SCALING CONDUCTANCE ON RANDOM FRACTAL*

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In the paper we use numerical simulations to show that superlocalization of electronic wave functions takes place on fractal objects also for energies E from the band. Finite size scaling of conductance g versus system size L reveals that $\langle \ln g \rangle$ scales as L^{d_ϕ}. The values of localization exponent d_ϕ we found in 2D are 1.138(3) for the state in the middle of the band $E = 0.5t$, and 1.144(3) for the state near the lower band edge $E = -3.5t$. These values are in good agreement with the conjecture $d_\phi = \zeta_l$, where ζ_l is the chemical length exponent.

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1. Introduction

A lot of physical systems exhibit fractal geometry at least over a limited range of length scales. One important example is the percolation cluster, which within the scale ξ_p — the percolation correlation length — behaves as a fractal. As the percolation threshold is approached, ξ_p diverges and the system has the fractal geometry even up to macroscopic scales. In 1987 Levy and Souillard [1] suggested that tortuous fractal geometry makes the spatial decaying of wave functions stronger than in Euclidean geometries. Namely, the mean amplitudes behave like

$$|\psi(r)| \sim \exp \frac{-r^{d_\phi}}{\xi_l}, \tag{1}$$

where r is the distance from the center of the wave function ψ, ξ_l is the localization length and d_ϕ is the localization exponent. It was then proven theoretically that for percolation cluster the localization exponent should

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lie inside the interval $1 \leq d_\phi \leq \zeta_l$ [2]. The upper bound of this interval is the exponent ζ_l which describes scaling of the average chemical length (the shortest path) l measured along the fractal between two points separated by Euclidean distance r

$$\langle l \rangle \sim r^{\zeta_l} . \tag{2}$$

The physical meaning of Eq. (1) is now more clear. Rewriting Eq. (1) as $|\psi(r)| \sim \exp(-\langle l \rangle / \xi_l)$ we conclude that electron, when put onto the fractal object, "feels" topological distance l rather then "air" distance r. This was rigorously proven for deep states on the percolation cluster for which the relation $d_\phi = \zeta_l$ is expected [2]. For states within the band only the inequality $1 \leq d_\phi \leq \zeta_l$ holds [2]. Less agreement concerns numerically obtained values of this exponent. Most numerical simulations are in accord with $d_\phi = 1$ *i.e.* no superlocalization is observed [3–5]. The only exception is that of Lambert and Hughes [6] which gives $d_\phi = \zeta_l$. It is now believed that this disagreement is caused by different kind of averages used by different authors [7–10]. Most of them use arithmetic averaging $\langle |\psi| \rangle$, whereas the proper average in order to observe superlocalization is either logarithmic average $\langle \ln |\psi| \rangle$ or average over few (typical) cluster configurations. Indeed in Ref. [6] the averaging of fractons was used. However, the typical average over few configurations taken by deVries *et al.* [3] still gives $d_\phi = 1$.

Almost all numerical studies use direct calculations of electron or fracton wave functions. Superlocalized wave functions make conductance "superlocalized"

$$g \sim |\psi(r)|^2 \sim \exp \frac{-2r^{d_\phi}}{\xi_l} \tag{3}$$

and one would expect that it is possible to study this phenomenon via calculations of the conductance. The only such approach was by Zhang and Sheng [11]. They used the finite size scaling method but did not find any evidence of superlocalization: $d_\phi = 1$ was obtained. On the one hand this result is not in contradiction to the theory since the calculations were performed for $E = 0.5t$ *i.e.* within the bound, where the theory says only $1 \leq d_\phi$. On the other hand the direct calculations of fractons inside the band by Bunde *et al.* [8] are consistent with $d_\phi = \zeta_l$.

Summing up the still open questions are:

(i) Is it possible to find superlocalization via calculations of the conductance?

(ii) Do states within the band obey or not the phenomenon of superlocalization? And if so,

(iii) how the energy influences the value of the localization exponent d_ϕ?

These are also the main topics of our paper. We use numerical simulations to answer the above questions. The paper is organized as follows. In the next section we describe details of numerical calculation. In Section 3 results of large-scale simulations performed on two dimensional percolation cluster are reported. Eventually, we end up with the concluding section.

2. Method of calculations

We consider site percolation on the square lattice in $d = 2$ space. The fraction $p = p_c = 0.593$ of the sites is randomly occupied by zero energies whereas the rest of them are removed. Linear size of the sample L is measured in units of lattice spacing. Perfect metallic electrodes are attached to opposite edges of the sample. Hard walls are assumed on the remaining two edges. For such a model one-electron tight-binding Hamiltonian is as follows:

$$H = \sum_n |n\rangle \varepsilon_n \langle n| + \sum_{n,m} |n\rangle t \langle m| \,, \tag{4}$$

where the second sum runs only over occupied nearest neighbor sites n and m and t is the hopping element. To calculate dimensionless conductance of the sample we use multichannel Landauer–Büttiker formula [12, 13]

$$g = 4 \frac{\sum_{i=1}^{m} T_i \sum_{i=1}^{m} v_i^{-1}}{\sum_{i=1}^{m} (1 + R_i - T_i) v_i^{-1}} \,, \tag{5}$$

where m is the number of quantum channels (modes) in the leads, T_i and R_i are calculated by summation the transmission and reflection matrices over m and v_i is velocity in the channel i. The transmission and reflection matrices have been calculated with the help of Green's function method [14].

