scaled as the inverse square of the frequency. So at low frequencies, we observe phonon-like modes with a localization length much larger than their wavelength, and with a low frequency spectral density of order one. In a few theoretical papers on this subject [23,24], it was contended that the situation at higher dimensions is analogous to that in electrons. We present here sufficient numerical evidence to show that this is not the case.

The vibration problem generally consists of a vector translation problem. A simpler version of the problem is the problem of scalar vibrations where there is a scalar translation at any point. This is a realistic problem in one and two dimensions (e.g., a membrane). However, scalar models are, as we shall see, interesting enough theoretically that we should start with a discussion of such models.
II. LOCALIZATION AND ELECTRONS

We shall review briefly presented some background on localization and its relation to the electronic case. The classical example for such phenomena is an electron in a disordered potential. An electron that obeys the Schrödinger equation with spatial disorder in the voltage is known to be localized for a strong enough disorder. We examine the equation

\[ i\hat{\psi}_j = \Delta \psi_j + V_j \psi_j, \]  

where \( j \) is the position, \( \Delta \) is the Laplacian operator on the relevant lattice, and the potential \( V_j \) is a random function. The variance of \( V \) affects the character of the eigenstates, the conductivity, and its dependence on the system size [1-10].

In one dimension and for any type of disorder all electronic states are localized: the wave-functions decay at large distances as

\[ \langle \psi(r)\psi(r + r_0) \rangle \sim \exp(-|r - r_0|/\xi), \]  

where \( \xi \) is the localization length, and \( r \) and \( r_0 \) are any given lattice points. This leads to an exponential localization of the conductivity.

In two dimensions the situation is marginal and depends to a large extent on the models. For any disorder in \( V_j \) the wave-functions form a multi-fractal set of the system. The multi-fractal exponent is weakly dependent on the energy. Above a certain critical disorder all electronic states are localized.

In three dimensions both extended and localized states exist. There is a critical energy \( E_c \) that defines the transition from localized to extended states. This transition is accompanied by a diverging correlation length \( \xi(E) \sim (E - E_c)^{-\nu} \), where \( \nu \) is a positive number. In three dimensions, states are extended below or above a mobility edge and localized below or above it. The electronic conductivity is expressed as \( \sigma \sim (E - E_c)^{\nu} \).

For electronic models with magnetic fields, there is also a localization transition in the two-dimensional case. Classical waves (photons and waves) were proposed to affect the character of the longitudinal modes, which have a role in vector models).

III. MODELS

A. Vibrations

We begin this section with a discussion of the phonon model. If there is a particle system that has a stable equilibrium, it is possible to displace it by \( \tilde{u}_i \) from the stable particle positions. If the \( \tilde{u}_i \) are small enough there is an elastic expansion around the equilibrium positions. Accordingly, vibration Hamiltonians of the following kind can be written as

\[ H = \frac{1}{2} \sum_{i,\alpha} m_i (\dot{u}_i^\alpha)^2 + \frac{1}{2} \sum_{i,j,\alpha,\beta} \Phi_{\alpha,\beta,i,j} u_i^\alpha u_j^\beta, \]  

where \( u_i^\alpha \) is the \( \alpha \) component of the translation in site \( i \), and \( \Phi \) represents the interaction terms.

We shall limit our discussion here to scalar elastic movements in an orthogonal direction to the state. (This will inhibit the interaction between the transversal and longitudinal modes, which have a role in vector models).

So the discrete elastic Hamiltonian can be given as

\[ H = \frac{1}{2} \sum_i m_i (\dot{u}_i)^2 + \frac{1}{2} \sum_{ij} K_{ij} (u_i - u_j)^2, \]  

where \( u_i \) represents elastic movements and \( K_{ij} \) represents the elastic constants.

