Phase diagram of the three-dimensional Anderson model of localization with random hopping

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Abstract. We examine the localization properties of the three-dimensional (3D) Anderson Hamiltonian with off-diagonal disorder using the transfer-matrix method (TMM) and finite-size scaling (FSS). The nearest-neighbor hopping elements are chosen randomly according to $t_{ij} \in [c - 1/2, c + 1/2]$. We find that the off-diagonal disorder is not strong enough to localize all states in the spectrum in contradistinction to the usual case of diagonal disorder. Thus for any off-diagonal disorder, there exist extended states and, consequently, the TMM converges very slowly. From the TMM results we compute critical exponents of the metal-insulator transitions (MIT), the mobility edge $E_c$, and study the energy-disorder phase diagram.

Keywords: disorder, localization, metal-insulator transition, random hopping

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1 Introduction

From the scaling hypothesis of localization \[1\] it is well known that in one (1D) and two dimensions (2D) almost all states of a non-interacting disordered quantum system are localized \[2\]. Delocalized states occur only for special choices of physical parameters. An example of such a model is provided by the Anderson model of localization with random hopping \[3\],

$$H = \sum_{i \neq j} t_{ij} |i\rangle \langle j| + \sum_{i} \epsilon_i |i\rangle \langle i| . \tag{1}$$

The hopping elements $t_{ij}$ between sites $i$ and $j$ are restricted to nearest neighbors and chosen randomly from the interval $[c - w/2, c + w/2]$. Thus $c$ represents the center and $w$ the width of the off-diagonal disorder distribution. The onsite potential energies $\epsilon_i$ are taken to be randomly distributed in the interval $[-W/2, W/2]$. We set the energy scale by keeping $w = 1$ fixed and use periodic boundary conditions.

In this work we will concentrate on the properties of the random hopping model in 3D. We study the density of states (DOS). Using TMM \[4\] together with FSS, we determine the mobility edge $E_c$ of the MIT separating extended from localized states. We find that the off-diagonal disorder is not strong enough to localize all states in the spectrum in contradistinction to the usual case of diagonal disorder.
2 Density of States

We have numerically computed the spectrum of the Hamiltonian (1) for 1000 samples, system size $N = M^3 = 10^3$ and various values of $c$. In Fig. 1 we show the resulting DOS for strong off-diagonal disorder $c = 0$ and moderate $c = 0.6$. For $c = 0$ the peak at energy $E = 0$ in the DOS of the finite system is well pronounced. It corresponds to a logarithmic singularity in the infinite system [5] as shown in Fig. 1 (left, inset). For larger values of $c$, the off-diagonal disorder becomes weaker and the DOS shows various sub-bands which reflect the spectral structure of the completely ordered model for $w, W = 0$. We remark that in the corresponding 2D model the smallest localization length and thus the strongest disorder was found at $c \approx 0.25$ [3].

![Fig. 1](image)

Fig. 1 Left: DOS for off-diagonal disorder with system size $10^3$ and $c = 0$; Inset: logarithmic behaviour of the DOS near the bandcenter. Right: DOS for $c = 0.6$; sharp lines correspond to the DOS of the ordered system at $w, W = 0$, scaled by $1/40$ for clarity. The binwidth in all cases is 0.01.

3 Determination of the mobility edge

The application of the TMM for the present case of random hopping relies on a reformulation of the Schrödinger equation [3] as

$$t_{jkn+1}^{||} \psi_{jkn+1} = (E - \epsilon_{jkn}) \psi_{jkn} - t_{jkn}^{||} \psi_{jkn-1} - t_{j+1kn}^{||} \psi_{j+1kn} - t_{j,kn}^{||} \psi_{j-1kn} - t_{j,k+1n}^{||} \psi_{jk+1n} - t_{j,kn}^{||} \psi_{jk-1n}$$

with $\psi_{jkn}$ corresponding to the wave function at site $(j, k, n)$, $t_{jkn}^{||}$, $t_{j+1kn}^{||}$, $t_{j,kn}^{||}$, $t_{j,k+1n}^{||}$, and $t_{j,kn}^{||}$ representing the hopping elements from site $(j-1, k, n)$ or $(j, k-1, n)$ respectively to site $(j, k, n)$ and $t_{jkn}^{||}$ the hopping element from $(j, k, n-1)$ to $(j, k, n)$. This equation may be written in matrix form as

