limit. This can be translated into a fractal Weyl law for the long-living states (which are associated to the universal fluctuations in the RMT regime). Such laws have been previously predicted by quantization of the classical repeller, based on the Gutzwiller trace formula for chaotic systems. We find that the effect can be explained on the mean-field level, which allows us to consider non-chaotic situations as well. Figure 4 demonstrates the mean-field correspondence of short-lived states with classical regions of fast escape for the case of a soft-chaotic system (the phase space is divided into stable and unstable regions).

Traditionally, semiclassics and random-matrix theory have been viewed as complimentary methods. It is good to see that they can be combined to open up new areas of applicability where each method by itself was at a failure.

[1] Ph. Jacquod, H. Schomerus, and C. W. J. Beenakker, Phys. Rev. Lett. **90**, 207004 (2003).

[2] J. Tworzydlo, A. Tajic, H. Schomerus, and C. W. J. Beenakker, Phys. Rev. B **68**, 115313 (2003).

[3] H. Schomerus and J. Tworzydlo, Phys. Rev. Lett. **93**, 154102 (2004).

[4] J. Tworzydlo, A. Tajic, H. Schomerus, P. W. Brouwer, and C.W.J. Beenakker, Phys. Rev. Lett. **93**, 186806 (2004).

3.1.21 Multiscaling in Anderson localization

Mikhail Titov and Henning Schomerus

Anderson localization is one of the most remarkable phase-coherent phenomena. It reveals itself in an exponential decay of the wave function of a classically free particle. This phenomenon is a result of multiple phase-coherent backward scattering, which is especially pronounced for a particle restricted to a single spatial dimension (to a line). Small fluctuations in the potential landscape do not affect the classical motion of a particle, while quantum-mechanically they can act as an effective potential barrier.

Unlike many other phase-coherent phenomena, Anderson localization cannot be understood within the well-developed framework of quasi-classical theory and requires a thorough theoretical investigation. At present, the detailed theory is limited to a simple class of one-dimensional non-interacting systems, which have many specific features of their own. It remains to be a challenge to distinguish the universal properties of these systems from those which are model-dependent.

In a series of recent works [1–4] we expand the existing theory of localization to a broader class of models. In particular we study the effects of lattice symmetry on the universal properties of the conductance, density of states, time-delay etc. The analytical method developed in Ref. [1] appears to be very successful in the scaling analysis of the universal fluctuations of these quantities. The general arguments given by Anderson, Thouless, Abrahams, and Fisher as early as in 1980 on the basis of scaling theory provide us with the conjecture that the conductance fluctuations in disordered metals are universally characterized by a single parameter. Our analytical approach

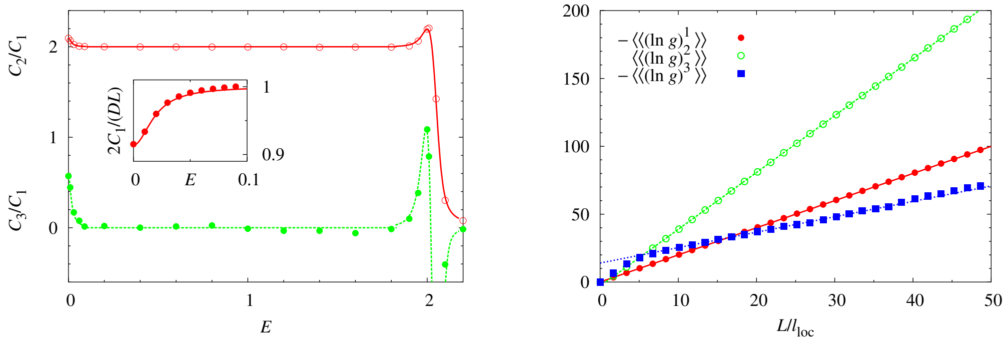

Figure 1: *Weak band-center and band-edge anomalies in the standard one-dimensional Anderson model with white-noise disordered potential. The left panel shows the coefficients* C_n *as the function of energy. The finite ratio* C_3/C_1 *indicates the violation of the single parameter scaling. The data points are the result of a numerical simulation of Ref. [2]. The curves are the analytical predictions of Ref. [1,2]. The right panel shows the first three cumulants of* $\ln g$ *at the band center as the function of system size* L*. The linear growth of the cumulants is the result of the central limit theorem. The slopes of the straight lines follow the predictions of Ref. [2].*

