Extended and localized phonons, free electrons, and diffusive states in disordered lattice models

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In this paper we propose that phonons, free diffusive electrons, and diffusion in two- and three-dimensional disordered lattice problems belong to a different class of localization than bonded electrons. This is manifested by three effects that can be observed numerically. First, there are extended states even at two dimensions, whereas there are no extended states in the usual electronic models. Second, the correlation length does not diverge at the mobility edges in three dimensions, and finally, the participation ratio of the extended states, decays to zero at this edge. This indicates zero electronic conductivity, in the extended region near the mobility edge. We show that low energy modes for these models can either have diverging localization lengths or are extended.

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It is well known that disorder in the properties of physical systems can induce localization effects on the relevant variables. A classic example for such phenomena is an electron in a disordered potential [1-10]. Specifically, an electron that obeys the Schrödinger equation, with spatial disorder in the potential, is known to be localized for a strong enough disorder, which affects the conductivity of an electronic system and its dependence on the system size. This subject has received enormous attention during the last three decades and is described in a numerous books and reviews [1-10].

In one dimension and for any kind of disorder, all electronic states are localized, i.e. the wave-functions decay at a large distance as $\exp(-|r - r_0|/\xi)$, where $\xi$ is the localization length, and $r$ and $r_0$ are local positions. This leads also to exponential localization of the electronic conductivity. In contrast, in two dimensions the situation is marginal. For any disorder the wave functions form a multi-fractal set in the system. In three dimensions there are localized and extended states separated by a mobility edge at an energy $E_c$. The correlation length diverges in the localized region as $\xi \sim (E - E_c)^{-\nu}$, and the conductivity is proportional to $(E - E_c)^\nu$ in the extended range [8]. Classical waves (photons and waves), are thought to behave similarly (see in [11]).

Specifically, there are three equivalent physical systems in which the disorder appears in a random Laplacian form and can cause dramatic effects. The first is vibration problems (or phonons) in disordered media. Examples for such problems are disordered solids, glasses, granular materials, packings, colloids, and polymers, where the geometrical disorder, connectivity and fluctuations in the elastic constants play a crucial role in determining the dynamics. The second is free electrons on a lattice, with randomness in their real, positive transmission coefficients. The third is the random diffusion problem.

The dynamical structure of all these problems is similar though the time-dependence, statistics, and physical properties are very different.

In the one-dimensional case, it is well known that phonons are localized [2,3,4]. However, the localization length of these systems is scaled, as the inverse square of the frequency. So at low frequencies, we observe phonon-like modes with a localization length that is much longer than their wave length, and with a low–frequency distribution function similar to the ordered one. In a few theoretical papers published on the subject [4,5], it was proposed that the situation in higher dimensions is analogous to the BE situation. We claim in this paper that there is sufficient numerical evidence that this is not the case.

We begin by demonstrating that the dynamical matrices of the three cases are equivalent within certain parameter limits. Then we analyze numerically a lattice problem that is similar to the models studied in the electronic case [1-10]. We used increasing lattice sizes to get information about the nature of the eigenstates as the system size is increased. The participation ratio (PR) of the states was used to measure the degree of localization. A localization transition between extended and localized states was observed in the spectra in two and three dimensions. However, the three–dimensional transitions are different from the bonded electron (BE) transition[1-10]. There is no divergence of the correlation length near the mobility edge $E_c$, (i.e. $\nu = 0$), and the volume of extended states (defined by the participation ratio) converges to zero at the mobility edge. This implies zero electronic conductivity near the mobility edge. Moreover, this can also have a major effect also on the heat conductivity for phonons in glasses where there are well–known anomalies (a plateau in heat conductivity in medium temperatures, see for example in [12]). Further-
more, in two dimensions there are three kinds of modes: extended, localized, and multi-fractal modes separated by mobility edges. We propose that the difference between these problems and the BEs is because that potential terms destroy the low–energy free structure of the free electrons and phonons.