There are two obvious constraints on the parameters. The first is the symmetry \( K_{ij} = K_{ji} \). The second is that \( H \) must be non-negative for all realizations of \( u \). This is a non-local demand for the elastic constants that is satisfied by a positive \( K_{ij} \). The single atom dynamics is defined by

\[ m_i \ddot{u}_i = \sum_j K_{ij} (u_i - u_j), \]
where \( m_i \) is the particle mass.

Assuming that \( u_i = \exp(i \omega t) \tilde{u}_i(\omega) \) we obtain an eigenvalue problem represented by

\[
-m_\omega^2 \tilde{u}_i = \sum_j K_{ij}(\tilde{u}_i - \tilde{u}_j).
\]  

(8)

Note that the eigenvalue problem is generally not symmetric because of the existence of the \( m_i \) terms.

B. Diffusion and ‘Free’ Quantum Particles

Free random diffusion has a similar dynamical form. We define particle densities \( \rho_i \) and random diffusivities \( D_{ij} \) between the nearby sites. The currents are \( J_{ij} = D_{ij}(\rho_i - \rho_j) \) and we obtain the random diffusion equation

\[
\dot{\rho}_i = \sum_j D_{ij}(\rho_i - \rho_j).
\]

(9)

Defining \( \rho_i(t, \mu) = \exp(-\mu t)\tilde{\rho}_i(\mu) \) results in a similar problem with \( \mu = -\omega^2 \). Since negative densities in \( \rho \) are not allowed, \( D_{ij} \) should be greater than zero. In contrast to the phonon model, there is no condition for detailed balance, and \( D \) does not have to be symmetric.

A free randomly moving quantum particle can be described by

\[
i \dot{\psi}_i = \sum_j M_{ij}(\psi_i - \psi_j)
\]

(10)

for arbitrary Hermitian \( M_{ij} \). For real and non-negative \( M \)s and for the linear solution \( \psi = \exp(iEt)\tilde{\psi}_i(E) \), we obtain a similar eigenvalue problem.

To summarize, the random realizations of these three linear models have the same linear dynamical structure, but only under the following conditions: the transmission coefficients \( M, D, \) and \( K \) are symmetric, real, and positive, and the phonon model is scalar and possesses a single mass. All these models are Positive Random Laplacian models. However, the time dependence, statistics and other properties are different. In this paper we use, unless stated otherwise, the phonon terminology.

The difference between these Random Laplacian models and the electronic models is already manifested in one dimension \([21,22]\). The single mass vibration model in one dimension can be mapped (see in the next section) to an electronic model with a disordered potential that decays with the square of the frequency. In higher dimensions, however, we are not aware of any solution. Since we know that this model is equivalent to the diffusion model, it is clear that for positive connection coefficients any density will diffuse to infinity. Therefore, the correlation length can either explode at low frequencies or the system can be extended.

IV. DEFINITION AND SIMULATION OF THE MODELS

A. Definitions

Here we focus on an equal mass (\( m_i \equiv 1 \)) model in a cubic lattice, of \( d \) dimensions, with a unit distance and size \( L \). We considered nearest neighbor interactions, with two elastic constants \( K_1 \) and \( K_2 \), with a ratio \( \alpha = K_2/K_1 \) between them, and a probability \( p \) to find \( K_1 \) and \( 1-p \) for \( K_2 \). Since \( \alpha < 1 \) is the same as \( \alpha > 1 \), we will discuss only the former limit. The normalization \( K_1 = 1 \) determines a scale of frequencies. This model was suggested in \([24]\) and simulated in \([30]\) for small \( \alpha \).

There are two simple limits for this model, namely, \( \alpha = 1 \), which is the ordered lattice limit, and \( \alpha = 0 \), which is for percolation. In the ordered lattice limit, all states are extended and ordered. The percolation limit, however, is more involved. Above the percolation threshold, we normally find phonons on a scale much larger than the percolation correlation length \([12]\). Below the percolation threshold, the system would be completely localized. For \( \alpha > 0 \), a different behavior exists. With extremely small values of \( \alpha \), there are fracton states together with phonons \([30]\). This is not the case were the values of \( \alpha \) are larger and \( p \) is not close to the percolation threshold.

