Spatial and Spectral Multifractality of the Local Density of States at the Mobility Edge

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We performed numerical calculations of the local density of states (LDOS) at disorder induced localization-delocalization transitions. The LDOS defines a spatial measure for fixed energy and a spectral measure for fixed position. At the mobility edge both measures are multifractal and their generalized dimensions \( D(q) \) and \( \tilde{D}(q) \) are found to be proportional: \( D(q) = d \tilde{D}(q) \), where \( d \) is the dimension of the system. This observation is consistent with the identification of the frequency-dependent length scale \( L_\omega \propto \omega^{-1/d} \) as an effective system size. The calculations are performed for two- and three-dimensional dynamical network models with local time evolution operators. The energy dependence of the LDOS is obtained from the time evolution of the local wavefunction amplitude of a wave packet, providing a numerically efficient way to obtain information about the multifractal exponents of the system.

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In the presence of disorder electronic states in phase-coherent systems can get localized. For dimensions \( d \geq 2 \) such a disordered system can exhibit a transition from localized to extended eigenstates as a function of energy or strength of the disorder, similar to continuous thermodynamic phase transitions \[1\]. This transition is accompanied by a diverging length scale \( \xi(E) \propto |E - E_c|^{-\nu} \) that can be identified for localized states with the localization length. Here \( E_c \) is the critical energy of the transition. On length scales shorter than \( \xi(E) \) the eigenstates exhibit strong fluctuations \[2\]. Sufficiently close to the transition the localization length exceeds the system size so that the wave functions fluctuate on all length scales up to the system size \( L \). The squared modulus of these critical eigenstates forms a multifractal measure \( \rho(r) = |\psi(r)|^2 \) \[3\]. The scaling behavior of multifractal measures is determined by an infinite set of exponents \( D(q) \), called generalized dimensions. The multifractal fluctuations lead to anomalous behavior of the diffusion coefficient \[4\].

The localization properties of the wavefunction are also reflected in the spectral properties of the system. Localized states correspond to a pure point like spectrum, extended states to an absolutely continuous spectrum, and critical states to a singular continuous spectrum. The latter kind of spectrum was observed in quasiperiodic systems \[5\], systems on incommensurate structures \[6\], in crystals in a magnetic field \[7\], and also in random one-dimensional systems \[8\]. For these systems the spectral measure excited by a wave packet is multifractal. Of particular interest has been the implications of the local spectra for dynamical properties \[9\]. Ketzmerick, Petschel, and Geisel \[10\] found that the return probability of a wave packet decays in time \( t \) asymptotically as \( t^{-\tilde{D}(2)} \), where \( \tilde{D}(2) \) is the correlation dimension of the associated spectral measure, the local density of states (LDOS).

The two aspects of spatial and spectral multifractality were brought together by Huckestein and Schweitzer who showed that enhanced return probability of wavepackets at the mobility edge of quantum Hall systems could be interpreted both from the spectral \[11\] as well as the spatial properties of the local density of states \[12\]. They showed that the generalized dimensions \( D(2) \) and \( \tilde{D}(2) \) characterizing the second moments of the spatial and spectral measures, respectively, are related by the spatial dimension \( d = 2 \) of the system, \( D(2) = d \tilde{D}(2) \). This follows from dynamical scaling by which the two-particle spectral function \( S(q, \omega) \) becomes a function of \( q L_\omega \) at criticality \[13\]. Here, \( L_\omega = (\rho(E_c)\omega)^{-1/d} \) can be interpreted as the system size with mean level spacing \( \omega \) and \( \rho(E_c) \) is the density of states at the mobility edge \[14\]. The length scale \( L_\omega \) introduced by the finite frequency \( \omega \) cuts off correlations and acts as an effective system size \[15\]. Recently, the same relation was shown to hold in three dimensional systems at the Anderson transition \[16\].

