Multifractal structure of eigenstates in the Anderson model with long-range off-diagonal disorder

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The spectrum of eigenvalues and the spatial structure of eigenstates for the Anderson model with long-range off-diagonal disorder ($V_{ij}=(\pm)/|\mathbf{R}_i-\mathbf{R}_j|^d$) is investigated numerically where $\mathbf{R}_i$ are Poisson-distributed random points in d-dimensional space. For this marginal case all states in the system are delocalized. Analyzing the scaling with system size of the inverse participation numbers for the most extended modes we find that these states exhibit a self-similar multifractal structure. The generalized dimensions, D_q, and the multifractal spectrum, $f(\alpha)$, are calculated. For $d=3$ the information dimension $D_1=2.65$ and the correlation dimension $D_2=2.33$ that characterizes the power-law behavior of the averaged two-particle Green function. The temporal autocorrelation function $C(t)$ built from the eigenstates of the most dispersive oscillator exhibits an nondiffusive algebraic decay $C(t)\sim t^{-\delta}$ with the exponent $\delta\equiv\tilde{D}_2=D_2/d$ reflecting the generalized multifractal dimension of the local density of states. [S0163-1829(98)02617-4]

Since the first paper of Anderson[1] on quantum localization of excitations in disordered systems our understanding of this difficult theoretical problem has progressed enormously. The disorder-induced localization-delocalization transition was found to manifest itself by a complex spatial behavior of the wave functions believed to have multifractal structure[2–5] at the localization threshold (or in finite size samples for localization lengths exceeding the sample size L).

Usually Hamiltonians with short-range, off-diagonal matrix elements are investigated. In the often used tight-binding model (also called Anderson model with diagonal disorder) the criterion of state localization in three-dimensional (3D) systems depends on the ratio between diagonal disorder and the off-diagonal transition matrix elements between neighboring states taken to be constant. In 1D and 2D systems, independent of this ratio, in the thermodynamic limit all states are localized in this model.[6]

From the above it seems interesting to investigate the opposite case: *long-range off-diagonal disorder* where for some distance dependence of the nondiagonal matrix elements, $V(R)$, all states are delocalized. For the 3D case this was proven for $V(R)$ falling off $\propto 1/R^3$ or slower[1] (see also Ref. 7). This dependence of transition matrix elements is characteristic for the dipole interaction between elastic defects in solids. It was shown recently that such an interaction between soft harmonic oscillators leads to the universal linear frequency dependence of the density of states above the boson peak in glasses.[8] It is remarkable that 95% vibrational states in glasses are usually neither localized nor propagating in the usual plane wave sense. These modes have been termed diffusons.[9] Their spatial structure is still a challenge to physicists in this field as well as for the *marginal* case of the Anderson model in general. A connected important problem is the diffusion of excitations in this model that in turn is relevant, e.g., for the thermal conduction. The 3D results can be extended to other dimensions 3 replacing $1/R^3$ by $1/R^d$.

A second motivation for this work is the increasing interest in statistical properties of large random matrixes, $N\times N$. We find drastic differences compared to the Wigner-Dyson random matrix theory for statistically independent off-diagonal matrix elements.[10] The triangle rule for distances implied in the $1/R^d$ law introduces specific correlations between the off-diagonal matrix elements causing in turn multifractal properties of the eigenstates. The distribution of the eigenvalues is also very different. In the Wigner semicircle the density of states at small energies is size dependent, $\propto 1/\sqrt{N}$. In our case it is size independent, i.e., it is finite in the thermodynamic limit.

In the present paper we study numerically the spectrum and eigenvector statistics of large $N\times N$ real symmetric matrixes $\hat{V}$ with purely off-diagonal disorder. Without loss of generality all diagonal matrix elements are set to zero. Off-diagonal disorder is introduced as $V_{ij}=(\pm 1)/|\mathbf{R}_i-\mathbf{R}_j|^d$. Here $\mathbf{R}_i$ are Poisson-distributed random points in d dimensional space ($d=1,2,3$), and the random sign, ± 1 provides for the average value $\langle V_{ij}\rangle=0$ corresponding to the interaction of randomly oriented electric or elastic dipoles.

