Localization in disordered structures: Breakdown of the self-averaging hypothesis

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We find that the relevant quantities describing the localization of electrons, vibrations, and random walks on random fractals are non-self-averaging. There exists a crossover distance $r_\times$ that increases logarithmically with the number N of configurations considered in the averages. For vibrations and electrons, the localization exponent changes from 1 below $r_\times$ to $d_{\min}$ above $r_\times$. For random walks, the exponent changes from $d_w/(d_w-1)$ to $d_{\min}d_w/(d_w-d_{\min})$, where d_w and $d_{\min}$ are the fractal dimensions of the random walk and the shortest path on the fractal, respectively. Our results explain the controversies regarding the localization exponent.

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It is well known (see, e.g., [1]) that in disordered structures, due to the absence of translational symmetry, electronic wave functions and vibrational excitations can be localized, i.e., the amplitudes of the wave functions and of the vibrational excitations decay with increasing distance from a localization center for certain energies E and frequencies ω, respectively. In recent years, the question of how electronic wave functions and vibrational excitations are localized in disordered self-similar structures has attracted much attention [2–7]. For a recent review see [8]. Closely related [7–11] to this problem is how the probability density of a random walker decreases with increasing distance r from the starting point of the random walk [10–17]. Apart from its principal relevance, the knowledge of the localization behavior in disordered self-similar systems is relevant for a large number of both experimental and theoretical issues, ranging from inelastic neutron and light scattering [18–20] to the thermally activated hopping conductivity in disordered systems [21,22] and to the viscous damping of fractons [23].

The law, however, that governs the decay of the localization functions (amplitudes of wave functions and vibrations, probability density of random walkers) has not been resolved yet. It is well accepted that asymptotically the mean localization functions decay proportional to $\exp[-\text{const}\times r^{d_\psi}]$ but different groups report on different localization exponents d_ψ. Here we show by both analytical and numerical calculations that the relevant localization functions are not self-averaged quantities and depend logarithmically on the number N of configurations taken into account in the averages. There exists a crossover distance $r_\times$ that increases logarithmically with N. Below and above $r_\times$, the averages are described by different localization exponents. This explains the puzzle regarding the values of the localization exponents [2–8,10–17].

To treat the three localization problems simultaneously, we introduce a function $\psi_i^{(\nu)}(r)$ which stands either for the amplitude $\phi_i^{(\nu)}(r,E)$ of the electronic wave function or for the amplitude $u_i^{(\nu)}(r,\omega)$ of the displacement of a vibrating particle, both on a site i at distance r from the localization center, or for the probability $P_i^{(\nu)}(r,t)$ to find a random walker (after t time steps) on a site i at distance r from its starting point; the upper index ν labels the configuration.

Our basic assumption is that the shortest-path distance ("chemical length") l rather than their Euclidean distance r between two points on the fractal is the relevant physical length in the problem, such that the fluctuations of $\psi_i^{(\nu)}(l)$ on sites i at fixed chemical distance l from the localization center are small, for both the same and different configurations. For simplicity we follow [5,10,11,15] and assume that

$$\psi_i^{(\nu)}(l)\cong\Psi(l)\sim\exp[-(l/\xi_l)^v]\ , \tag{1}$$

where $v=1$ for fractons and electrons and $v=d_w/(d_w-d_{\min})$ for random walks on the fractal. Here, d_w describes how the root mean square displacement $\langle R(t)\rangle\sim t^{1/d_w}$ of a random walker changes with time t and $d_{\min}$ is the fractal dimension of the shortest path on the fractal, $\langle l(r)\rangle\sim r^{d_{\min}}$. Relation (1) is rigorous for random walks, localized wave functions, and localized vibrations on linear chains with a single defect, with $v=2$ for random walks. It has been argued in [2] that (1) with $v=1$ holds also for electronic wave functions localized around deep impurities on percolation clusters. Computer simulations [15] have shown that (1) holds also for random walks on percolation cluster, and it is believed that (1) is also a good approximation for fractons in percolation clusters (see also the discussion in [5]).