We treated the eigenvalue problem numerically using the LAPACK package for real symmetric banded systems for the equal mass model. Specifically, we used a cubic system of size \( L \), where the distance between particles is unity. Most of our simulations were performed under free boundary conditions. However, we verified that the simulations were not changed under periodic boundary conditions. For this propose, we computed a set of eigenvalues \( \omega_i \)s, and eigenvectors denoted as \( \bar{u}_r(\omega_i) \), where \( r \) is the lattice position. To verify the accuracy, we checked some examples for which the answers were known and compared the results of other codes to our computation.

B. The One-Dimensional Case

The one-dimensional problem on an ordered lattice is a classic example \([29]\). Eigenstates can be written as

\[
u_k = \exp(i(kr + \omega(k)t)).
\]

(11)

If the lattice is disordered the states can no longer be written as periodic modes and thus the problem becomes localized. This general problem was solved in \([21,21,22]\) and it is localized with a localization length that is proportional to \( \omega^{-2} \). We thought that it would be useful to test our code on this system to check both the numerical code and the dependence of our results on the system.
size. The solution of the theoretical model in one dimension can provide some insight as to why this model is so different from the bonded electronic model; therefore we present it in detail in Appendix A.

Considering the above, we simulated the one-dimensional problem. Figure 1 displays our results for the participation ratio, which is as noted previously, proportional to the correlation length. This curve also shows an $\omega^{-2}$ dependence of the correlation length. As the system size is enlarged, wider regions of such behavior can be observed in the curve. For a definite system size $L$, there is a cutoff in the frequency that is defined by $L \sim \omega_c^{-2}$. Below this cutoff the correlation length is larger than $L$. Since $\omega_c \sim L^{-0.5}$ and the number of states is proportional to $L$, there are $L^{0.5}$ free states in such a system. This can be observed in the plateaus on the right-hand side of the curve.

C. Two-Dimensional Models

We now analyze the previous model in two dimensions. As mentioned previously, for the electronic model in two dimensions, any degree of variation in $V$ generates fractal exponents $D(2)$. These effects are observed in system sizes between 16 and 50. A transition in scaling for low noise levels can be easily observed.

In the two-dimensional positive Laplacian case we were unable to distinguish any failure of normal scaling for small values of noise. Therefore, unlike the electronic case, a small disorder has no effect whatsoever on the scaling described by the participation ratio. For smaller values of $\alpha$, localization is indeed observed. In Figure 2 presents numerical results of systems with parameters $p = 0.4$ and $\alpha = 0.1$. Figure 2a shows the density of states divided by $\omega$. A boson peak with a center around $0.6 - 0.65$ is visible. Figure 2b presents $I^4$ as a function of $\omega$ for different system sizes. At low frequencies there are extended modes whose participation ratio scales with the system size. There is a well-defined mobility gap at $\omega_c$, separating the extended and quasi-localized states. Below the mobility edge the participation ratio can be written as

$$I^4(\omega) \sim |\omega - \omega_c|^2.$$

All the states near the mobility edge are extended, though their volumes may be very small. The density of states in the extended region is close to the classical density $N(\omega) \sim \omega$. To analyze these states, we calculated the exponent $D(2)$. Figure 2c shows the dependence of $D(2)$ on $\omega$. Five scaling regimes of $D(2)$ are visible. The multi-fractality of these states can be verified either by calculating the dependences of $I^{2p}$ or calculating of the distribution function of $u_r$ and from point-point correlations. The transitions in $D(2)$ are sharp within our numerical accuracy. Thus, there is a sharp transition between the multi-fractal and extended states in this model at $\omega_c = 0.63 \pm 0.03$. Note that this is also the position of the boson peak.