We place N random points, s (in the following called oscillators) according to Poisson statistics in a d-dimensional ''cube'' of size $L=N^{1/d}$ ($100\leqslant N\leqslant 10000$) thus keeping the average concentration of oscillators constant. Diagonalizing the matrix $\hat{V}$ we find a set of N orthonormal eigenvectors $e_s(j)$ with

$$\sum_{s=1}^{N} e_s^2(j)=\sum_{j=1}^{N} e_s^2(j)=1 \tag{1}$$

and corresponding eigenvalues, ω_j. This is repeated until the relative variance of the average values, discussed in the fol-

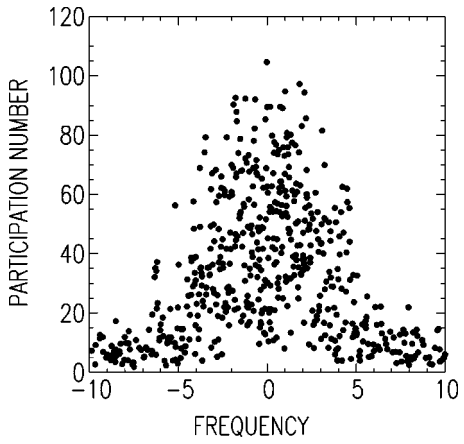

FIG. 1. Participation numbers versus frequency for a 3D system of 800 oscillators.

lowing, has dropped well below the percent level, i.e., for the smaller systems typically for several hundred configurations.

As the usual measure of localization of the states j we calculate for each realization of $\hat{V}$ the participation ratio

$$P_j=\left(N\sum_{s=1}^{N} e_s^4(j)\right)^{-1}. \tag{2}$$

The product $NP_j\equiv N_j$, the participation number, shows how many oscillators participate in the mode j (frequency ω_j). Figure 1 shows the participation numbers N_j versus frequencies ω_j for a 3D system of 800 oscillators. Striking are the strong fluctuations of N_j for small ω_j. Here we are mainly interested in the mode j_m (frequency ω_m) with the maximal participation number (ratio) which is the most extended one in the system. An example of the spatial structure of the eigenvector of such a mode in a 1D system of 1000 oscillators is shown in Fig. 2. For a given number N of oscillators, the fluctuations of the maximum participation number N_m from sample to sample are relatively small. After averaging it can, therefore, be used as a characteristic quantity of systems with given N.

To study the multifractal properties of the eigenstates we investigate the scaling with N (or equivalently system size

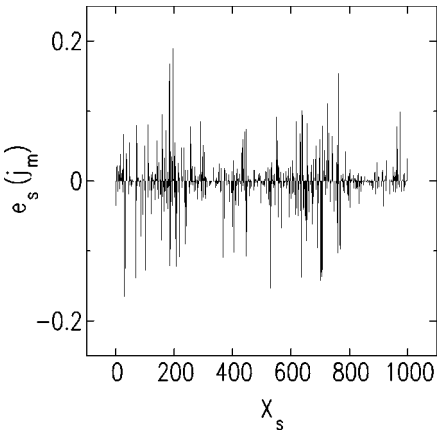

FIG. 2. The most extended mode in a one-dimensional system of 1000 oscillators.

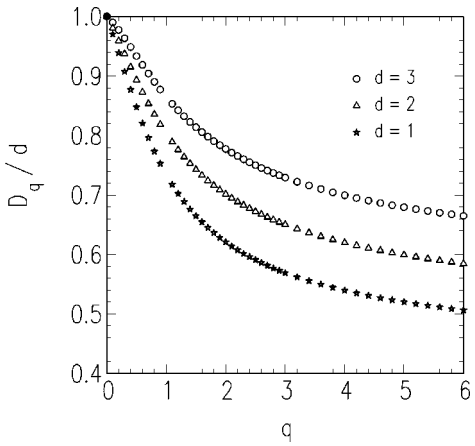

FIG. 3. Generalized dimensions for the most extended eigenstates as function of q for one-, two- and three-dimensional systems.

