Localization of electronic states in amorphous materials: recursive Green’s function method and the metal-insulator transition at $E \neq 0$

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1 Introduction

Traditionally, condensed matter physics has focused on the investigation of perfect crystals. However, real materials usually contain impurities, dislocations or other defects, which distort the crystal. If the deviations from the perfect crystalline structure are large enough, one speaks of disordered systems. The Anderson model [1] is widely used to investigate the phenomenon of localisation of electronic states in disordered materials and electronic transport properties in mesoscopic devices in general. Especially the occurrence of a quantum phase transition driven by disorder from an insulating phase, where all states are localised, to a metallic phase with extended states, has lead to extensive analytical and numerical investigations of the critical properties of this metal-insulator transition (MIT) [2–4]. The investigation of the behaviour close to the MIT is supported by the one-parameter scaling hypothesis [5, 6]. This scaling theory originally formulated for the conductance plays a crucial role in understanding the MIT [7]. It is based on an ansatz interpolating between metallic and insulating regimes [8]. So far, scaling has been demonstrated to an astonishing degree of accuracy by numerical studies of the Anderson model [9–13]. However, most studies focused on scaling of the localisation length and the conductivity at the disorder-driven MIT in the vicinity of the band centre [9, 14, 15]. Assuming a power-law form for the d.c. conductivity, as it is expected from the one-parameter scaling theory, Villagonzalo et al. [6] have used the Chester-Thellung-Kubo-Greenwood formalism to calculate the temperature dependence of the thermoelectric properties numerically and showed that all thermoelectric quantities follow single-parameter scaling laws [16, 17].

In this chapter we will investigate whether the scaling assumptions made in previous studies for the transition at energies outside the band centre can be
reconfirmed in numerical calculations, and in particular whether the conductivity $\sigma$ follows a power law close to the critical energy $E_c$. For this purpose we will use the recursive Green’s function method [18, 19] to calculate the four-terminal conductance of a disordered system for fixed disorder strength at temperature $T = 0$. Applying the finite-size scaling analysis we will compute the critical exponent and determine the mobility edge, i.e. the MIT outside the band centre. A complementary investigation into the statistics of the energy spectrum and the states close to the MIT can be found in Chapter [20]. An analysis of the mathematical properties of the so-called binary-alloy or Bernoulli-Anderson model is done in Chapter [21].

2 The Anderson Model of Localisation and its Metal-Insulator Transition

The Anderson model [1, 2] is widely used to investigate the phenomenon of localisation of electronic states in disordered materials. It is based upon a tight-binding Hamiltonian in site representation

$$H = \sum_i \epsilon_i |i\rangle \langle i| + \sum_{i \neq j} t_{ij} |i\rangle \langle j|,$$

(1)

where $|i\rangle$ is a localized state at site $i$ and $t_{ij}$ are the hopping parameters, which are usually restricted to nearest neighbours. The on-site potentials $\epsilon_i$ are random numbers, chosen according to some distribution $P(\epsilon)$ [22, 23]. In what follows we take $P(\epsilon)$ to be a box distribution over the interval $[-W/2, W/2]$, thus $W$ determines the strength of the disorder in the system. Other distributions have also been considered [2, 3, 24].

For strong enough disorder, $W > W_c (E = 0)$, all states are exponentially localized and the respective wave functions $\Psi(r)$ are proportional to $e^{-(r-r_0)/\xi}$ for large distances $|r-r_0|$. Thus, $\Psi$ is confined to a region of some finite size, which may be described by the so-called localisation length $\xi$. In this language extended states are characterised by $\xi \rightarrow \infty$. Comparing $\xi$ with the size $L$ of the system one can distinguish between strong and weak localisation, for $\xi \ll L$ and $L < \xi$, respectively. Here we also assume that the phase-relaxation length $\ell_\Phi \gg L$. Otherwise, the effective system size is determined by $\ell_\Phi$.

It turns out that the value of the critical disorder strength $W_c$ depends on the distribution function $P(\epsilon)$ and the dimension $d$ of the system. In absence of a magnetic field and for $d \leq 2$ all states are localized\(^3\), i.e. $W_c = 0$ [7, 8].

\(^3\)We note that the phrase weak localization in the context of the scaling theory is often used with a specific meaning, namely the onset of localization in large 2-dimensional samples, where the conductance decreases logarithmically with scale [2, 7].