To obtain the mean localization functions, one first averages $\psi_i^{(\nu)}(r)$ over all $N_r^{(\nu)}$ sites i at distance r from the localization center in the νth configuration, according to

$$\Psi^{(\nu)}(r)=\frac{1}{N_r^{(\nu)}}\sum_{i=1}^{N_r^{(\nu)}}\psi_i^{(\nu)}(r)\ . \tag{2}$$

Assuming that among the $N_r^{(\nu)}$ sites $N_l^{(\nu)}(r)$ sites are at chemical distance l from the center and employing Eq. (1), we can write $\Psi^{(\nu)}(r)=(1/N_r^{(\nu)})\sum_l N_l^{(\nu)}(r)\Psi(l)$. Averaging over N configurations and replacing the sum by an integral yields the localization function of interest,

$$\langle \Psi(r) \rangle_N = \int_{l_{\min}(r,N)}^{\infty} \phi(l|r;N)\Psi(l)dl \ , \tag{3}$$

where $\phi(l|r;N)$ is the average of $N_l^{(\nu)}(r)/N_r^{(\nu)}$ over N configurations for a range dl near l, and $l_{\min}$ is defined as $\phi(l|r;N)=0$ for $l<l_{\min}$.

Equation (3) reveals that averaging the localization functions involves both a simple arithmetic average $[\phi(l|r;N)]$ that is independent of N for large N and a minimization procedure $[l_{\min}(r,N)]$. Naturally, the minimum value $l_{\min}(r,N)$ depends strongly on N, and this causes, as we shall see below, the breakdown of self-averaging and scaling at large distances r. The average $\phi(l|r;N)$ can be written as [5] (see also [24])

$$\phi(l|r;N)\equiv\phi(l|r)=\frac{C_1}{l}\left[\frac{r}{l^{1/d_{\min}}}\right]^g \times\exp\left[-C_2\left[\frac{r}{l^{1/d_{\min}}}\right]^{\tilde{\delta}}\right] \tag{4}$$

with $\tilde{\delta}=d_{\min}/(d_{\min}-1)$. For linear fractals generated by random walks (RW structures), we have $C_2=d/2$, $d_{\min}=2$, and $g=d-2$. For percolation clusters, where $d_{\min}\cong 1.13$ in $d=2$ and $d_{\min}\cong 1.34$ in $d=3$ [11], one has $g\cong 1.35$ in $d=2$ and $g\cong 1.5$ in $d=3$. We found that C_2 is nearly independent of d: $C_2\cong 0.5$ for site percolation and $C_2\cong 1.2$ for bond percolation, on both square and simple cubic (sc) lattices [17]. For fixed r, $\phi(l|r)$ has a maximum at $l_{\max}(r)=\alpha_{\max}r^{d_{\min}}$, with $\alpha_{\max}=[\delta C_2/(g+d_{\min})]^{d_{\min}-1}$.

To determine $l_{\min}(r,N)$ (for RW and percolation structures) we have performed Monte Carlo simulations. We found [Fig. 1(a)] that $l_{\min}$ decreases monotonically with N until the absolute minimum $l_{\min}\equiv r$ is reached, according to

$$l_{\min}(r,N)=\begin{cases} r, & r\ll r_c(N) \ , \\ \alpha_{\min}(N)r^{d_{\min}}, & r\gg r_c(N) \end{cases} . \tag{5}$$

To determine the crossover value $r_c(N)$ analytically we note that the probability W_N of finding a RW structure or a percolation structure at the critical concentration p_c with $l=r=r_c$ in a square or sc lattice with coordination number z is $W_N\equiv 1/N=zp^{r_c}$, with $p=1/z$ for RW structures and $p=p_c$ for percolation clusters. This yields

$$r_c(N)=\begin{cases} (\ln z+\ln N)/\ln z, & \text{RW structure} \ , \\ (\ln z+\ln N)/\ln(1/p_c), & \text{percolation} \ . \end{cases} \tag{6}$$

To determine $\alpha_{\min}(N)$ we assume scaling, $l_{\min}(r,N)=r_c g(r/r_c)$. In order to satisfy (5), we must require $g(x)=x$ for $x\ll 1$ and $g(x)=g_1 x^{d_{\min}}$ for $x\gg 1$. This yields