L) of the generalized inverse participation numbers of these maximally extended modes j_m

$$M_q=\left\langle \sum_{s=1}^{N} [e_s^2(j_m)]^q \right\rangle_N \propto N^{-(q-1)D_q/d}=L^{-(q-1)D_q}. \tag{3}$$

Here and in the following angular brackets denote averaging over the samples with given number N. If the generalized dimension D_q depends on q one speaks of a multifractal structure of the eigenstates.[11] Figure 3 shows the functions D_q/d for $d=1,2,3$ obtained from our numerical simulation. Nonzero values of D_2 imply delocalization of the most extended states in the system. A plane-wave-like state would give a constant value $D_q/d=1$. In the multifractal analysis one usually calls D_2 the correlation dimension.[12] We obtain values of 0.62, 1.40, and 2.33 for the 1D, 2D, and 3D cases, respectively. The corresponding values for the information dimension D_1 are 0.74, 1.61 and 2.60. For a disordered electron system near the Anderson transition D_2 determines the exponent in the power law behavior of the averaged two-particle Green function.[4] In our case, using the scale independence of the density of states (see below), we can derive for this function a similar relation valid for the most extended states in our system:

$$\overline{|G^+(r,\omega_m)|^2}\propto L^{-d}(L/r)^{d-D_2}, \quad r\ll L. \tag{4}$$

Knowing the functional form of D_q one can calculate the multifractal spectrum $f(\alpha)$, related by a Legendre transformation[13] to the exponent in Eq. (3), $\tau_q=(q-1)D_q$,

$$f(\alpha)=\alpha\cdot q-\tau_q \tag{5}$$

with $\alpha=d\tau_q/dq$. In the single fractal case ($D_q=D=\text{const}$) the function $f(\alpha)$ consists of only one point (D,D) in the $(f(\alpha),\alpha)$ plane. The physical meaning and the significance of the function $f(\alpha)$ can be understood from the following consideration. Let us introduce the distribution function of the eigenvector amplitudes for the most extended modes, $e_s^2(j_m)$, in the ensemble

$$P_N(x)=\frac{1}{N}\left\langle \sum_{s=1}^{N} \delta(x-e_s^2(j_m)) \right\rangle_N . \quad (6)$$

The generalized inverse participation numbers can then be expressed as

$$M_q=N\langle x^q\rangle=N\int_0^1 P_N(x)x^q dx. \quad (7)$$

Changing to a new variable, $\alpha=-d\ \ln x/\ln N$, and the corresponding distribution function, $\mathcal{P}_N(\alpha)d\alpha\leftrightarrow P_N(x)dx$, and setting $\mathcal{P}_N(\alpha)=\rho_N(\alpha)N^{f(\alpha)/d-1}$ (Ref. 13) we obtain

$$M_q=\int_0^\infty d\alpha\,\rho_N(\alpha)N^{[f(\alpha)-q\alpha]/d}. \quad (8)$$

For $N\to\infty$ the main contribution to the integral in Eq. (8) will originate from that value α where $f(\alpha)-q\alpha$ is extremal, provided that $\rho_N(\alpha)$ is a smooth function of α which does not vanish at this particular α-value. The extremeness condition $q=f'(\alpha)$ is the reverse of the Legendre transformation Eq. (5) whence using $(q-1)D_q=q\alpha(q)-f(\alpha(q))$ we regain Eq. (3). Thus, $f(\alpha)$ determines the distribution function of the squared oscillators amplitudes (or their energies) for the most extended state. In general, as well as in our case, $f(\alpha)$ is a convex function of α with a single maximum at $\alpha_{\max}$ and can be approximated by parabola near this maximum. This implies that the distribution function $P_N(x)$ is almost log-normal. This fundamental property was first discovered in disordered electron systems for mesoscopic conductance fluctuations.[14]

Another interesting quantity analogous to the participation number is the *dispersion number*

$$K_s=\left(\sum_{j=1}^{N} e_s^4(j)\right)^{-1}. \quad (9)$$

It measures in how many modes j the oscillator number s effectively participates. Again we are interested in the oscillator s_m with the maximal K_m in each sample. Again K_m fluctuates only weakly between the samples. Obviously if the oscillator with maximum dispersion number is excited it will lose its energy more rapidly than the others. Therefore, ''diffusion'' of energy from this oscillator will be fastest in the system.

