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Are the phases in the Anderson model long-range correlated?

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Abstract

We investigate the local cumulative phases at single sites of the lattice for time-dependent wave functions in the Anderson model in $d = 2$ and 3. In addition to a local linear trend, the phases exhibit some fluctuations. We study the time correlations of these fluctuations using detrended fluctuation analysis. Our results suggest that the phase fluctuations are long-range correlated, decaying as a power law with time. It seems that the exponent depends on the degree of disorder. In $d = 3$, close to the critical disorder $w_c = 16.5$, the correlation exponent exhibits a maximum value of $\alpha \approx 0.6$ which is significantly above random fluctuations ($\alpha = 0.5$).

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The Anderson model is the standard model for transport in weakly disordered solids, e.g. compounds, amorphous semiconductors or semiconductors with impurities [1]. Anderson wave functions are known to be always localized in $d = 2$, while there is a localization–delocalization transition in $d = 3$ at the critical disorder $w_c \approx 16.5$ [2]. The wave functions were found to be multifractal at the critical point [3,4]. The localization behavior and the multifractality also show up in the behavior of time-dependent wave functions, e.g. when considering a diffusing wave packet [5,6]. But up to now only the probability densities $|\psi_n(t)|^2$ at site n have been investigated, not the phases of the time-dependent wave functions. In this paper, we investigate, for the first time, the

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local phases $\varphi_n(t)$. We find that they are long-range correlated in time. The correlations seem to be most pronounced at the critical point in $d = 3$.

We consider the Schrödinger equation in tight-binding approximation for the wave function of a quantum particle on (a) a regular square lattice and (b) a simple cubic lattice. The wave function amplitudes ψ_n for the lattice sites n satisfy the tight-binding equation $E\psi_n = \varepsilon_n\psi_n + \sum_\delta V_{n,n+\delta}\psi_{n+\delta}$, where the sum runs over all nearest-neighbor sites $n+\delta$ of site n, and E is the eigenvalue. The local potentials ε_n are chosen randomly in an uncorrelated way from the interval $[-w/2, w/2]$, where w is the disorder parameter.

Here, we consider the time-dependent tight-binding Schrödinger equation, $i(d/dt)\psi_n(t) = \varepsilon_n\psi_n(t) + \sum_\delta V_{n,n+\delta}\psi_n(t)$. The choice $\hbar = 1$ determines the unit of time. We assume no hopping disorder, $V_{n,n+\delta} = 1$ for nearest-neighbor sites n and $n + \delta$ and $V = 0$ elsewhere. We numerically calculate the local amplitudes $\psi_n(t)$ for the wave function by integration of the time-dependent equation using a Rung–Kutta method. The complex functions $\psi_n(t)$ can be separated into their absolute amplitudes and their phases, $\psi_n(t) = |\psi_n(t)|\exp[i\varphi_n(t)]$. We are interested in the phases and their dependences on time. In order to avoid the (somehow artificial) jumps in the time dependence of the phases $\varphi_n(t)$ due to the restriction of their values to $[0, 2\pi]$ we consider the cumulative phases here. The cumulative local phases are continuous functions of time since their values are not taken modulo 2π. The results for the integration of the time-dependent Schrödinger equation are similar for different kinds of initial conditions if equilibrium is reached and the disorder is not too strong. Therefore, we set $|\psi_n(t = 0)| = \text{const.}$ for all sites n, since equilibrium is reached relatively fast in that case. The phases $\varphi_n(t = 0)$ are taken randomly distributed, and the constant is chosen according to the normalization condition $\sum_n |\psi_n|^2 = 1$.

Fig. 1 shows typical results for the local phases $\varphi_n(t)$ as function of time. In addition to the linear trend the phases exhibit large fluctuations. The linear trend is trivial: If we disregard the hopping terms in the time-dependent Schrödinger equation the remaining diagonal term gives just this linear time dependence, $\varphi_n(t) = \varphi_n(0) - \varepsilon_n t$. Thus, the slope of the linear increase is directly related to the local potential ε_n. The fluctuations of the local phases, in contrast, are not trivial, since they are due to accumulation of phase from different paths through the system. Now the question arises whether these fluctuations are just random, i.e. the deviation of $\varphi_n(t)$ from the linear trend is like a random walk, or whether the fluctuations are somehow correlated?

