Real-Space Scaling Studies of Localization

Patrick A. Lee
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 15 March 1979)

The Anderson model of localization in two dimensions is studied with use of a numerical implementation of real-space renormalization-group transformations. A critical parameter W/V is found which separates localized and extended behavior, the latter being characterized by scaling toward strong coupling.

There has been considerable recent interest toward producing a scaling theory of electronic localization in disordered systems. In particular, Thouless and co-workers[1-3] have stressed that when two pieces of material are put together the properties of the wave function of the combined system may be determined entirely by the conductance of each subsystem. This point of view was further developed in a recent paper by Abrahams, Anderson, Licciardello, and Ramakrishnan.[4] These authors write down a single-parameter scaling equation

$$\partial \ln g / \partial \ln L = \beta(g), \tag{1}$$

where $g = G/(e^2/\hbar)$ is the dimensionless conductance which is a function of the linear dimension L of the sample. It is clear that $\beta(g)$ approaches $d-2$ for large g. The two dimensional case is particularly interesting. Abrahams *et al.* assume that β is monotonic and regular. It then follows that β is always negative and scaling is toward the weak-coupling limit. Consequently Abrahams *et al.* concluded that all states are localized in two dimensions.

The purpose of this work is to implement numerically the renormalization program discussed by Thouless and by Wegner.[5] For definiteness I study the Anderson[6] model on a square lattice,

$$H = \sum_i \epsilon_i |i\rangle\langle i| + V \sum_{\mathrm{NN}} (|i\rangle\langle j| + \mathrm{c.c.}), \tag{2}$$

where ϵ_i is distributed randomly between $-W/2$ and $W/2$, and V is a constant hopping matrix element between nearest neighbors (NN). Previous numerical work has involved diagonalization of the secular matrix for samples of increasing sizes.[1,7] Instead I start by diagonalizing 200 $L = 4$ samples with noninteracting boundary conditions. The basis set is truncated from sixteen states to M states closest to a given energy (chosen to be the band center in this paper). The eigenvalue and the wave function on the border sites are stored. Next I divide the 200 samples into four groups and pick a sample at random out of each group to put together to form an $L = 8$ sample. The coupling between state α in cell i and state β in the neighboring cell j can be calculated from the border wave function. These coupling constants are denoted $V_{\alpha\beta}'(L)$ with $L = 4$ in this case. A $4M \times 4M$ secular matrix can now be set up and diagonalized. Again the basis is truncated, this time from $4M$ to M states, and their energies and wave functions on the border of the $L = 8$ sample are stored. One can visualize this pictorially as "tracing" over the internal borders. This is repeated until 200 $L = 8$ samples are generated. The process is iterated with the storage requirement increasing linearly with L. In the calculation presented here, L goes up to 256.

It should be apparent that the present scheme is similar in spirit to Wilson's solution of the Kondo problem.[8] The only approximation in this scheme is the truncation of the basis set. This should be a reasonable approximation as long as $V'(L)/\tilde{W}(L) \ll 1$, where $\tilde{W}(L)$ is the average spacing between energy levels of the $L \times L$ system. The discarded energy levels (labeled δ) can be included by perturbation theory[9] and contribute the following correction to the secular matrix:

$$\delta V_{\alpha,\beta}' = \sum_\delta V_{\alpha,\delta}' V_{\delta,\beta}'/(E - E_\delta). \tag{3}$$

We note that after a single iteration, V' is random in sign and varies over several orders of magnitude. Thus for $\alpha \neq \beta$, $\delta V_{\alpha\beta}'$ is a fluctuation quantity and is small compared with $V_{\alpha\beta}'$. This is especially true for states near the band center because the energy denominator is at least $\sim M\tilde{W}/2$. Since we are dealing with a random system the small random correction can be thought of as changing the system to a slightly different member of the statistical ensemble. There is, however, one systematic correction. The diagonal elements $\delta V_{\alpha,\alpha}'$ are not random in sign and are proportional to $-E$ on the average. Physically the discarded states produce a compression of the states that are retained. Indeed from the

numerical work I find that $\tilde{W}$ does not decrease by a factor of 4 per iteration as it should. I have simply uniformly compressed the M eigenvalues at the beginning of each iteration so that $W'(L) = r(L)\tilde{W}(L)$ produces the correct density of states. I have chosen $M = 6$ in the data presented here and $r(L)$ is found to be between 0.8 and 0.9.

