Effect of short-range order on transport in one-particle tight-binding models

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We investigate transport properties of topologically disordered three-dimensional one-particle tight-binding models, featuring site-distance-dependent hopping terms. We start from entirely disordered systems into which we gradually introduce some short-range order by numerically performing a pertinent structural relaxation using local site-pair interactions. Transport properties of the resulting models within the delocalized regime are analyzed numerically using linear response theory. We find that even though the generated order is very short ranged, transport properties such as conductivity or mean free path scale significantly with the degree of order. Mean free paths may exceed the site-pair correlation length. It is furthermore demonstrated that while the totally disordered model is not in accord with a Drude- or Boltzmann-type description, moderate degrees of order suffice to render such a picture valid.

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I. INTRODUCTION

Since its introduction the Anderson model has been a paradigm in the investigation of disordered quantum systems [1]. However, most existing amorphous materials are not amorphous due to disordered on-site potentials on a periodic lattice (Anderson model) but feature a spatially disordered site configuration. A model class for such systems has been introduced and to some extent analyzed by Lifshitz [2]. In both system classes the phenomenon of Anderson localization occurs, i.e., at some (or all) energies energy eigenstates extend only over a finite spatial range called the localization length. Three-dimensional systems may feature localized and extended states that are energetically separated by the mobility edges. The lowest- (and highest-) energy eigenstates of an energy band are usually localized at all nonzero degrees of disorder, while the states in the center of the spectrum may be delocalized [1]. There also exists a degree of disorder at which all eigenstates become localized, called the Anderson transition. While there is an enormous amount of literature on Anderson transitions [1,3], mobility edges, [4–11] and localization lengths [1,12], there seems to be less work on the quantitative description of transport behavior (conductivities, diffusion constants, mean free paths, etc.) in the delocalized regime. This is probably due to the fact that electronic transport on the macroscopic scale in doped semiconductors or glassy systems is almost always dominated by thermally activated hopping processes between localized energy eigenstates at the lower band edge [5,13,14]. At feasible temperatures in standard materials the Fermi distribution simply gives only non-negligible probability to localized states at the lower band edge (highly doped but weakly compensated semiconductors may be an exception here [13,15]). However, transport mediated by the delocalized center of the spectrum, which is the subject of the present paper, may be of importance for electronic conduction in amorphous metals or phononic heat conduction in amorphous materials [16]. Many of the quantitative results on transport in the delocalized regime are either on extremely weakly disordered systems, i.e., crystals comprising some defects [17–20], or on the Anderson model [21–23]. These investigations find localized and/or diffusive behavior in the limit of large time and length scales. Remarkably diffusive and even weakly localized behavior has been found on finite time scales (at high frequencies) also in strictly periodic (quantum) systems of the Lorentz gas type [24–26]. However, the present paper addresses truly nonperiodic systems and finds ballistic behavior (mean free path) for the short and diffusive behavior on the long length scale. Recently results on transport within the delocalized regime in some Lifshitz models featuring completely random site configurations have been reported in Ref. [27]. Both transport types, i.e., hopping (though not thermally activated) and band or Drude transport, have been found, which provides an alternative to the widespread belief that transport phenomena within the delocalized regime in disordered systems may generally be described using a Drude or Boltzmann approach [15]. The present paper is along the lines of Ref. [27] and extends the studies to Lifshitz models that are not completely random but feature some short-range order in the site configuration. We find that even weak short-range order affects transport properties strongly.

The paper is organized as follows. We start by introducing our models and their specific parameters in Secs. II and III. Then we compute in Sec. IV the dependence of their conductivities (at high temperatures and low fillings) on the amount of short-range order. After briefly commenting on localization and short-range order in Sec. V we address the Einstein relation and mean free paths defined on the basis of an Einstein relation in Sec. VI. By considering models featuring different length scales of the hopping amplitudes we find some universality of the transport properties in Sec. VII. We close with a summary in Sec. VIII.

II. MODEL OF GENERATION OF SHORT-RANGE ORDER

Even the most amorphous solids are spatially not completely random but feature some short-range order on an atomic scale. As this order becomes more pronounced the amorphous system gradually passes over to a crystal. Many of

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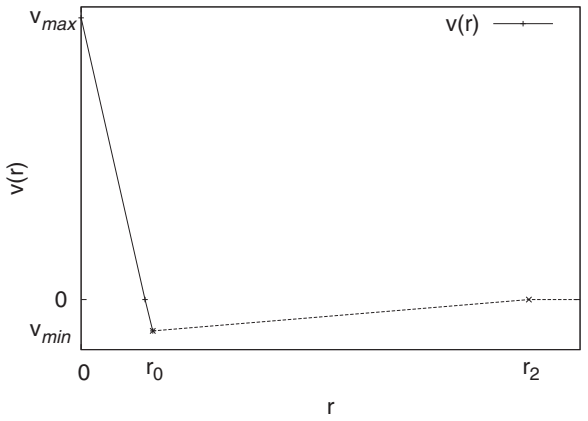

FIG. 1. Polygon pair-interaction potential $v(r)$ used in the structural relaxation algorithm (1) to generate short-range order.

