Renormalization-group study of Anderson localization

Eytan Domany* and Sanjoy Sarker†
Department of Physics, FM-15, University of Washington, Seattle, Washington 98195
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A renormalization-group method is used to study localization of electrons in a random system. A position-space method yields a localization edge in three dimensions. In two dimensions our results indicate localization even for small randomness in agreement with Abrahams, Anderson, Licciardello, and Ramakrishnan; however we cannot rule out the existence of a localization edge.

The localization of electrons moving in a random potential[1] has attracted considerable attention[2] ever since the problem was first posed by Anderson.[1] In recent years, various authors have attempted to construct a scaling theory of localization,[3,4] and to address the issue on the basis of renormalization-group arguments.[5] The latest development was reported by Abrahams *et al.*[6] who presented a scaling theory for the dimensionless conductance $2\hbar G/e^2$. They conclude that in two dimensions all states are localized; while in three dimensions a localization edge is expected.

In what follows we present a renormalization-group study of the problem; although our results indicate agreement with the predictions of Abrahams *et al.*,[6] we cannot rule out the existence of a localization edge in two dimensions.

We consider the Hamiltonian

$$H=\sum_i \epsilon_i |i\rangle\langle i| - \sum_{\langle i,j\rangle} (|i\rangle\langle j| + |j\rangle\langle i|) \quad , \tag{1}$$

where $\langle i,j\rangle$ are nearest-neighbor sites of a d-dimensional hypercubic lattice. The independent, random site energies ϵ_i are taken from a *Gaussian* distribution of width σ and zero average, e.g.,

$$\langle \epsilon_i \rangle = 0, \quad \langle \epsilon_i \epsilon_j \rangle = \sigma^2 \delta_{ij} \quad . \tag{2}$$

The hopping element was chosen to be $t=1$ in Eq. (1); this choice sets the energy scale, and does not affect the eigenstates of H. The problem of interest is whether the eigenstates of Eq. (1), especially those with energies near the band center, $E=0$, are localized or extended. For $\sigma=0$ all states are extended, and for $\sigma \to \infty$ all are localized. The manner in which the localization length L varies with σ depends on the dimensionality of the system. In three dimensions we find that states at the band center are localized for $\sigma > \sigma_c$, with the localization length L diverging according to a power law $L \sim (\sigma - \sigma_c)^{-\nu}$, $\nu > 1$ as σ approaches $\sigma_c \simeq 7$ from above. In two dimensions, although we cannot rule out the existence of such σ_c, our results are consistent with localization for all values of σ, with L diverging exponentially for small σ, i.e., $L \sim \exp(1/a\sigma)$.

Our method uses perturbation theory to map the Hamiltonian (1) onto a new Hamiltonian, characterized by a new width σ' of the random distribution. The central problem is to establish this mapping, and to determine how σ scales under the renormalization-group transformation; namely, to estimate the function $\sigma' = f(\sigma)$. The main part of this work utilizes an application of position-space renormalization-group ideas. This method is expected to yield reliable results when σ is not too small.

Our approach is based on a version of perturbation theory.[7] The Hamiltonian H is written as the sum of two terms,

$$H = H_0 + H_1 \quad . \tag{3}$$

A certain set of the eigenstates of H_0 is included in a "model space" D. If ψ is an eigenstate of H with energy E, the projection of ψ onto D, denoted $\psi_D = P_D \psi$, satisfies the equation

$$H_D \psi_D = E \psi_D \quad . \tag{4}$$

The operator H_D is defined only in the subspace D, and is given by

$$H_D = H_0 + V_D \quad , \tag{5}$$

where V_D is the solution of the operator equation

$$V_D = H_1 + H_1 \frac{1-P_D}{E-H_0} V_D \quad . \tag{6}$$

If E, an exact eigenvalue of H, is known, one can, in principle, construct V_D and by solving Eq. (4) find the projections of the corresponding eigenstates ψ onto the model space D.

For an infinite lattice the spectrum of Eq. (1) forms a continuum, and we can choose any value of E near the band center to study the corresponding eigenstates. A realistic application of perturbation theory will expand V_D and keep terms to some finite order in H_1 (the present work is based on neglecting all second- and higher-order terms). This way an operator $V_D^{\text{approx.}}$ is defined, which is used in Eqs. (4)

and (5) instead of V_D. Whether such an approximation yields reasonably good eigenstates ψ_D, depends on the choice of H_0 and the model space D. If H_0 is such that its eigenstates reasonably approximate the eigenstates of H, low-order truncation of V_D can yield reasonable results. It is also important to include in D all eigenstates of H_0 with energies close to the energy E, thereby avoiding small values of the energy denominator in Eq. (6). When many states with energy near E are excluded from D, the approximation of replacing V_D by H_1, say, is not expected to yield reliable estimates of ψ_D.