In case at $t=0$ all amplitudes are zero but for one oscillator s, whose complex amplitude $A_s(t=0)=1$ one has

$$A_s(t)=\sum_j e_s^2(j)e^{i\omega_j t}. \quad (10)$$

A temporal autocorrelation function $C(t)$ was defined in Ref. 15 by smoothing of the probability to be in the initial state at time t

$$C_s(t)=\frac{1}{t}\int_0^t dt'|A_s(t')|^2\sim t^{-\delta}. \quad (11)$$

Conventional diffusive behavior gives $\delta=d/2$. However, if the corresponding spectral measure is multifractal, then

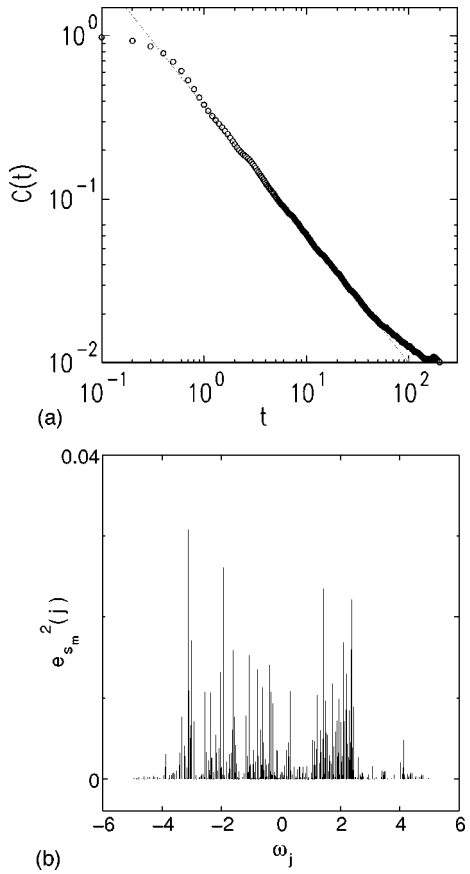

FIG. 4. (a) Temporal autocorrelation function of the most dispersive oscillator ($K_m=102$) in a 3D system of 1000 oscillators. (b) Local density of states for this oscillator.

$\delta=\tilde{D}_2$, with $\tilde{D}_2$ the correlation dimension of the associated spectral measure, the local density of states (LDOS) for oscillator s.[15]

For a two-dimensional disordered electron system in a strong magnetic field it was found that at the mobility edge the generalized dimensions D_2 and $\tilde{D}_2$ characterizing the second moments of the spatial and spectral measures, respectively, are related to each other, $\tilde{D}_2=D_2/d$ (with $d=2$).[16] Recently this result was generalized to $3d$ systems.[17] For our Hamiltonian we find that the same relation is valid in all three dimensions. As an example we show in Fig. 4(a) the function $C(t)$ for the oscillator with maximal dispersion number in a 3D system of 1000 oscillators. A least square fit gives for the slope, $\delta\approx 0.79$, very close to the ratio $D_2/3\approx 0.78$ found for this dimension. Fig. 4(b) shows the LDOS for this oscillator exhibiting multifractal properties. For a 2D system we obtained, $\delta=0.72$. This means that in 3D and 2D systems the decay of the autocorrelation function is slower than for conventional diffusion. For 1D systems the situation is different, $\delta=0.61$, and the decay is faster.