D. Three-Dimensional Models

The same kind of model was also simulated in three dimensions. Figure 3a presents the density of states divided by $\omega^2$. A boson peak is observed at $\omega \approx 0.6$. Extended states and a localization transition to a fully localized state were observed (see Fig. 3b). Because of insufficient statistics, it is unclear whether there are quasi-localized states for this problem. Again, the scaling of the extended eigenstates near the localized regime behaves as

$$I^4 \sim |\omega - \omega_c|L^3.$$  \hspace{1cm} (12)

The states in the extended regime behave similarly to those in two dimensions. Note that in this model the states up to a scale of $\omega \approx 0.65$ have a flat global scaling (see in Fig 3b).

The phase transition from localized to delocalized states is different from that of the electrons. Specifically, there is no divergence of the localization length, as is observed in the electronic models, so $\xi \sim (\omega - \omega_c)^0$. This also indicates zero ‘conductivity’ below the transition and will have an important effect on low heat conductivity in glasses [14]. The phonon volume in the extended regime shows a second order behavior similar to that observed for the volume of the infinite cluster in percolation models.

Let us now compare in detail comparison of our numerical results with the theory. Note that both theoretical works [23,24] are based on approximations. Here, comparison of a numerical simulation with theory is possible, even for a system with a limited scale. The basic concept used in our simulations is the following: if there is an increase in the system size, localization lengths that are not dependent on the system size will appear in the simulation when the system scale becomes large enough. This is indeed what was observed in our one-dimensional computation. As the system size is increased, there is a decreased lower zone of frequency where participation ratios depend on system size, and an increased range where they fit the theoretical predictions. This effect does not occur in two and three dimensions. There is a clear localization transition in two dimensions, but the states above it, even those with the smallest normalized participation ratios, continue to scale with the system size. A two-dimensional scaling length $\xi \sim \exp(-\omega^{-2})$ was predicted in [24]. This indicates that above a cutoff given by $L \sim \xi$, all states would scale with the system size and there would be a shift in the cutoff when $L$ is increased. Both effects were not observed in our calculations.
V. SCATTERING AND EIGENVECTOR STRUCTURE

A. The Two-Dimensional System

As observed before the scattering of phonons and the shape of the scattering is an extremely interesting issue. We can expect to observe at least three scaling ranges in the shape of the spectra. Figure 4 presents shapes of various wave-functions (left) and the square of their Fourier transform \( F(\vec{k}, \omega)(\text{right}) \). Figure 4a shows for \( \omega \approx 0.1 \) a well-defined periodic mode together with a well-defined peak in Fourier space. As the frequency is increased, there is an increase in scattering. This is manifested in the creation of local domains with different directions and the existence of rings in Fourier space. At higher frequencies (\( \omega \approx 2 \)), the shapes become localized. Figure 5 gives examples of the radially integrated Fourier transform \( F(|\vec{k}|, \omega) \) for the shapes presented in Figure 4.

To quantify these effects, we measured the peak values of \( k_0 \), which is scaled linearly with \( \omega \) below the localization edge. Therefore, as stated before, they appear to be phononic. Above this edge over a limited region we find that \( \omega \sim k^{0.85\pm0.3} \). Next, we assumed that the Fourier transforms can be represented as

\[
F(k, \omega) = \frac{\Gamma^2}{(k-k_0)^2 + \Gamma^2}.
\]

We make a fit with this expression to try to determine the amount of scattering.

Fits with this expression are reasonably good up to a value of \( \omega \approx 1 \). Figure 6a shows the linear dependence of \( k_0 \) at a frequency up to \( \omega_b \approx 0.65 \). Above this range the Lorentzian fits are less good because of the existence of larger tails at large ks. In this range we observe (see Fig. 6a) a transition to an anomalous dependence of the wave vector \( \omega \sim k^{0.8\pm0.05} \). Figure 6b shows the width \( \Gamma \) as a function of \( \omega \). In the smaller range scale, for small frequencies up to a scale of \( \omega = 0.2 \pm 0.05 \), the width is constant, since the system is not large enough to create scattering at these wavelengths. Above this value up to \( \omega_b = 0.65 \), we obtain a dependence of \( \Gamma \sim \omega^\mu \) with \( \mu \), where \( \mu = 1.7 \pm 0.2 \). In the second frequency range there is a smaller exponent, \( \mu = 1.1 \pm 0.1 \).