\(^4\)Strictly speaking, this is only true if $H$ belongs to the Gaussian orthogonal ensemble [25].
For systems with $d = 3$ the value of $W_c$ additionally depends on the Fermi energy $E$. The curve $W_c(E)$ separates localized states ($W > W_c(E)$) from extended states ($W < W_c(E)$) in the phase diagram [22,23,26]. If instead of $E$ the disorder strength is taken as a parameter, there will be a critical energy $E_c(W)$ — also called the mobility edge — and states with $|E| < E_c$ are extended and those with $|E| > E_c$ localized yielding the same phase boundary in the $(E,W)$-plane. At the mobility edge, states are multifractals [27]. The separation of localized and extended states is illustrated in Fig. 1, which shows a schematic density of states (DOS) of a three-dimensional (3D) Anderson model. Since for $T = 0$ localized states cannot carry any electric current, the system shows insulating behaviour, i.e. the electric conductivity $\sigma$ vanishes for $|E| > E_c$ or $W > W_c$. Otherwise the system is metallic. Therefore, the transition at the critical point is called a disorder-driven MIT.

For the MIT in $d = 3$ it was found that $\sigma$ is described by a power law at the critical point [2],

$$\sigma(E) = \begin{cases} \sigma_0 \left| 1 - \frac{E}{E_c} \right|^{-\nu}, & |E| < E_c \\ 0, & |E| > E_c \end{cases}$$

(2)

with $\nu$ being the universal critical exponent of the phase transition and $\sigma_0$ a constant. The value of $\nu$ has been computed numerically by various methods [2,9–11] and was also derived from experiments [28,29]. The results range from 1 to 1.6, depending on the distribution $P(\epsilon)$ and the computational method [3] used.

**Fig. 1.** Typical DOS of a 3D Anderson model for fixed $W < W_c$. The states in the grey regions are localized, otherwise they are extended. The mobility edges are indicated at $\pm E_c$. Also indicated is the power-law behaviour of $\sigma(E)$ (dashed lines) close to $\pm E_c$ according to (2).
Moreover, Wegner [30] was able to show that for non-interacting electrons the d.c. conductivity $\sigma$ obeys a general scaling form close to the MIT,

$$\sigma(\varepsilon, \omega) = b^{2-d} \sigma(b^{1/\nu} \varepsilon, b^{z} \omega) .$$

(3)

Here $\varepsilon$ denotes the dimensionless distance from the critical point, $\omega$ is an external parameter such as the frequency or the temperature, $b$ is a scaling parameter and $z$ is the dynamical exponent. For non-interacting electrons $z = d$ [31]. Assuming a finite conductivity for $\omega = 0$, one obtains from (3)

$$\sigma(\varepsilon, 0) \propto \varepsilon^{\nu(d-2)},$$

(4)

where $\varepsilon = |1 - E/E_c|$. With $d = 3$ this gives (2).

### 3 Computational Method

An approach to calculate the d.c. conductivity from the Anderson tight-binding Hamiltonian (1) is the recursive Green’s function method [18, 19, 23]. It yields a recursion scheme for the d.c. conductivity tensor starting from the Kubo-Greenwood formula [32]. Moreover, this method allows to compute the density of states and the localization length as well as the full set of thermoelectric kinetic coefficients [33]. Parallel implementations of the method are advantageous [34,35]. The method is therefore a companion to the more widely used transfer-matrix method [36,37] or iterative diagonalisation schemes [38,39].

#### 3.1 Recursive Green’s Function Method

Let $\mathbf{H} = \sum_{ij} H_{ij} |i\rangle\langle j|$ denote our hermitian tight-binding Hamiltonian. The single particle Green’s function $\mathbf{G}^\pm (z)$ is defined as [40] $(z^\pm - H)\mathbf{G}^\pm = \mathbf{1}$ where $z = E \pm i\gamma$ is the complex energy and the sign of the small imaginary part $\gamma$ distinguishes between advanced and retarded Green’s functions, $\mathbf{G}^- (E - i0)$ and $\mathbf{G}^+ (E + i0)$, respectively [40]. Equivalently, $\mathbf{G}^\pm$ can be represented in the basis of the functions $|i\rangle$,

$$(z^\pm \delta_{ij} - H_{ij})G^\pm_{ij} = \delta_{ij} ,$$

(5)

where $G^\pm_{ij}$ is the matrix element $\langle i|G^\pm|j\rangle$. We note that for a hermitian Hamiltonian $G^\pm_{ij} = (G^\mp_{ji})^*$.