One of the important characteristics of the energy spectrum is the density of states (DOS) $g(\omega)$

$$g(\omega)=\frac{1}{N}\left\langle \sum_{j=1}^{N} \delta(\omega-\omega_j) \right\rangle_N . \quad (12)$$

Usually this function is non critical and scale independent in the limit $L\to\infty$. Figure 5 shows $g(\omega)$ for 3D system with

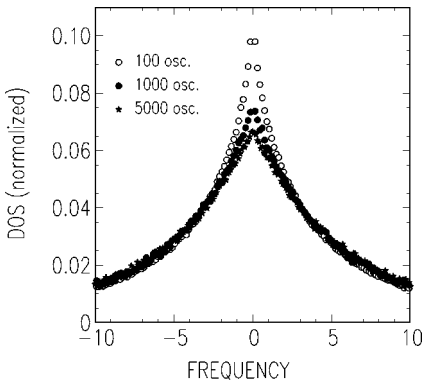

FIG. 5. Density of states for a 3D system of 100, 1000, and 5000 oscillators.

100, 1000, and 5000 oscillators. For large N the DOS does no longer depend on the system size. Using this property one can introduce a length $L_\omega=(g(0)\omega)^{-1/d}$ (Ref. 18) that can be taken as the size of the system whose mean level spacing equals ω at small ω. In our case existence of such a length might be a consequence of the invariance under the transformation $(\mathbf{r},t)\rightarrow(b\mathbf{r},b^d t)$ due to $V(R)\propto R^{-d}$.[19] Therefore, $1/L_\omega^d\propto\omega$ and $g(\omega)\rightarrow$ const for $\omega\rightarrow 0$. If this holds, then comparing the scaling behaviors of M_q and $C(t)$ leads to the relation $\tilde{D}_2=D_2/d$ observed in our computer experiment. However for more definite conclusion one needs investigate the same problem for $V(R)\propto R^{-\mu}$ with $\mu\neq d$.

To conclude, we investigated numerically the spatial structure of delocalized states in the marginal case of the Anderson model with long-range off-diagonal disorder corresponding to the important dipole interaction. Because of the long-range correlations in the system these delocalized states have multifractal spatial structure causing anomalous diffusion of excitations in this system.

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[1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[2] F. Wegner, Z. Phys. B **36**, 209 (1980).
[3] C. Castellani and L. Peliti, J. Phys. A **19**, L429 (1986).
[4] M. Janssen, Int. J. Mod. Phys. B **8**, 943 (1994).
[5] V. I. Fal'ko and K. B. Efetov, Phys. Rev. B **52**, 17 413 (1995).
[6] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
[7] L. S. Levitov, Europhys. Lett. **9**, 83 (1989).
[8] V. L. Gurevich, D. A. Parshin, J. Pelous, and H. R. Schober, Phys. Rev. B **48**, 16 318 (1993).
[9] J. Fabian and P. B. Allen, Phys. Rev. Lett. **77**, 3839 (1996).
[10] M. L. Metha, *Random Matrices and the Statistical Theory of Energy Levels* (Academic, New York, 1967).
[11] For the average participation number and its higher moments we find a similar scaling behavior. There the generalized dimensions depended weakly on the system size N. It proves that different states have a similar multifractal structure but with slightly different spectra of generalized dimensions. Therefore, multifractality holds for the whole spectrum of energies, but in general, the multifractal dimensions are a function of energy and participation number.
[12] H. G. E. Hentschel and I. Procaccia, Physica D **8**, 435 (1983).
[13] T. C. Hasley, M. H. Jensen, L. P. Kadanoff, I. Procaccia, and B. I. Shraiman, Phys. Rev. A **33**, 1141 (1986).
[14] B. L. Altshuler, V. E. Kravtsov, and I. V. Lerner, Phys. Lett. A **134**, 488 (1989).
[15] R. Ketzmerick, G. Petschel, and T. Geisel, Phys. Rev. Lett. **69**, 695 (1992).
[16] B. Huckestein and L. Schweitzer, Phys. Rev. Lett. **72**, 713 (1994).
[17] B. Huckestein and R. Klesse, Phys. Rev. B **55**, R7303 (1997).
[18] J. T. Chalker and G. J. Daniell, Phys. Rev. Lett. **61**, 593 (1988).
[19] L. S. Levitov, Phys. Rev. Lett. **64**, 547 (1990).