Superdiffusive Transport and Metal-Insulator Transition in Two Dimensions

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Through numerical simulations and diagrammatical calculation, we find a metal-insulator transition in 2D disordered systems where the scattering impurities are fractally correlated. The transition is accessible through the variation of either the Fermi energy or the impurity scattering strength, and in the metallic regime the electronic transport is shown to be superdiffusive in nature.

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It is now widely accepted that the marginal spatial dimension for wave localization is two [1], i.e., all waves are localized in random media with dimensionality two or one. An important assumption underlying this result is that the geometric correlation length ζ of the inhomogeneities is finite so that the medium is macroscopically homogeneous. In the past decade, however, many examples of disordered systems were found in which ζ , while not infinite, could reach the scale of macroscopic samples [2]. For such materials the violation of the macroscopic homogeneity assumption thus raises the possibility of altered localization behavior. In one scenario, where the electron or the wave is confined on fractal objects, it has been suggested that the localized wave functions may decay faster than exponential, i.e., superlocalized [3]. In this work, we study the effects of random impurity potentials which are fractally correlated. Instead of confining the electron or wave, however, the impurities are embedded in an otherwise homogeneous 2D host medium and act as wave scatterers. Through both numerical simulations and diagrammatical calculation, we show that novel phenomena can result in such systems. In particular, there can be a metal-insulator (or localization-delocalization) transition both as a function of scattering potential strength and as a function of Fermi energy (or wave frequency), and in the metallic regime the transport is found to be superdiffusive in nature.

Consider the tight-binding Hamiltonian

$$H = \sum_i \epsilon_i a_i^\dagger a_i + t \sum_{\langle ij \rangle} a_i^\dagger a_j, \quad (1a)$$

where ϵ_i denotes the site energy, given by

$$\epsilon_i = \begin{cases} W, & \text{for the impurity sites,} \\ 0, & \text{for the host sites,} \end{cases} \quad (1b)$$

$a_i^\dagger$ (a_i) is the creation (annihilation) operator for site i , t denotes the hopping matrix element, taken to be 1 below, and $\langle ij \rangle$ denotes nearest-neighbor ij pairs. The host medium is taken to be a simple square lattice, with the impurity sites chosen as members of a random fractal, constructed as a critical percolation network generated by the random occupation of sites at probability $p = p_c \cong 0.593$, and then reverting the isolated clusters to the host medium.

The 2D percolative network is known to have fractal dimension [2] ~ 1.89 . For finite-sized $L \times L$ samples, we

retain only those configurations in which the networks are percolating in both the x and y directions.

The electronic transport characteristics of the model are obtained by evaluating the transmission probability T of $L \times L$ samples when each is attached to perfect leads [4,5]. Here T is given by

$$T = \text{Tr} t t^\dagger = \sum_{i=1}^{L_0} T_i, \quad (2a)$$

with L_0 denoting the number of propagating channels of the leads given by the number of k_x 's that yield real values for $E = 2(\cos k_x a + \cos k_y a)$ for $k_y = \pi n/(L+2)a$,

FIG. 1. Conductance variation as function of sample size L for various values of W . The Fermi energy is 0.5. Solid lines denote the simulation results calculated by the recursive Green's-function method, averaged over 3500 configurations for $L=15$ to 200 configurations for $L=90$. Dashed lines are calculated from solving the self-consistent diagrammatic theory. Classical 2D conductance (purely diffusive) would be a flat line (L independent). Ballistic transport is represented by a linear dependence on L . The vertical axis is linear for the delocalized regime and logarithmic for the localized regime.

$n=1,2,\dots,L+1$, with a being the lattice constant, and

$$T_i = \sum_{j=1}^{L_0} |t_{ij}|^2. \quad (2b)$$

t_{ij} is the transmission amplitude between site j at one end of the sample and site i at the other. It is calculated by

$$|t_{ij}|^2 = v_i v_j |G_{ij}^+(L+2,0)|^2, \quad (2c)$$

where $G_{ij}^+(n,n')$ is the retarded Green's function with source at n' of the x coordinate of channel j and receiver at n of channel i . Positions 0 and $L+2$ are located inside the incoming and outgoing sides of the leads, respectively, and $v_i = \partial E / \partial k_x$ evaluated at $k_x(i)$. G_{ij}^+ is evaluated by using the recursive Green's-function technique [6]. The conductance G may be related to T by $G = (e^2/h)T$, or, for high-transmission samples, by the more accurate multichannel-Landauer formula [5].