3. Finite size scaling

The calculations we have performed use the finite size scaling technique. The conductance g was calculated for increasing lattice size L. The calculations have been done for two energies inside the band, one in the middle of the band, $E = 0.5t$, and the other for deeper states near the lower band edge, $E = -3.5t$. The population of the samples in both cases was 50000, so it took more than a week to collect one set of the data in the range from $L = 4$ to $L = 80$ with unit step. Results of these simulations are shown in Fig. 1 where $\langle \ln g \rangle$ is plotted versus L. The curvature one may observe in these plots indicates deviations from "pure" exponential localization. Indeed, fitting with Eq. (3) gives localization exponent: $d_\phi = 1.144(3)$ for $E = -3.5t$ and $d_\phi = 0.138(3)$ for $E = 0.5t$. In order to ensure whether

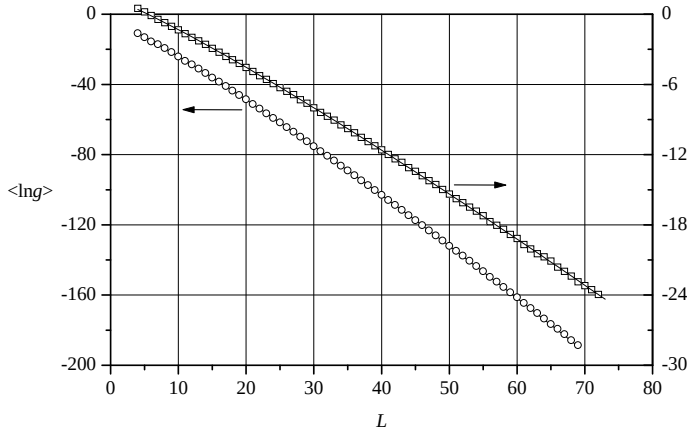

Fig. 1. Averaged logarithm of conductance $\langle \ln g \rangle$ versus size L of the lattice. Calculations are made for for $E = -3.5t$ (circles) and for $E = 0.5t$ (squares). In both cases the population of the samples was 50000. Lines are the fit to Eq. (3). The fitting parameters are $d_\phi = 1.144(3)$, $\xi_l = 0.68(1)$, for $E = -3.5t$ and $d_\phi = 0.138(3)$, $\xi_l = 5.13(6)$, for $E = 0.5t$.

the measured exponents are not the effect of finite size of our samples we have repeated the fittings in the ranges $L > 20$ and $L > 30$. In both cases the change of d_ϕ was less than 5%. This strongly supports the existence of superlocalization on percolation cluster and proves that it is possible to observe it via calculations of conductance.

Our estimates of exponent d_ϕ are very close to the upper bound ζ_l of theoretically acceptable values of this exponent. For the latter the recent estimates are $\zeta_l = 1.13$ [15], and 1.15 [16, 17]. Thus we may conclude that the conjecture $d_\phi = \zeta_l$ is valid also for the states inside the band.

The case of $E = 0.5t$ was also the matter of calculations of Zhang and Sheng [11]. So the direct comparison of numerical data is possible. In general their data, while the same as ours for small sizes, (for $L = 15$ both they and we have $\langle \ln g \rangle \simeq -2.8$) are a bit larger than ours for large sizes. For $L = 75$ they have $\langle \ln g \rangle \simeq -21.5$ whereas our value is -24. This is reflected in slightly different values of localization length calculated from the data. They found $\xi_l = 3.30$ comparing to our value of $\xi_l = 5.13$. As we have already mentioned also the values of exponent d_ϕ are different. We think that these discrepancies are caused mainly by relatively small population of the samples they used to calculate the averages.

4. Conclusions

The main conclusion is that the conjecture $d_\phi = \zeta_l$, which originally was derived for the states that are deep below the band of extended states, holds also for the states inside the band. Another conclusion is that the phenomenon of superlocalization can be observed in the size dependence of the conductance. To our knowledge our simulations are the first which confirm these conclusions so clearly. To end up let us mention that the phenomenon we have discussed above is not of minor importance. This is because of its relevance to variable range hopping (VRH). The superlocalized behavior of electronic wave functions leads to the conclusions that VRH on fractal objects is described by the relation $\sigma \sim \exp(-(T_0/T)^\gamma)$ with $\gamma = d_\phi/(d_\phi + D)$, D is the fractal dimension [18] rather than ordinary Mott's law with exponent $\gamma = 1/(1+d)$.

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