Turning now to the Hamiltonian (1), note that for large σ all eigenstates of Eq. (1) are expected to be localized. Thus in this regime, it is appropriate to break the lattice into cells, and include in H_0 all elements of Eq. (1) that connect sites i,j *within* the same cell. Hopping elements that connect sites in *neighboring* cells are included in H_1. This separation of H is the basis of our position-space method, details of which are given below. The eigenvalues and eigenstates of H_0 are found numerically. To complete the definition of our procedure, we have to specify how the model space D is constructed. The choice of which states are to be included in D, depends on the energy E whose corresponding eigenstates we wish to study. If a cell contains b^d sites, b^d states per cell are generated. Of these, we include one from each cell in D; the state whose energy E_α is closest to E is chosen. If α,β stand for the selected cell states, we obtain, using $V_D \approx H_1$,

$$H_D = \sum_\alpha \epsilon_\alpha |\alpha\rangle\langle\alpha| - \sum_{\langle\alpha,\beta\rangle} t_{\alpha\beta}(|\alpha\rangle\langle\beta| + |\beta\rangle\langle\alpha|) , \quad (7)$$

where $\langle\alpha,\beta\rangle$ are nearest-neighbor cells, and $t_{\alpha\beta} = \langle\alpha|H_1|\beta\rangle$. In this new Hamiltonian not only the site energies ϵ_α are random, but also the hopping elements $t_{\alpha\beta}$. We now follow the spirit of renormalization-group treatments of random spin systems, approximating the generated $t_{\alpha\beta}$ distribution by a simpler one. Two choices were considered. The *first* replaces $t_{\alpha\beta}$ by a uniform $t_{\rm eff}$. However, one has to note that the variables $t_{\alpha\beta}$ will be generated with randomly selected signs. Sign$(t_{\alpha\beta})$ is determined by the signs of the cell states $|\alpha\rangle, |\beta\rangle$ that are chosen arbitrarily by the computer. The Hamiltonian (7) is invariant under a trivial gauge transformation generated by flipping the sign of any set of the cell states; only the frustration[8] of a plaquette of cells has physical significance. We investigated various measures of $t_{\rm eff}$, and chose to work with $t_{\rm eff} = \langle|t_{\alpha\beta}|\rangle$. Replacement of $t_{\alpha\beta}$ by $t_{\rm eff}$ in Eq. (7) reduces the randomness in the Hamiltonian, so that the "true" randomness is probably larger than what our estimate will yield. On the other hand, by working only in the model space D, some channels of possible propagation of the electron are discarded, thereby increasing the possibility of localization, which amounts to an effective increase of σ.

To put H_D in the form given by Eqs. (1) and (2), we divide Eq. (7) by $t_{\rm eff}$; however, we also have to shift the origin of energy by the average value of ϵ_α. For general E, $\langle\epsilon_\alpha\rangle \neq 0$, although for the band center ($E=0$) we get $\langle\epsilon_\alpha\rangle = 0$. After these manipulations the state ψ_D satisfies the equation $H'\psi_D = E'\psi_D$, where H' has the form (1). The new width σ' of the random site energy distribution and the new eigenvalue E' are given by

$$\sigma' = (\langle\epsilon_\alpha^2\rangle - \langle\epsilon_\alpha\rangle^2)^{1/2}/t_{\rm eff} , \quad (8a)$$

$$E' = (E - \langle\epsilon_\alpha\rangle)/t_{\rm eff} . \quad (8b)$$

Equations (8a) and (8b) constitute the recursion relations of our renormalization-group procedure. It should also be noted that, for small E the distribution of the site energies generated by our procedure was found to be reasonably approximated by a Gaussian distribution, even when the initial ϵ_i were taken from a uniform distribution over an interval $[-w/2, w/2]$. The *second* approximation of the $t_{\alpha\beta}$ distribution assigns to each bond the value $t_{\rm eff}$ with probability p or $-t_{\rm eff}$ with probability $1-p$. The value of p is determined by requiring that the probability of frustration of a basic plaquette is the same as that of the actual $t_{\alpha\beta}$ distribution (for details see below). With this parametrization the Hamiltonian (1), Eq. (2) is mapped onto

$$\mathcal{H} = \sum_i \epsilon_i |i\rangle\langle i| + \sum_{\langle ij\rangle} \eta_{ij}(|i\rangle\langle j| + |j\rangle\langle i|) , \quad (9)$$

where ϵ_i are distributed according to Eq. (2) and η_{ij} according to

$$P(\eta_{ij}) = p\,\delta(\eta_{ij}-1) + (1-p)\delta(\eta_{ij}-1) . \quad (10)$$

We found that starting with the Hamiltonian (1) (i.e., $p=1$) after a few iterations we map onto $p=\frac{1}{2}$, and this value does not change with further iterations.