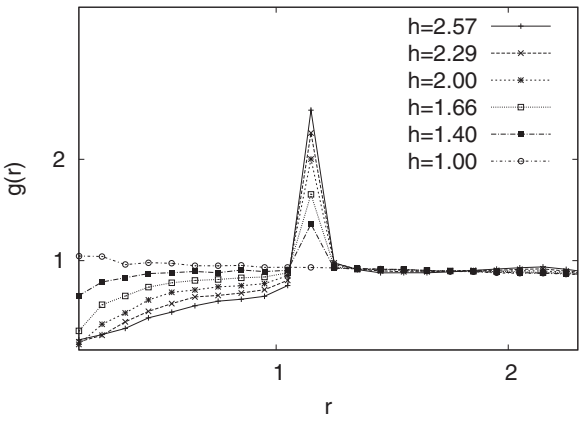

FIG. 2. Pair-correlation function $g(r)$ after different run times of the structural relaxation algorithm (1). Obviously, short-range order is gradually generated; the most frequent site distance is stable at $r = 1.12$. Based on this figure, the height of the first peak h is used to quantify the degree of short-range order. Note that the second peak is hardly visible for all degrees of order.

those intermediate structures actually exist. It is the purpose of this paper to investigate the effect of increasing order in initially completely (nonphysically) disordered systems on transport properties. The systems will be modeled by quantum tight-binding models featuring intersite distance-dependent hopping amplitudes (see Sec. III). Thus the site configuration eventually affects the transport properties. Indeed, as will become clear below, changing the topological order of the atomic sites has a substantial effect on the transport quantities such as mean free paths and conductivities. The case of a distribution of fully disordered sites was extensively investigated in Ref. [27]. Thus, in this paper we generate some short-range order in the following straightforward way: We start by producing a set of $N = L^3$ three-dimensional position vectors $\vec{r}_j$ by drawing each Cartesian coordinate (x_j, y_j, z_j) of each vector independently from a uniform distribution on the interval $[0, L]$, i.e., within a cube of volume L^3 in real space. This guarantees a uniform site distribution with unit density. Now short-range order is produced based on pair-interaction potentials $v(|\vec{r}_{ij}|)$, where $|\vec{r}_{ij}| = |\vec{r}_i - \vec{r}_j|$ denote interatomic distances between sites i and j. We schematically mimic the relaxation that would occur through the minimization of the total interaction energy $V := \sum_{ij} v(|\vec{r}_{ij}|)$ with respect to the site positions $\vec{r}_j$ for particles in viscous fluid. Routinely one could use a structural relaxation algorithm with a typical interatomic potential such as Morse; however, due to the curvature of such potentials, the most frequent site distance grows while order is numerically generated. Since we intend to exclusively focus on the effect of the degree of order, we want to keep other parameters such as density and most frequent site distance fixed. Thus we employ a rather simple pair-interaction potential that is essentially a polygon (see Fig. 1). The parameters $r_0 = 1.12$, $r_2 = 8$, $v_{\min} = -20$, and $v_{\max} = 140$ control the short-range repulsion and the long- (intermediate-) range attraction. The choice $r_0 = 1.12$ guarantees that throughout the lattice relaxation the value of the site density $\rho = 1$ remains unchanged even if close packing would be reached (which of course practically never happens). This kind of simple polygon potential may not be very realistic, but it suffices to continuously generate a first peak in the pair-site correlation function at r_0 (see Fig. 1). Thus we define our lattice relaxation by the following gradient descent method:

$$x_{\mathbf{i}}^{n+1} = x_{\mathbf{i}}^{n} - \lambda \left.\frac{\partial V}{\partial x_{\mathbf{i}}}\right|_{\{x_{\mathbf{i}}^{n}\}}. \tag{1}$$

Here $\mathbf{i},\mathbf{j}$ label the Cartesian components of all position vectors, i.e., $\mathbf{i},\mathbf{j} = 1, \ldots, 3N$, and n denotes the step number of the minimization algorithm. The parameter λ has to be adequately defined such that the algorithm is stable. This kind of algorithm of course will not lead to a global minimum of the potential; rather it will move the atomic sites such that the potential energy is locally minimized. Up to a certain limit a desired degree of short-range order may now simply be generated by iterating (1) for a pertinent number of steps. Figure 2 illustrates the corresponding generated short-range order by displaying the pair-correlation function $g(r)$:

$$g(r) = \frac{1}{4\pi r^2 \rho dr} \sum_{ij} \mathrm{rect}\left(\frac{|\vec{r}_{ij}| - r}{dr}\right), \tag{2}$$

where $\mathrm{rect}(\cdots)$ denotes the standard rectangular function.

For small dr the quantity $\sum_{ij} \mathrm{rect}[(|\vec{r}_{ij}| - r)/dr]$ should be proportional to dr, thus the correlation function $g(r)$ is independent of the specific choice of dr. Unfortunately, statistical effects also become more pronounced for smaller dr since our sample is finite. Thus calculating $g(r)$ with sufficient precession may require large samples. We found, however, that satisfactory results may be produced from samples comprising no more than 24^3 sites.