If $\mathbf{H}$ contains only nearest-neighbour hopping matrix elements, (5) can be simplified using a block matrix notation. This is equivalent to considering the system as being built up of slices or strips for 3D or 2D, respectively, along one lattice direction. In what follows all quantities written in bold capitals are matrices acting in the subspace of such a slice or strip. For 2D and 3D these
Fig. 2. Scheme of the recursive Green’s function method for a 3D system. The new Green’s function $G^{(N+1)}$ can be calculated from the old Hamiltonian $H_N$ (light grey), the new slice Hamiltonian $H_{N+1}$ (dark grey) and the coupling $t_N$ (solid arrows).

are matrices of size $M \times M$ and $M^2 \times M^2$, respectively, where $M$ is the lateral extension of the system (cf. Fig. 2). The left hand side of (5) is then given as

$$
\begin{pmatrix}
\ddots & \ddots & \vdots & \vdots & \\
0 & -H_{i,i-1} (z\pm I - H_{ii}) & 0 & \cdots & \\
\vdots & 0 & -H_{i+1,i} (z\pm I - H_{i+1,i+1}) & -H_{i+1,i+2} & 0 \\
0 & \cdots & \ddots & \ddots & \\
\end{pmatrix}
\times
\begin{pmatrix}
\ddots & \ddots & \vdots & \vdots & \\
G_{i-1,j}^\pm & \ddots & \vdots & \vdots & \\
\vdots & \ddots & \ddots & \vdots & \\
G_{i,j}^\pm & \ddots & \vdots & \vdots & \\
\vdots & \ddots & \ddots & \ddots & \\
\end{pmatrix},
$$

(6)

where $i$ and $j$ now label the slices or strips. From this expression one can easily see that (5) is equivalent to

$$
(z\pm I - H_{ii}) G_{ij}^\pm - H_{i,i-1} G_{i-1,j}^\pm - H_{i,i+1} G_{i+1,j}^\pm = I \delta_{ij}.
$$

(7)

Using the hermiticity of $H$ we define the hopping matrix $t_i \equiv H_{i,i+1}$ (and hence $t_i^\dagger = H_{i,i-1}$) connecting the $i$th and the $(i+1)$st slice. Now, we consider adding an additional slice to a system consisting of $N$ slices. The Hamiltonian of this larger system can be written as [19]

$$
H^{(N+1)} \rightarrow H_{ij} + t_N + t_N^\dagger + H_{N+1,N+1} (i,j \leq N).
$$

(8)

The first and the last terms describe the uncoupled $N$-slice and the additional 1-slice system. Using $t_N$ as an "interaction" the Green’s function $G^{(N+1)}$ of the coupled system can be calculated via Dyson’s equation [19, 40],

$$
G_{ij}^{(N+1)} = G_{ij}^{(N)} + G_{iN}^{(N)} t_N G_{Nj}^{(N+1)} (i,j \leq N).
$$

(9)
In particular, we have

\[ G^{(N+1)}_{N+1,N+1} = \left[ z^2 \mathbf{I} - H_{N+1,N+1} - t_N G^{(N)}_{NN} t_N \right]^{-1} \]  
(10a)

\[ G^{(N+1)}_{ij} = G^{(N)}_{ij} + G^{(N)}_{iN} t_N G^{(N+1)}_{N+1,N+1} t_N^\dagger G^{(N)}_{Nj} (i,j \leq N) \]  
(10b)

\[ G^{(N+1)}_{i,N+1} = G^{(N)}_{iN} t_N G^{(N+1)}_{N+1,N+1} (i \leq N) \]  
(10c)

\[ G^{(N+1)}_{N+1,j} = G^{(N+1)}_{N+1,N+1} t_N^\dagger G^{(N)}_{Nj} (j \leq N) \]  
(10d)

With (10) the Green’s function can be obtained iteratively. Additionally, there are two kinds of boundary conditions which must be considered: across each slice and at the beginning and the end of the stack. The first kind does not present any difficulty and usually hard wall or periodic boundary conditions are employed. The second kind of boundary is connected to some subtleties with attached leads which will be addressed in Section 6.

3.2 Density of States and D.C. Conductivity

The DOS is given in terms of Green’s function by [40]

\[ \rho(E) = -\frac{1}{\pi \Omega} \mathrm{Im} \, \mathrm{Tr} \, G^+ = -\frac{1}{\pi N M^2} \mathrm{Im} \sum_{i=1}^{N} \mathrm{Tr} \, G^+_i \]  
(11)

and the d.c. conductivity \( \sigma \) is

\[ \sigma = \frac{2e^2 \hbar}{\pi \Omega m^2} \mathrm{Tr} \left[ p \, \mathrm{Im} \, G^+ \, p \, \mathrm{Im} \, G^+ \right] . \]  
(12)

Here, \( \Omega \) denotes the volume of the system and \( m \) the electron mass. Using for the momentum the relation \( p = \frac{\hbar m}{\hbar} [H, x] \) one can rewrite (12) in position representation

\[ \sigma = \frac{e^2 4}{\hbar N M^2} \mathrm{Tr} \left\{ \gamma^2 \sum_{i,j} G^+_i x_j \, G^-_j x_i - i \gamma \sum_{i} \left( G^+_i - G^-_i \right) x_i^2 \right\} , \]  
(13)

where \( x_i \) is the position of the \( i \)th slice.

