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Anderson Localization in Two Dimensions

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The conductance for a two-dimensional tight-binding model with on-site disorder is calculated numerically with use of the Kubo formula. For weak disorder logarithmic localization is observed, in agreement with the scaling theory. The magnetoresistance is found to be negative in both the logarithmic and exponential localization regimes. Results for a model with random complex hopping matrix elements are also presented.

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In the last two years, significant advances have been made in understanding the scaling behavior of Anderson localization.[1,2] Much of the work has been based on the idea[3] that the behavior as a function of length scale L is determined by a single scaling variable, the dimensionless conductance at scale L, $g(L)=\Gamma(L)/(e^2/\hbar)$, where $\Gamma(L)$ is the conductance of a system with linear dimension L. The renormalization-group differential recursion relation which describes the changes in g as a function of length scale can be written as $d\ln g/d\ln L=\beta(g)$. The β function has been computed in two dimensions by perturbation theory in powers of g^{-1} for weak disorder. For spinless electrons it is found[4] that $\beta(g)=-(2\pi^2 g)^{-1}+O(g^{-4})$ where the absence of the zeroth-order term is unique to two dimensions (2D) and suggests that two is the lower critical dimensionality for the Anderson transition. In 2D, localization is predicted for any amount of disorder, since g always decreases as a function of L corresponding to insulating behavior. For weak disorder, however, the effects of localization will only decrease $g(L)$ logarithmically.

Numerical tests of these ideas have so far been based on rather small sample sizes and are not conclusive.[5-7] In particular, an approximate numerical study of the scaling behavior by one of us[8] failed to show the expected logarithmic localization in 2D. More recently several other approximate numerical calculations have come out in support of the one-parameter scaling theory.[9,10] The present work is aimed at helping to resolve the controversy.

We consider a tight-binding Anderson model on a 2D square lattice,

$$H=\sum_{j,k} V_x{}^{jk} a_{j+1,k}{}^{\dagger} a_{j,k} + V_y{}^{jk} a_{j,k+1}{}^{\dagger} a_{j,k} + \text{c.c.} + \sum_{j,k} E_{j,k} a_{j,k}{}^{\dagger} a_{j,k}, \tag{1}$$

where j and k label the sites in the x and y directions and E_{jk} is a random site energy distributed uniformly between $\pm W/2$. We initially take $V_x=V_y=1$. The parameter W thus provides a measure of the disorder. The frequency-dependent conductance of an $L\times L$ sample is given by the Kubo formula

$$\Gamma(\omega)=(\pi/\omega L^2)\int dE' \sum_{\alpha,\beta} |\sum_j \langle\alpha|J(j)|\beta\rangle|^2 \delta(E'+\omega-E_\beta)\delta(E'-E_\alpha), \tag{2}$$

where the current operator is $J(j)=ie\sum_k V_x{}^{jk}(a_{j,k}{}^{\dagger}a_{j-1,k}-\text{c.c.})$ and $|\alpha\rangle, |\beta\rangle$ are the eigenstates of the system with $E_\alpha<E<E_\beta$, where E is the Fermi energy. For an isolated sample the eigenvalues are discrete and $\Gamma(\omega)$ consists of a series of δ functions so that some procedure for averaging over ω must be introduced.[7,11] Furthermore the numerical computation of the current matrix elements is time consuming. We thus take a somewhat different approach by extending the disordered sample to infinity in the $\pm x$ directions by affixing an ordered tight-binding lattice on each side. We take periodic boundary conditions in the y direction for all x, and apply an electric field in the x direction *only* in the disordered region. The energy spectrum will now be continuous and the $\omega\to 0$ limit of the conduc-

tance can be taken. Current conservation immediately implies that the matrix element $\langle\alpha|J(j)|\beta\rangle$ is independent of j. The sum over j in Eq. (2) is hence trivially done.

