One-Parameter Scaling of Localization Length and Conductance in Disordered Systems

A. MacKinnon and B. Kramer
Physikalisch-Technische Bundesanstalt, D-3300 Braunschweig, Federal Republic of Germany
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The localization length for disordered systems is calculated with a new recursive method. The scaling behavior of the conductance is determined. The assumptions about the β function made in recent analytical work are confirmed. Only localized states are found for two dimensions. In three dimensions there is an Anderson transition at a critical disorder of $W_c = 16 \pm 0.5$ with critical exponents for the conductivity and the localization length of $s = \nu = 1.2 \pm 0.3$, respectively.

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Recent theoretical studies of localization have been focused on the scaling behavior of the conductance[1,2] and on numerical investigations of the electronic states and the conductivity.[3-5] There is considerable inconsistency, particularly between analytical and numerical results in two dimensions. Here scaling theory predicts, under certain assumptions, localization for any disorder,[2] the dependence of the conductance as a function of the spatial dimensions of the sample changing from exponentially to logarithmically decreasing at some critical disorder. The predictions from numerical data range from the existence of an Anderson transition[4,5] to localization for any disorder but with a power-law decrease of the states for weak disorder,[6] and logarithmic scaling of the conductance.[7] However, in all of the numerical calculations the error bars, if taken seriously, were such that no definite conclusion was possible.[5]

We present numerical results for the localization length and the conductivity in two and three dimensions, the accuracy of which exceeds that of the earlier work by orders of magnitude. Moreover, the accuracy is quantitatively controllable and only limited by the accuracy of the computer since the method used is an implementation of exact analytical relations. The data support the assumptions made in the scaling theory of Abrahams *et al.*[2] and indicate that for $d < 3$ only localized states exist independent of the degree of disorder, whereas for $d = 3$ there is an Anderson transition at a finite critical disorder with a continuous drop of the conductivity.

We consider a system of length N in, say, the x direction, and lateral dimensions M^{d-1} in the y and z directions described by the usual Anderson tight-binding Hamiltonian with site diagonal matrix elements, which are rectangularly distributed with width W. The off-diagonal matrix elements are taken as unity between nearest neighbors and zero otherwise. Boundary conditions are periodic in the y and z directions. For N large compared with M the system is essentially one dimensional. Thus, we may define a localization length λ depending on M and W via the transmission coefficient, i.e.,

$$\lambda^{-1} = \lim_{N \to \infty} [2(N-1)]^{-1} \ln \mathrm{Tr} |\langle 1|G(N)|N\rangle|^2. \quad (1)$$

Here $\langle 1|G(N)|N\rangle$ denotes the M^{d-1}-dimensional matrix of the resolvent $[E - H(N)]^{-1}$ between the site states in the first and Nth slice of the system.

The matrix elements of the resolvent may be obtained from recursion relations.[7-9] The simplest possibility is to calculate the inverse of $\langle 1|G(N)|N\rangle$, A_N, from

$$A_N = (E - H_N)A_{N-1} - A_{N-2}, \quad (2)$$

which involves the Hamiltonian H_N of the Nth isolated slice of the system. This is faster than the method of Ref. 7, because it involves no matrix inversion, but it tends to numerical instability. Since the eigenvalues of A_N rise exponentially with N at different rates, the smallest of them is lost when its ratio to the largest becomes comparable with the accuracy of our computer. The smallest eigenvalue, however, contributes dominantly to $\langle 1|G(N)|N\rangle$. This problem can be overcome by regularly multiplying Eq. (2) from the right-hand side by $\langle 1|G(N)|N\rangle$. The numerical implications of this can be tested by varying the frequency of this operation. In practice, in order to maintain an accuracy of the localization length of 1%, it is sufficient at every tenth iteration, on a machine with a word length of 48 bits. The statistical accuracy of λ can be controlled by noting that as $N \to \infty$ its variance is given by $\langle \Delta\lambda^2(N)\rangle = 2\langle \lambda(N)\rangle / N$ (for fixed M).[10] We have checked this by calculating $\Delta\lambda^2$ simultaneously with λ in each step. N was increased until $\Delta\lambda/\lambda$

$=1\%$ was reached. For $W=5$ in two dimensions and $M=32$ this required $N=3\times10^5$, but convergence is somewhat faster for $\lambda \ll M$.