In Fig. 1, the solid lines give the sample-size variation of the calculated dimensionless conductance $g = G/(e^2/h)$ at $E=0.5$. The dashed lines are the results of diagrammatic evaluations to be described later. It is seen that for $W \lesssim W_c \approx 2.9 \pm 0.5$, $\langle g \rangle$ increases with L , indicating a delocalized behavior; whereas for $W > W_c$, $\langle \ln g \rangle$ decreases with L , indicating a localized behavior. For reference, the classical 2D conductance, i.e., pure diffusive behavior, is noted to be sample-size independent, and the ballistic transport behavior is generally characterized by linear variation of T with L since in that case T is directly proportional to the number of channels. Therefore the intermediate behavior of the delocalized regime, $0 < W$

$\lesssim W_c$, is indicative of superdiffusive transport that interpolates between diffusive and ballistic behavior. If we denote $g(L) \sim D(L) \propto L^s$, then the mean-square displacement $L^2 = D(L)\tau \propto L^s \tau$, or $L^2 \propto \tau^{2/(2-s)}$, where s varies between 0 and 1 depending on the values of W and E . For $E=0.5$, $s \approx 0.43$ and 0.33 for $W=1$ and 2 , respectively. For $W > W_c$, on the other hand, the variation of $\langle \ln g \rangle$ with L is also nonlinear, indicating a subexponential localization behavior.

The superdiffusive transport and the transition between the localized and delocalized behaviors can also be studied in the space-time domain by directly solving the time-dependent Schrödinger's equation $i\partial\psi/\partial\tau = H\psi$, where the time τ is the units of $\hbar/t$ and H is given by Eq. (1). The diffusion constant D may then be evaluated as $D = d\langle r^2 \rangle / d\tau$ as a function of τ . Besides offering a consistency check, the space-time simulation also offers the possibility of studying much larger sample sizes.

We have carried out time-domain simulations on 800×800 samples by using the unconditionally stable numerical scheme developed by de Raedt [7]. For comparison, we have also calculated the cases where the distribution of impurities is homogeneous. A wave packet with $\langle E \rangle = 0$ is created at the center of the square, by using the projection operator method [8]. Figure 2 shows the calculated variation of $D = d\langle r^2 \rangle / d\tau$ as a function of time for three different values of $W=1, 1.5$, and 2 . In each case the impurities are distributed both fractally and homogeneously with the same overall density. It is noted

FIG. 2. Time dependence of $d\langle r^2 \rangle / d\tau$ for three values of W evaluated from simulations of a single 800×800 configuration. Each pair of curves represents one case in which the scattering impurities are fractally correlated (denoted by F) and another case in which the impurities are homogeneously distributed with the same overall density (denoted by H).

that for the homogeneous cases, denoted by H , D is a slightly decreasing function of τ since the waves are localized, but the localization lengths are large due to the low density of scatterers. As a result the behavior is nearly diffusive, with $D \approx \text{const}$. For the fractal-impurities case, on the other hand, D is noted to be a monotonically increasing function of τ for $W < 3$. The values of s deduced for $W=1,2$ are 0.36 and 0.3, respectively. These results are consistent with the recursive Green's-function calculations.

As opposed to the homogeneous-impurities case, where in 2D all waves are localized, for impurities arranged with fractal symmetry a metal-insulator transition can occur in 2D through the variation of either the Fermi energy E or the scattering barrier height W , or both. In Fig. 3 we show the phase diagram calculated by the recursive Green's-function method as described above. For a fixed $W=3.6$, the drastic conductance changes as a function of E , are illustrated in Fig. 4 as one crosses from the insulating regime to the conducting regime and then to the insulating regime again. The steepness of the conductance variation is noted to increase as the sample size increases. Thus for field-effect transistors it may be en-

visioned that based on the present metal-insulator transition phenomenon, one can have a gate-voltage-controlled switch (through the variation of Fermi energy) if the scattering impurities can be arranged in a fractal pattern.