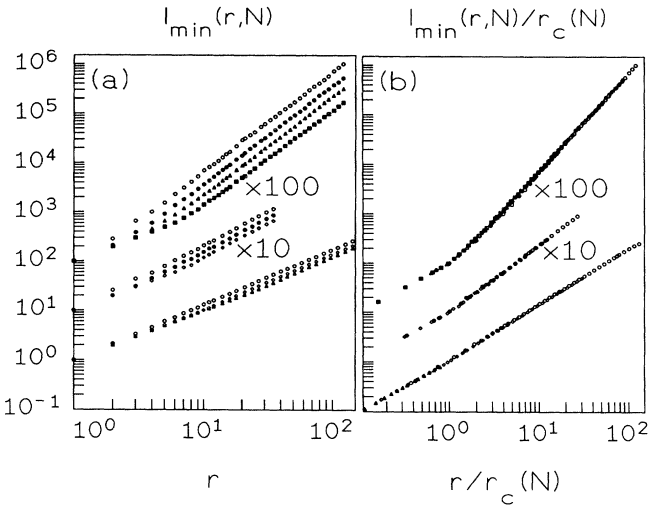

FIG. 1. (a) The minimum distance $l_{\min}(r,N)$ vs r for (from top to bottom) (a1) RW structures on the sc lattice [$N=1$ (circle), 5 (full circle), 50 (triangle), and 10 000 (full square)], (a2) bond percolation on the sc lattice [$N=1$ (circle), 10 (full circle), and 1000 (diamond)], and (a3) site percolation on the square lattice [$N=1$ (circle), 100 (diamond), and 250 000 (full triangle)]. For N below 10 000, averages have been performed over typically 100 sets of N configurations. (b) Scale plot of $l_{\min}/r_c$ vs r/r_c for the same structures and the same N values as in (a).

$$\alpha_{\min}(N)=g_1 r_c^{1-d_{\min}} \ . \tag{7}$$

Figure 1(b) shows $l_{\min}/r_c$ versus r/r_c for the same N values as in Fig. 1(a). The data collapse supports strongly the scaling ansatz, and shows that $g_1\cong 1$ for both percolation structures and $g_1\cong 0.8$ for the RW structure.

Using (4)–(7), the integral (3) can be calculated analytically. For $l_{\min}(r,N)<l<l_{\max}(r)$, the integrand in (3) is the product of two exponential functions $\Psi\phi\sim\exp[-C_2(r/l^{1/d_{\min}})^{\tilde{\delta}}-(l/\xi_l)^v]\equiv\exp[-\eta(l)]$, which shows a steep maximum at $l^*=\xi_r^{d_{\min}}(r/\xi_r)^{u/v}$, with $\xi_r^{d_{\min}}=\xi_l\{C_2/[v(d_{\min}-1)]\}^{1/v}$ and $u=vd_{\min}/[1+v(d_{\min}-1)]$. Applying the method of steepest descent, we obtain (see also [5,15])

$$\ln\langle \Psi(r) \rangle_N \sim -\eta(l^*)\sim -\left[\frac{r}{\xi_r}\right]^u . \tag{8}$$

For electrons and fractons, $u=1$ and ξ_r is proportional to the standard localization length. For random walks, $u=d_w/(d_w-1)$ and ξ_r is proportional to $\langle R(t) \rangle$.

By definition, (8) holds only for $l_{\min}(r,N)<l^*<l_{\max}(r)$, and this restriction determines the r regime $r_1<r<r_\times(N)$ where (8) is valid. We find

$$r_1=\xi_r[(g+d_{\min})/C_2\tilde{\delta}]^{1/u} \ , \tag{9a}$$

$$r_\times(N)=\xi_r g_1^{-1/[u(d_{\min}-1)]} r_c^{1/u}(N) \ . \tag{9b}$$

For $r>r_\times(N)$, the integrand in (3) is peaked sharply at $l=l_{\min}(r,N)$, and

$$\ln\langle\Psi(r)\rangle_N \sim -[l_{\min}(r,N)/\xi_l]^v \sim -r_c(N)^{v(1-d_{\min})}(r/\xi_r)^{vd_{\min}}, \quad r > r_\times(N) . \tag{10}$$

Equations (8)–(10) suggest the scaling ansatz

$$\ln\langle\Psi(r)\rangle_N = -[r_\times(N)^u] f(r/r_\times(N)) \tag{11}$$

with $f(x)\sim x^u$ for $x \ll 1$ and $f(x)\sim x^{d_{\min}v}$ for $x \gg 1$.

This scaling behavior of the localization functions represents the main result of this paper. Equations (8)–(11) show that at large distances r the relevant length scale increases *logarithmically* with the number N of configurations, and conventional scaling and self-averaging breaks down. Below $r_\times(N)\sim r_c(N)^{1/u}$ $\langle\Psi(r)\rangle_N$ is independent of N and described by the exponent u, while above $r_\times$, $\langle\Psi(r)\rangle_N$ depends logarithmically on N and is described by the exponent $vd_{\min}$. For fractons and electrons, $u=1$ and $vd_{\min}=d_{\min}$, while for random walks $u=d_w/(d_w-1)$ and $vd_{\min}=d_{\min}d_w/(d_w-d_{\min})$.