The scaling behavior of the system is monitored by studying the quantity $v(L) = \langle V'(L)\rangle / W'(L)$, where $\langle V'\rangle$ denotes a geometric mean of the absolute value of $V_{\alpha\beta}'$. The quantity $v(L)$ looks like a generalization of the initial V/W and it is tempting to interpret it as the scaling variable.[5] However, we know that v cannot be the only variable because by itself it is insufficient to determine the scaling behavior of the model. This is because there exists important correlation between $V_{\alpha\beta}'$ and $V_{\alpha\beta'}'$ when β and β' belong to two different neighboring cells. The state α may have large amplitude near one corner of the cell leading to large $V_{\alpha\beta}'$ and small $V_{\alpha\beta'}'$. Failure to include this correlation leads to completely wrong behavior of the model. However, $v(L)$ still provides a valuable monitor of the system and it is instructive to look at the quantity

$$d\ln v / d\ln L = \beta'(v). \tag{4}$$

This is obtained numerically from $[\ln v(2L) - \ln v(L)]/\ln 2$ for a variety of initial V/W values and the results are shown in Fig. 1(a). We see that for $W/V \geq 6$, v scales toward weak coupling and β' becomes increasingly negative whereas for $W/V \leq 5.8$ scaling is toward strong coupling. The solid line is a guide to the eye. It crosses the x axis at $v = 0.11$, an indication that the truncation of basis is a reasonable approximation up to the "fixed point." For $v > 0.11$ scaling is toward strong coupling. The following simple argument shows that β' should approach 0.5 for large v. If we start with large V/W the wave function must initially be extended even for samples large compared with the mean free path λ. When two such samples are put together $V_{\alpha\beta}'$ is the sum of the product of the wave functions on the opposite borders. Each wave function is $\sim L^{-1}$ from the normalization and we are summing L/λ quantities that fluctuate in sign and magnitude. We thus conclude that $V_{\alpha\beta}' \sim VL^{-2}(L/\lambda)^{1/2}$. Hence $v = V'/W' \propto L^{1/2}$ and $\beta' = \frac{1}{2}$. Of course, the basis truncation approximation breaks down when v becomes large, and we have discarded data for $v \gtrsim 0.5$.

A second monitor of the scaling behavior is Thouless's sensitivity to boundary condition $\langle \Delta E\rangle$.[1-3] This is defined as the geometric mean

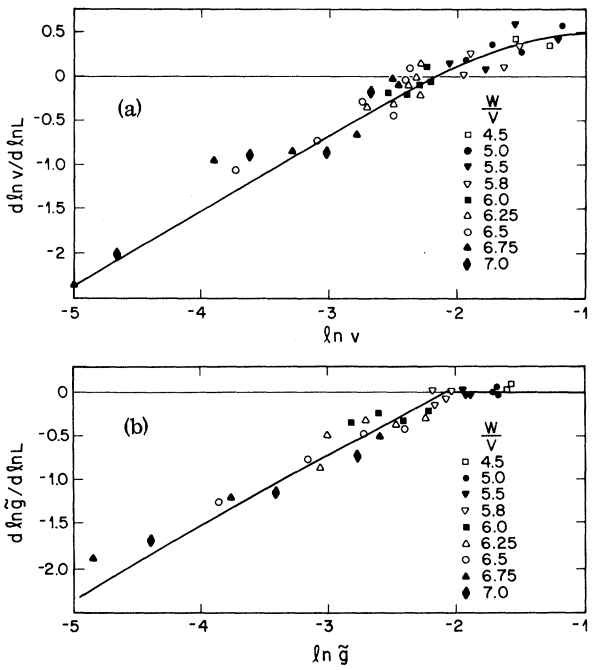

FIG. 1. (a) The scaling function β' vs $\ln v$ obtained from $\ln v(L) - \ln v(L/2)$ with L up to 256 for a variety of W/V. The solid line is a guide to the eye. (b) The scaling function β vs $\ln \tilde{g}$.

of the shift in the eigenvalues if a sample is subject to periodic and then antiperiodic boundary conditions. It is straightforward within our scheme to calculate this quantity at each iteration. Licciardello and Thouless[2] have argued that $\tilde{g}$ defined as $\langle \Delta E\rangle / 1.45\tilde{W}$ equals g, the conductance divided by $e^2/\hbar$. The quantity $\tilde{g}$ is a more attractive candidate for the scaling variable because $\langle \Delta E\rangle$ contains the correlation across the two opposing borders of the sample. Its scaling behavior is similar to that of v when the latter scales toward weak coupling. However, if $\tilde{g}$ is related to the conductance it can only remain constant, even if v scales toward infinity. This is shown in Fig. 1(b). The solid line is again a guide to the eye: It intersects the x axis at $\tilde{g} = 0.13$ and remains zero for larger values of $\tilde{g}$. I do not believe that it is correct to interpret this as a line of fixed point as in the two-dimensional x-y model,[10] because other parameters like v are scaling toward strong coupling. This behavior of β contradicts the smooth behavior postulated by Abrahams *et al.*,[4] and I disagree with their conclusion that all states are localized in two dimensions.