The physics of our model may be intuitively understood as resulting from the competition of two long-range effects: the coherent backscattering and the fractal correlation. For homogeneous 2D samples, the coherent backscattering effect diverges logarithmically as a function of L in the weak scattering limit. In the case of fractal scatterers, however, the density decays as a power law, and therefore one expects the delocalization tendency to always prevail. This is the source of the superdiffusive behavior. On the other hand, when the scattering becomes strong, i.e., W large, the wave function can decay exponentially in areas where the local density of scatterers is high. Yet, due to the decreasing density of scatterers further out, there can always be leakage at the exponential-tail end of the wave function. This is evidenced by the sublinear decay of $\langle \ln g \rangle$ for $W > W_c$. An interesting question is whether such small leakage, when combined with the linear increase in the number of channels as L increases, can eventually result in the metallic behavior for $W > W_c$ at extremely large L . To investigate this possibility, we have carried out diagrammatic

FIG. 3. Phase diagram as a function of W and E calculated from recursive Green's-function simulations. The bars indicate estimated error for each point. The transition in behavior is obtained by many runs at different W and E , each averaged over 200–3000 configurations depending on the sample size. The dashed line indicates the cross section examined by Fig. 4.

FIG. 4. Fermi-energy dependence of $\exp[\langle \ln g \rangle]$ at $W=3.6$, for two sample sizes. The phenomenon of metal-insulator transition is clearly demonstrated by the sharp variations of the conductance as one crosses the mobility edges.

calculations on a simplified model that takes into account only the power-law correlation of the scatterer density but not the connectivity that is inherent in the fractal critical percolation network. We assume that scatterers are correlated within distance L , and uncorrelated beyond L . The average density of scatterers, $n(L)$, is set equal to that of the average of a $L \times L$ critical percolation network. That is,

$$\langle \epsilon_i \epsilon_j \rangle = n(L) W^2 C(R_{ij}), \quad (3a)$$

$$C(R_{ij}) = \begin{cases} 1, & i=j, \\ a/|R_{ij}|^{0.11}, & i \neq j; |x_{ij}|, |y_{ij}| \leq L/2, \\ n(L), & \text{otherwise,} \end{cases} \quad (3b)$$

where $a=0.5736$ and the exponent 0.11 are numerical constants obtained by fitting to the critical-percolation-network density variation.

Given the correlation function of the scatters, the diagrammatic calculation of the single-particle Green's function, the diffusion constant, and its renormalization due to the coherent backscattering effect follows standard procedures [9,10]. The dimensionless conductance is given by the Vollhardt and Wölfle form [11]:

$$g_L(E) = D_L(E) \rho(E) [1 + (L/\xi_L)] \exp(-L/\xi_L), \quad (4a)$$

where the subscript L denotes the quantity as pertaining to that of a $L \times L$ finite-sized sample,

$$D_L(E) = \frac{1}{4\pi} D_B(E) \beta(E) \ln[1 + q_L^2 \xi_L^2(E)], \quad (4b)$$

$$\xi_L(E) = q_u^{-2} \left[\exp \left(\frac{4\pi}{\beta(E)} \right) - 1 \right], \quad (4c)$$