Our approach enables us to shed light onto the different types of averaging procedures used in the literature. The "typical" average $\langle\Psi_{\rm typ}(r)\rangle \equiv \exp\langle\ln\Psi^{(\nu)}(r)\rangle$ with $\Psi^{(\nu)}(r)$ from (2) corresponds to the case $N=1$ in (9)–(11) [25]. This average, introduced in [5], must be distinguished from the "quenched" average $\langle\Psi_Q(r)\rangle \equiv \exp\langle\ln\psi_i^\nu(r)\rangle$ introduced earlier [2]. The quenched average can be calculated directly [2] from (1), $\langle\ln[\psi_i^{(\nu)}(r)]\rangle \sim -\langle[l_i(r)/\xi_l]\rangle^v \cong -[l_{\max}(r)/\xi_l]^v \sim -(r/\xi_r)^{vd_{\min}}$, and shows no crossover. While $\langle\Psi_Q(r)\rangle$ suppresses even the fluctuations on the same configuration, the typical average $\langle\Psi_{\rm typ}(r)\rangle$ suppresses only the fluctuations between *different* configurations and therefore describes the "typical" localization behavior of one configuration. Note that the same asymptotic behavior (both averages are governed by the same exponent $vd_{\min}$) has different origins. The typical averages is dominated by $l_{\min}(r,1)$, while the quenched average is dominated by $l_{\max}(r)$, and thus, for large r, is of several orders of magnitudes lower than the typical average.

To test our predictions (8)–(11), we have performed Monte Carlo simulations (with quadruple precision) of random walks on RW structures in the sc lattice and on site percolation clusters on the square lattice, where according to (9b) the crossover behavior can be more easily observed than for fractons. Figure 2 shows $\ln\langle P(r,t)\rangle_N$ for several N values and, in addition, $\ln\langle P_{\rm typ}(r,t)\rangle$, for both structures. The N-dependent crossover is clearly seen. The slopes of the curves correspond to our predictions: $d_\psi=\frac{4}{3}$ and 4 for RW structures [curve (a)] and $d_\psi=1.53$ and 1.86 for percolation in $d=2$ [curve (b)]. Figure 3 shows the data of Fig. 2 in scaled form, $\ln\langle P_{\rm typ}\rangle/[r_\times(1)]^u$ versus $r/r_\times(1)$ and $\ln\langle P\rangle_N/[r_\times(N)]^u$ versus $r/r_\times(N)$, for $N>1$. The excellent data collapse is in perfect agreement with (8)–(11) and confirms also that the typical average $\langle P_{\rm typ}\rangle$ corresponds to $\langle P(r,t)\rangle_{N=1}$, as predicted.

Our results can resolve the controversy [$d_\psi=1$ or $d_{\min}$ for electrons and fractons, $d_\psi=d_w/(d_w-1)$ or $d_w d_{\min}/(d_w-d_{\min})$ for random walks] regarding the values of the localization exponents in the literature [2–8,10–17]. According to (9b) and (6), the crossover distance $r_\times(N)$ decreases with increasing dimension, and is lower for bond than for site percolation. In [3–5], the exponent $d_\psi=1$ has been observed for electrons and fractons in site percolation clusters on the square lattice, with localization lengths greater than 11 (corresponding to $\xi_r>46$). While in [5] typical averages (corresponding to

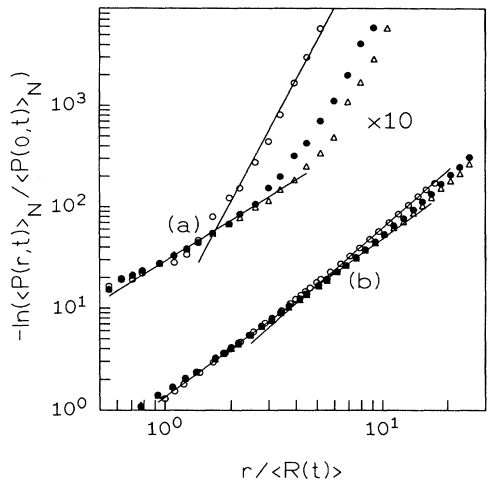

FIG. 2. Logarithm of the mean probability density $-\ln[\langle P(r,t)\rangle_N/\langle P(0,t)\rangle_N]$ of random walks vs $r/\langle R(t)\rangle$ for (a) RW structures [$t=10\,000$, $N=25$ (full circle), and 250 (triangle)] and (b) site percolation clusters on the square lattice [$t=400$, $N=5$ (full circle) and 50 (triangle)], compared with the typical probability density $-\ln[\langle P_{\rm typ}(r,t)\rangle/\langle P_{\rm typ}(0,t)\rangle]$ (circle); $\langle R(t)\rangle$ is the rms displacement.

