Localization of Waves in Fractals: Spatial Behavior

Pedro de Vries,[1] Hans De Raedt,[1,2] and Ad Lagendijk[1,3]

[1]*Natuurkundig Laboratorium, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands*

[2]*Physics Department, University of Antwerp, Universiteitsplein 1, B-2610 Wilrijk, Belgium*

[3]*Foundation for Fundamental Research on Matter (FOM)–Institute for Atomic and Molecular Physics, Kruislaan 407, 1098 SJ Amsterdam, The Netherlands*

(Received 9 January 1989)

Localization of a quantum particle on two-dimensional percolating networks is investigated numerically. Solving the time-dependent Schrödinger equation for particular initial wave packets we study the spatial behavior of eigenstates for two tight-binding models: the quantum percolation model and the fracton model. At the lower band edge of the fracton model localization lengths agree with theoretical scaling predictions. We address the question concerning the existence of superlocalization. Our results show no indication for superlocalized behavior of eigenstates.

PACS numbers: 71.50.+t, 63.50.+x

The characterization of the spatial behavior of excitations on random fractal structures has recently received much theoretical and experimental interest.[1-5] Because of geometric disorder in such systems the concept of localization can be applied.[6] The question arises, however, whether fractal geometry changes the usual exponential behavior associated with Anderson localization. The precise form of the spatial decay of states is still unknown. Assuming the asymptotic decay of localized wave functions (or vibrational amplitudes with frequency $\omega=\sqrt{E}$) to behave like

$$|\Psi(r;E)| \propto l(E)^{-D/2}\exp\{-\tfrac{1}{2}[r/l(E)]^{d_\phi}\}, \qquad (1)$$

where l is the localization length and D is the fractal dimension,[7] several different theoretical values have been given for the exponent d_ϕ. Lévy and Souillard predict[1] $d_\phi=d_w/2>1$, where d_w describes the anomalous diffusion of a (classical) random walker:[8] $\overline{r^2}\propto t^{2/d_w}$. Their result implies that states on a fractal are *superlocalized*. Other arguments[2] relate d_ϕ to the static exponent ζ_c characterizing the (chemical) distance measured along the fractal.[8] Values of the localization exponent for a realization should lie in the interval $1\le d_\phi\le\zeta_c$. Averaging over all configurations would then result in regular exponential behavior $d_\phi=1$.[2] It has also been argued[3] that $d_\phi=\tilde{\zeta}$, where $\tilde{\zeta}=d_w-D$ describes the scaling with distance of the resistivity between two points.[8] The resistivity exponent is always smaller than the chemical-length exponent.

In the present Letter we present a numerical study of the localization properties of a quantum particle moving on two-dimensional percolating networks. Predicted values for the exponent d_ϕ on these structures resulting from the diffusion and chemical-length exponent are 1.43 and 1.13, respectively.[1,2,8] The resistivity exponent in two dimensions is smaller than unity: $\tilde{\zeta}=0.975$.[8] Two tight-binding models defined on these networks are investigated. For both models we compute the energy dependence of the localization length and show that localized states decay asymptotically with $d_\phi\simeq 1$. For the fracton model the power-law behavior for the localization length at the lower band edge is found to be in agreement with theoretical scaling arguments. Naturally, the above results also hold for classical waves.

We consider "infinite" site-percolating clusters at the percolation threshold $p_c=0.593$ on $L\times L$ square lattices. It is well known that such a structure exhibits fractal characteristics on all length scales with a fractal dimension $D=91/48$.[7] The two tight-binding Hamiltonians we study are

$$H_1=-V\sum_{\langle i,j\rangle} t_{ij}(c_i^\dagger c_j+c_j^\dagger c_i), \qquad (2)$$

$$H_2=H_1+V\sum_{i=1}^{N} z_z c_i^\dagger c_i, \qquad (3)$$

where in H_1 the summation is over nearest neighbors, $c_i^\dagger$ (c_i) creates (annihilates) a particle at site i, V is the interaction constant (set equal to unity in the following), $t_{ij}=0$ or 1 depending on the absence or presence of a nearest neighbor, and z_i is the coordination number of site i. The first Hamiltonian (2) corresponds to the quantum percolation problem, which has been studied extensively.[9,10] It describes the motion of a particle on an AB alloy where the B sites are energetically forbidden and can be regarded as an Anderson Hamiltonian in which the site energies are chosen randomly to be 0 with probability p_c and ∞ with probability $1-p$. Therefore, behavior similar to the Anderson model could be expected. At the classical threshold p_c all quantum states should be localized with a finite localization length depending weakly on energy. This model can also be considered to possess correlated off-diagonal disorder (uncorrelated disorder corresponds to bond percolation).