$q_L = 1/L$ is the lower cutoff wave vector due to the finite sample size and $q_u = \text{const}/l$ (with l the mean free path) is the upper cutoff wave vector, $D_B(E)$ is the diffusion constant calculated in the classical Boltzmann theory, $\rho(E)$ is the density of states, and $\beta(E)$ is a function given by $4n(L)W^2/v_F^2$ (with v_F the Fermi velocity) in the homogeneous-scatterer case. For correlated scatterers $\beta(E)$ is somewhat more complicated and is given by Eq. (24) in Ref. [9]. For numerical evaluation of Eq. (4a), we have chosen $q_u = 0.2/l$. The dashed lines in Fig. 1 depict the sample-size variation of $g_L(E)$ for $E=0.5$ and various values of W . It is seen that the behavior is qualitatively similar to that obtained by numerical simulation, thus providing further confirmation of the metal-insulator transition phenomenon. Since $d(\ln g_L)/dL$ is a decreasing function of L for $W > 2$, one can ask if there is a value of L at which $d(\ln g_L)/dL$ changes sign. The accurate numerical solution of the self-consistent theory is possible up to $L \approx 250$, and $d(\ln g_L)/dL$ is found to be strictly negative in this regime for $W \geq 2$. However, by approximating $C(R_{ij}) = 1/n(L)$ for $i=j$ and 0 for $i \neq j$, the self-consistent equations may be solved analytically. It is found that for $W=2$, $d(\ln g_L)/dL$ can change sign at $L = L_0 \approx 5 \times 10^4$. Moreover, L_0 increases exponentially as W increases. That means if we consider only the effect of density decay, then for $L > L_0$ the small leaks of the ex-

ponential details of the quasilocized states can combine to delocalize. However, the effect of connectivity, which is neglected in the diagrammatical calculation, is certain to push the crossover point to even higher values of L , if not to infinity. Therefore, until that point is resolved, the limiting $L \rightarrow \infty$ behavior remains an open question. What may be concluded from the calculation is that, even if there is a finite crossover point L_0 , that sample size is extremely large and increases exponentially with W .

In summary, a metal-insulator transition has been found in 2D disordered systems in which the impurity scatterers are fractally correlated. The transport behavior in the metallic regime is shown to be superdiffusive. The effect of the scatterer density correlation is further analyzed by diagrammatical calculations with results which confirm qualitatively the picture obtained by numerical simulations. The question about the $L \rightarrow \infty$ limiting behavior is examined, with the conclusion that even if there is a crossover in behavior, it has to occur at transcendently large sample sizes. An experimental verification of the present phenomenon would be important not only scientifically but may also demonstrate potential applications, e.g., in field-effect transistors.

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- [1] See, for example, P. A. Lee and T. V. Ramakrishnan, *Rev. Mod. Phys.* **57**, 287 (1985).
- [2] Percolation network at the threshold is one example, see D. Stauffer, *Introduction to Percolation Theory* (Taylor & Francis, Philadelphia, 1985). Diffusion-limited aggregates constitute another example, see T. A. Witten and L. M. Sander, *Phys. Rev. B* **27**, 5606 (1983). Our model is noted to differ from that of S. John and M. J. Stephen [*Phys. Rev. B* **28**, 6358 (1983)], where $\langle \epsilon_i \epsilon_j \rangle = \gamma C(r_{ij})$ [see our Eq. (3a)] but γ is a constant so that the density of scatterers is homogeneous. In our case γ is sample-size dependent.
- [3] Y. E. Levy and B. Souillard, *Europhys. Lett.* **4**, 233 (1987); A. B. Harris and A. Aharony, *Europhys. Lett.* **4**, 1355 (1987).
- [4] R. Landauer, *IBM J. Res. Dev.* **1**, 223 (1957).
- [5] M. Buttiker, Y. Imry, R. Landauer, and S. Pinhas, *Phys. Rev. B* **31**, 6207 (1985).
- [6] P. A. Lee and D. S. Fisher, *Phys. Rev. Lett.* **47**, 882 (1981).
- [7] H. de Raedt, *Comput. Phys. Rep.* **7**, 1 (1987).
- [8] D. Weaire and A. R. Williams, *J. Phys. C* **10**, 1239 (1977).
- [9] Q. J. Chu and Z. Q. Zhang, *Phys. Rev. B* **39**, 7120 (1989).
- [10] W. Xue, P. Sheng, Q. T. Chu, and Z. Q. Zhang, *Phys. Rev. Lett.* **63**, 2837 (1989).
- [11] D. Vollhardt and P. Wölfle, *Phys. Rev. Lett.* **48**, 699 (1982).