Defining a quantity that sensibly parametrizes the degree of order in general is a formidable task of it own. Here we exclusively focus on the dependence of the transport properties on the peak height of the pair-correlation function, i.e., $h = \max[g(r)]$ [which occurs due to our specific potential $v(r)$ always at $r = 1.12$]. This peak height assumes the value $h = 1$ for the completely disordered system, which has been addressed in detail in Ref. [27], and in principle increases to infinity for a long-range-order crystal. In this sense it may be viewed as a simple indicator for the degree of topological order in a system.

III. MODEL OF TIGHT-BINDING HAMILTONIAN

Based on the short-range-order site structure described in the previous section we now specify the Hamiltonian of the model. The latter is a one-particle tight-binding Hamiltonian

$$\hat{H} = \sum_{jk} H_{jk} \hat{a}_j^\dagger \hat{a}_k, \tag{3}$$

where $\hat{a}_i^\dagger$ and $\hat{a}_i$ denote the annihilation and creation operators. The function H_{jk} describes the dependence of the overlap or hopping amplitudes on the positions of the respective sites. We consider isotropic overlap, thus H_{jk} essentially depends on the distance s_{jk} between site j and site k. Here we specifically choose H_{jk} to be a Gaussian function

$$H_{jk} := \exp\left(\frac{-4s_{jk}^2}{\pi \tilde{l}^2}\right). \tag{4}$$

The Gaussian function decrease is not intended to specifically address any real amorphous material. It is rather motivated by numerical feasibility: Since the system is disordered there are localized states at the edges of the energy spectrum. Those tend to become fewer with increasing $\tilde{l}$. For technical reasons we intend to focus on models with a negligible number of localized states (see Sec. V). However, for reliable results on transport from exact diagonalization on systems featuring large $\tilde{l}$ large sample sizes are needed. In Ref. [27] similar systems (but featuring no short-range order) have been investigated. There it was found that for the Gaussian function H_{jk} a range of $\tilde{l}$ may be found for which localization and finite-size effects (at $L = 24$) are both negligible. Such a range of $\tilde{l}$ does not exist, e.g., for exponentially decreasing hopping amplitudes as considered, e.g., in Refs. [3,4,12]. Further, $\tilde{l}$ parametrizes the mean overlap length. In the completely disordered system, i.e., for random sites, we have

$$\frac{1}{N} \sum_{jk} s_{jk} |H_{jk}| = \tilde{l}. \tag{5}$$

The distances s_{jk} are, due to the usage of periodic boundary conditions, somewhat complex functions. They may be defined as

$$s_{jk} := \sqrt{d_{jk}^2(x) + d_{jk}^2(y) + d_{jk}^2(z)}, \tag{6}$$

where the d are essentially the Cartesian components of $\vec{r}_j - \vec{r}_k$. To account for periodic boundary conditions they are specifically defined as

$$d_{jk}(\alpha) = \begin{cases} |\alpha_j - \alpha_k|, & |\alpha_j - \alpha_k| < \frac{L}{2} \\ L - |\alpha_j - \alpha_k|, & |\alpha_j - \alpha_k| > \frac{L}{2}, \end{cases} \tag{7}$$

where α is one of the Cartesian coordinates, i.e., $\alpha = x, y, z$. Thus the distance s_{jk} is essentially the shortest distance between the sites j and k under periodic closure of the sample.

IV. CURRENT DYNAMICS AND CONDUCTIVITY

Now we investigate the dependence of the conductivity on h, i.e., different degrees of short-range order. We employ linear response theory, i.e., the Kubo formula. In the limit of high temperatures and low fillings (routinely described within the framework of the grand canonical ensemble) the dc conductivity is given as [28,29]

$$\sigma_{\mathrm{dc}} = \sigma(t \to \infty), \quad \sigma(t) = \frac{f}{T} \int_0^t \frac{1}{N} \mathrm{Tr}\{\hat{J}(t')\hat{J}(0)\} dt', \tag{8}$$

where f is the filling factor (mean number of particles per site at equilibrium), trace and current operators refer to the one-particle sector only, and $\hat{J}(t)$ denotes the current operator in the Heisenberg picture. Furthermore, T is the temperature and we set $k_B = 1$ and $\hbar = 1$; we set the charges of the particles to unity, i.e., $q = 1$. Now of course an appropriate current operator has to be defined. In the context of periodic systems and next-neighbor hoppings this is often done by considerations based on the continuity equation for the particle density [30–33]. Here we choose a definition of the the current that is based on the velocity in, say, the x direction. Eventually this choice will be justified by the agreement of the results with the diffusion constant in the sense of an Einstein relation (see Sec. VI). The velocity operator reads

$$\hat{v} = i[\hat{H}, \hat{x}]. \tag{9}$$

Here $\hat{x}$ is an x-position operator and is defined as

$$\hat{x} = \sum_{i=1}^{N} x_i \hat{n}_i, \quad \hat{n}_i := \hat{a}_i^\dagger \hat{a}_i, \tag{10}$$

where x_i is the x coordinate of the position of site i. Thus the operator $\hat{v}$ may also be written as

$$\hat{v} = \mathrm{i} \sum_{ij} (x_j - x_i) H_{ij} \hat{a}_i^\dagger \hat{a}_j. \tag{11}$$