For $\sigma=\infty$ all states are localized, and for $\sigma=0$ it has been shown[9] that there exists a finite range of energies near the band center with all states extended (although the off-diagonal elements are random). The recursion relations (8a) and (8b) are supplemented by one for p; however, the line $p=\frac{1}{2}$ was found to be invariant, and therefore on this only Eqs. (8a) and (8b) are needed.

Since for the band-center equation (8b) yields $E'=E=0$, this line is a trajectory of the renormalization-group transformation. On this line it is sufficient to study the recursion relation (8a), that yields $\sigma'=f(\sigma)$. An unstable fixed point of this relation corresponds to a critical randomness σ_c, above which the system flows to the localized ($\sigma\to\infty$) regime, while for $\sigma<\sigma_c$ it flows to $\sigma=0$. For $\sigma\gtrsim\sigma_c$ the states are localized over a length given by

$L = L_1(\sigma - \sigma_c)^{-\nu}$, where $\nu = \ln b/\ln\Lambda$, with $\Lambda = [df(\sigma)/d\sigma]_{\sigma_c}$, and b is the linear cell size. Stability of this fixed point in the E direction means that the same exponent characterizes the divergence of the localization length of all states as the mobility edge is approached. The mobility edge itself $E_c(\sigma)$ is given by the sepratrix that flows into the fixed point $(\sigma_c, 0)$. The recursion relation (8a), for $E = 0$, was studied extensively in two and three dimensions. We worked with cells of 3^d sites ($b = 3$). In 2-D samples of 900 cells were generated for each σ; in three dimensions the sample size was 512. These cells were arranged in *five different ways* to form a 30×30 (2-D) or $8 \times 8 \times 8$ (3-D) lattice, that was used to determine σ'. To study the flow of p, for each lattice the fraction of frustrated squares was calculated, and the new p was fixed to yield the same frustration probability. The function $f(\sigma)$ was determined using both ways of approximating the $t_{\alpha\beta}$ distribution; for the second approximation Eq. (10) was also used (with $p = \frac{1}{2}$) to generate the original random cells. The results of these procedures are shown in Figs. 1 and 2. In two dimensions we obtain $\sigma' > \sigma$ for all σ (except $\sigma = 0$). In three dimensions the numerical results do indicate a fixed point for $\sigma \approx 7$. These results may be viewed as evidence for the absence of localization in two dimensions, and presence thereof in three dimensions. However, this perturbative approach is certain to break down for small σ. In that regime the eigenstates are either extended, or localized over a scale much larger than any realistic choice of b. Moreover, for small σ each cell will contain more than one state with $\epsilon_\alpha \approx 0$. Since the number of these nearly degenerate states increases when a large cell is created from b^d small cells, increasing the number of states that are assigned to D (say, from one to three) will not resolve the problem of degeneracy. This, in turn, will cause the perturbation series for V_D to be very slowly convergent. Thus for small enough σ, truncation after first order in H_1 is not expected to yield a good representation of V_D. Therefore we are reluctant to accept the small-σ part of our curves as valid. However, we do believe that the results shown in Figs. 1 and 2 represent a good approximation of $f(\sigma)$ for $\sigma > 1$.

In two dimensions, the analysis of Abrahams

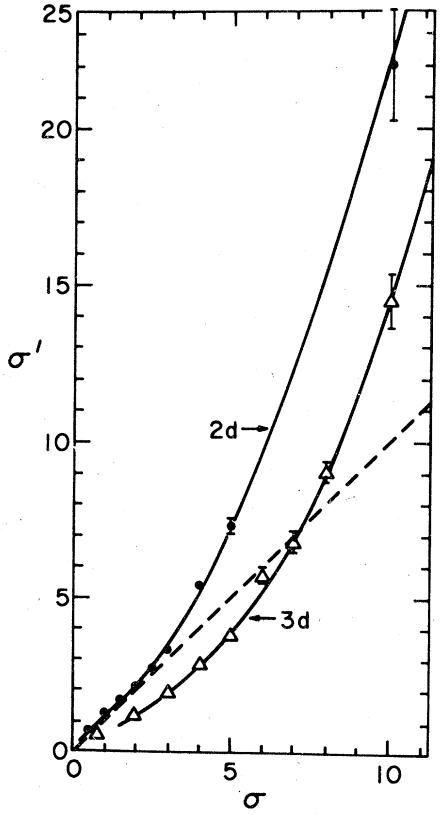

FIG. 1. σ' vs σ, in two and three dimensions. Results based on representing the hopping elements $t_{\alpha\beta}$ by a uniform t_{eff}. In two dimensions no fixed point is found, while in three dimensions we get $\sigma_c \approx 7$.