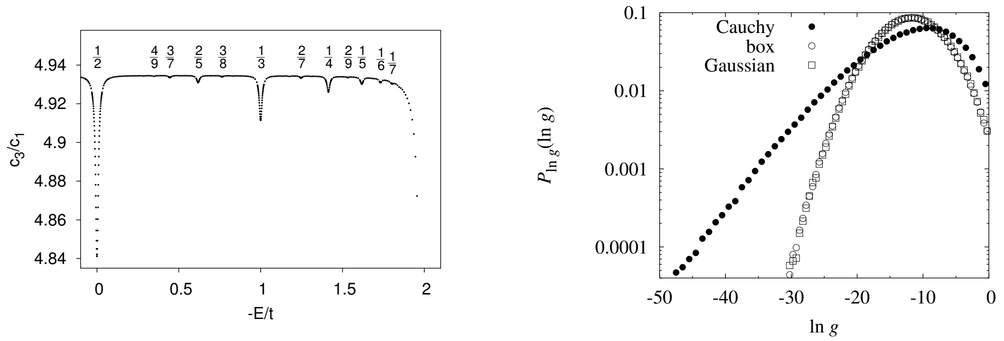

Figure 2: *The figure illustrates the multiscaling in the Anderson model with Cauchy disorder (Lloyd model). The left panel shows the ratio* C_3/C_1 *according to the analytical result of Ref. [4]. The ratio reveals anomalies at energies* $E = -2t\cos(\pi p/q)$ *with* p *and* q *integers. The corresponding rational number* p/q *is indicated in the figure. The right panel shows the distribution function of the logarithm of the conductance obtained numerically in Ref. [4] from the Anderson model with Cauchy disorder (full circles), box disorder (open circles), and Gaussian disorder (open squares). The deviation from the parabolic form for the case of Cauchy disorder is a signature of multiscaling.*

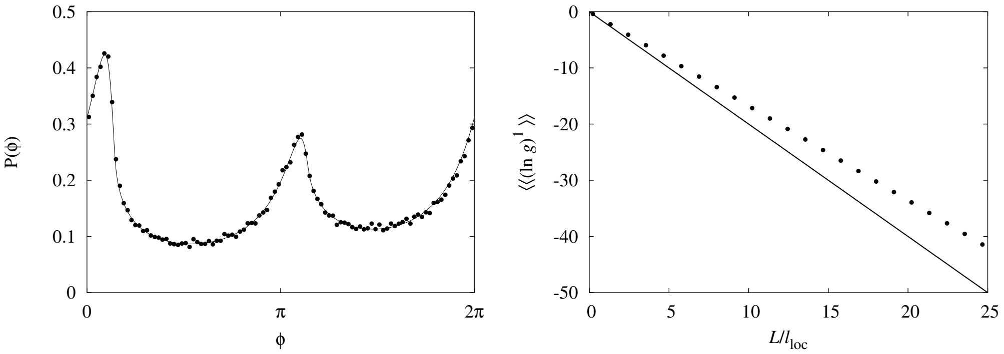

Figure 3: *This figure refers to an Anderson model with correlated disorder (correlation length: three lattice constants) at energy $E = 1$ (quarter band). The left panel shows the non-uniform distribution of the phase of the reflected wave, obtained from numerical simulations (filled circles) and our analytical theory (solid curve). The right panel show the mean of $\ln g$ from the numerical simulations (filled circles), which clearly deviate from the prediction of perturbation theory (solid line).*

allows to find and explain important situations where such single parameter scaling fails.

The violation of the single parameter scaling is shown to be related to the lattice symmetry of the model and can be essentially enhanced if disorder is short-range correlated. It turns out that a specific disordered potential can have different effects on the wave-functions at different energies. In one dimension this leads to a partial delocalization of certain states on the lattice. A well-known example is the Dyson singularity in the localization length (affecting also other quantities, such as the density of states) which is caused by the presence of a completely delocalized state at the band center. It emerges in systems where the potential disorder is absent and only hopping integrals fluctuate. The existence of similar effects in lattice models with potential disorder and the ensuing deviations from single-parameter scaling is an entirely new development [1–4].