The interpretation of such an operator as the velocity or current is not in entire agreement with periodic boundary conditions. A (slow) transition of probability from, say, the right edge of the sample ($x = L$) to the left edge of the sample ($x = 0$) would give rise to very high negative velocities; however, within the concept of periodic boundary conditions such a transition should correspond to low positive velocities (across the boundary). Thus, in order to obtain a suitable current operator we modify the above velocity operator (11) such that it features the same structure for transitions arising from the periodic closure as it already exhibits for transitions within the sample:

$$\hat{J} = \sum_{ij} J_{ij} \hat{a}_i^\dagger \hat{a}_j,$$

$$J_{ij} = \begin{cases} i[x_j - x_i] H_{ij}, & |x_j - x_i| < \frac{L}{2} \\ \mathrm{sgn}(x_j - x_i)(i[L - |x_j - x_i|] H_{ij}), & |x_j - x_i| > \frac{L}{2}. \end{cases} \tag{12}$$

Equipped with this definition for the current, we may now simply calculate the current autocorrelation function appearing in (8). We do so using standard numerically exact diagonalization routines. Within a reasonable computing time we are able to treat samples up to a size of $L = 24$. In order to be able to compare the key features of the dynamics of the current autocorrelation functions for various degrees of order and model sizes to each other we compute a kind of normalized current autocorrelation function $j'(t) := \mathrm{Tr}\{\hat{J}(t)\hat{J}(0)\}/\mathrm{Tr}\{\hat{J}^2(0)\}$.

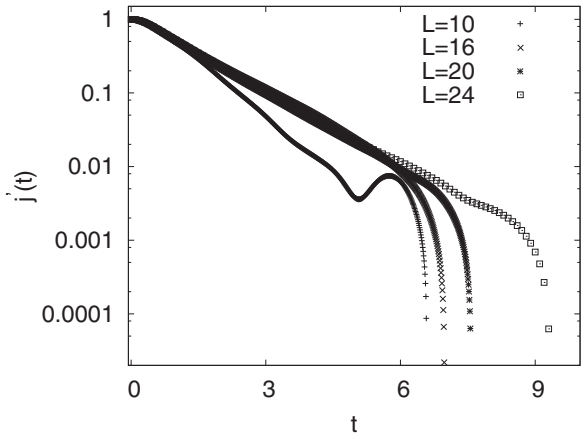

FIG. 3. Normalized current autocorrelation function $j'(t)$ for mean overlap length $\tilde{l} = 1.3$ and short-range order quantified by $h = 2.57$ for increasing sample sizes L. Since the graphs coincide in regions where they are substantially different from zero, for, say, $L \geqslant 16$, data can reliably be expected to contain negligible finite-size effects at $L = 24$. Moreover, the linear dependence of the current autocorrelation function on time in the logarithmic plot suggests an exponential decay, which indicates Boltzmann transport.

Before analyzing conductivity and transport behavior, we briefly address finite-size effects and numerical limitations. We find that for all models discussed in the present paper sample sizes of $L = 24$ are sufficient to get rid of significant finite-size effects. This is illustrated exemplarily in Fig. 3. The normalized current correlation functions $j'(t)$ for the different sample sizes above, say, $L = 16$ coincide for the relevant initial times, at which $j'(t)$ is substantially different from zero, hence the finite-size effects are indeed negligible. For $L = 24$ a matrix of dimension $d \approx 14\,000$ has to be diagonalized and a corresponding correlation function has to be computed. This is numerically feasible but demanding on standard computers. In order to analyze conductivity we plot the scaled conductivity $\sigma_{\mathrm{dc}} T/f$ for various generated short-range orders at fixed mean overlap length $\tilde{l} = 1.3$ against h (see Fig. 4).

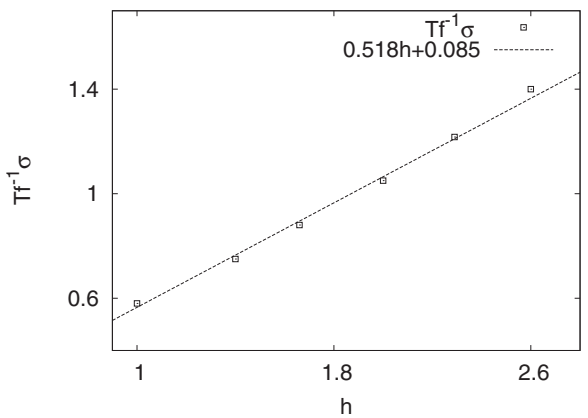

FIG. 4. Scaled conductivity $Tf^{-1}\sigma_{\mathrm{dc}}$ [or diffusion constant D (see Sec. VI)] for mean overlap length $\tilde{l} = 1.3$ as a function of the degree of order h starting from the fully disordered model $h = 1$. The conductivity appears to scale linearly with respect to h; the dashed line is the corresponding fit.