This transition approximately overlaps the change between extended and multi-fractal modes : \( \omega_b = \omega_c \). For the higher frequencies, the states are more localized and fits to Eq. [14] are not good.

B. The Three-Dimensional Case

We performed the same type of fit in this case as in the two-dimensional case. The results are presented in Figure 7. Here the range in Fourier space is smaller (one decade) and this makes some of our estimates inaccurate. As in the two-dimensional case, we observe for small \( \omega \) values a range of constant peak width. For larger values of \( \omega \) there is a range with a very sharp rise, which can be fitted to \( \Gamma \sim (\omega - \omega_c)^{3.5\pm0.5} \). For \( \omega_b \sim 0.66 \) there is a crossover to anomalous scattering. When \( \omega_b \) is further increased, there is a transition to localized states. We noted that this usually occurs in glassy models where the transition to a strong scattering transition happens within the extended range.

Note that the dependence on \( \Gamma \) that we would obtain in optical Rayleigh scattering is \( \Gamma \sim \omega^{d+1} \), though this is not the same type of problem for the phonons [15]. Our results in two dimensions are not consistent with this. In three dimensions they might be consistent with such scattering.

In two dimensions the transition between normal and anomalous scattering is exactly the point where the localization transition and the boson peak is observed. All these effects are clumped together in two dimensions. In three dimensions there are two transitions: the first is the localization edge \( \omega_c \) and the second is at the transition between normal and anomalous scattering and the boson peak at \( \omega_b \). This is a strong indication that in three dimensions, the strong scattering effects begin before the localization edge effects do. This is also in accord with the commonly accepted situation as indicated by the literature on glasses.

C. Relation to Experiments and General Discussions on Glasses

In actual experiments the dynamical correlations are measured by

\[
S(\vec{k}, \omega) = \int_{-\infty}^{\infty} dt \exp(-i\omega t) < \sum_{i,j} \exp(ik \cdot (r_i(t) - r_j(0))) >,
\]

where the average is done in time at the relevant measurement temperatures. If we have a complete knowledge of the eigenvectors we can transform this expression to

\[
S(\vec{k}, \omega) = \frac{1}{\mathcal{F}} \sum_l \delta(\omega - \omega_l) N(\omega, T) \left[ \sum_{ij} e_i^l \cdot e_j^l \cdot k \exp(ik(r_i^0 - r_j^0)) \exp(-W_{ij}) + h.o.t. \right]
\]

where the es are eigenvectors, \( N(\omega, T) \) is the distribution function and the \( Ws \) are the Debye-Waller factors. The basic components in this sum are

\[
G(\vec{k}, \omega_l) = k^2 F(\vec{k}, \omega_l).
\]
Usually the sum is done over some range in $\omega$, so it represents some average over the modes. In the normal scaling region the results we get from both kinds of fits are in accord. In two dimensions the fits can fail because of the existence of a longer tail in the Fourier transforms.

In this paper we showed that indeed as speculated in the literature there in 3 dimensions there is a cross over frequency between anomalously scattered waves and weak scattering in which the width of the square of the fourier scales as $\omega^{3.5\pm0.5}$. The scale of this crossover is not the Ioffe-Rogel scale so we don’t know if it makes any sense to use this terminology. The conclusions from such a theory to transport is not clear. The reader can read some thoughts about it and some references from the glass literature in [7]. The transport situation for states below the cross over should be discussed using different theoretical measures then ours. Nonlinear effects cannot be approximated using our method.

We note that if there are nonlinear scattering effects associated with vibrations at low temperatures (like two-level systems), they will be observed in scattering experiments but not in harmonic analysis. Furthermore if there are lifetime effects they will not be observed in such an experiment.