In order to answer this question we have investigated the correlations of the phases using the detrended fluctuation analysis (DFA) that can systematically overcome the linear trend in the phase data. Descriptions of the DFA can be found elsewhere [7–9]. The correlation of the detrended phase shifts $\phi_n(t) = \varphi_n(t) - \varphi_n(t-1) + \varepsilon_n$ at time scale τ is characterized by the (auto)correlation function $C(\tau) = \langle\phi_n(t)\phi_n(t+\tau)\rangle = [1/(T-\tau)]\sum_{t=1}^{T-\tau}\phi_n(t)\phi_n(t+\tau)$ for a time series of total length T. If the detrended phase shifts $\phi_n(t)$ are uncorrelated, $C(\tau)$ is zero for positive τ. For short-range correlations $C(\tau)$ decays exponentially. Since a direct calculation of $C(\tau)$ is hindered by the nonstationarities in the data, we study the fluctuation $F(\tau)$ as function of the time scale τ instead. The fluctuation $F(\tau)$ is defined as the standard deviation of the phase

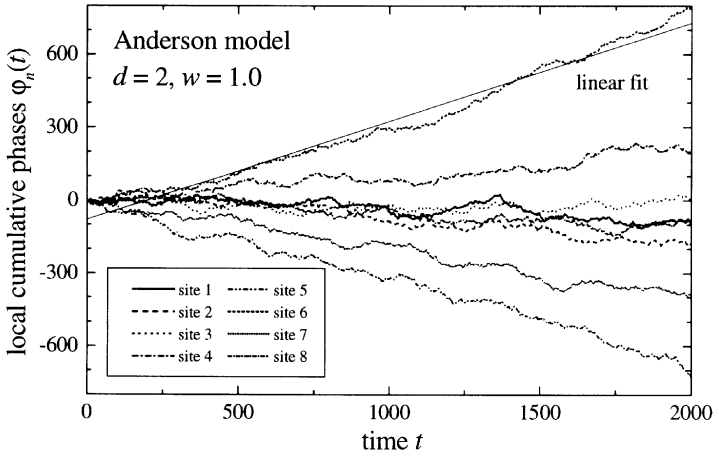

Fig. 1. Cumulative time-dependent local phases $\varphi_n(t)$ for the Anderson model in $d=2$ for eight (randomly chosen) sites n. System size is 30×30; and the disorder parameter is $w=1$. In addition to the linear trends the phases exhibit large fluctuations.

profiles $\varphi_n(t)$ from linear fits in segments of length τ [7–9]. For the relevant case of long-range power-law correlations, where $C(\tau)\sim\tau^{-\gamma}$ with $0<\gamma<1$, the fluctuations increase by a power law $F(\tau)\sim\tau^{\alpha}$. According to random walk theory (see e.g. [10,11]) the exponent α is related to γ by $\alpha=1-\gamma/2$. For uncorrelated data (as well as for short-range correlations represented by exponentials $C(\tau)\sim\exp(-\tau/\tau_{\rm p})$ or $\gamma\geqslant 1$), we have $\alpha=\frac{1}{2}$. The data are long-range correlated if α is significantly larger than $\frac{1}{2}$.

Our numerical procedure was as follows: First, we extracted phase records $\varphi_n(t)$ from the time-dependent wave functions in the Anderson model for each site n. The resonable time scales are limited by (i) diffusion time $\tau_D=L^2/D$ and (ii) reoccurance time. By Fourier transform of $\psi_n(t)$ we checked that reoccurance time is larger than the time scales τ considered. Then we calculated the fluctuation $F(\tau)$ for several time scales τ and determined the exponent α from the successive slopes of $\log F(\tau)$ versus $\log\tau$. The results for the Anderson model in $d=2$ and 3 are shown in Fig. 2. We find that the fluctuations of the phase records are long-range correlated. The scaling exponent α is significantly larger than the value $\alpha=\frac{1}{2}$ for random data, but its precise value depends significantly on the disorder strength w. For time-dependent Anderson wave functions in $d=2$, α reaches its maximum $\alpha\approx 0.57$ for $w\approx 8$, for which the system size is approximately equal to the localization length of the wave functions. In $d=3$, the correlation exponent α reaches its maximum for $w\approx 18$, which is quite close to the critical disorder $w_{\rm c}\approx 16.5$. Note that the maximum correlation exponent α is still not reached in the finite time series in Fig. 2b for large disorder (localized modes), while α seems to decay for small disorder (extended modes).

