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

Abdellah Khodja\textsuperscript{1,1}\textsuperscript{*} and Jochen Gemmer\textsuperscript{1}\textsuperscript{†}

\textsuperscript{1}Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, D-49069 Osnabrück, Germany

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 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.

PACS numbers: 05.60.Gg, 72.80.Ng, 66.30.Ma,

I. INTRODUCTION

Since its introduction the Anderson model has been a paradigm in the investigation of disordered quantum systems \cite{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 extend analyzed by Lifshitz \cite{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 which are energetically separated by the mobility edges. The lowest (and highest) energy eigenstates of an “energy band” are usually localized at all non-zero degrees of disorder, while the states in the center of the spectrum may be delocalized \cite{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 \cite{1,3}, mobility edges \cite{4,5,27} and localization lengths \cite{1,10}, 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 \cite{5,32}. 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 \cite{5,19}). However, transport mediated by the delocalized center of the spectrum, which is the subject of the paper at hand, may be of importance for electronic conduction in amorphous metals or phononic heat conduction in amorphous materials \cite{11}. Much of the quantitative results on transport in the delocalized regime are either on extremely weakly disordered systems, i.e., crystals comprising some defects \cite{12,15} or on the Anderson model \cite{16,18}. 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 timescales (at high frequencies) also in strictly periodic (quantum) systems of the Lorentz gas type \cite{26,28,29}. However, the paper at hand addresses truly non-periodic systems and finds ballistic behavior (mean free path) on the short and diffusive behavior on the long lengthscale. Recently results on transport within the delocalized regime in some Lifshitz models featuring completely random site configurations have been reported in Ref. \cite{9}. Both transport types 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 \cite{19}. The paper at hand is along the lines of Ref. \cite{9} and extends the studies to Lifshitz models which 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 at hand is organized as follows: we start by introducing our models and their specifying parameters in Sec. \textsuperscript{II} and \textsuperscript{III}. Then we compute in Sec. \textsuperscript{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. \textsuperscript{VII}, we address the Einstein relation and mean free paths defined on the basis of an Einstein relation in Sec. \textsuperscript{V}. By considering models featuring different length scales of the hopping amplitudes we find some universality of the transport properties in Sec. \textsuperscript{VII}. We close with
II. MODEL: 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 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 inter-site distance-dependent hopping amplitudes, cf. Sec. \[\text{III}\]. 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 like mean free paths conductivities, etc. The case of fully disordered sites distribution was extensively investigated in Ref. \[\text{[9]}\] and in principle increases to infinity for a long range order.

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 generated based on pair-interaction potentials of increasing order in initially completely (nonphysically) disordered systems featuring unit density. Now short range order is generated 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 which 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, etc. But, 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, most frequent site distance, etc. fixed. Thus we employ a rather simple pair interaction potential which is essentially a polygon, see Fig. \[\text{I}\]. The parameters \(r_0 = 1.12, r_2 = 8, v_{\text{min}} = -20, v_{\text{max}} = 140\) 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 is 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 \(r_0\), cf. Fig. \[\text{I}\]. Thus we define our lattice relaxation by the following gradient descent method:

\[x_i^{n+1} = x_i^n - \lambda \frac{\partial V}{\partial x_i}|_{\{x_i^n\}}\]  

(1)

here \(i, j\) label the Cartesian components of all position vectors, i.e., \(i, j = 1, \ldots, 3N\) and \(n\) denotes the step-number of the minimization algorithm. The parameter \(\lambda\) has to be adequately defined such that the algorithm is stable. This kind of algorithm will of course not lead to a global minimum of the potential, it will rather 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 \(\text{(1)}\) for a pertinent number of steps. Fig. \[\text{II}\] illustrates the corresponding generated short range order by displaying the pair correlation function \(g(r)\):

\[g(r) = \frac{1}{4\pi r^2 \rho dr} \sum_{ij} \text{rect}\left(\frac{|\vec{r}_{ij}| - r}{dr}\right)\]  

(2)

(here \(\text{rect}(\cdots)\) denotes the standard rectangular function.)

For small \(dr\) the quantity \(\sum_{ij} \text{rect}\left(\frac{|\vec{r}_{ij}| - r}{dr}\right)\) 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 precision 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 its own. Here we exclusively focus on the dependence of the transport properties on the “peak-height” of the pair correlation function, i.e., \(h = \text{max}(g(r))\) (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. \[\text{[9]}\] and in principle increases to infinity for a long range
ordered crystal. In this sense it may be viewed as a simple indicator for the degree of topological order in a system.