Starting from these relations and using the iteration scheme (10) one can derive recursion formulae to calculate the properties for the \((N+1)\)-slice system. The results are expressed in terms of the following auxiliary matrices
The derivation can be simplified assuming the new slice to be at $x_{N+1} = 0$. This leads, however, to corrections for the matrices $B_N$ and $C_N^\pm$ because the origin of $x_i$ has to be shifted to the position of the current slice in each iteration step. The corrections are

$$B_N' = B_N + iC_N^+ + iC_N^- + \frac{1}{2}t_N^\dagger (R_N - R_N^\dagger) t_N,$$ \hspace{1cm} (15a)

$$C_N'^\pm = C_N^\pm - \frac{1}{2}t_N^\dagger (R_N - R_N^\dagger) t_N.$$ \hspace{1cm} (15b)

Here we have used the identity

$$\gamma \sum_{i=1}^{N} G_{Ni}^+ G_{iN}^- = \frac{1}{2} (G_{NN}^+ - G_{NN}^-) = \frac{1}{2} (R_N - R_N^\dagger) = -\text{Im} R_N.$$ \hspace{1cm} (16)

The derivation of the recursion relations is given in Refs. [18, 19, 23, 41], it yields the following expressions

$$s^{(N+1)}_\rho = s^{(N)}_\rho + \text{Tr} \{ R_{N+1} (F_N + I) \},$$ \hspace{1cm} (17a)

$$s^{(N+1)}_\sigma = s^{(N)}_\sigma + \text{Tr} \{ \text{Re} (B_N R_{N+1}) + C_N^+ R_{N+1} C_N^- R_{N+1} \},$$ \hspace{1cm} (17b)

$$R_{N+1} = \left[ z^\dagger I - H_{N+1} R_{N+1} - t_N^\dagger R_N t_N \right]^{-1},$$ \hspace{1cm} (17c)

$$B_{N+1} = t_{N+1}^\dagger R_{N+1} \left[ B_N + 2 C_N^+ R_{N+1}^\dagger C_N^- \right] R_{N+1} t_{N+1},$$ \hspace{1cm} (17d)

$$C_{N+1}^+ = t_{N+1}^\dagger R_{N+1} C_N^+ R_{N+1}^\dagger t_{N+1},$$ \hspace{1cm} (17e)

$$C_{N+1}^- = t_{N+1}^\dagger R_{N+1} C_N^- R_{N+1}^\dagger t_{N+1},$$ \hspace{1cm} (17f)

$$F_{N+1} = t_{N+1}^\dagger R_{N+1} (F_N + I) R_{N+1} t_{N+1}.$$ \hspace{1cm} (17g)

The DOS and the d.c. conductivity are then given as
\[ \rho^{(N+1)}(E) = \frac{1}{\pi(N+1)M^2} s^{(N+1)}_\rho, \quad (18) \]
\[ \sigma^{(N+1)}(E) = \frac{\epsilon^2}{h} \frac{4}{(N+1)M^2} s^{(N+1)}_\sigma. \quad (19) \]

For a comparison with the scaling arguments, we convert the conductivity into the two-terminal conductance as
\[ g_2 = \sigma \frac{M^2}{L} \quad (20) \]
with \( L = N + 1 \). In distinction to the usual use of the recursive scheme which constructs a single sample with \( L \gg M \), we shall have to use many different cubic samples with \( L = M \).

We note that it is also possible to calculate the localisation length \( \xi(E) \) by the Green’s function method. The value of \( \xi(E) \) is connected to the matrix \( G^{+}_{1N+1} \),
\[ \frac{1}{\xi(E)} = - \lim_{\gamma \to 0} \lim_{N \to \infty} \frac{1}{2N} \ln \left| \text{Tr} G^{+}_{1N}(E) \right|^2. \quad (21) \]
The recursion relation for \( \xi^{(N+1)}(E) \) is
\[ \frac{1}{\xi^{(N+1)}(E)} = - \frac{1}{N+1} s^{(N+1)}_\xi, \quad (22a) \]
\[ s^{(N+1)}_\xi = s^{(N)}_\xi + \ln \left| \text{Tr} G^{+(N+1)}_{N+1} \right|. \quad (22b) \]

4 Finite-Size Scaling

For finite systems there can be no singularities induced by a phase transition and the divergences at the MIT are always rounded off [42]. Fortunately, the MIT can still be studied using a technique known as finite-size scaling [2]. Here we briefly review the main results taking the dimensionless four-terminal conductance \( g_4 \) of a large cubic sample of size \( L \times L \times L \) as an example. We note that similar scaling ideas can also be applied to the reduced localisation length \( \xi/L \). In order to obtain \( g_4 \) of the disordered region only, we have to subtract the contact resistance due to the leads. This gives
\[ \frac{1}{g_4} = \frac{1}{g_2} - \frac{1}{\mathcal{N}}. \quad (23) \]
Here \( \mathcal{N} = \mathcal{N}(E) \) is the number of propagating channels at the Fermi energy \( E \) which is determined by the quantization of wave numbers in transverse direction in the leads [43, 44].