We introduce the Green's function $G^{(\pm)}=(E-H\pm i\eta)^{-1}$ and $2iG''=G^{(-)}-G^{(+)}$. Defining $\Gamma=\Gamma(\omega=0)$, Eq. (2) simplifies to

$$\Gamma=(e^2/\pi)\,\mathrm{Tr}[G''(j_0,j_0')G''(j_0'-1,j_0-1)+G''(j_0-1,j_0'-1)G''(j_0',j_0) - G''(j_0,j_0'-1)G''(j_0',j_0-1)-G''(j_0-1,j_0')G''(j_0'-1,j_0)], \quad (3)$$

where the trace is over the site index k and the j_0, j_0' are arbitrary. For j_0 and j_0' chosen to be on opposite sides and far away from the disordered region we have shown elsewhere[12] that Eq. (3) is equivalent to

$$\Gamma=(e^2/2\pi\hbar)\,\mathrm{Tr}(t^\dagger t), \quad (4)$$

where t is the transmission matrix relating incoming waves on one side of the disordered region to "transmitted" waves on the other side. One can compute t using a transfer-matrix technique which is in principle more efficient than calculating the Green's functions in Eq. (3) (the cost is $\propto L^3$ vs L^4), but the matrix inversion necessary to obtain t rapidly becomes singular, limiting this method to relatively small L, but providing a useful check to the calculations described below.

We should mention a shortcoming of our choice of boundary condition. By applying a field, E, only in the disordered region a current is generated in the ordered "wire" that is spatially nonuniform, i.e.,

$$J(x,t)=(ELe^2/2\pi\hbar)\textstyle\sum_{ab}|t_{ab}|^2\exp(i\omega|x|/v_a-i\omega t),$$

where v_a is the velocity in channel a. This gives rise to density fluctuations that must be screened out in a charged system. It has recently been shown[13,14] that in the single-channel case, application of a spatially uniform out-of-phase field in the wire produces a uniform total current so that the Landauer formula $\Gamma=(e^2/2\pi\hbar)|t|^2/(1-|t|^2)$ is obtained. It is unclear at present how to generalize this result to many channels (i.e., a finite-width strip) but the expectation is that in the limit of large channel number the correction to Eq. (4) will be small.

We compute the Green's functions by a recursive method[11] which builds up the sample in the x direction one column at a time, starting from the left with a system in which all sites $j>j_0$ are deleted. The Green's function $G^L(j_0)\equiv G_{kk'}{}^L(j_0,j_0)$ for the last column obeys the matrix recursion relation

$$G^L(j_0)=[G^0(j_0)^{-1}-V_x{}^2G^L(j_0-1)]^{-1}, \quad (5)$$

where $G^0(j_0)$ is the Green's function for the isolated j_0th column. Similarly we introduce $G^R(j_0)$ as the first-column Green's function for a system in which all sites $j<j_0$ are deleted. It is easy to show that

$$G(j,j)=[G^0(j)^{-1}-V_x{}^2G^R(j+1)-V_x{}^2G^L(j-1)]^{-1} \quad (6)$$

and $G(j,j+1)=G(j,j)V_xG^R(j+1)$. We have assumed V_x to be a constant in the above discussion, but this condition can easily be relaxed.

Initially G^L is computed for a semi-infinite system of a perfect lattice and then, by repeated use of Eq. (5), G^L is computed for the left-hand side plus the disordered region. Finally another semi-infinite perfect system is attached to the right with use of Eq. (6). The conductance is then calculated from Eq. (3) with $j_0=j_0'$ just outside the disordered region.

The logarithm of the dimensionless conductance is computed for M different samples with fixed W and E. The mean $\overline{\ln g}$ and the rms deviation $\Delta\ln g$ are then calculated with typically $M=200$ for $L=16$ and 32 and $M=100$ for $L=64$. The results for $W=4$, $E=0$ (band center) are shown in the inset in Fig. 1. The error bars are statistical, given by $\pm(\Delta\ln g)/\sqrt{M}$. We see that $\overline{\ln g}$ decreases upon doubling of L in at least qualitative agreement with the logarithmic localization predicted by the scaling theory. For the same value of W, the previous calculation by Lee[8] showed metallic behavior, i.e., $\overline{\ln g}$ independent of L. That calculation was approximate in that the basis set was truncated with each doubling of L, and can be viewed as an approximation valid for strong disorder. Apparently systematic errors were sufficiently large at $W=4$ to produce the wrong answer. It is worth noting that Stein and Krey[7] computed the conductance using the Kubo formula for isolated samples and obtaining $\ln g=-1.65$ for $W=4$ independent of L. Due to var-