We discuss these effects in terms of the self-averaging behavior of the logarithm of the conductance g. In one-dimension, $\ln g$ is an additive quantity in the sample length n (measured in units of the lattice constant). The fluctuations of $\ln g$ are shown to fulfill the central limit theorem, which predicts a linear growth of cumulants with the system size $\langle\langle(-\ln g)^j\rangle\rangle = C_j n + \mathcal{O}(1)$, where the coefficients C_j are proven to be universal. In the simplest model of white-noise potential disorder the single parameter scaling predicts $C_2 = 2C_1$ with all other coefficients vanishing, $C_j = 0$ for $j \geq 3$. However, small deviations from such behavior can be observed in the vicinity of the band center and of the band edge [2]. The ratios C_2/C_1 and C_3/C_1 are plotted at Fig. 1. The finite value of the ratio C_3/C_1 demonstrates the violation of single parameter scaling.

The possibility to observe Anderson localization of electrons is limited to low dimensional systems at low temperatures. However, a similar phenomena (dynamical localization) exists in optical lattices. In experiments on atoms driven by a regular train of laser pulses, the probability distribution function of atoms in momentum space is seen to relax from an initial Gaussian into an exponential profile, demonstrating the absence of diffusion in momentum direction.

The widely used model which captures many essential details of the experiments is the kicked rotator, which in turn has been mapped onto the Anderson model with an effectively random Cauchy-distributed potential (Lloyd model). The wave-function profile Ψ in the localized regime is again characterized by the coefficients C_j in the central limit theorem, $\left\langle\left\langle(\ln|\Psi|^2)^j\right\rangle\right\rangle = C_j n + \mathcal{O}(1)$, with the only difference that n counts the number of laser pulses (kicks). We demonstrate in Ref. [4] that the lattice model with Cauchy disorder gives rise to multiscaling behavior. Some of our results are presented in Fig. 2.

Work in progress indicates that the anomalies of the wave-function fluctuations are greatly enhanced if the disordered potential has finite-range correlations. As an example, we consider a model of disorder with correlations over three lattice sites. As shown in Fig. 3, at energy $E = 1$ the phase of the reflected wave is not uniformly distributed, and the localization length departs from the perturbative estimate. Both observations violate the basic assumptions of single-parameter scaling.

[1] H. Schomerus and M. Titov, Phys. Rev. E **66**, 066207 (2002).

[2] H. Schomerus and M. Titov, Phys. Rev. B **67**, 100201(R) (2003).

[3] H. Schomerus and M. Titov, Eur. Phys. J. B **35**, 421 (2003).

[4] M. Titov and H. Schomerus, Phys. Rev. Lett. **91**, 176601 (2003).

3.1.22 Electrical response of molecular chains from density functional theory

Stephan Kümmel, Leeor Kronik, and John P. Perdew

Molecular chains are systems that consist of a linear sequence of molecular units. Such chains are important in different fields and contexts, ranging from biochemistry to plastics fabrication. Among the many classes of molecular chains, conjugated chains, i.e., chains with alternating single and double bonds, are of particular interest in the field of molecular electronics and nonlinear optics. The prototypical example of a conjugated chain is polyacetylene, the electronic structure of which is schematically depicted in Fig. 1. The valence electrons in such a chain show a very high mobility along the backbone of the chain, but very little perpendicular to it. This leads to a fast, large, and directional electrical response in the linear as well as in the nonlinear regime. Therefore, hopes are high that materials based on such chains can be used as alternatives to inorganic solids for non-linear optics tasks such as frequency doubling of lasers, and also to build advanced nonlinear optics devices.

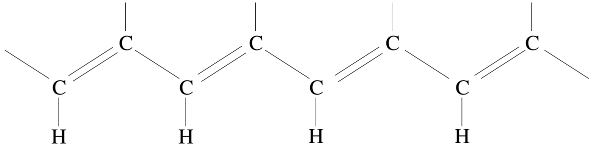

Figure 1: *Schematical sketch of the electronic structure of the conjugated chain trans-polyacetylene.*