The plot clearly suggest a linear dependence of the conductivity on the peak height of the site pair-correlation function. The corresponding fits yield for the respective conductivities

$$\sigma_{\mathrm{dc}}(\tilde{l} = 1.3) = \frac{f}{T}(0.518h + 0.085). \tag{13}$$

This equation implies that for increasing short-range order the conductivity increases significantly. If the most frequent site distance is only twice more frequent that any other long-range distance, the conductivity is roughly doubled compared to the completely random model. This means that even in the regime of amorphous systems a slight increase of order will affect transport properties substantially. Furthermore, considerations based on Fig. 5 may indicate a transition from a non-Drude to Boltzmann- or Drude-type transport. If one computes a current-correlation function from a Drude model or a Boltzmann equation (in the relaxation-time approximation) one always obtains an exponential decay of the current. Thus, in order for some (quantum) dynamics to be in accord with a Drude-type model, it must yield an exponentially decaying current-correlation function. In the present model, however, exponentially decaying current-correlation functions only appear at a certain degree of short-range order. To illustrate this we plot the normalized current-correlation function $j'(t)$ in Fig. 5 for $h = 1$ (complete disorder) and $h = 2.57$. At $h = 1$ the curve agrees well with a Gaussian fit. Such a decay of the current cannot result from a Boltzmann equation. The latter may yield multiexponential decay if behavior beyond the relaxation time approximation is taken into account, but no Gaussian relaxation. However, at the short-range order specified by $h = 2.57$ the decay gradually passes over to an exponential as illustrated by the respective exponential fit. This implies a transition from non-Drude to Drude transport.

Note that this transition occurs still in the strongly disordered regime; even at $h = 2.57$ the system its far away from a crystal containing some impurities. The existence of this transition may be supported by an investigation of the

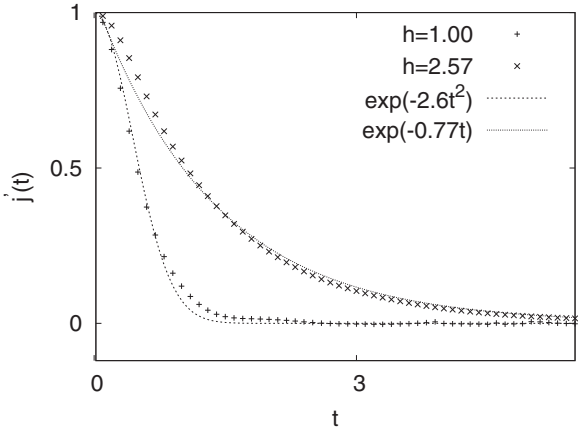

FIG. 5. Normalized current correlation function $j'(t)$ at mean overlap length $\tilde{l} = 1.3$ as a function of time t for the fully disordered model $h = 1$ and the short-range-order model $h = 2.57$. At $h = 1$ the decay appears to be approximately Gaussian, whereas at $h = 2.57$ it is dominantly exponential (see Fig. 3), which indicates Boltzmann transport.

dependence of a mean free path on the short-range order. Such an investigation is presented in Sec. VI.

V. LOCALIZATION

In Ref. [27] it was found, using methods based on the inverse participation ratio, that in the topological fully disordered model ($h = 1$) at mean overlap length $\tilde{l} \geqslant 1.3$ almost the entire spectrum is delocalized. For smaller overlap lengths more and more energy eigenstates become localized. The Anderson transition, at which the entire spectrum is localized, occurs roughly at $\tilde{l} \approx 0.6$. The same work furthermore reports that the conductivity scales as a power law with mean overlap lengths in the fully delocalized regime, i.e., for $\tilde{l} \geqslant 1.3$,

$$\sigma_{\mathrm{dc}}(h = 1.00) = \frac{f}{T} 0.17 \tilde{l}^{4.83}. \tag{14}$$

In the present paper we computed the conductivity for even smaller mean overlap lengths $\tilde{l} < 1.3$ (see Fig. 6).

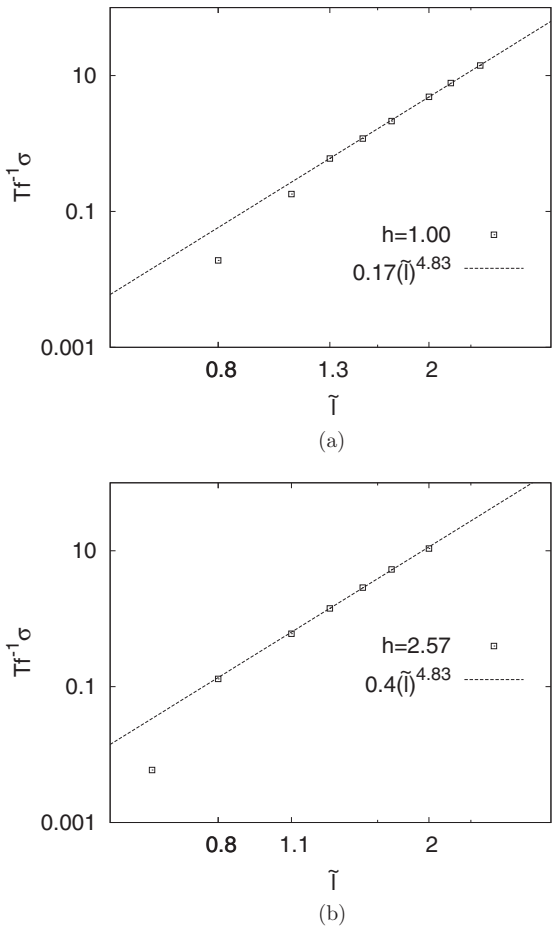

FIG. 6. Double logarithmic plot showing (a) the scaled conductivity $Tf^{-1}\sigma_{\mathrm{dc}}$ for the fully disordered model $h = 1$. Already at overlap lengths as long as $\tilde{l} = 1.1$ there are deviations from the power law. This indicates localization of substantial parts of the spectrum. Also shown is (b) the scaled conductivity $Tf^{-1}\sigma_{\mathrm{dc}}$ at $h = 2.57$. The power law is fulfilled down to the overlap length $\tilde{l} = 0.8$, which indicates that almost all states are delocalized at an overlap length as short as $\tilde{l} = 0.8$