Near the MIT one expects a one-parameter scaling law for the dimensionless conductance [7, 30, 42]
Localization of electronic states in amorphous materials

\[ g_4(L, \varepsilon, b) = F \left[ \frac{L}{b}, \chi(\varepsilon)b^{1/\nu}, \phi(\varepsilon)b^{-y} \right], \quad (24) \]

where \( b \) is the scale factor in the renormalisation group, \( \chi \) is a relevant scaling variable and \( \nu > 0 \) is the critical exponent. The parameter \( \varepsilon \) measures the distance from the mobility edge \( E_c \) as in (2). However, recent advances in numerical precision have shown that in addition to corrections to scaling due to the finite sizes of the sample need to be taken into account so that the general scaling form is

\[ g_4(L, \varepsilon, b) = F \left[ \frac{L}{b}, \chi(\varepsilon)b^{1/\nu}, \phi(\varepsilon)b^{-y}, \phi'(\varepsilon)b^{-y} \right], \quad (25) \]

where \( \phi \) is an irrelevant scaling variable and \( y > 0 \) is the corresponding irrelevant scaling exponent. The choice \( b = L \) leads to the standard scaling form

\[ g_4(L, \varepsilon) = F \left[ L^{1/\nu}\chi(\varepsilon), L^{-y}\phi(\varepsilon) \right], \quad (26) \]

with \( F \) being related to \( F \). For \( E \) close to \( E_c \) we may expand \( F \) up to order \( n_R \) in its first and up to order \( n_I \) in its second argument such that

\[ g_4(L, \varepsilon) = \sum_{n'=0}^{n_1} \phi^{n'} L^{-n'y} F_{n'}(\chi L^{1/\nu}) \quad \text{with} \quad (27a) \]

\[ F_{n'}(\chi L^{1/\nu}) = \sum_{n=0}^{n_R} a_{n'n} \chi^n L^{n/\nu}. \quad (27b) \]

Additionally \( \chi \) and \( \phi \) may be expanded in terms of the small parameter \( \varepsilon \) up to orders \( m_R \) and \( m_I \), respectively. This procedure gives

\[ \chi(\varepsilon) = \sum_{m=1}^{m_R} b_m \varepsilon^m, \quad \phi(\varepsilon) = \sum_{m'=0}^{m_I} c_{m'} \varepsilon^{m'}. \quad (28) \]

From (26) and (27) one can see that a finite system size results in a systematic shift of \( g_4(L, \varepsilon = 0) \) with \( L \), where the direction of the shift depends on the boundary conditions [42]. Consequently, the curves \( g_4(L, \varepsilon) \) do not necessarily intersect at the critical point \( \varepsilon = 0 \) as one would expect from the scaling law (24). Neglecting this effect in high precision data will give rise to wrong values for the exponents.

Using a least-squares fit of the numerical data to (27) and (28) allows us to extract the critical parameters \( \nu \) and \( E_c \) with high accuracy. One also obtains the finite-size corrections and can subtract these to show the anticipated scaling behaviour. This finite-size scaling analysis has been successfully applied to numerical calculations of the localisation length and the conductance within the Anderson model [3, 14].

\[ ^5 \text{The choice of } b \text{ is connected to the iteration of the renormalisation group [42].} \]
5 MIT at $E = 0.5\, t$ for varying disorder

5.1 Scaling of the Conductance

We first investigate the standard case of varying disorder at a fixed energy [14]. We choose $t_{ij} \neq 0$ for nearest neighbours $i, j$ only, set $t_{ij} = t$ and $E = 0.5\, t$ which is close to the band centre. We impose hard wall boundary conditions in the transverse direction. For each combination of disorder strength $W$ and system size $L$ we generate an ensemble of 10000 samples. The systems under investigation are cubes of size $L \times L \times L$ for $L = 4, 6, 8, 10, 12$ and 14. For each sample we calculate the DOS $\rho(E, L)$ and the dimensionless two-terminal conductance $g_2$ using the recursive Green’s function method explained in Section 3. Finally we compute the average DOS $\langle \rho(E, L) \rangle$, the average conductance $\langle g_4(E, L) \rangle$ and the typical conductance $\exp(\ln g_4(E, L))$.