Let us define the equivalent models that we study. The first is the discrete random elastic Hamiltonian

\[ H = \frac{1}{2} \sum_{ij} K_{ij} (u_i - u_j)^2, \]  

where \( u_i \) represents scalar elastic movements and \( K_{ij} \) represents the elastic constants. Though the \( u_i \) are generally vectors, we will limit our discussion here to scalars. There are two obvious constraints on the parameters. The first is the symmetry \( K_{ij} = K_{ji} \). The second is that for all realizations of \( u_i \), the Hamiltonian is non-negative. This is a non-local requirement for the realizations of the elastic constants that can be trivially satisfied by non-negative \( K_{ij} \) which is used. The single atom dynamics is defined by

\[ m_i \ddot{u}_i = \sum_{ij} K_{ij} (u_i - u_j), \]  

where \( m_i \) is the particle mass. Assuming that \( u_i = \exp(i\omega t) \bar{u}_i(\omega) \) we obtain an eigenvalue problem

\[-m_i \omega^2 \bar{u}_i = \sum_{ij} K_{ij} (\bar{u}_i - \bar{u}_j).\]  

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

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

Defining \( \rho_i(t, \mu) = \exp(-\mu t) \bar{\rho}_i(\mu) \) we obtain a similar eigenvalue problem with \( \mu = \omega^2 \). Since negative densities in \( \rho \) are not allowed, \( D_{ij} \geq 0 \).

A free randomly moving quantum particle is described by

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

for arbitrary hermitian \( M_{ij} \). For real and non-negative \( M \)’s we again obtain a similar equation, for \( \psi = \exp(iEt) \bar{\psi}_i(E) \). These linear models have the same linear dynamical structure for the phonon case when the masses are the same, and in the diffusive case where the diffusion constants are symmetric. However, the time dependence, the statistics and other properties are different. In this paper we use, unless stated otherwise, the phonon terminology.

Let us concentrate on an equal mass \( (m_i = 1) \) model in a cubic lattice, in \( d \) dimensions, with a unit distance and size \( L \). We consider the nearest neighbors' 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 only discuss this limit. The normalization \( K_1 = 1 \) defines a scale of frequencies. This model was suggested in [14] and was simulated in [17] for small \( \alpha \).

We can calculate the density of states \( N(\omega) \) and the eigenvectors \( \bar{u}_r(\omega) \). The participation ratio is our main measure for the nature of the states. It is defined as

\[ I_4(\omega) = \left( \sum_r \bar{u}_r^4(\omega) \right)^{-1}, \]

where the summation encompasses all lattice sites. If a state is localized, the non-normalized PR is not dependent on the system size. However for extended eigenstates the PR is scaled as \( L^d \) [8]. If the states are multi-fractal, as is reported for electronic states in two dimensions, the PR is scaled as \( L^\beta \) with \( \beta < d \). Another measure of the localization is the behavior of the correlation length and the conductivity near the mobility edge.

There are two simple limits for this model. Namely, \( \alpha = 1 \), which is the ordered lattice limit, and \( \alpha = 0 \), which is the percolation case. With \( \alpha = 1 \), all states are extended and ordered. The percolation limit however, is more involved. Above the percolation threshold it is expected to see phonons on a scale much larger than the percolation correlation length [14], and fractal excitations called fractons, below this length [16]. Below the percolation threshold, the system would be completely localized. The two–and three–dimensional percolation cases were recently studied in [18]. Different behavior is observed for \( \alpha > 0 \). Fractons with phonons were observed for the case of extremely small \( \alpha [17] \).

The eigenvalue problem is treated numerically using the LAPACK package with real symmetric banded systems for the equal mass model. For the variable mass model we used a special routine for real–banded systems. Specifically, we used a cubic system of size \( L \), where the distance between particles is unity. Most of our simulations were done for free boundary conditions. However, we verified that the periodic boundary conditions did not change them. We computed a set of eigenvalues \( \omega_i \), and eigenvectors denoted as \( \bar{u}_r(\omega_i) \), where \( r \) is the lattice position.

We simulated the one dimensional case to check our method. The numerical results here are completely in accord with the theoretical predictions. We found that the PR scales in the low frequency regime as \( \omega^{-2} \), with a lower frequency cutoff whose size is reduced with an increase in system size.
FIG. 1. The density of states $N(\omega)$ for $p = 0.4$ and $\alpha = 0.1$. Note the two distinct peaks that are typical to the two-component system.

In the two-dimensional case, we observed that for small values of $\alpha$, localization effects are observed over a wide range of $p$s. Figures 1-3 present numerical results from a system with parameters $p = 0.4$ and $\alpha = 0.1$. Figure 1 shows the density of states.

FIG. 2. The participation ratio $I_4$ in a two-dimensional system for $p = 0.4$, $\alpha = 0.1$ and various system sizes. 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 $\omega \sim 0.6$.