III. MODEL: TIGHT-BINDING HAMILTONIAN

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

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

(3)

$$\hat{a}_j^\dagger, \hat{a}_j$$ denotes 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:

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

(4)

The Gaussian decrease is not intended to be 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 $l$. For technical reasons we intend to focus on models with a negligible amount of localized states, cf. Sec. IV. However, for reliable results on transport from exact diagonalization on systems featuring large $l$ large sample sizes are needed. In Ref. [8] similar systems (but featuring no short range order) have been investigated. There it has been found that for Gaussian $H_{jk}$ a range of $l$ may be found for which localization as well as finite-size effects (at $L = 24$) are both negligible. Such a range of $l$ does not exist, e.g., for exponentially decreasing hopping-amplitudes as considered e.g., in Refs. [3, 4, 10]. $l$ parametrizes the mean overlap length. In the completely disordered system, i.e., for random sites we have:

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

(5)

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

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

(6)

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

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

(7)

where $\alpha$ 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 $j, k$ 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:

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

(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, furthermore $\hat{J}(t)$ denotes the current operator in the Heisenberg picture. $T$ is the temperature and we set $k_B = 1$, $\hbar = 1$, furthermore 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 $\rho = 30, 31, 32$. Here we choose a definition of the current which is based on the “velocity” in, say, $x$-direction. Eventually this choice will be justified by the agreement of the results with the diffusion constant in the sense of an Einstein relation, cf. Sec. VII. The velocity operator reads:

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

(9)
Here $\hat{x}$ is a $x$-position operator and it is defined as

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

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

$$\dot{v} = i \sum_{ij} (x_j - x_i) \hat{H}_{ij} \hat{a}_i \hat{a}_j^\dagger$$  \hspace{1cm} (11)

The interpretation of such an operator as 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. But 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:

$$\hat{J} = \sum_{ij} J_{ij} \hat{a}_i \hat{a}_j^\dagger$$  \hspace{1cm} (12)

This equation implies that for increasing short range order the conductivity increases significantly. If the most frequent site distance is only twice more frequent than any other long range distance, the conductivity is roughly appearing in [S]. We do so using standard numerically exact diagonalization routines. Within 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 auto-correlation functions for various degrees of order and model sizes to each other we compute a kind of “normalized” current auto-correlation function, $j'(t) := \text{Tr}\{J(t)J(0)\}/\text{Tr}\{J^2(0)\}$. Before analyzing conductivity and transport behavior, we briefly address finite-size effects and numerical limitations. We find that for all models discussed in the paper at hand 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 $d \approx 14000$ 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 $\dot{f} T^{-1} \sigma_{dc}$ for various generated short range orders at fixed mean overlap length $\bar{l} = 1.3$ against $h$, see Fig. 4. 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:

$$\sigma_{dc}(\bar{l} = 1.3) = \frac{f}{T} (0.518h + 0.085).$$  \hspace{1cm} (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 than any other long range distance, the conductivity is roughly

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Normalized current auto-correlation function $j'(t)$ for mean overlap length $\bar{l} = 1.3$ 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 $L \geq 16$, data can reliably be expected to contain negligible finite-size effects at $L = 24$. Moreover, the linear dependence of the current auto-correlation function on time in the logarithmic plot suggest an exponential decay which indicates Boltzmann transport.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Scaled conductivity $T \dot{f}^{-1} \sigma_{dc}$ (or diffusion constant $D$, see Sec. VI) for mean overlap length $\bar{l} = 1.3$ as function of the the degree of order $h$ starting from the fully disordered model $h = 1$. The conductivity appears to scale linearly w.r.t. $h$, the dashed line is the corresponding fit.}
\end{figure}
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 of transport. If one computes a current-correlation function from a Drude model or a Boltzmann equation (in relaxation-time approximation) one always obtains an exponential decay of the current. Thus, in order for some (quantum) dynamics to be in accord with Drude-type of model, it must yield an exponentially decaying current-correlation function. In the model at hand, 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 multi-exponential 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 dependence of a mean free path on the short range order. Such an investigation is presented in Sec. VI.