The results for the different conductance averages are shown in Figs. 3 and 4 together with respective fits to the standard scaling form (26). Shown are the best fits that we obtained for various choices of the orders of the expansions (27, 28). The expansion orders and the results for the critical exponent and the critical disorder are given in Table 1. In Fig. 5 we show the same data as in

![Graph showing the average dimensionless conductance vs disorder strength for $E = 0.5\, t$. System sizes are given in the legend. Errors of one standard deviation are obtained from the ensemble average and are smaller than the symbol sizes. Also shown (solid lines) are fits to (26) for $L = 8, 10, 12$ and 14.]

Fig. 3. Average dimensionless conductance vs disorder strength for $E = 0.5\, t$. System sizes are given in the legend. Errors of one standard deviation are obtained from the ensemble average and are smaller than the symbol sizes. Also shown (solid lines) are fits to (26) for $L = 8, 10, 12$ and 14.

Figs. 3 and 4 after the corrections to scaling have been subtracted indicating that the data points for different system sizes fall onto a common curve with
two branches as it is expected from the one-parameter scaling theory. The results for the conductance averages and also the critical values are in good agreement with transfer-matrix calculations [9, 14].

5.2 Disorder Dependence of the Density of States

The Green’s function method enables us to compute the DOS of the disordered system. It should be independent of $L$. Figure 6 shows the average DOS at $E = 0.5 \, t$ for different system sizes. There are still some fluctuations present. These can in principle be reduced by using larger system sizes and increasing the number of samples. The fluctuations will be particularly inconvenient when trying to compute $\sigma(E)$.

The reduction of the DOS with increasing disorder strength can be understood from a simple argument. If the DOS were constant for all energies
its value would be given by the inverse of the band width. In the Anderson model with box distribution for the on-site energies the band width increases linearly with the disorder strength $W$. The DOS in the Anderson model is not constant as a function of energy, nevertheless let us assume that for energies in the vicinity of the band centre the exact shape of the tails is not important. Therefore,

$$\rho(W) \propto \frac{1}{B + \alpha W},$$

shows a decrease of the DOS with $W$. Here $B$ is an effective band width taking into account that the DOS is not a constant even for $W=0$. The parameter $\alpha$
allows for deviations due to the shape of the tails. In Fig. 6, we show that the data are indeed well described by (29).

6 Influence of the Metallic Leads

As mentioned in the introduction most numerical studies of the conductance have been focused on the disorder transition at or in the vicinity of the band centre. Let us now set $E = -5t$ and calculate the conductance averages as before. The results for the typical conductance are shown in Fig. 7a. Earlier studies of the localization length provided evidence of a phase transition around $W = 16.3t$ although the accuracy of the data was relatively poor [23]. Surprisingly, in Fig. 7a there seems to be no evidence of any transition nor of any systematic size dependence. The order of magnitude is also much smaller than in the case of $E = 0.5t$, although one expects the conductance at the MIT to be roughly similar.

The origin of this reduction can be understood from Fig. 8, which shows the DOS of a disordered sample and a clean system (i.e. without impurities and therefore without disorder) such as in the metallic leads. As already pointed out in Ref. [19], the difference between the DOS in the leads and in the disordered region may lead to false results for the transport properties. Put to an extreme, if there are no states available at a certain energy in the
Fig. 7. System size dependence of the logarithm of the typical conductance for fixed energy $E = -5t$. Errors of one standard deviation are obtained from the ensemble average and are smaller than the symbol sizes. The lines are guides to the eye only. The upper plot was calculated using the metallic leads "as they are", i.e. the band centre of the leads coincides with the band centre in the disordered region. In the lower plot the band centre of the leads was "shifted" to the respective Fermi energy.

leaves, e.g. for $|E| \geq 6t$, there will be no transport regardless of the DOS and the conductance in the disordered system at that energy. The DOS of the latter system becomes always broadened by the disorder. Therefore, using the standard setup of system and leads, it appears problematic to investigate transport properties at energies outside the ordered band. Additionally, for energies $3t \lesssim |E| < 6t$ the DOS of the clean system is smaller than the disorder broadened DOS. Thus the transport properties that crucially depend on the DOS might be also changed in that energy range. The problems can be overcome by shifting the energy of the disordered region while keeping the Fermi energy in the leads in the lead-band centre (or vice versa). This
Localization of electronic states in amorphous materials

Fig. 8. DOS of a clean system (full black line) and a disordered system (grey) with $W = 12t$ and $L = 21$, obtained from diagonalising the Hamiltonian (1). The dashed lines indicate the band edges of the ordered system.

is somewhat equivalent in spirit to applying a gate voltage to the disordered region and sweeping it — a technique similar to MOSFET experiments. The results for the typical conductance using this method are shown in Fig. 7. One can see some indication of scaling behaviour and also the order of magnitude is found to be comparable to the case of $E = 0.5t$. Another possibility of avoiding the DOS mismatch is choosing a larger hopping parameter in the leads [45], which results in a larger bandwidth, but also a lower DOS.

