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Localization in Disordered Two-Dimensional Systems

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The question of localization is examined by employing the localization function method in the limit of infinitesimal disorder for a square-lattice tight-binding model. Within numerical accuracy we find that the localization function equals to 1 within the band; this strongly indicates that all eigenstates become localized for nonzero disorder.

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Recently there has been considerable discussion about the existence or nonexistence of extended electronic states in two-dimensional (2D) disordered systems.[1]

The purpose of this paper is twofold. First we present two theorems concerning the localization function method,[2] $L(E)$, which is based on Anderson's original approach[3,4]; these theorems are very useful because they allow the elimination of some additional approximations associated with the $L(E)$ method. Second, we report results for the $L(E)$ function in a 2D system with infinitesimal disorder. The localization function $L(E)$ which is less (more) than one in the regions of the spectrum consisting of localized (propagating) eigenstates is given by

$$L(E)=\lim_{N\to\infty}\Big|\sum_j V^{N+1}t_j^{(N)}(E)\Big|^{1/N}=\lim_{N\to\infty}\Big|\sum_j V^{N+1}G_{n_1}^{0}G_{n_2}^{0,n_1}\cdots G_{n_N}^{0,n_1,\ldots,n_{N-1}}\Big|^{1/N}, \tag{1}$$

where V is the off-diagonal matrix element V_{ij} of the tight-binding Hamiltonian

$$H=\sum_i \epsilon_i|i\rangle\langle i|+\sum_j{}' V_{ij}|i\rangle\langle j|,$$

and

$$G_{n_i}^{0,n_1,\cdots}(z)=\langle n_i|(z-H^{0,n_1,\cdots})^{-1}|n_i\rangle; \tag{2}$$

the superscripts $0, n_1, \ldots$ denote that $\epsilon_0=\epsilon_{n_1}=\cdots=\infty$. Finally the summation over j in Eq. (1) is over all sets of sites $\{n_1, n_2, \ldots, n_N\}$ which form self-avoiding paths starting and ending at site 0.

The calculation of $t_j^{(N)}\equiv G_{n_1}^{0}\cdots G_{n_N}^{0,n_1,\ldots,n_{N-1}}$ is greatly facilitated by two theorems for $t_j^{(N)}(z)$, which are stated below (the proofs will be presented elsewhere): Theorem 1 states that

$$t_j^{(N)}(z)=\prod_i(z-\tilde{E}_i^{\,j})/\prod_i(z-E_i), \tag{3}$$

where $\tilde{E}_i^{\,j}$ are the eigenvalues of $H^{0,n_1,\ldots,n_N}$ and E_i are the eigenvalues of H^0; the proof is based on the fact that the poles of each G in the $t_j^{(N)}(z)$ are canceled by the zeros of the previous G. Theorem 2 states that

$$t_j^{(N)}(z)=\det\{G_j^{(N)}\}/G_{00}, \tag{4}$$

where the elements of the matrix $G_j^{(N)}$, G_{nm}, are the Green's functions $G_{nm}=\langle n|(z-H)^{-1}|m\rangle$, and the sites n, m belong to the self-avoiding path j. Equation (4) is valid for both open and closed self-avoiding paths. Theorem 2 is proved either by induction or by starting from Theorem 1. Up to now $t_j^{(N)}(z)$ was approximated by $(G_{n_1}^{0})^N$ in order to avoid the very tedious calculations of Green's functions with many sites excluded. Equation (4), which expresses $t_j^{(N)}$ in terms of Green's functions with no sites excluded, greatly simplifies the calculation of $t_j^{(N)}$ and makes the approximation $t_j^{(N)}\approx(G_{n_1}^{0})^N$ unnecessary. In the present case of infinitesimal disorder, G_{nm} are the periodic Green's functions, which can be calculated very accurately; thus we avoid here another usual source of approximation, namely that of replacing G_{nm} by an appropriate average (e.g., the coherent-potential-approximation average).