In this letter, we show that at the mobility edge the spatial and spectral structures of the LDOS are intimately related: their respective generalized dimensions \( D(q) \) and \( \tilde{D}(q) \) are proportional,

\[
D(q) = d \tilde{D}(q),
\]

where \( d \) is the space dimension of the system. This relation, generalizing the result of ref. \[17\] to arbitrary \( q \), is a consequence of the length scale \( L_\omega \) acting quite generally as an effective system size, not only for correlation functions but also for moments of the LDOS. We test the relation numerically for two- and three-dimensional network models \[18\]. Introducing a time evolution into
these models \[18\] allows us to calculate the LDOS by studying the time evolution of wave packets. This provides a new efficient method to obtain the multifractal exponents of the LDOS without the need to diagonalize large matrices.

Before motivating the relation \[\text{(3)}\] let us define our multifractal analysis. We study a normalized multifractal density \(\rho(x)\) on a \(d\)-dimensional domain \(\Omega\). Here, \(\Omega\) is the two- or three-dimensional space or the one-dimensional energy axis, depending on whether we study the spatial or spectral aspect of the LDOS. We study the scaling of the box probabilities with respect to the box sizes \(l\). \(\Omega_i(l)\) is the volume of the \(i\)th of \(N_l = (L/l)^d\) non-overlapping hypercubes of linear size \(l\) covering the whole domain \(\Omega\) of linear size \(L\). For a multifractal density the averaged \(q\)th moments, \(\langle P^q(l,L) \rangle = N_l^{-1} \sum_{i=1}^{N_l} (P_i(l))^q\), show power law dependence on \(l/L \ll 1\) for all real \(q\),

\[
\langle P^q(l,L) \rangle \propto \left( \frac{l}{L} \right)^{d+\tau(q)} .
\] (3)

The distinguishing feature of a multifractal is that the exponents \(\tau(q) \equiv (q-1)\tilde{D}(q)\) are a non-linear function of \(q\). A multifractal is thus described by a non-countable set of exponents \(D(q)\). If the multifractal measure is taken from a statistical ensemble, the system average over the box probabilities can be replaced by an ensemble average for a single box.

The LDOS is given by \(\rho(r,E) = \sum_\alpha \delta(E-E_\alpha)|\phi_\alpha(r)|^2\), where the sum runs over the quantum numbers \(\alpha\) with corresponding eigenstates \(\phi_\alpha\). At energies \(E\) close to the mobility edge \(E_c\) the LDOS exhibits multifractal properties on length scales between microscopic lengths, like the lattice constant \(a\) or the elastic mean free path, and the system size \(L\) or the correlation length \(\xi(E)\). The corresponding lower and upper energy scales are the mean level spacing \(\Delta = \rho(E_c)^{-1}L^{-d}\) and \(E_\xi \propto L^{-\nu}\), respectively. For energies \(\omega\) less than \(E_\xi\) the correlation length \(\xi(\omega)\) exceeds the system size \(L\).

We now argue that the existence of a single frequency-dependent length scale \(L_\omega\) implies the relation \[\text{(3)}\]. Consider box probabilities of the LDOS with respect to both space and energy

\[
P_i(l,\omega) = \int_{\Omega_i(l)} d^d x \int_{E_i + \frac{\omega}{L}}^{E_i + \frac{\omega}{l}} dE \rho(r,E) ,
\] (4)

where we consider an energy interval in the critical region described above. For energies \(\omega\) less than the mean level spacing \(\Delta\) these box probabilities scale like single eigenfunctions, \(P^q(l,\omega) \propto (l/L)^{d+\tau(q)}\). For energies larger than the mean level spacing, we expect the disorder average of the moments of these box probabilities to scale with the same exponents but with the system size \(L\) replaced by a frequency-dependent effective system size \(L_\omega\),

\[
\langle P^q(l,\omega) \rangle \propto \left( \frac{l}{L_\omega} \right)^{d+\tau(q)} .
\] (5)

In principle, the frequency-dependent length scale introduced in eq. \[\text{(3)}\] could depend on \(q\). However, if we assume that there exists only one such length scale, then we can identify \(L_\omega\) with \((\rho(E_c)\omega)^{-1/d}\) by considering the first moment

\[
\langle P_1(l,\omega) \rangle = \rho(E_c)\omega^d \propto \left( \frac{l}{L_\omega} \right)^d .
\] (6)