7 The MIT outside the band centre

Knowing the difficulties involving the metallic leads and using the "shifting technique" explained in the last section, we now turn our attention to the less-studied problem of the MIT at fixed disorder. We set the disorder strength to $W = 12t$ and again impose hard wall boundary conditions in the transverse direction [14]. We expect $E_c \approx 8t$ from the earlier studies of the localization length [23]. Analogous to the transition for varying $W$ we generate for each combination of Fermi energy and system size an ensemble of 10000 samples (except for $L = 19$ and $L = 21$, where 4000 and 2000 samples, respectively, were generated) and examine the energy and size dependence of the average and the typical conductance, $\langle g_4 \rangle$ and $\exp(\ln g_4)$, respectively.

7.1 Energy Dependence of the DOS

Before looking at the scaling behaviour of the conductance we have to make sure that the "shifting technique" indeed gives the right DOS outside the
ordered band. Additionally, we have to check the average DOS for being independent of the system size. In Fig. 9 we show the DOS obtained from diagonalisation of the Anderson Hamiltonian with 30 configurations (using standard LAPACK subroutines) and the Green’s function calculations. The Green’s function data agree very well with the diagonalisation results, although there are still bumps around \(E = -8.2t\) for small DOS values. The average DOS for different system sizes is shown in Fig. 10. For large energies the DOS is nearly independent of the system size. However, close to the band edge one can see fluctuations because in the tails there are only few states and thus many more samples are necessary to obtain a smooth DOS.

7.2 Scaling Behaviour of the Conductance

The size dependence of the average and the typical conductance is shown in Fig. 11. We find that for \(E/t \leq -8.2\) the typical conductance is proportional to the system size \(L\) and the constant of proportionality is negative. This corresponds to an exponential decay of the conductance with increasing \(L\) and is characteristic for insulating behaviour. Moreover, the constant of proportionality is the localisation length \(\xi\). We find that \(\xi(E)\) diverges at some energy,
which indicates a phase transition. This energy dependence of $\xi$ is shown in Fig. 12.

For $E/t \geq -8.05$, $\langle g_4 \rangle$ is proportional to $L$. This indicates the metallic regime and the slope of $\langle g_4 \rangle$ vs $L$ is related to the d.c. conductivity. We fit the data in the respective regimes to the standard scaling form (26). The results for the critical exponent and the mobility edge are given in Table 2. The obtained values from both averages, $\langle g_4 \rangle$ and $\langle \ln g_4 \rangle$, are consistent. The average value of $c = 1.50 \pm 0.18$ is in agreement with results for conductance scaling at $E/t = 0.5$ and transfer-matrix calculations [9, 14].

![Graph showing DOS vs energy for different system sizes and $W = 12t$ calculated with the recursive Green’s function method. The data are averaged over 10000 disorder configurations except for $L = 21$ when 2000 samples have been used. The lines are guides to the eye only. Error bars are obtained from the sample average.](image)

**Table 2.** Best-fit estimates of the critical exponent and the mobility edge for both averages of $g_4$ using (26) with $n_R = m_l = 0$. The system sizes used are $L = 11, 13, 15, 17, 19, 21$. 

| $\langle g_4 \rangle$ | $-8.2$ | $-7.4$ | $3$ | $2$ | $1.60 \pm 0.18$ | $-8.14 \pm 0.02$ |
|-----------------------|--------|--------|-----|-----|----------------|------------------|
| $\langle \ln g_4 \rangle$ | $-8.8$ | $-7.85$ | $3$ | $2$ | $1.58 \pm 0.06$ | $-8.185 \pm 0.012$ |
Fig. 11. System size dependence of the 4-point conductance averages $\langle g_4 \rangle$ and $\langle \ln g_4 \rangle$ for $W = 12t$ and Fermi energies as given in the legend. Error bars are obtained from the ensemble average and shown for every second $L$. The dashed lines in the metallic regime indicate the fit result to (30) using the parameters of Table 2. In the insulating regime, linear functions for $\langle \ln g_4 \rangle = -L/\xi + c$ have been used for fitting.