There is still one point which makes the calculation of $L(E)$ very difficult: The Green's functions for an infinite system have to be evaluated at $z = E + is$ as $s \to 0$, while the localization function $L(E)$ must be obtained at a real energy E. One can easily show from Eq. (3) that

$$\lim_{s\to 0} |t_j^{(N)}(E+is)| = |t_j^{(N)}(E)|.$$

Thus our method allows a calculation of the magnitude of $t_j^{(N)}(E)$ but not of its sign. The latter is needed because of the summation in Eq. (1). To temporarily avoid this difficulty we calculated first the quantity $L^*(E)$:

$$L^*(E) = \lim_{N\to\infty} [\sum_j V^{N+1} |t_j^{(N)}(E)|]^{1/N}. \quad (5)$$

Clearly $L^*(E) \geq L(E)$. The equality holds for E at the band edge (or outside it) as can be seen from Eq. (3). The assumption of strong correlations[2] puts $L^*(E) = L(E)$ everywhere. We shall reexamine later this assumption. To calculate $\lim_{N\to\infty}[\sum_j |t_j^N(E)|]^{1/N}$ we have followed three equivalent yet distinct approaches in order to check the accuracy of our extrapolation to $N \to \infty$.

First Method.—We explicitly calculated $\det\{G_j^{(N)}\}$ for all self-avoiding closed paths (polygons) up to order $N = 14$. The calculations are facilitated because many different paths give (because of symmetry considerations) the same value for $\det\{G_j^{(N)}\}$. E.g., to obtain the contribution of the 16 464 self-avoiding polygons of order $N = 14$ one needs to evaluate only 86 distinct determinants of order 14×14. Having $\sum_j |t_j^{(N)}(E)|$, we define

$$(L^*)_N \equiv V[\sum_j |t_j^{(N)}(E)| / \sum_j |t_j^{(N-2)}(E)|]^{1/2}.$$

It turns out that $(L^*)_N$ vs $1/N$ is almost a straight line (except at $E = 0$); thus $L^* = \lim_{N\to\infty}(L^*)_N$ is obtained rather accurately by linear extrapolation.

Second Method.—Taking into account that $(M_N)^{1/N} \to K$ as $N \to \infty$, where M_N is the total number of self-avoiding polygons and K is the connectivity of the lattice ($K = 2.639$ for the square lattice), we can write

$$L^*(E) = KV \lim_{N\to\infty} \langle |t_j^{(N)}(E)| \rangle^{1/N}; \quad (6)$$

the brackets indicate the average over all j of order N. We have calculated as in the previous method the quantity $\langle |t_j^{(N)}(E)| \rangle^{1/N}$ up to $N = 14$. We found that it becomes weakly dependent on N as N increases (except at $E = 0$); thus the $N \to \infty$ limit can be obtained rather accurately.

Third Method.—We have estimated $\langle |t_j^{(N)}(E)| \rangle^{1/N}$ in Eq. (6) from a sample of M randomly generated open self-avoiding paths of order N (N up to 100; $M = 10$–100). Again the results are almost independent of N for large N and one can easily extrapolate to $N = \infty$.

The Green's functions G_{nm} for the square lattice were calculated by some well-known recursion relations.[5] At the center and the edges of the band, special care is needed because of the singularities of G_{nm}. Also for $|E| \geq 4V$ the recursion relations develop numerical instabilities which can be avoided by using asymptotic expansions for G_{nm} (for large $|n-m|$). Details will be presented elsewhere.

In Fig. 1 we present our results for $L^*(E)$ vs E according to the three methods above. A test of the accuracy of our calculation is the behavior of $L^*(E)$ for $E \geq 4V$, where $L^*(E) = L(E)$; $L(E)$ must approach monotonically 1 as $E \to 4V^+$. Figure 1 shows that this is actually the case within a 1% numerical uncertainty. This is the first time that such accuracy has been obtained without the use of adjustable parameters. There is a precipitous drop of $L^*(E)$ at $E = 0$ (from 2.33 ± 0.05 at $E/2V = 0.005$ to 1.4 ± 0.4 at $E = 0$). Furthermore the *estimated* error at $E = 0$ is more than an order of magnitude larger than the estimated er-