In a two-component system we observe two distinct peaks in the distribution function. At low frequencies the density of states is linear in $\omega$, so the states are phonon-like. Figure 2 presents $I_4(\omega)$ as a function of $\omega$. At low frequencies there are extended modes whose PR scales with the system size. There is a well-defined mobility gap at $\omega_c$, separating the extended and multifractal states. The PR below it is $I_4(\omega) \sim (\omega_c - \omega)L^2$. To analyze these states we calculated the exponent $\beta$. This is shown in Fig. 3 where the scaling exponent $\beta$ of $I_4$ versus $L$ is presented as a function of $\omega$. Five scaling regimes of $\beta$ are visible in the curve. There is a marked transition between the extended state $\beta = 2$ and the state with $\beta = 1$, within our numerical accuracy. Thus, there is a sharp mobility gap between the multi-fractal and extended states in this model.

The same behavior was observed for a very wide set of parameters for $\alpha < 0.5$, and the probabilities between 0.2 and 0.8. A phase diagram of those limits will be published in a forthcoming paper. The same effects were also observed for continuous distributions of the elastic constants.

The same kind of model was also simulated in three dimensions, where we observed a localization transition (see Fig. 4). The scaling of the extended eigenstates is again $I_4(\omega) \sim |\omega - \omega_c|L^3$. Above the mobility edge all states are localized. There is no divergence in the correlation length near the transition $\xi \sim (\omega - \omega_c)^\nu$ ($\nu = 0$). Therefore this localization transition is different from that of BE. One would expect to see no power law contribution to the zero conductivity of free electrons near the $E_c$. This result is related to the decay of the PR near $E_c$. States with a low PR cannot transfer current effectively, because according to the Kubo-Greenwood formula, the conductivity is related to overlaps between wave functions. This is also a clear indication for zero conductivity in the two-dimensional case (see Fig. 5). Indeed, calculations of conductivity in such systems will reveal a strong dependence of the conductivity on $E$ but will probably show only slight or no dependence of the conductivity on the system size. Moreover, this will also have an important effect on the heat conductivity in glasses.

A common feature of all these models is the existence a minimal zero energy state. This is a sign for the existence
of ‘free’ states in a low–frequency region. To show that the localization length should diverge, let us consider the random quenched model of diffusion with minimal diffusivity. Any local density will diffuse to infinity with a minimal effective diffusion constant (above the minimal value of $D$). If all states are localized, no diffusion to infinity would be possible, since the initial condition is expanded by eigenstates of the problem. Therefore the correlation length should either diverge at low frequencies or the system will be extended.

Let us now make a detailed comparison using the theory. Note that both theoretical works \cite{14, 15} are based on approximations which also fail in the electronic case \cite{8}. One can compare a numerical simulation with the theory even for a system with a limited scale. The basic concept used in our simulation is the following: if there is an increase in the system size, localization lengths that do not depend on the system size will appear in the simulation when the system scale becomes large enough. This is what is observed in numerics in one dimension. As the system size is increased, there is a decreased lower zone of frequency where PRs depend on system size, and an increased range where the PRs fit the theoretical predictions. Interestingly, this kind of effect does not occur in two and three dimensions. Specifically, there is a clear localization transition in two dimensions, but the states above it, even the ones with the smallest normalized PRs continue to scale with the system size. A two–dimensional scaling length $\xi \sim \exp(-\omega^{-2})$ was predicted in \cite{14}. This indicates that above a cutoff given by $L \sim \xi$, all states would scale with the system size and that there would be a shift in the cutoff when $L$ is increased. Both effects were not observed in our numerics. In three dimensions it was claimed that a blowup of the correlation exponent occurred with a similar exponent in the electronic case \cite{14}. This was also not observed. The results of \cite{14} for three dimensions can also be tested, since they are detailed, and there is no agreement. Note that for larger system sizes, there might be difficulties in scalings; this is the common danger of numerical work.

All the effects discussed in this paper seem to be conserved for different masses and also for different continuous probability distributions for the $K$s.

The findings presented here raised the following questions that are currently under study. What is the theory of the observed transition? What is the effect of adding the mass and vector properties to the phonon translations? What is the nature of the transition between bonded and free electrons? How does the electrical and heat conductivity depend on the energy? What is the connection of those effects to real glasses?

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\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{fig4.png}
\caption{The normalized PR in three dimensions for $p = 0.8$, $\alpha = 0.1$. The solid line is for $L = 8$, dotted for $L = 16$, and dashed $L = 22$. The curves are averaged in frequency to reduce the fluctuations. An average of 6 runs was used for $L = 8$. The extended modes are observed below $\omega \sim 1$.}
\end{figure}

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