7.3 Calculation of the D.C. Conductivity

Let us now compute the d.c. conductivity from the conductance $\langle g_4(E, L) \rangle$. From Ohm’s law, one naively expects the macroscopic conductivity to be the ratio of $\langle g_4(E, L) \rangle$ and $L$. There are, however, several complications. First, the mechanism of weak localisation gives rise to corrections to the classical behaviour for $g_4 \gg 1$. Second, it is a priori not known if this relation still holds in the critical regime. And third, the expansion (27) does not yield a behaviour of the form $g_4 \propto \epsilon^{\nu}$.

In order to check our data for consistence with the anticipated power law (2) for the conductivity $\sigma(E)$ in the critical regime, we assume the following
Fig. 12. Localisation length (for \( E < E_c \)) and correlation length (for \( E > E_c \)) vs energy obtained from a linear fit to \( \langle \ln g_4 \rangle = \mp \frac{L}{\xi} + \text{const.} \), respectively. The error bars close to the transition have been truncated (arrows), because they extend beyond the plot boundaries.

The scaling law for the conductance,

\[
\langle g_4 \rangle = f(\chi^\nu L),
\]

which results from setting \( b = \chi^{\nu} \) in (24). Due to the relatively large error bars of \( \langle g_4 \rangle \) at the MIT as shown in Fig. 11, we might as well neglect the irrelevant scaling variable. Then we expand \( f \) as a Taylor series up to order \( n_R \) and \( \chi \) in terms of \( \varepsilon \) up to order \( m_R \) in analogy to (27b) and (28). The best fit to our data is determined by minimising the \( \chi^2 \) statistic. Using \( n_R = 3 \) and \( m_R = 2 \) we obtain for the critical values, \( \nu = 1.58 \pm 0.18 \) and \( E_c/t = -8.12 \pm 0.03 \). These values are consistent with our previous fits. The linear term of the expansion of \( f \) corresponds to the conductivity close to the MIT.

To estimate the quality of this procedure we also calculate the conductivity from the slope of a linear fit to \( \langle g_4 \rangle \) throughout the metallic regime, and from the ratio \( \langle g_4 \rangle/L \) as well.

The resulting estimates of the conductivity are shown in Fig. 13. We find that the power law is in good agreement with the conductivity obtained from the linear fit to \( \langle g_4 \rangle = \sigma L + \text{const.} \) for \( E \leq -7t \). In this range it is also consistent with the ratio of \( \langle g_4 \rangle \) and \( L \) for the largest system computed \((L = 21)\). Deviations occur for energies close to the MIT and for \( E > -7t \). In the critical regime one can argue that for finite systems the conductance will always be larger than zero in the insulating regime because the localisation length becomes eventually larger than the system size.
Fig. 13. Conductivity $\sigma$ vs energy computed from $\langle g_4 \rangle / L$ for $L = 21$ (□), a linear fit with $\langle g_4 \rangle = \sigma L + \text{const.}$ ($\bullet$) and a fit to the scaling law (30) (solid line). The dashed line indicates $E_c/t = -8.12$. Error bars of $\langle g_4 \rangle / L$ represent the error-of-mean obtained from an ensemble average and are shown for every third $E$ value. The dashed line indicates the position of $E_c$ and the inset shows the region close to $E_c$ in more detail.

8 Conclusions

We computed the conductance at $T = 0$ and the DOS of the 3D Anderson model of localisation. These properties were obtained from the recursive Green’s function method in which semi-infinite metallic leads at both ends of the system were taken into account.

We demonstrated how the difference in the DOS between the disordered region and the metallic leads has a significant influence on the results for the electronic properties at energies outside the band centre. This poses a big problem for the investigation of the MIT outside the band centre. We showed that by shifting the energy levels in the disordered region the mismatch can be reduced. In this case the average conductance and the typical conductance were found to be consistent with the one-parameter scaling theory at the transition at $E_c \neq 0$. Using a finite-size-scaling analysis of the energy dependence of both conductance averages we obtained an average critical exponent $\nu = 1.59 \pm 0.18$, which is in accordance with results for conductance scaling at $E/t = 0.5$, transfer-matrix calculations [9, 11, 14, 26] and diagonalisation studies [10, 12]. However, a thorough investigation of the influence of the leads is still lacking. It would also be interesting to see if these effects can be related to studies of 1D multichannel systems with impurities [46].
We calculated the d.c. conductivity from the system-size dependence of the average conductance and found it consistent with a power-law form at the MIT [47]. This strongly supports previous analytical and numerical calculations of thermoelectric properties reviewed in Ref. [3]. Similar results for topologically disordered Anderson models [48–50], random-hopping models [37,51–53] and the interplay of disorder and many-body interaction [54–57] have been reported elsewhere.

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