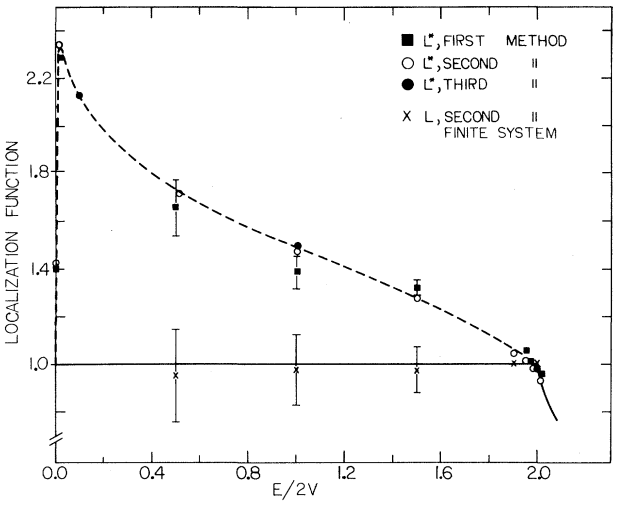

FIG. 1. The localization function $L(E)$ (solid line) and its upper limit $L^*(E)$ (dashed line) vs E for a square lattice in the limit of infinitesimal disorder. At the center ($E = 0$) and the edges ($E = \pm 4V$) of the band, $L^*(E) = L(E) = 1$. The points (solid square, open circle, and solid circle) represent results for $L^*(E)$ according to three different methods (see text) and the crosses are results for $L(E)$ from finite systems; bars indicate estimated errors.

rors at other energies. Finally, according to arguments to be presented below, the actual value of $L(E)$ at $E=0$ is 1.

The precipitous drop of $L^*(E)$ at $E=0$ has two causes: First, for a lot of paths j (closed or open), $t_j^{(N)}(0)$ was exactly zero. As a matter of fact, for large N it was difficult to find a path for which $t_j^{(N)}(0)$ was not zero. Second, even when $|t_j^{(N)}(0)|$ was different from zero, it was substantially less than the value of the same diagram at, e.g., $E/2V=0.005$.

We found that the vanishing of $t_j^{(N)}(0)$ is associated with at least one of the eigenvalues $\tilde{E}_i^j$ being zero [see Eq. (3)]; these zero eigenvalues correspond to localized chainlike eigenfunctions which terminate at appropriate points of the path j as discussed by Kirkpatrick and Eggarter[6] and Yoshino and Okazaki.[7] Thus one sees that the $E=0$ Kirkpatrick–Eggarter localization, which is associated with a special type of disorder,[6] is related to the localization of the eigenfunctions at $E=0$ for any kind of disorder.

The reduced values of the nonzero $t_j^N(0)$ can be explained by the following argument: The Green's function $G_{nm}(E+is)\sim|n-m|^{-1/2}$ when $|n-m|\gg R(E)$ and E inside the band; for $|n-m|\lesssim R(E)$, G_{nm} is of the same order of magnitude as G_{00}. The length $R(E)\to\infty$ as $E\to 0$; thus $G_{nm}(0)/G_{00}(0)$ remains appreciable for any distance $|n-m|$. This property (which implies strong multiple-scattering effects) cause both a very slow convergence as N increases [which explains the large estimated errors of $L^*(0)$] and a reduction of the value of $\det\{G_j^{(N)}\}$.

We found out that all $t_j^{(N)}(is)$ [apart from a common factor $G_{00}(is)$] are real and for a given N all have the same sign; thus $L(0)=\lim_{s\to 0}L(is)=\lim_{s\to 0}L^*(is)$. But the localization function $L(is)$ is less than one for $s\neq 0$ because the renormalization perturbation expansion[2] always converges outside the band.[2] Hence $L(0)\leq 1$. Actually the equality sign holds because as the disorder approaches zero the eigenstates at $E=0$ must tend to extended Bloch states.