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

V. COMMENT ON LOCALIZATION

In Ref. [9] it was found, using methods based on the inverse participation ratio, that in the topological fully disordered model ($h = 1$) at mean overlap length $l \geq 1.3$ 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 ($\tilde{l} \geq 1.3$):

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

(14)

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

Figure 6: (double logarithmic plot) Panel (a) shows the scaled conductivity $Tf^{-1}\sigma_{dc}$ at mean 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. Panel (b) shows the scaled conductivity $Tf^{-1}\sigma_{dc}$ 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
beginning \( \tilde{l} \approx 1.3 \), 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 \([3, 9]\). We now use those findings to produce a rough estimate for the localization properties of the various short range ordered models. To those ends 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 ordered 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 ordered 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 suggest 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 ordered models is, however, beyond the scope of the paper at hand and thus 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 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 \([34]\) (and references therein). Recently it has been reported that the Einstein relation holds for periodic, interacting, 1-d quantum systems at high temperatures. It is claimed to hold even for finite times, thus taking the form

\[
D(t) = \frac{T}{\epsilon^2} \sigma(t) \quad (15)
\]

here \( D(t) \) is the (time-dependent) diffusion constant, \( \epsilon^2 \) is the uncertainty (variance) of the transported quantity per site at the respective equilibrium \([34]\). In Ref. \([9]\) it has been demonstrated that (15) also holds for completely disordered systems of the type considered in the paper at hand. Furthermore an analytical argument for the validity of (15) has been presented which does not depend on the topological structure at all. However, since this argument is not conclusive we investigate in the following numerically whether (15) also holds for short range ordered 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 \( \epsilon^2 = f \) \([24]\). Thus if one hypothetically accepts the validity of (15) also for the systems at hand, one gets from inserting (8):

\[
D(t) = \int_0^t \frac{1}{N} \text{Tr}\{\hat{J}(t')\hat{J}(0)\} dt' \quad (16)
\]

If a diffusion equation holds, the derivative w.r.t. time of the density is the (time-dependent) diffusion constant, \( h \), i.e., at the point at which substantial parts of the spectrum become localized. Those deviations in-
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 a good agreement during an initial time period. This period obviously increases with system size. More specifically, Fig. 7 suggests 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 short range ordered systems at hand.

The coincidence of $D_1(t)$ and $D_2(t)$ allows for a definition of a mean free path $\lambda$ on the basis of $D_2(t)$ which is, as demonstrated above computationally less demanding. The mean free path is introduced as follows: If the particle was completely ballistic (infinite mean free path) the current auto-correlation function would never decay and the time-dependent diffusion coefficients in the sense of \cite{6} would always increase linearly. The time-dependent diffusion coefficients of the models at hand increase linearly at the beginning, cf. 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 \cite{7} 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 \cite{24}. However in the Drude regime this definition roughly coincides with traditional mean free path. The so defined mean free paths $\lambda$ are displayed in Fig. 8 for short range ordered models featuring different $h$ (but fixed $\hat{l} = 1.3$). 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 disordered 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 ballistic motion of particles is not necessarily restricted to the range of order as often assumed. These findings suggest that transport behavior for these short range ordered 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 alike the dynamics of a particle in a periodic lattice featuring some impurities or a system of quasi free, 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 over-damped Brownian particle or the thermally activated hopping transport which may occur in the localized regime of amorphous or /and doped semiconductors \cite{8}. 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 \cite{35, 36} and both transport-types in the three-dimensional Anderson model \cite{10, 21}. Note that while any dynamics featuring a finite mean free path yield diffusive behavior described by some conductivity like 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.

![Mean free path as function of degree of short range order](image)

**Figure 8:** Mean free path $\lambda$ as function of the degree of short range order $h$ at the mean overlap length $\hat{l} = 1.3$. Obviously the mean free path increases significantly with increasing short range order.

VII. TRANSPORT BEHAVIOR FOR VARYING OVERLAP LENGTHS

Until now we studied solely the effect of increasing short range order $h$ at fixed mean overlap length $\hat{l} = 1.3$. The latter is the shortest $\hat{l}$ at which almost all energy eigenstates are delocalized, even for the completely disordered model \cite{8}. Our method is not suitable to investigate even shorter $\hat{l}$ since it does not resolve w.r.t energy (high temperature limit). The investigation of larger $\hat{l}$ 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, $\hat{l}$. We use the same method as described in the previous Sections, e.g., linear response theory. The results are displayed in Figs. 9 and 10.

![Power law dependence](image)

Obviously, Fig. 9 exhibits a power-law dependence of the conductivity on $\hat{l}$, with the same exponent for all $h$. More specifically Fig. 10 suggests the following form of the conductivity within the investigated range of $h, \hat{l}$:
\[ \sigma_{dc}(\tilde{l}, h) = \frac{f}{T} (0.146h + 0.024) \tilde{l}^{4.83}, \] (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 \( \lambda \). Fig. 10 suggests:

\[ \lambda(\tilde{l}, h) = (0.42h)^{2.68}, \] (21)

VIII. SUMMARY AND CONCLUSION

We investigated the transport behavior of a class of quantum systems which may be described as three-dimensional, topologically short range ordered, 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 Schroedinger equation for finite samples comprising up to \( \approx 14000 \) 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 mean free path appear to be product functions w.r.t. to those parameters indicates a kind of universality. The scaling with order is such that mean free paths which 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.