In conclusion, the localization–delocalization transition in the Anderson model does also show up in the correlation of the cumulative phases at single sites of time-dependent wave functions. Analyzing the fluctuations of the phases by DFA we find that maximum long-range correlations occur close to the critical point in $d=3$. Further research

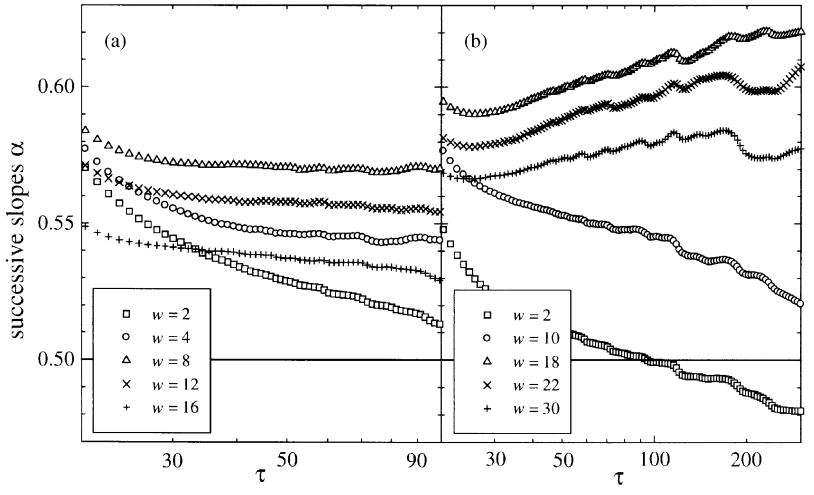

Fig. 2. Successive slopes $\alpha = d\log F(\tau)/d\log \tau$ for the fluctuation $F(\tau)$ of the local cumulative phases in the Anderson model in (a) $d = 2$ and (b) $d = 3$. The linear system sizes are $L = 60$ in (a) and $L = 20$ in (b). $F(\tau)$ has been averaged over all sites and (a) seven and (b) four configurations. The symbols correspond to different degrees of disorder. $\alpha > \frac{1}{2}$ indicates long-range correlations in the phase time series. We checked that the time scale τ is always smaller than diffusion time and reoccurance time.

work is necessary to determine the physical origin of the long-range correlations we find numerically.

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References

[1] B. Kramer, A. MacKinnon, Rep. Prog. Phys. 56 (1993) 1469.
[2] A. MacKinnon, B. Kramer, Z. Phys. B 53 (1983) 1.
[3] M. Schreiber, H. Grussbach, Phys. Rev. Lett. 67 (1991) 607.
[4] H. Grussbach, M. Schreiber, Phys. Rev. B 51 (1995) 663.
[5] B. Huckestein, L. Schweitzer, Phys. Rev. Lett. 72 (1994) 713.
[6] R. Ketzmerick et al., Phys. Rev. Lett. 79 (1997) 1959.
[7] C.K. Peng et al., Phys. Rev. E 49 (1994) 1685.
[8] S.V. Buldyrev et al., Phys. Rev. E 51 (1995) 5084.
[9] E. Koscielny-Bunde et al., Phys. Rev. Lett. 81 (1998) 729.
[10] A.-L. Barabasi, H.E. Stanley, Fractal Concepts in Surface Growth, Cambridge University Press, 1995.
[11] M.F. Shlesinger, B.J. West, J. Klafter, Phys. Rev. Lett. 58 (1987) 1100.