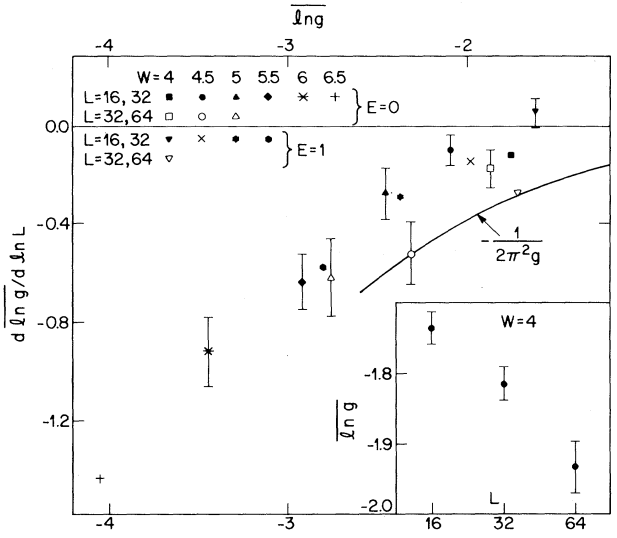

FIG. 1. Numerically calculated scaling function for the Anderson model showing the dependence of the logarithm of the conductance g on length scale L.

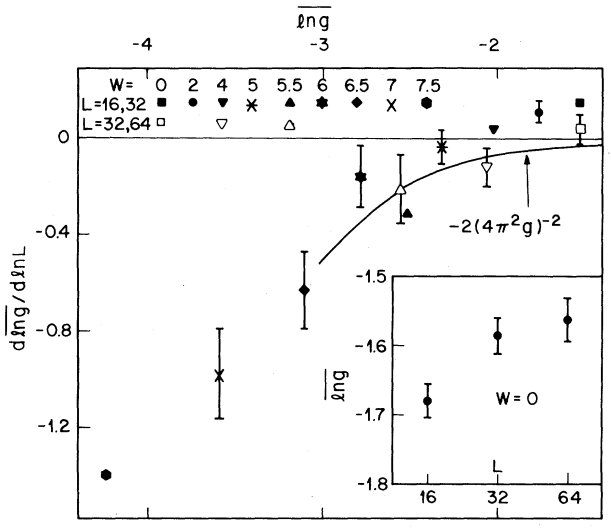

FIG. 2. Scaling function for the Anderson model with random complex hopping matrix element.

ious approximations their calculations are effectively cut off at relatively small L, so that the agreement with the present result is reasonable. We further note that Eq. (4) most likely underestimates the conductance and requires corrections of order l/L (l is the mean free path) to account for boundary resistance and the effects of current in the perfect regions. Since these corrections would probably lead to smaller underestimates of the conductance for larger systems, we believe that our observed decrease in $\overline{\ln g}$ with increasing L is a slight underestimate.

By calculating the differences $\overline{\ln g(2L)} - \overline{\ln g(L)}$ for various values of W we construct the numerical scaling function shown in Fig. 1. Note the similarity between the data for $E=0$ and 1. The open symbols are obtained from $L=64$ and $L=32$ samples and are quite consistent with the perturbative result $\beta=(2\pi^2 g)^{-1}$. The solid symbols are from $L=32$ and $L=16$, and may overestimate β for the reasons discussed above, especially in the large-g limit when l/L is large. These corrections appear to be small for $\ln g \lesssim -3$.