IX. ACKNOWLEDGEMENTS

We thank H. Niemeyer for fruitful discussions.

[1] 50 Years of Anderson Localization, edited by E. Abrahams (World Scientific Publishing Company, 2010)

[2] I. M. Lifshitz, Adv. Phys. 13, 483 (1964)
[3] J. D. Bauer, V. Logovinsky, and J. L. Skinner, J. Phys. C: Solid State Phys. 21, 993 (1988)
[4] D.J. Priour, Phys. Rev. B 85, 014209 (2012)
[5] S. Knief, W. von Niessen, and T. Koslowski, Phys. Rev. B 58, 4459 (1998)
[6] H. Grussbach and M. Schreiber, Phys. Rev. B 51, 663 (1995)
[7] R. Atta-Fynn, P. Biswas, P. Ordejon, and D.A. Drabold, Phys. Rev. B 69, 085207 (2004)
[8] B. I. Shklovskii and A. L. Efros, Electronic properties of doped semiconductors (Springer, 1984)
[9] A. Khodja, H. Niemeyer, and J. Gemmer, Phys. Rev. E 87, 052133 (2013)
[10] J.J. Krich, and A. Aspuru-Guzik, Phys. Rev. Lett 106, 156405 (2011)
[11] A. Amir, Y. Oreg, and Y. Imry, Phys. Rev. Lett. 105, 070601 (2010)
[12] I. Mertig, E. Mrosan, and P. Ziesche, Multiple Scattering Theory of Point Defects in Metals: Electronic Properties, Teubner-Texte zur Physik, Vol. 11 (Leipzig, 1987)
[13] J.P. Dekker, A. Lodder, and J. van Ek, Phys. Rev. B 57, 12719 (1998)
[14] N. Papanikolaou, N. Stefanou, and C. Papastaikoudis, Phys. Rev. B 49, 16117 (1994)
[15] T. Vojta, I. Mertig, and R. Zeller, Phys. Rev. B 46, 15761 (1992)
[16] R. Steinigeweg, H. Niemeyer, and J. Gemmer, New Journal of Physics 12, 113001 (2010)
[17] P. Markos, Acta Physica Slovaca 56, 561 (2006)
[18] B. Kramer and A. MacKinnon, Rep. Prog. Phys. 56, 1469 (1993)
[19] B. L. Altshuler and A. G. Aronov, Electron–Electron Interactions in Disordered Systems, ed. A. L. Efros and M. Pollak, (Elsevier, Amsterdam, 1985)
[20] A. Rodriguez, A. Chakrabarti, and R.A. Romer, Phys. Rev. B 86, 085119 (2012)
[21] J. Brndiar and P. Markos Phys. Rev. B 74, 153103 (2006)
[22] B. Bulka, M. Schreiber, and B. Kramer, Z. Phys. B 66, 21 (1987)
[23] R. Steinigeweg, J. Gemmer, H.-P. Breuer, and H.-J. Schmidt, Eur. Phys. J. B 69, 275 (2009)
[24] R. Kubo, M. Toda, and N. Hashitsume, Statistical Physics II: Nonequilibrium Statistical Mechanics (Springer, Berlin, 1991)
[25] J. Jaeckle, Einführung in die Transporttheorie (Vieweg, Braunschweig, 1978)
[26] P. Gaspard, Phys. Rev. E 53, 4379 (1996)
[27] X. Zotos, Phys. Rev. Lett. 82, 1764 (1999)
[28] C. Tian, A. Larkin, Phys. Rev. Lett. 95, 246601 (2005)
[29] C. Tian, Phys. Rev. Lett. 102, 243903 (2009)
[30] F. Heidrich-Meisner, A. Honecker, D.C. Cabra, and W. Brenig, Phys. Rev. B 68, 134436 (2003)
[31] J. Benz, T. Fukui, and A. K. C. Scheeren, J. Phys. Soc. Jpn. Suppl. 74 (2005)
[32] M. Nardone, M. Simon, I.V. Karpov, and V.G. Karpov, J. Appl. Phys 112, 071101 (2012)
[33] J. Gemmer, R. Steinigeweg, , and M. Michel, Phys. Rev. B 73, 104302 (2006)
[34] R. Steinigeweg, H. Wichterich, and J. Gemmer, Europhys. Lett. 88, 10004 (2009)
[35] R.L. Weaver, Phys. Rev. E 73, 036610 (2006)
[36] M. Michel, G. Mahler, and J. Gemmer, Phys. Rev. Lett. 95, 180602 (2005)