As noted before, there is no actual available data for the normal scaling range, neither in real glasses nor in the numerical simulations, because of various experimental and numerical difficulties, so it is impossible to compare our results with experimental data. We hope that in due time this will be possible.

VI. CONCLUSIONS

In this paper we focused on the relatively simple case of the scalar vibration model. This can be demonstrated experimentally, for example, on a membrane. There are nontrivial predictions on the localization in such a system. We observed that the eigenvectors for these models are strongly scattered and that there are strong scattering regions in the extended regime when the problem is in two and three dimensions. The dependences of the width of the Fourier transforms of the modes do not seem to be in accord with naive Rayleigh scattering estimates in two dimensions.

We find that in the two-dimensional system there is only one critical scale that is observed by a localization edge, a boson peak, and a shift in the scattering and the dependence of $\omega$ on $k$. On the other hand, in the three dimensional system there are at least two scattering scales and three scattering regimes. The first one is the localization edge and the second is the scattering edge where scattering becomes large. The second scale overlaps with the boson peak. A similar picture about Silicon glass is given in [14] even though we do not agree with many of the statements in this paper about the nature of the states. This subject will be discussed in more detail in another paper where the transport coefficients will be calculated.

Introducing of vector disorder and structural disorder will induce further complications, consisting of interactions between longitudinal and transversal modes. The existence of mass disorder is another strong mechanism for introducing more scattering, especially in the optical bands. This subject is especially interesting because the representation of systems with mass disorder is equivalent to a Schrödinger equation with a correlated potential. This will be discussed in another paper [25]. Another subject that remains largely untreated in our paper is the definition of electrical and thermal conductivities. Kubo and transport formulas can be used to estimate the dependence of these conductivities on temperature and elastic disorder [12], this will be done in another study.

We demonstrated that a set of models has a different behavior with the effect of noise than bonded electrons. This is manifested in two main ways: (1) the phonon models seem to be delocalized in two dimensions, and (2) they have a percolative behavior as a function of the frequency. The scale of the mode diverges as the distance from the critical points times the system volume.

We focused on the relatively simple case where the movements are scalar. This can be realized experimentally, for example, on a membrane. There are nontrivial predictions for such a system. Introducing of vector disorder and structural disorder will induce further complications, consisting of interactions between longitudinal and transversal modes and possibly soft modes (to be discussed elsewhere). The existence of mass disorder is another strong mechanism for introducing more scattering, especially in the optical bands. Notably, the eigenvectors for these models are strongly scattered and there are strong scattering regions in the extended region in two and three dimensions.

Another subject that remains largely untreated in this paper is the definition of electrical and thermal conductivities. Kubo formulas can be used to estimate the dependence of these conductivities on temperature and elastic disorder [12], which will be done in another study.

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APPENDIX A: THE ONE-DIMENSIONAL VIBRATION PROBLEM

It was shown in [21,22] that the phonon model is equivalent to the electronic model with a rescaled interaction $V_i \omega^{-2}$. We shall briefly repeat the arguments because, first, we can use them to solve this problem and second, because it is reasonable to assume that there is an analogous effect at higher dimensions.

The one-dimensional equation can be written as

$$\omega^2 \bar{u}_i = K_i (\bar{u}_i - \bar{u}_{i+1}) + K_{i-1} (\bar{u}_{i-1} - \bar{u}_i). \quad (A1)$$

This model can be solved through the following transformations: if we define $Q_n = K_i (\bar{u}_i - \bar{u}_{i+1})$, the equation is transformed to

$$Q_{n+1} - 2Q_n + Q_{n+1} = -\Omega/K_n Q_n, \quad (A2)$$

where $\Omega = -\omega^2$. This is a Schrödinger equation with a potential that scales down with the frequency. Eigenvalues explode exponentially as

$$Q_n = \exp(n\gamma(\Omega)). \quad (A3)$$

An equivalent equation for $R_n = Q_{n+1}/Q_n$ can be written as

$$R_n = 2 + \Omega/K_i - 1/R_{n-1}. \quad (A4)$$

We can now write an equation for the probability distribution $P(R)$ in the steady state. Here we get

$$P(R) = \frac{p}{2+\Omega/K_1 - 1/R} P(2 + \Omega/K_1 - 1/R) + \frac{1-p}{2+\Omega/K_2 - 1/R} P(2 + \Omega/K_2 - 1/R). \quad (A5)$$