The scaling of the spectral measure defined by the LDOS follows from eq. \[\text{(3)}\] by choosing the spatial box size \(l\) of the order of the microscopic length scale \(\ell\), below which the wavefunctions become smooth functions of coordinate. The scaling of the spectral measure with respect to energy defines the exponents \(\tilde{r}(q) \equiv (q-1)\tilde{D}(q)\),

\[
\langle P^q(\ell,\omega) \rangle \propto \left( \rho(E_c)\ell^d \omega \right)^{1+\tilde{r}(q)/d} \propto \omega^{1+\tilde{r}(q)} ,
\] (7)

leading to eq. \[\text{(3)}\].

For our computations, we consider two normalized measures, the spatial measure \(\rho(r) = |\psi_\alpha(r)|^2\) and the spectral measure \(\tilde{\rho}(E) = A^{-1}\rho(r_0,E)\). The spatial measure is normalized since the eigenfunctions are normalized, and the spectral measure is explicitly normalized on an energy interval \(E\), satisfying \(E \ll E_\xi\). To support the validity of eq. \[\text{(3)}\] we now present results of numerical calculations. Fig. \[\text{(3)}\] shows the functions \(D(q)\) and \(2\tilde{D}(q)\) calculated for a two-dimensional network model at the quantum Hall critical point \[\text{[13,18]}\]. The functions

\[\text{FIG. 1. Generalized dimensions } D(q)/2 \text{ (○) and } \tilde{D}(q) \text{ (□) for a two-dimensional network model at the quantum Hall critical point. Systems of size } 150 \times 150 \text{ (○) and } 200 \times 200 \text{ (□) were used and the statistical uncertainties are smaller than the symbol sizes.}\]
agree within the error bars. In order to check the dependence on the spatial dimension $d$ of the system we study a three-dimensional network introduced recently [7]. In contrast to the two-dimensional network here a band of extended states appears. At the mobility edge of this system we again find good agreement with eq. (1) as seen in Fig. 3.

We now describe our new numerical method of obtaining the LDOS. We use two- and three-dimensional network models, describing the integer quantum Hall effect [10] and the so called quantum Hall-insulator [17], respectively. Both models are extended to dynamical network models by providing them with a unitary time evolution operator $U$ for discrete microscopic time steps [18]. Within these models the evolution—involving full quantum interference—of arbitrary initial states can be obtained easily by iterative application of $U$. In particular, the time evolution of a state $\psi$ initially sharply peaked at coordinate $r_0$ yields the temporal Green’s function $G(r_0,r_0;t)$. The LDOS is then the Fourier transform of this quantity. This provides an efficient method of calculating the LDOS, without the need to diagonalize the operator $U$ or the associated Hamiltonian.

Starting point of our calculations is the 2D-network model introduced by Chalker and Coddington [10] to describe non-interacting spinless electrons in the integer Quantum Hall regime. It exhibits a localization-delocalization-transition characteristic for the QHE: except for the critical energy $E_c$ all states are localized, with a localization length $\xi \propto |E-E_c|^{-\nu}$, $\nu = 2.3$. Origin of the model and exact definitions can be found in refs. [10] and [18], here we give only a brief description restricted to our purposes.

The network consists of $2 \times 2$ scattering matrices as nodes which are arranged on a square lattice and connected by one-dimensional unidirectional channels, called links. The scattering matrices contain coefficients $t_{lm}$ describing transitions from electron states on incoming links $\psi_l$ to outgoing link states $\psi_m$. At the critical point the transmission amplitudes are of constant value $T_{ml} = |t_{ml}|^2 = 1/2$, while the disorder is given by randomly distributed arguments of the coefficients $t_{ml}$.