In Fig. 2 is shown the behavior of $\ln \tilde{g}$ vs L for

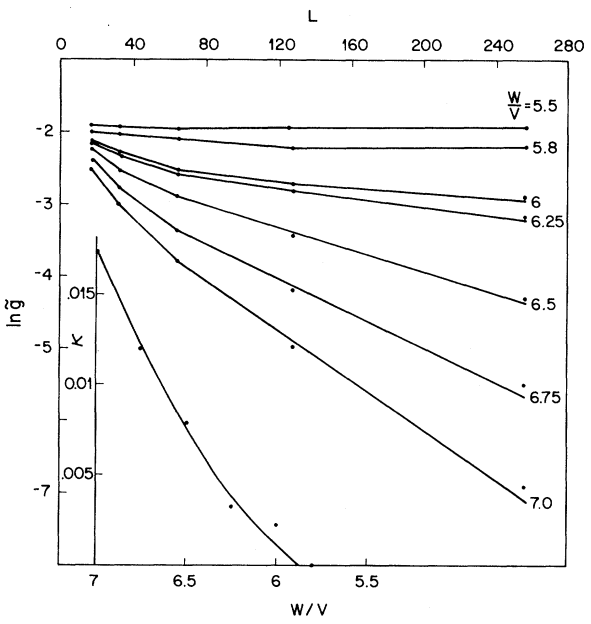

FIG. 2. Plots of $\ln\tilde{g}$ vs L. The slope of the straight-line portion gives the inverse localization length κ which is shown in the inset vs W/V.

several W/V. In particular for $W/V=6$ the values for $L=8$, 16, and 32 decrease in a manner consistent with that obtained by Licciardello and Thouless[1] by diagonalization of the secular matrix up to $L=34$, an observation which led these authors to speculate that all states are localized in two dimensions. My present result indicates that the critical W/V is between 5.8 and 6.0. For $W/V>6.0$ we can see a systematic deviation from exponential decrease for larger L. An explanation may be that the precise numerical factor relating conductance and $\tilde{g}$ provided by Licciardello and Thouless[2] is based on the assumption that the distribution of the individual energy shift ΔE upon boundary condition change is Lorentzian. I have compiled histograms of the distribution on a logarithmic scale. For $\tilde{g}\geq 0.13$ the distribution scales toward a fixed form upon iteration which is not quite Lorentzian because it has a tail on the small-ΔE side; nevertheless, its full width at half height is very close to that of a Lorentzian. When the scaling is toward weak coupling the distribution broadens continuously and develops a long tail for small ΔE. It is likely that the relation between conductance and $\tilde{g}$ is not a constant ratio. If we simply take the slope of the straight lines drawn in Fig. 2 as an inverse localization length κ we can plot κ vs W/V as shown in the inset. There is too much uncertainty in this kind of a plot to extract the exponent in $\kappa\sim[W/V-(W/V)_c]^{\nu}$, but perhaps it is safe to say that $\nu>1$.

In conclusion, I find that in the Anderson model in two dimensions there exists a critical W/V of between 5.8 and 6 that separates scaling toward extended or localized states at the band center. The conductance may be a good scaling variable on the localized side. However, its scaling equation will be expected to exhibit an unusual behavior (a kink in the β function) because of the added constraint that the conductance must stay constant even when the coupling matrix elements are scaling toward infinity. While the precise behavior of β is subject to numerical uncertainty the scaling of v toward strong coupling for large $\tilde{g}$ is such a striking effect that there is little doubt of its validity. This means that when four cells are put together the resulting eigenfunctions are complicated linear combinations of eigenfunctions of each individual cell, surely a signature of extended states.[11]

I thank P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan for keeping me informed as their work progressed and for helpful discussions.

[1]D. C. Licciardello and D. J. Thouless, J. Phys. C 8, 4157 (1975).
[2]D. C. Licciardello and D. J. Thouless, J. Phys. C 11, 925 (1978).
[3]D. J. Thouless, Les Houches Lectures, 1978 (unpublished).
[4]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).
[5]F. J. Wegner, Z. Phys. B 25, 327 (1976).
[6]P. W. Anderson, Phys. Rev. 109, 1492 (1958).
[7]S. Yoshino and M. Okazaki, J. Phys. Soc. Jpn. 43, 415 (1977).
[8]K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).
[9]P. Löwdin, J. Chem. Phys. 19, 1396 (1951).
[10]H. G. Schuster, Z. Phys. B 31, 99 (1978).
[11]D. J. Thouless, Phys. Rev. Lett. 39, 1167 (1977).