The second Hamiltonian (3) has an additional random diagonal part. The site energies are proportional the local coordination number which obviously is a random

quantity. This model can be mapped exactly onto a master equation describing a classical random walker on percolating networks or onto the vibrational problem of such structures: the fracton model.[3,10,11] It is for these classical problems that most work concerning fractal dynamics has been done so far. The on- and off-diagonal disorder are highly correlated, so behavior different from (2) can be expected for this model. The density of states at the lower band edge is proportional to $E^{(\bar{\bar{d}}-2)/2}$, where according to the Alexander-Orbach conjecture[11-15] the spectral or fracton dimensionality $\bar{\bar{d}}$ is equal to $\frac{4}{3}$. The localized excitations in Eq. (3) are termed fractons.[11] The scaling model[3,11] predicts that fractons are described by *one* single length. The localization length $l(E)$ is then proportional to the wavelength $\lambda(E)$ and scales accordingly,[3,11]

$$l(E) \propto E^{-\bar{\bar{d}}/2D}. \tag{4}$$

In contrast to the Anderson model the localization length increases with decreasing energy. In fact, the ground state with $E=0$ is a uniform extended state. We have, for the first time, verified the scaling prediction (4).

The localization behavior of both models is obtained by solving the time-dependent Schrödinger equation using a numerical algorithm based on Trotter-Suzuki product formulas, developed previously by one of us.[16] The numerical scheme is explicit and unconditionally stable, guaranteeing that all errors remain bounded independent of the time step. The global root-mean-square error on the wave function is fourth order in the time step. This algorithm permits an efficient and accurate computation of the time development of wave packets on large lattices ($>10^4$ sites) and for times T sufficiently long to discriminate localized behavior.[16] Different types of initial wave packets were constructed in order to compute either localization lengths or probability distributions. Let us mention in passing that we have also computed[17] the density of states for both models and found agreement with theory and previous calculations.

Our approach to study the energy dependence of the localization length is to calculate inverse participation ratios[18] (IPR) $\mathcal{P}_n^{-1}$ defined by $\mathcal{P}_n^{-1}(E) = \sum_{i=1}^{N} |\phi(\mathbf{r}_i;E)|^{2n}$, which are a measure of the effective number of sites covered by a normalized eigenstate ϕ. For localized states the participation number $\mathcal{P}_2(E)$ goes like $l(E)^D$; the proportionality constant depends on the precise shape of the wave function. We employ a technique developed by Weaire and Williams[18] to compute weighted band averages $\langle \mathcal{P}_n^{-1} \rangle$ in terms of time-averaged quantities of a state $\Psi(t)$ chosen suitably random at $t=0$. The energy interval contributing to IPR can be varied by applying the projection operator[18] $[1-(H-E_0)^2/E_{\max}^2]^m$ ($E_{\max}$ is an upper bound to the spectrum) to the initial wave function and adjusting E_0 and m.

In Fig. 1 participation numbers ($n=2$) as a function of energy are shown for the two models. If follows that the participation numbers are much smaller than the lattices sizes (100×100 and 200×200) used; hence finite-size effects are unimportant. For the quantum percolation model we find a smooth behavior as a function of energy. The results are an even function of energy. All states are localized with a finite localization length $l \approx 1$–5. Calculations of the density of states have shown that at the center of the band two inner tails are present,[9,17] which explains why l decreases for $|E| \to 0$.

The fracton model exhibits a power-law behavior at

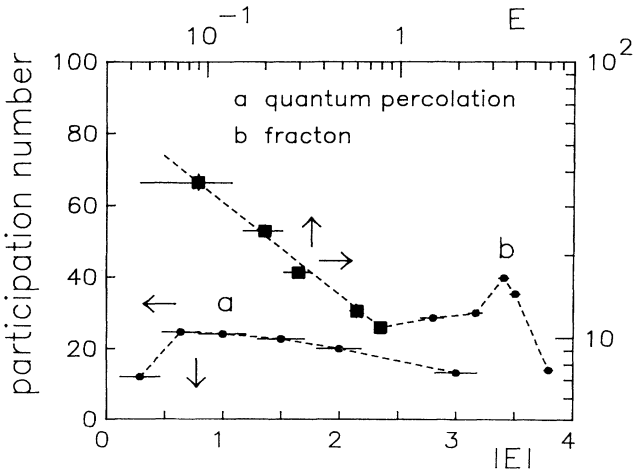

FIG. 1. Participation numbers ($n=2$) as a function of energy. Bars on the energy are determined by the parameter m. ●, averaged data from six runs on 100×100 lattices with mean size $N=3400$. ■, single run on a 200×200 lattice with size $N=12064$. Error bars not shown have size of symbols. Lines are guides to the eye.