Obviously, deviations from the power law appear right below $\tilde{l} \approx 1.3$, i.e., at the point at which substantial parts of the spectrum become localized. Those deviations increase rapidly for decreasing mean overlap length. Thus we interpret the deviations from the power law (14) as a consequence of increasing localization. This is supported by investigations based on inverse participation ratio [4,27]. We now use those findings to produce a rough estimate for the localization properties of the various short-range-order models. To that end we compute the conductivities for different mean overlap lengths for $h = 2.57$ and use the deviation from the power law as an indicator for the onset of substantial localization. Indeed, Fig. 6(b) shows that for the short-range-order model the conductivity satisfies the power law (14) down to $\tilde{l} \approx 0.8$. Below that deviations from the power law arise. Thus we conclude that the onset of substantial localization occurs in this short-range-order model at an even lower mean overlap length, namely, $\tilde{l} \approx 0.8$. This fits into the overall picture since one expects in the limit of fully ordered systems (crystals) delocalization to occur for arbitrarily small overlap length $\tilde{l}$. This finding suggests that probably also in the respective localized regime localization lengths are longer in the presence of short-range order. A conclusive statement on this as well as on the universality class of the short-range-order models is, however, beyond the scope of the present paper and thus is left for further research.

VI. EINSTEIN RELATION AND MEAN FREE PATHS

Apart from the conductivity the diffusion coefficient is another important transport quantity. According to the Einstein relation, conductivity and the diffusion constant should be proportional to each other. However, the validity of the Einstein relation and the limits of its applicability have been much debated subjects and continue to be so in the context of quantum systems (see, e.g., [34] and references therein). It has been reported that the Einstein relation holds for periodic, interacting, one-dimensional quantum systems at high temperatures. It is claimed to hold even for finite times, thus taking the form

$$D(t) = \frac{T}{\epsilon^2} \sigma(t), \tag{15}$$

where $D(t)$ is the (time-dependent) diffusion constant and ϵ^2 is the uncertainty (variance) of the transported quantity per site at the respective equilibrium [34]. In Ref. [27] it was demonstrated that (15) also holds for completely disordered systems of the type considered in the present paper. Furthermore, an analytical argument for the validity of (15) has been presented that does not depend on the topological structure at all. However, since this argument is not conclusive we investigate numerically in the following whether (15) also holds for short-range-order systems. In our case the transported quantity is the particle density. In the limit of high temperatures and low fillings the equilibrium fluctuations scale as $\epsilon^2 = f$ [28]. Thus, if one hypothetically accepts the validity of (15) also for the systems at hand, one gets from inserting (8)

$$D(t) = \int_0^t \frac{1}{N} \mathrm{Tr}\{\hat{J}(t')\hat{J}(0)\} dt'. \tag{16}$$

If a diffusion equation holds, the derivative with respect to the time of the spatial variance of the diffusing quantity equals twice the diffusion constant [34]. We analyze numerically the dynamics of this variance using an initial state of the form

$$\rho(0) = \frac{1}{Z}\exp\left(-\frac{\left(\hat{x}-\frac{L}{2}\right)^2}{2}\right),$$
$$Z = \mathrm{Tr}\left\{\exp\left(-\frac{\left(\hat{x}-\frac{L}{2}\right)^2}{2}\right)\right\}, \tag{17}$$

i.e., a state in which the probability is more or less concentrated in a thin slab of a thickness on the order of one, perpendicular to the x axis in the middle of the cubic sample. We calculate the increase of the variance of this state and take a derivative with respect to time, thus obtaining directly a diffusion constant, which we call $D_1(t)$,

$$D_1(t) = \frac{1}{2}\frac{d}{dt}\mathrm{Tr}\{\hat{x}^2(t)\rho(0)\}. \tag{18}$$

[Note that the particle density does not drift, hence $\frac{d}{dt}\mathrm{Tr}\{\hat{x}(t)\rho(0)\} = 0$.] We compare this to the right-hand side of (16), which should equal the diffusion coefficient if the Einstein relation holds; thus we call this quantity $D_2(t)$:

$$D_2(t) = \int_0^t \frac{1}{N}\mathrm{Tr}\{\hat{J}(t')\hat{J}(0)\}dt'. \tag{19}$$

If the Einstein relation holds $D_1(t)$ and $D_2(t)$ should coincide.