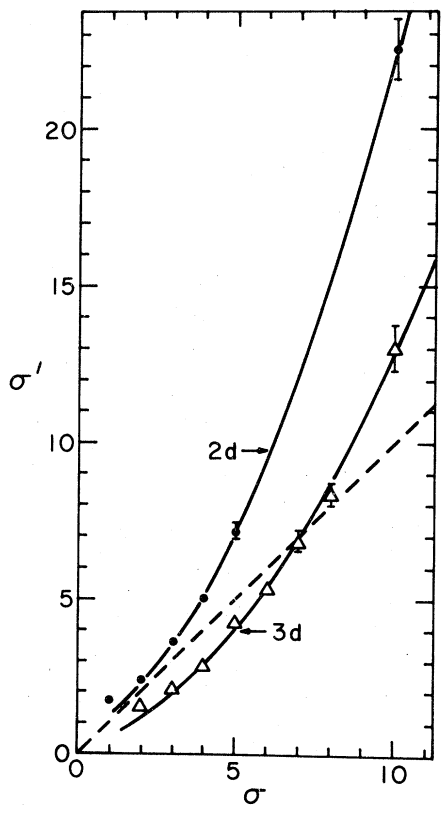

FIG. 2. σ' vs σ, in two and three dimensions. Results based on hopping elements with random signs [Eqs. (9) and (10) with $p = \frac{1}{2}$]. No fixed point in two dimensions; in three dimensions, $\sigma_c \approx 7$.

et al.[6] implies that the randomness is marginal near the $\sigma=0$ fixed point. It can be, however, marginally stable or marginally unstable, depending on the sign of the second-order coefficient in the expansion

$$f(\sigma)\approx\sigma+a_2\sigma^2+O(\sigma^3)\ . \tag{11}$$

At this point it seems that we do not have sufficient information to determine the sign of a_2 in an unambiguous manner, since our position-space method clearly breaks down for low σ. Nevertheless, since our results in three dimensions do show a fixed point, we believe that the absence thereof in two dimensions can serve as an indication of agreement with Abrahams *et al.* In this case, the differential recursion relations obtain from Eq. (12),

$$\frac{d\sigma}{dl}=\bar{a}\sigma^2+O(\sigma^3)$$

leads to the form $L\sim\exp(1/a\sigma)$ for the localization length L.

In three dimensions the randomness is irrelevant near the $\sigma=0$ fixed point, i.e., $f(\sigma)\approx a_1\sigma+O(\sigma^2)$ with $a_1<1$. This is indeed consistent with our numerical findings which show a fixed point for $\sigma_c\approx 7$. The statistical error in our present procedure does not allow a precise determination of ν; values of $1.25<\nu<1.75$ are consistent with the data.

It is difficult to make direct comparison with results derived by other methods since most workers use the rectangular site energy distribution of width w. If, however, we associate with σ a value of w that yields the same second moment, i.e., $w_c\approx\sigma_c(12)^{1/2}$, our result could be interpreted as $w_c\approx 24$. Analytic work by Licciardello and Economu[10] gave for the simple cubic lattice the values 62, 32, and 14.5 for three different criteria of localization, of which they consider 14.5 the most reliable. They also quote an upper bound of 24, attributed to numerical analysis of Schönhammer and Brenig.[11] Other numerical estimates for w_c/Z (where Z is the number of nearest neighbors on the lattice), evaluated for the diamond lattice,[11–13] yield $w_c/Z\approx 2$.

As to the exponent ν, the values reported in the literature[5,14] correspond to a definition $L\sim(E-E_c)^{-\nu'}$, which is different than ours. Most values for ν' are in the range 0.6–0.75. Stein and Krey[13] estimate $\nu_w=0.66\pm0.05$, and although their definition of ν_w coincides with ours, the numerical value is not in agreement.

An important question we plan to address in the future concerns the stability of the $E=0$ fixed point. If it is unstable, the exponent ν' is expected to differ from our ν.

The numerical method presented above can be improved by studying larger cell sizes, and, to a certain extent, by increasing the number of states assigned to D from each cell. Inclusion of second- and higher-order terms in V_D may turn out to be important to achieve significant improvement.

Recently we received a report by Lee who studied the 2-D problem by a closely related method, and does find a localization edge.[15]

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*Present address: Dept. of Electronics, Weizmann Inst. of Science, Rehovot, Israel.

†Present address: LASSP, Clark Hall, Cornell Univ., Ithaca, N. Y. 14853.

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