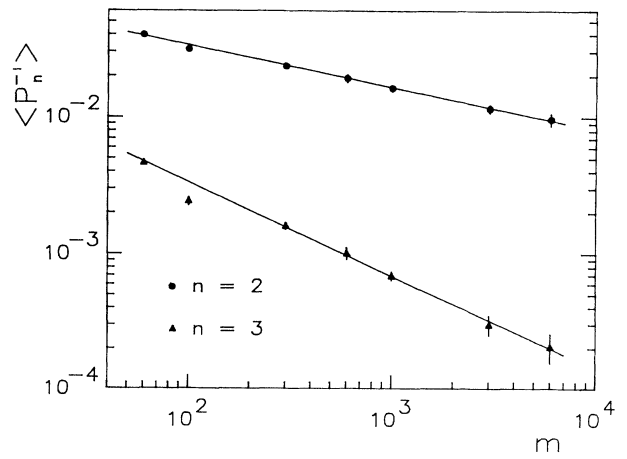

FIG. 2. $\langle \mathcal{P}_n^{-1} \rangle_m$ for $n=2$ and $n=3$ as a function of the projection parameter m with $E_0=0$. Averaged data from three runs on 200×200 lattices with mean size $N=12000$. Lines are fits to the data.

the lower band edge in accordance with theory.[3,11] Using Eq. (4) we find for the fracton dimensionality $\bar{\bar{d}}=1.12\pm0.11$. To improve on this result we have calculated inverse participation ratios for $n=2$ and $n=3$ as a function of the projection parameter m with $E_0=0$ which are presented in Fig. 2. Now only states with $E\ll0.1$ contribute to the IPR. Computations for 70×70, 100×100, and 200×200 lattices show that convergence as a function of lattice size has been achieved for the m values covered. It can be shown analytically,[17] assuming Eq. (4) to be valid, that $\langle\mathcal{P}_n^{-1}\rangle\propto m^{-\bar{\bar{d}}(n-1)/4}$ for $m\gg1$. From the data we compute, respectively, $\bar{\bar{d}}=1.23\pm0.12$ and $\bar{\bar{d}}=1.38\pm0.12$ for $n=2$ and $n=3$. We conclude that indeed the localization length scales as $E^{-\bar{\bar{d}}/2D}$.

We now turn to the problem of spatial decay of eigenstates. In order to reduce information we study one-dimensionally integrated probability distributions $I(x)=\sum_y|\Psi(x,y)|^2$ and $I(y)=\sum_x|\Psi(x,y)|^2$ of wave packets Ψ from which the behavior of eigenstates is inferred. At $t=0$ wave packets are constructed in the center of the lattice either by putting the particle on one site (calculation of the Green's function) or by diagonalizing a 19×19 subsystem. In the former case eigenstates with energies from the whole spectrum can contribute to the wave packet. In the latter case the energy uncertainty as measured by $\sigma_E^2=\langle H^2\rangle-\langle H\rangle^2$ can be reduced greatly, so that participating eigenstates lie substantially in a small energy interval. The time development is such that initially wave packets expand rapidly. For time (in units of $1/V$) varying between 300 and 1000, diffusionlike behavior, $l(t)^2\propto t$, can be found.[17] Eventually, the wave packets localize and the measured localization lengths (slowly) saturate to values well below system sizes (also see Fig. 1). Below we present results from wave packets calculated up to $t=10000$.

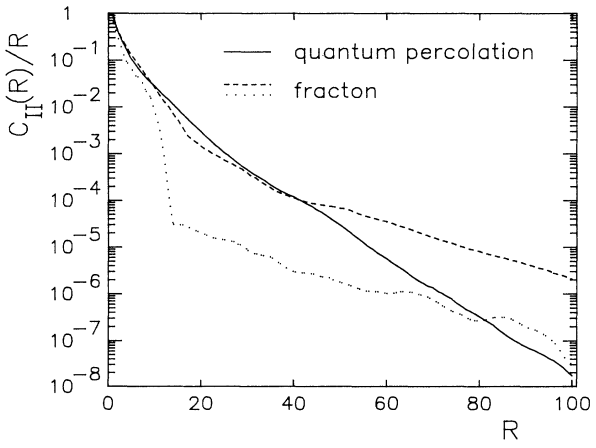

FIG. 3. Autocorrelation functions of probability distributions on 200×200 percolating clusters. C_{II} is normalized at $R=0$.

In general the envelope of wave packets need not correspond to the envelope of the contributing eigenstate. This is certainly true for wave packets formed from extended states. For a spectrum with finite localization lengths, as is the case of the quantum percolation model, we argue that the asymptotic decay of wave packets is similar to that of its constituents and is determined by some typical large l. For the fracton model this argument only strictly holds for packets with components that do not lie at the lower band edge. However, for the times covered we have observed similar decay properties for wave packets that have started on one site, and thus also consist of eigenstates with $E\approx0$.