We calculated the localization length $\lambda(W, M)$ for $d=2$ with $4<W<15$ and $M=1, 2, 4, 8, 16, 32$, and for $d=3$ with $10<W<28$ and $M=1-7$. Because of the periodic boundary conditions our data for $M=1$ do not agree for $d=2$ and 3, and are different from the $d=1$ limit.[11] In order to investigate the behavior of λ with *large* M we introduced a scale change $M \to M/\lambda_\infty(W)$, where the scaling parameter $\lambda_\infty(W)$ depends only on the disorder. Minimizing the variance of the $\ln[\lambda_\infty(W)/M]$ values which correspond to a given value of $\lambda(W, M)/M$, we found the following scaling laws:

$$\lambda(W, M)/M = f_d(\lambda_\infty(W)/M), \tag{3}$$

which are shown in Fig. 1. $d=2, 3$ means two-dimensional (2D) and three-dimensional (3D), respectively. No assumption about the form of f_d was made, except that the exponent of M in the left-hand side of Eq. (3) was fixed at 1, since only this yielded scaling within the accuracy of the raw data. For $d=1$ the scaling function is $f_1(x)=x$, trivially. The scaling laws of Fig. 1 are the most important result of this work and lie at the heart of the following discussion. We investigate first the meaning of $\lambda_\infty(W)$.

We first note that f_2 is monotonically increasing with $\lambda_\infty(W)/M$, whereas f_3 is singular at $\lambda(W, M)/M=0.65\pm0.1$ such that for $W>16$ the data scale on the lower branch, whereas for $W\leq16$ they scale on the upper branch. Since $f_2(x)\sim x$ as $x \to 0$ we identify $\lambda_\infty(W)=\lim_{M\to\infty}\lambda(W, M)$. The same holds for the lower branch of f_3. Thus, $\lambda_\infty(W)$ is the (finite) localization length in the infinitely large systems. In 2D the data do not show singular behavior down to $W=4$. Any Anderson transition would have to occur at $W<4$. This is in contrast to the recent work by Pichard and Sarma.[6] They interpret their data as showing a transition to power-law localization at $W=6$. We believe that this discrepancy is due to the restriction of their calculations for $d=2$ to $M<16$. In 3D the above interpretation of $\lambda_\infty(W)$ as a localization length is only valid above the critical disorder of $W_c=16\pm0.5$. In the upper branch of f_3 we observe that $\lambda(W, M)/M$ increases with increasing M. From Fig. 1 we deduce for $W<W_c$ and large M approximately