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T_n \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}, \quad T_n = \begin{pmatrix} [t_{n+1}^{||}]^{-1} (E - H_{\perp}) + [t_{n+1}^{||}]^{-1} [t_{n+1}^{||}]^{-1} & 0 \\ 1 & 0 \end{pmatrix}$$

(3)
with $\psi_n = (\psi_{11n}, \ldots, \psi_{1Mn}, \psi_{21n}, \ldots, \psi_{Mn})$ denoting the wave function in the $n$th slice, $H_n$ the Hamiltonian in the $n$th slice, and the matrix $t_n$ connecting the $(n-1)$th with the $n$th slice. As usual, the localization length $\lambda = 1/\gamma_{\text{min}}$ is computed from the smallest Lyapunov exponent $\gamma_{\text{min}}$ of the $2M^2$ eigenvalues $\exp(\pm \gamma_i)$ of $\Gamma = \lim_{K \to \infty} (\tau_K^\dagger \tau_K)^{1/2K}$. Here, $\tau_K = T_1 T_2 \cdots T_{K-1}$. Assuming the validity of one-parameter scaling close to the MIT, we expect the reduced localization lengths $\lambda(M)/M$ to scale onto a scaling curve $\lambda(M)/M = f(\xi/M)$ with scaling parameter $\xi$.

In Fig. 2 we show the results up to $M = 14$ at $c = 0$ and $W = 0$. The crossing between extended states at $E \lesssim 1.28$ and localized states at $E \gtrsim 1.28$ is clearly visible. The mobility edge is thus $E_c \approx 1.28$. The inset zooms into the MIT region, where one can see an $M$-dependent shift of the crossing point towards smaller $E$ for increasing $M$. Due to this finite size effect, which is supposed to vanish for $M$ large enough, we take non-linear and non-universal corrections to FSS [7] into account. The FSS curve constructed from these data in Fig. 2 shows two branches similarly to the FSS curves in the Anderson model of localization with pure diagonal disorder [6]. However, in contradistinction to the model with diagonal disorder, we find that the off-diagonal disorder at $c = 0$ is not strong enough to localize all the states.

Analysing data for larger values of $c$, we find increasing localization lengths. Consequently the mobility edge increases with increasing $c$. In Fig. 3 we show the results up to $c = 1$. For larger $c$ the transition observed for $c = 0$ in Fig. 2 becomes less easy to detect and we obtain reasonably accurate crossings for large $M$ only. The crossing becomes sharp again when varying $W$ instead of $E$. This allows us to determine the critical exponents $\nu_E$ and $\nu_W$ of the scaling parameter $\xi \propto |E - E_c|^\nu_E$ and $\xi \propto |W - W_c|^\nu_W$. In agreement with recent results in the Anderson model with pure diagonal disorder [6] we find $\nu_E = 1.61 \pm 0.07$ and $\nu_W = 1.54 \pm 0.03$. 

**Fig. 2** Left: Reduced localization length $\lambda/M$ as function of energy $E$ at $c = 0$ and $W = 0$ as obtained by TMM with 0.1% accuracy. Note the MIT at $E_c \approx 1.28$. Inset: Enlarged region close to the MIT, only every second data point indicated by a symbol, the error bar shown separately. Right: FSS curve for the TMM data from the left panel.
Fig. 3 Phase diagram of the Anderson model of localization with off-diagonal disorder $c$ as obtained from TMM with 1% accuracy. The values of $E_c$ are indicated by diamonds. Squares represent the numerically determined upper band edge $E_B$ for a system with $10^3$ sites averaged over 1000 samples. The straight dashed line is the band edge $E_{\text{max}}$ for the infinite system corresponding to a constant $t = c + 1/2$. The difference between $E_B$ and $E_{\text{max}}$ occurs due to exponential tails of the DOS which cannot be resolved by our calculations. States with $|E| < E_c$ are extended (dark gray), whereas states with $E_c < |E| \leq E_B$ are localized (light gray).

4 Conclusions

We have investigated the DOS and the localization properties of the Anderson model of localization with off-diagonal disorder. Our results show that in 3D a finite part of the spectrum close to the band center remains extended even for the strongest off-diagonal disorder $c = 0$, whereas in 1D and 2D the off-diagonal disorder has non-localized states only for $E = 0$. FSS is possible and we determine the mobility edge separating extended and localized states in the off-diagonal disorder vs. energy phase diagram. The obtained critical exponents of the MITs are in agreement with prior results for the model with only diagonal disorder [7, 8] and convincingly support the universality.

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