What is happening at other energies? The real question is whether or not the signs of each $t_j^{(N)}(E)$ produce enough cancellations as to reduce $L(E)$ from its upper-limit value $L^*(E)$ to 1. To examine this question we considered finite systems (25×25, 51×51, 101×101 sites) with no disorder and rigid boundary conditions for which we calculated explicitly the Green's functions G_{nm} at *real* energies E. Thus, by employing Eq. (4), we were able to obtain $t_j(E)$ for all self-avoiding polygons up to order 14. Using the first or the second method, we calculated both $L^*(E)$ and $L(E)$. Because we are dealing with real energies, the errors associated with the $N\to\infty$ extrapolation were significantly larger than before for most of the energies inside the band (see Fig. 1). The values of L^* (not shown in Fig. 1) were consistent with the previous ones. $L(E)$ was found considerably less than $L^*(E)$ and, within numerical uncertainties, equal to one for E within the band. As the disorder increases from zero, one expects that $L(E)<1$ for all E (implying that all eigenstates are localized); $L^*(E)$ would also decrease except for $E\approx 0$ where the sharp peak would tend to disappear. On the basis of numerical work in finite samples,[8] we conjecture that $L^*(E)<1$ implies strong localization while $L(E)<1<L^*(E)$ implies very weak localization which is not revealed in the numerical work. It is possible that $L(E)<L^*(E)$ for a d-dimensional system when $d\leq 2$, while for $d>2$ $L(E)\approx L^*(E)$. Let us point out that for $d\leq 2$ (and only for $d\leq 2$) a closed self-avoiding path separates the space into two disjoint regions, one inside and one outside. As a result of this topological property the eigenvalues $\tilde{E}_i^j$ of $H^{0,n_1,\ldots,n_N}$ (see Theorem 1) can be separated into two groups: The first group is associated with eigenfunctions outside the closed path (scattering-type eigenfunctions) while the second group is associated with the eigenstates trapped inside the closed path. We suspect that this second weakly correlated group, which is absent for $d>2$, may be responsible for strong sign cancellation in $|\sum_j t_j^{(N)}|$ and thus may be responsible for the localization in all disordered d-dimensional systems (with $d\leq 2$).

In conclusion, we have significantly improved the $L(E)$ method, and we have demonstrated that for 2D lattices the eigenstates become localized for any nonzero disorder.

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Hybrid Quantum Oscillations in a Surface Space-Charge Layer

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The transconductance of an accumulation layer on n-type InAs is studied in a magnetic field $\vec{H}$ parallel to the layer. Structures are observed, nonperiodic in $1/H$, corresponding to mixed electric and magnetic subbands. The effect promises a simple, sensitive method of probing the shape of the self-consistent potential in surface space-charge layers with multiply occupied subbands.

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We report the observation of quantum oscillations in a surface space-charge layer for the crossed-field geometry. In this geometry the magnetic field $\vec{H}$ is applied parallel to the space-charge layer, in contrast to the usual configuration in which both electric and magnetic fields are normal to the layer. For the usual configuration, electric and magnetic quantization is decoupled, leading to complete quantization of the two-dimensional electron gas.[1] For the crossed-field geometry, electric and magnetic quantization is mixed, giving hybrid subbands whose dispersion depends on the relative strengths of electric and magnetic fields.[2] The number of observable oscillations in our experiment corresponds to the number of electric subbands occupied at $H = 0$; thus a space-charge layer with multiply filled subbands is best suited for studying the effect.

The accumulation layer on low-concentration n-type InAs is such a multiply filled system.[3,4] Because of the small (isotropic) effective mass ($m^* = 0.024 m_e$)[5] the space-charge layer is ~100 Å thick in the usual density range (~10^{12} cm^{-2}). In relatively modest magnetic fields ($\lesssim 10$ T), the cyclotron radius achieves a comparable value, so that a perturbation approach[6] is not expected to be applicable.

Effects of a parallel magnetic field on a space-charge layer have been observed in other experiments. In a fixed, high-density accumulation layer on n-type InAs, Tsui[7] used a tunneling technique to observe the decrease of the binding energy of the (single) bound state with increasing magnetic field. In this high-density case (i.e., strong electric field) perturbation theory[6] predicted the observed H^2 dependence. Beinvogl, Kamgar, and Koch[8] observed the (plasma-shifted) intersubband resonant frequency to increase with magnetic field for an accumulation layer on (100) Si. Their result, expected qualitatively from perturbation theory,[6] was analyzed quantitatively by Ando.[2,9] Although the effect of H on the occupied ground-state subband can be treated as a small perturbation, the excited (unoccupied) subbands are severely distorted by the magnetic field. In PbTe this strong-field condition is easily realized for all subbands, and recently[10] inversion-layer cyclotron resonance was shown to behave three dimensionally in a parallel magnetic field. The present experiment is capable of describing features of the hybrid subbands not directly accessible by these other methods.

Our sample is a (100) epitaxial layer of InAs ($n \approx 2\times10^{15}$ cm^{-3}) overlaid with a SiO_2 insulating layer and a gate electrode. Further details may be found elsewhere.[3,4] We monitor the low-temperature (4.2 K) transconductance $d\sigma/dV_G$ of the induced accumulation layer as a function of V_G and H. (σ is the channel conductivity and V_G is