The localization exponents are defined as

$$\gamma(\Omega) = \frac{1}{n(R)} \int P(R) dR. \quad (A6)$$

For small values of couplings or frequency the solution is defined by a fixed-point solution. Using the average value of the map $b = \Omega \bar{A}$, $\bar{A} = (p/K_1 + (1-p)/K_2)$ we get

$$\bar{R} = 1 + \frac{b}{2} + \left( b + \frac{1}{4} b^2 \right)^{1/2}, \quad (A7)$$

which can be expanded to

$$\bar{R} - 1 = b^{1/2} + \frac{b}{2} + O(b^{3/2}). \quad (A8)$$

The localization length follows

$$\xi = 8/b = \frac{8}{\bar{A}} \omega^{-2}. \quad (A9)$$

These results can be tested in a simulation as we here, mainly, to test the simulation.
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FIG. 1. Log-log scale of the participation ratio $I^4$ (proportional to $\xi$) as a function of system size for one-dimensional systems with $\alpha = 0.1$ and $p = 0.4$, for sizes 128-8192 with jumps of factor two. We observed that the curves decay as $\omega^{-2}$, as the bold line illustrates. As the system size is increased, this scaling range also increases. Note that the upper cutoffs are defined by $L \sim \omega_c^{-2}$. Below $\omega_c$, $I^4$ is proportional to the system size.
FIG. 2. (a) The density of states $N$, for $p = 0.4$ and $\alpha = 0.1$, divided by $\omega$ for a system size $L = 100$. The peak is the extra number of states relative to the linear normal distribution, which is called the boson peak. (b) The participation ratio is $I^4$. The curves are averaged over equal intervals of $\omega$ of size 0.05 to reduce the $I^4$ fluctuations. The extended modes are seen below $\omega \sim 0.63$. (c) The scaling exponent $D(2)$ is shown as a function of the frequency $\omega$. The curve is averaged over intervals of frequencies $\omega$ in order to reduce the noise in $I^4$. 
FIG. 3. (a) The density of states $N$, for $p = 0.8$ and $\alpha = 0.1$, divided by $\omega^2$ for a three-dimensional system with a size of $L = 22$. The peak is the extra number of states relative to the linear normal distribution, which is called the boson peak. (b) The participation ratio $I^4$ normalized by $L^3$ with the same parameters. The solid line is for $L = 8$, dotted for $L = 16$, and dashed for $L = 22$. The curves are averaged to reduce the fluctuations. For the system with $L = 8$, we ensemble the average of 6 runs to reduce fluctuations. The extended modes are observed below $\omega \sim 1$ by their collapse into one curve.
FIG. 4. We present the two-dimensional shapes and Fourier transforms of the states of the $100^3$ system with $p = 0.4$ and $\alpha = 0.1$ for $\omega = 0.1(a), 0.2(b), 0.6(c), 1.0(d), 2.0(e)$.

FIG. 5. The radially averaged squares of the two-dimensional Fourier transforms $F(k)$ for the previous $\omega$s are shown.
FIG. 6. The length $k_0$ of the Fourier transforms as a function of $\omega$ (a) and the width $\Gamma$ of the peak (b) for the same two-dimensional system.
FIG. 7. The length $k_0$ of the Fourier transforms as a function of $\omega$ (a) and the width $\Gamma$ of the peak (b) for the three-dimensional system with $p = 0.8$, $\alpha = 0.1$, and $L = 22$. 