The results are displayed in Fig. 7. Although finite-size effects are much more pronounced for $D_1(t)$ than for $D_2(t)$, there is good agreement during an initial time period. This period obviously increases with system size. More specifically, Fig. 7 suggest that the time during which $D_1(t)$ and $D_2(t)$ coincide becomes arbitrarily long for arbitrarily large systems Thus we conclude that the Einstein relation is valid for coherent one-particle transport in the present short-range-order systems.

The coincidence of $D_1(t)$ and $D_2(t)$ allows for a definition of a mean free path λ on the basis of $D_2(t)$ that is, as

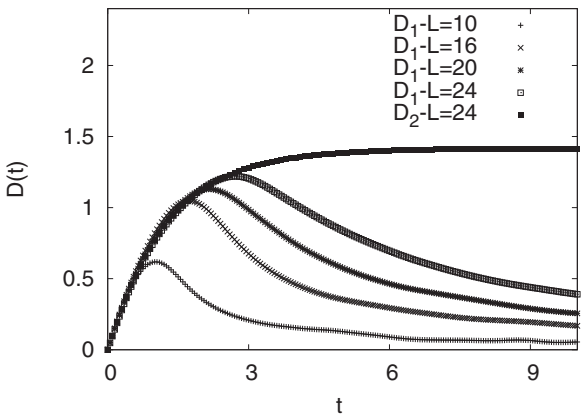

FIG. 7. Comparison of two methods to calculate (time-dependent) diffusion coefficients: $D_1(t)$ from (18) and $D_2(t)$ from (19). The data address the generated short-range order quantified by $h = 2.57$ and mean overlap length $\tilde{l} = 1.3$. Obviously, finite-size effects are more pronounced for $D_1(t)$; however, $D_1(t)$ appears to coincide with $D_2(t)$ up to increasing times for increasing sample sizes. This coincidence implies the validity of an Einstein relation.

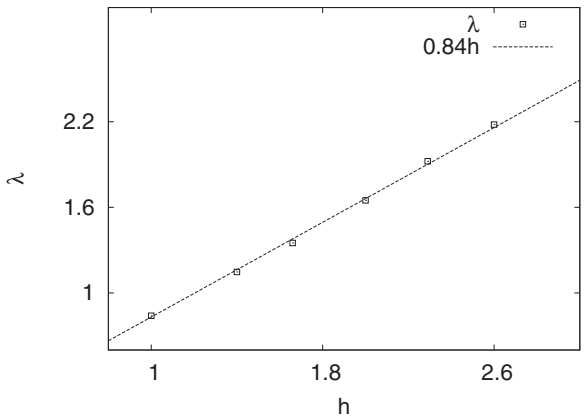

FIG. 8. Mean free path λ as a function of the degree of short-range order h at the mean overlap length $\tilde{l} = 1.3$. Obviously, the mean free path increases significantly with increasing short-range order.

demonstrated above, computationally less demanding. The mean free path is introduced as follows: If the particle were completely ballistic (infinite mean free path) the current autocorrelation function would never decay and the time-dependent diffusion coefficients in the sense of (16) would always increase linearly. The present time-dependent diffusion coefficients of the models increase linearly at the beginning (see Fig. 7), but reach a final plateau after that initial period. We define, somewhat arbitrarily, the ballistic period as the period before the diffusion coefficient has reached 90% of its eventual value. Now we call the mean free path the square root of the increase of the spatial variance of an initial state of type (17) during this ballistic period. So the mean free path is roughly the initial increase of width of an initially narrow probability distribution up to the point where the fully diffusive dynamics begins. In this way a mean free path may be defined even in the non-Drude regime where traditional notions of mean free paths do not apply [28]. However, in the Drude regime this definition roughly coincides with traditional mean free path. The so-defined mean free paths λ are displayed in Fig. 8 for short-range-order models featuring different h (but fixed $\tilde{l} = 1.3$). The mean free path appears to increase linearly with h. Although the generated topological order is small and the structure is still near a fully disorder model, the mean free path increases substantially with respect to h. In the Drude regime this may be viewed as corresponding to a decrease of the scattering cross section. This leads to the remarkable situation that the mean free path exceeds the range of the order, e.g., at $h = 2.57$, recall that the most frequent site distance has been kept fixed at $r_0 = 1.12$ and a second peak is hardly visible in Fig. 2. Thus we conclude that the ballistic motion of particles is not necessarily restricted to the range of order as often assumed. These findings suggest that the transport behavior for these short-range-order models may be described by a Drude model or a Boltzmann equation for, say, $h > 2.6$, as already indicated in Sec. IV. This Drude transport is then much like the dynamics of a particle in a periodic lattice featuring some impurities or a system of quasifree, weakly interacting particles. At $h = 1$, however, the mean free path is below the most frequent site distance $r_0 = 1.12$. This non-Drude transport is comparable to the dynamics of an overdamped

Brownian particle or the thermally activated hopping transport that may occur in the localized regime of an amorphous and/or doped semiconductor [13]. Again, this is in accord with the findings in Sec. IV. It may be worth pointing out that both transport types have also been found in other one-particle quantum systems, e.g., non-Boltzmann transport in modular quantum systems [35,36], and both transport types in the three-dimensional Anderson model [9,21]. Note that while any dynamics featuring a finite mean free path yield diffusive behavior described by some conductivity like that displayed in Fig. 4 on the macroscopic scale, the concrete size of the mean free path will alter transport through structures that are on the order of the mean free path significantly. Thus transport through thin films or nanostructures may quantitatively depend on the mean free path.