For the two models and for both kinds of initial states the probability distributions $I(x)$ and $I(y)$ show two basic structures. It follows that the majority of the probability is localized in "microclusters" which are attached to the macroscopic cluster by a few bonds and which contain the initial starting point(s). This feature has also been demonstrated by recent calculations on the fracton model.[15,19] This structure can be regarded as some kind of "random cavity" and essentially determines the localization length as calculated above with IPR. The second basic structure is the asymptotic behavior showing exponential-like tails. For a particular geometry these two structures do not change into another continuously: The borders of the microscluster are reflected in a pronounced decrease in the I values as a function of x or y. Evidently, the tails are anisotropic and may also show steps and small "plateaus" depending on the local geometry.

To compute d_ϕ we first calculate the autocorrelation function $C_{II}(R)$ of $\frac{1}{2}[I(x)+I(y)]$ to average out fluctuations. If I behaves exponentially with localization length l, C_{II} goes like $R\exp(-R/l)$ for large R. In Fig. 3 autocorrelation functions $C_{II}(R)/R$ are shown. The solid and dashed curves correspond to the case that the particle is put on one site at $t=0$ for the quantum percolation and fracton model, respectively. The solid (dashed) curve is computed from an average of ten (five) runs. For the dotted curve one initial wave packet was constructed by diagonalization with energy $\langle H\rangle=0.19$ and energy uncertainty $\sigma_E=0.05$ using the fracton model. The sharp decrease in probability is clearly seen in this case. All curves show exponential-like behavior. A best fit on the data for quantum percolation gives $d_\phi=0.99\pm0.05$. For the fracton model we find $d_\phi=1.00\pm0.04$. Our results are not in agreement with the predictions $d_\phi=d_w/2=1.43$ and $d_\phi=\zeta_c=1.13$, and, in fact, do not support the idea of superlocalization on fractal lattices.

Discussions with S. Alexander, E. Courtens, and R. Orbach are gratefully acknowledged. This work is part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (FOM), which is

financially supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO), and is partially supported by the Supercomputer Project of the Belgian National Science Foundation (NFWO). We are grateful to Control Data (The Netherlands) for granting us computer time on the Cyber 205.

[1]Y. E. Lévy and B. Souillard, Europhys. Lett. **4**, 233 (1987).

[2]A. Brooks Harris and A. Aharony, Europhys. Lett. **4**, 1355 (1987).

[3]A. Aharony, S. Alexander, O. Entin-Wohlman, and R. Orbach, Phys. Rev. Lett. **58**, 132 (1987).

[4]Y. Tsujimi, E. Courtens, J. Pelous, and R. Vacher, Phys. Rev. Lett. **60**, 2757 (1988).

[5]A. Boukenter, E. Duval, and H. M. Rosenberg, J. Phys. C **21**, 541 (1988).

[6]B. Souillard, in *Chance and Matter,* Proceedings of the Les Houches Summer School, Session XLVI, edited by J. Souletie, J. Vannimenus, and R. Stora (Elsevier, Amsterdam, 1987).

[7]D. Stauffer, *Introduction to Percolation Theory* (Taylor & Francis, London, 1985).

[8]S. Halvin and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987); H. J. Herrmann and H. E. Stanley, J. Phys. A **21**, L829 (1988); J.-M. Normand, H. J. Herrmann, and M. Hajjar, J. Stat. Phys. **52**, 441 (1988).

[9]S. Kirkpatrick and T. P. Eggarter, Phys. Rev. B **6**, 3598 (1972).

[10]I. M. Sokolov, Usp. Fiz. Nauk **150**, 221 (1986) [Sov. Phys. Usp. **29**, 924 (1986)], and references therein.

[11]S. Alexander and R. Orbach, J. Phys. (Paris), Lett **43**, L625 (1982).

[12]S. J. Lewis and R. B. Stinchcombe, Phys. Rev. Lett. **52**, 1021 (1984).

[13]I. Webman and G. S. Grest, J. Phys. (Paris), Lett. **45** L1155 (1984).

[14]S. N. Evangelou, Phys. Rev. B **33**, 3602 (1986).

[15]K. Yakubo and T. Nakayama, Phys. Rev. B **36**, 8933 (1987).

[16]H. De Raedt, Comp. Phys. Rep. **7**, 1 (1987).

[17]P. de Vries, H. De Raedt, and A. Lagendijk (to be published).

[18]D. Weaire and A. R. Williams, J. Phys. C **10**, 1239 (1977); D. Weaire and V. Srivastava, J. Phys. C **10**, 4309 (1977).

[19]K. Yakubo, T. Nakayama, and R. Orbach (private communication).