It has been shown that the leading logarithmic divergence in perturbation theory is destroyed by terms in the Hamiltonian which break time-reversal symmetry, such as spin-flip scattering[16] or a magnetic field.[17] There is a disagreement on the next leading term which either vanishes[18] or is given by $\beta(g) \approx -2/(4\pi^2 g)^2 + O(g^{-4})$.[19] To test this case we have performed calculations with $V_x=1$ and $V_y{}^{jk}=\exp(i\theta_{jk})$, where θ_{jk} is a random phase.[20] The results for purely off-diagonal disorder, $W=0$, are shown in the inset in Fig. 2. The increase in g between $L=16$ and 32 may be due to finite-size effects. Comparison with the inset in Fig. 1 shows that the two cases with similar g show very different scaling behavior. A scaling function is constructed as before and shown in Fig. 2. Again the open symbols which are obtained from scale changes between $L=32$ and 64 are consistent with the perturbative result. The uncertainties in our computation are such that we cannot hope to distinguish between a smooth nonzero β function and the existence of a line of fixed points, but it is clear that the complex hopping case is described by a very different β function than the real hopping case.

Lastly, we present some calculations of magnetoresistance. A uniform magnetic field B normal to the plane can be introduced by taking $V_x=1$ and $V_y{}^{kj}=\exp(iBj)$ in Eq. (1), where B is measured in units of $\hbar c/a^2 e$ (a is the lattice spacing). The results for $W=4$ are shown in Fig. 3(a). For a given L we observe a negative magnetoresistance. For a sufficiently large field we find that the logarithmic localization is destroyed. The conductance change for $B=0.1$ as L varies from 16 to 64 is similar to the complex hopping case. This is again consistent with predictions based on the perturbation theory.[17] Interestingly the negative magnetoresistance persists into the exponentially localized regime as shown in Fig.

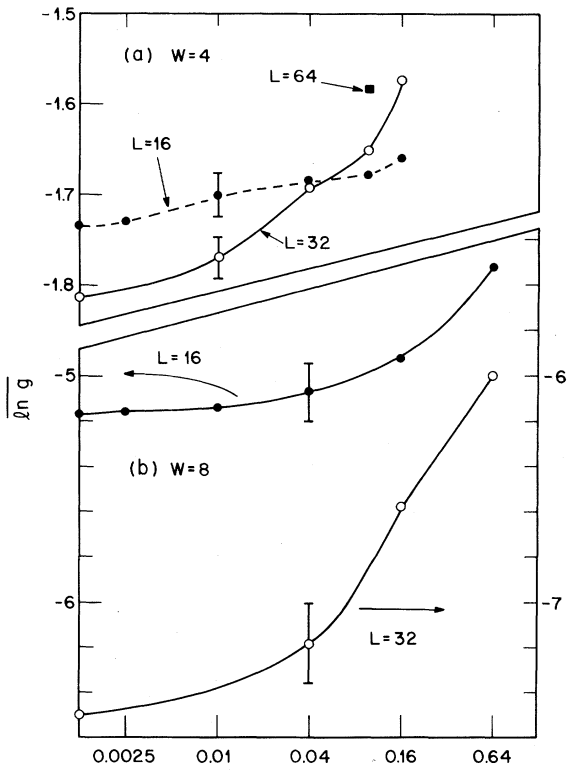

FIG. 3. Conductance vs magnetic field B measured in units of $\hbar c/ea^2$.

3(b) for $W=8$. This suggests that the localization length *increases* with increasing magnetic field. We speculate that this occurs when the Landau radius $(eB/\hbar c)^{-1/2}$ becomes comparable with the localization length. Apparently the time-reversal-noninvariant nature of the magnetic field delocalizes the electrons.

Experimentally a negative magnetoresistance has been observed in metal-oxide-semiconductor field-effect transistors[21-23] in the low-field regime and in clean copper films[24] but not in alloy films.[25,26] Note that a theory based on electron-electron interactions[17,27] predicts logarithmic corrections to the conductivity similar in form to the localization theory. A negative magnetoresistance is, however, probably the best indicator of the presence of localization effects, since the interaction theory predicts only positive magnetoresistance.[17] It appears that a theory that takes into account both localization and interaction effects as well as various symmetry-breaking processes is necessary to explain the experiments.

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