VII. TRANSPORT BEHAVIOR FOR VARYING OVERLAP LENGTHS

Until now we have studied solely the effect of increasing short-range order at fixed mean overlap length $\tilde{l} = 1.3$. The latter is the shortest $\tilde{l}$ at which almost all energy eigenstates are delocalized, even for the completely disordered model [27]. Our method is not suitable to investigate even shorter $\tilde{l}$ since it does not resolve with respect to energy (the high-temperature limit). The investigation of larger $\tilde{l}$ is, however, to some extent possible. Thus in this section we investigate the dependence of transport parameters on both the amount of order h and the mean overlap length $\tilde{l}$. We use the same method as described in the previous sections, i.e., linear response theory. The results are displayed in Figs. 9 and 10.

Obviously, Fig. 9 exhibits a power-law dependence of the conductivity on $\tilde{l}$, with the same exponent for all h. More specifically, Fig. 10 suggests the following form of the conductivity within the investigated range of h and $\tilde{l}$:

$$\sigma_{\mathrm{dc}}(\tilde{l},h) = \frac{f}{T}(0.146h + 0.024)\tilde{l}^{4.83}. \tag{20}$$

This product form indicates a kind of universality: Whatever the amount of short-range order is, the scaling with the mean overlap length is always the same and vice versa. A similar situation is found for the scaling of the mean free path λ. Figure 10 suggests

$$\lambda(\tilde{l},h) = (0.42h)\tilde{l}^{2.68}. \tag{21}$$

Whether or not this universality holds for even more different model types is a tentative subject for further research.

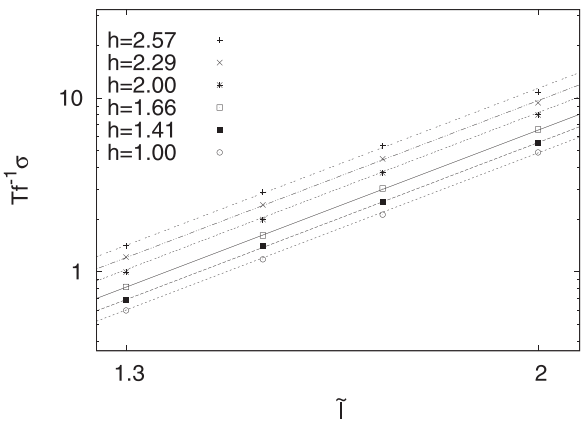

FIG. 9. Scaled conductivities $Tf^{-1}\sigma_{\mathrm{dc}}$ as functions of mean overlap length $\tilde{l}$ for various degrees of short-range order parametrized by h on a double logarithmic scale. For all h the conductivities appear to follow the same power law with respect to $\tilde{l}$; the dashed lines are the corresponding fits. This points in the direction of a universality.

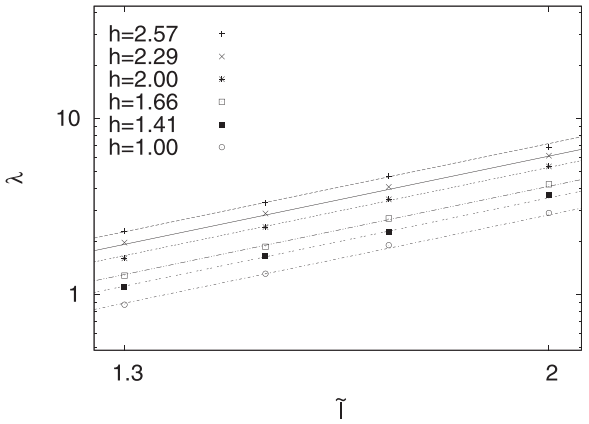

FIG. 10. Mean free paths λ as functions of mean overlap length $\tilde{l}$ for various degrees of short-range order parametrized by h on a double logarithmic scale. For all h the mean free paths appear to follow the same power law with respect to $\tilde{l}$; the dashed lines are the corresponding fits. This points in the direction of a universality.

VIII. CONCLUSION

We investigated the transport behavior of a class of quantum systems that may be described as three-dimensional topologically short-range-order one-particle tight-binding models. These models are meant to be very simplified descriptions of amorphous materials in the delocalized regime. Conductivity and mean free paths at low fillings and high temperatures have been determined essentially by evaluating the Kubo formula using numeric solutions of the Schrödinger equation for finite samples comprising up to approximately 14 000 sites. Conductivities and mean free paths are found to scale linearly with a measure of the (low) amount of order and as a power law with the mean overlap length of the hopping amplitudes. The fact that conductivity and the mean free path appear to be product functions with respect to those parameters indicates a kind of universality. The scaling with order is such that mean free paths that exceed the range of order are reached at comparatively low degrees of order. This is interpreted as a transition towards a Boltzmann or Drude type of transport, i.e., almost free, weakly scattered particles, in a rather amorphous regime. We furthermore verified the validity of an Einstein relation for those systems and found explicit hints that increasing order pushes the Anderson transition towards shorter mean overlap lengths. The latter findings are in accord with generic expectations.

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