States (or wave functions) $\psi$ on the network are $N$-dimensional complex vectors $\psi = \{\psi_l\}_{l=1,2,...,N}$, where the $l$-th component denotes the complex amplitude on link $l$. The network operator $U$ is defined by its action on single link states $e_l = \{\delta_{lk}\}_{k=1,...,N}$,

$$U e_l = t_{ml} e_m + t_{nl} e_n,$$  

where $t_{ml}$ and $t_{nl}$ are the transmission coefficients from an incoming link $l$ into two outgoing links $m$ and $n$ at a node [18].

Here we use $U$ as the time evolution operator in discrete time steps for states on the network. To motivate this, consider a particle at critical energy $E_c$ in the incoming link $l$ of node $j$, that is described by the state $\psi(0) = e_l$. After a characteristic time $\tau$ (we choose $\tau = 1$ in the following) the incident wavepacket has passed the scatterer and thereby split into two outgoing packets in the channels $m$ and $n$ (see fig. 1 in ref. [18]). This process corresponds just to the acting of $U$ on $\psi(0)$ as seen in Fig. 3.

$$\psi(0) \rightarrow \psi(1) = U \psi(0) = t_{ml} e_m + t_{nl} e_n.$$

Since this happens in the same way at all scatterers we generalize relation (3) to the time evolution of an arbitrary state and define

$$\psi(t + n) = U^n \psi(t),$$  

for integer $n$. With the latter definition the original static network becomes a quantum-dynamical model of a disordered system. We can relate the eigenvectors $\{\Phi^{\omega}\}$ with eigenvalues $\{e^{-i\omega}\}$ of $U$ to eigenfunctions and energy spectrum of a Hamiltonian $H$ by identifying [9,20]

$$U = \exp(-iH\tau).$$  

To obtain the LDOS $\tilde{\rho}_l(\omega) = \sum_{\omega'} \delta(\omega - \omega')|\phi^{\omega'}|^2$ (the sum runs over all eigenvalues $\omega'$ of $H$) at link $l$, we calculate numerically the temporal Green’s function $G(l,l;t) = \langle \psi_l | U^t | \psi_l \rangle$. In terms of the eigenstates of $U$ the Green’s function is given by

$$G(l,l;t) = \sum_{\omega} |\langle \psi_l | \phi^{\omega} \rangle|^2 e^{-i\omega t} = \int d\omega \tilde{\rho}_l(\omega) e^{-i\omega t}.\quad (11)$$

Hence the LDOS $\tilde{\rho}_l(\omega)$ can be obtained by an inverse Fourier transform of $G(l,l;t)$, which on the other hand can be generated iteratively according to (4).
each finite time $T$ for a quantum Hall system of $200 \times 200$ nodes. Due to the finite time $T$ (16384 iterations) of the Fourier transform each $\delta$-function in the LDOS is broadened into a peak of width $\Delta \omega = 2\pi/T$.

$$\tilde{\rho}_l(\omega) = \frac{1}{2\pi} \int dt G(l, l; t)e^{i\omega t} = \frac{1}{\pi} \text{Re} \int_0^\infty dt G(l, l; t)e^{i\omega t}. \quad (12)$$

Fig. (3) shows as an example the energy dependence of the LDOS obtained in that way.

The three-dimensional network investigated here is very similar to the one studied by Chalker and Dohmen \[17\]. It is built out of layered two-dimensional networks with additional inter-layer couplings, that we choose slightly different from Chalker and Dohmen \[20\].

In conclusion, we studied numerically the spatial and spectral multifractal measures defined by the local density of states (LDOS) at the mobility edge of two- and three-dimensional disordered electron systems. We have presented evidence that both of these measures are equivalent, as the ratio of their respective generalized dimensions $D(q)$ and $\tilde{D}(q)$ is simply given by the dimension of the system. This result is interpreted as a consequence of the occurrence of a single energy-dependent length scale $L_\omega = (\rho(E_\omega)\omega)^{-1/d}$ acting as the effective system size. The numerical calculations were performed for two- and three-dimensional network models. These model, endowed with a discrete time evolution, turned out to be especially suitable for determining the LDOS as a function of energy.

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