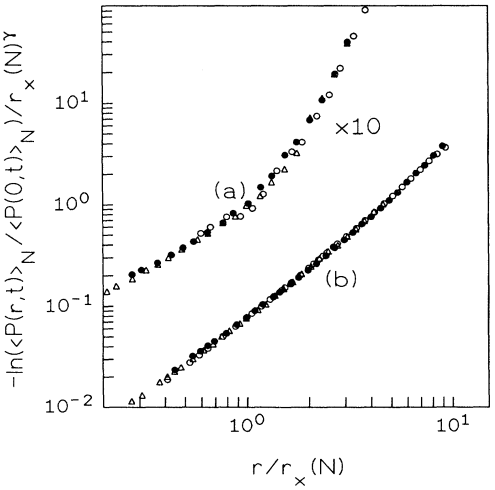

FIG. 3. Scale plots $-\ln[\langle P(r,t)\rangle_N/\langle P(0,t)\rangle_N]/r_\times^u(N)$ vs $r/r_\times(N)$ and $-\ln[\langle P_{\rm typ}(r,t)\rangle/\langle P_{\rm typ}(0.t)\rangle/r_\times^u(1)]$ vs $r/r_\times(1)$ for (a) RW structures on the sc lattice and (b) site percolation clusters on the square lattice, both for the same N values as in Fig. 2.

$N=1$) have been considered, averages with $N=5$ and 10 have been studied in [3,4]. All calculations have been performed for $r<100$, corresponding to $r/\xi_r<2.3$ well below $r_\times(1)/\xi_r\cong 2.6$, and this explains the result $d_\psi=1$. For random walks on the same system the corresponding exponent $d_\psi=d_w/(d_w-1)$ has been observed [15]. Although the crossover is considerably lower for random walks, it could not be recognized in [15], since the simulations have been performed for too large N [$N=1400, r_\times(1400)/\xi_r\cong 7$]. So far the exponent $d_\psi=\upsilon d_{\min}$ has only been observed numerically [6] for quenched averages of fractons, where the crossover is absent. According to (6), superlocalization ($d_\psi>1$ for electrons and fractons) should become more important in $d=3$, in particular when the relevant physical quantities are characterized by the behavior of single fractons or electrons. This is probably the case for depolarized Raman scattering and for the Mott hopping conductivity [21], where indeed superlocalization has been reported to occur [18, 22].

The formalism used in this paper can also be applied to discuss the short-distance regime $r<r_1$: We obtained [26] $\langle\psi(r)\rangle_N\simeq\langle\psi(0)\rangle[1-\text{const}\times(r/\xi_l)^g]$, with ξ_l from (1) and g from (4).

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[25] For a single configuration (ν) the product of $\phi^{(\nu)}\Psi^{(\nu)}$ shows, for not too small r, either a saddle point at $l^{*(\nu)}>l^{(\nu)}_{\min}$ or is peaked sharply at $l^{(\nu)}_{\min}$. If the probability for the occurrence of the saddle is denoted by $N_\times(r)/N$ one obtains $\langle\ln\Psi\rangle\equiv 1/N\sum_{j=1}^{N}\ln\Psi^{(\nu)}(r)\sim 1/N\{\sum_{j=1}^{N_\times(r)}\eta^{(\nu)}[l^{*(\nu)}(r)]+\sum_{j=N_\times(r)+1}^{N}\eta^{(\nu)}[l^{(\nu)}_{\min}(r)]\}$. Assuming $1/N\sum_{j=1}^{N}\eta^{(\nu)}[l^{*(\nu)}(r)]=\eta(l^*)$ and $1/N\sum_{j=1}^{N}\eta^{(\nu)}[l^{(\nu)}_{\min}(r)]=\eta[l_{\min}(r,1)]$, we obtain $\langle\ln\Psi\rangle\sim(N_\times/N)\eta(l^*)+[(N-N_\times-1)/N]\eta[l_{\min}(r,1)]$. For small r, where $N_\times/N\cong 1$, the first term dominates and we recover (8), while for large r, where $N_\times/N\ll 1$, the second term dominates and we recover (10) with $N=1$. The crossover occurs at a distance $\bar{r}_\times$ where $\eta[l^*(\bar{r}_\times)]=\eta[l_{\min}(\bar{r}_\times,1)]$, yielding $l^*(\bar{r}_\times)=l_{\min}(\bar{r}_\times,1)$. This condition for $\bar{r}_\times$ is identical to (9b) with $N=1$. For a detailed discussion we refer to Ref. [17].
[26] Y. Dräger, St. Russ, and A. Bunde (unpublished).