$$\lambda(W, M)/M \sim M/\lambda_\infty(W). \tag{4}$$

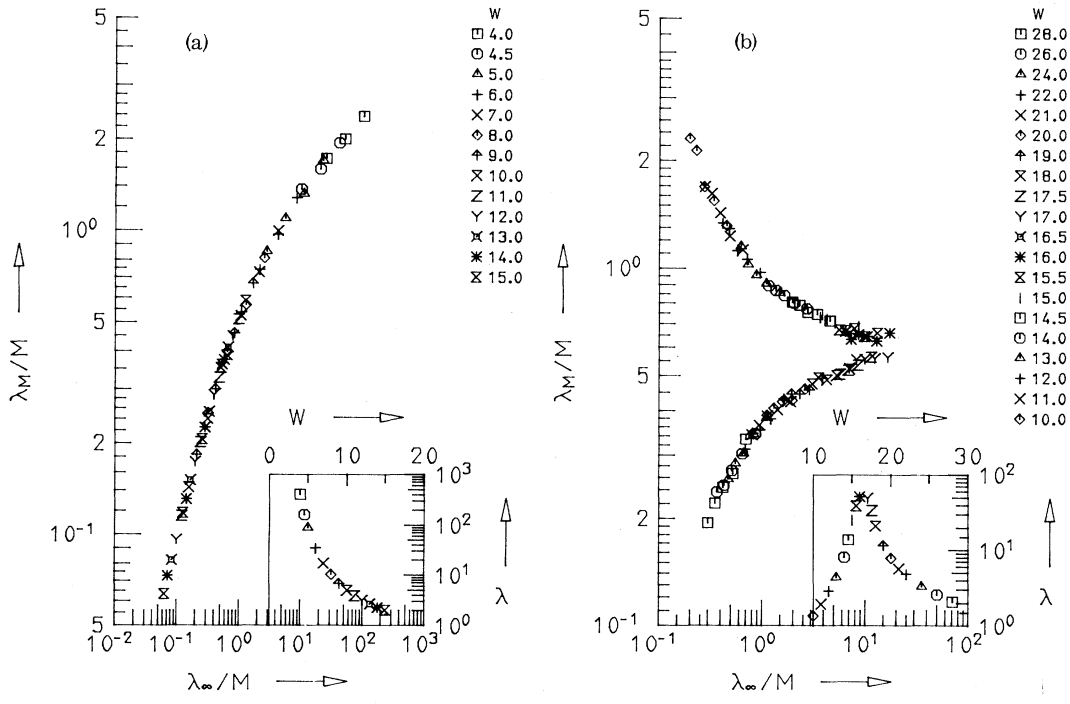

FIG. 1. Scaling function λ_M/M vs λ_∞/M for the localization length λ_M of a system of thickness M for (a) $d=2$ ($M\geq4$) and (b) $d=3$ ($M\geq3$). Insets show the scaling parameter λ_∞ as a function of the disorder W.

What does $\lambda_\infty(W)$ mean in this case? The transmission coefficient T of a very long bar may be written as

$$T = \exp[-2N/\lambda(W, M)]. \quad (5)$$

Taking Landauer's relation between the conductance g and T as valid[12,13] we have for large g

$$g \sim M^2/N\lambda_\infty(W). \quad (6)$$

Comparison with the classical relations between g and the conductivity σ of a rod of length N cross section M^2 yields finally

$$\sigma(W) = 1/\lambda_\infty(W). \quad (7)$$

The data for λ_∞ as a function of the disorder are shown in the insets in Fig. 1. For $d=3$ the critical exponents ν and s for the localization length and the conductivity were determined. They were found to be equal and $s=\nu=1.2\pm0.3$, the error bar resulting mainly from the uncertainty in the position of W_c. In view of the intrinsic difficulties in a numerical determination of these exponents we consider our result as in good agreement with those of Vollhardt and Wölfle,[14] who derived analytically $\nu=s=1$. For $d=2$ we find it very difficult to assign a power-law behavior for $\lambda_\infty(W)$ as W decreases. A fit by an essential singularity of the kind proposed in Ref. 14 turned out to be successful, implying that $\lambda_\infty(W) \sim [\exp(\text{const}/W^2)]/W^2$. However, the data are also consistent with $\lambda_\infty(W) \sim \exp(\text{const}/W)$.

We may calculate the scaling behavior of the conductance of a very long bar using

$$d\ln g = \frac{\partial \ln g}{\partial \ln N} d\ln N + \frac{\partial \ln g}{\partial \ln M} d\ln M. \quad (8)$$

Eliminating one length scale by setting $d\ln N = d\ln M$, i.e., N/M remains constant, and assuming g to depend only on T, i.e., $g=G(T)$, we obtain

$$\beta(g) \equiv \frac{d\ln g}{d\ln M} = \beta_1(g)\frac{d\ln f_d(x)}{d\ln x}. \quad (9)$$

Here $x=\lambda_\infty(W)/M$ and $\beta_1(g)$ is the β function of the case where $\lambda(W, M)$ is independent of M, i.e., $d=1$. The result (7) suggests that, in the conducting regime, the relative values of M and N are unimportant. This is also true for $\lambda_\infty(W) \ll M$ in the localized regime. Therefore we take $N=M$ in what follows.

Since, as noted earlier, there is a critical value of $\lambda(W,M)/M$ in 3D; there are also critical values of T and correspondingly g above which they scale to the limit of extended states for increasing M, and below which they scale to zero. This is in accord with the predictions of Ref. 2. Since $\beta_1(g)$ does not change its sign, the behavior of β_d is solely determined by the second factor in Eq. (9) and the exact definition of $G(T)$ is not very important. Since we have a large number of points in Fig. 1 and $f_d(x)$ is smooth we may calculate the derivative in Eq. (9) very accurately. Results, which were obtained with use of the Landauer form of $G(T)$, are shown in Fig. 2. They are consistent with those of Ref. 2. In particular, $f_d(x) \sim x$ for $f_d \to 0$ in all dimensions gives $\beta_d(g) \sim \ln g$, which is characteristic of localization. In the limit of large g, which corresponds to $f_d \to \infty$, we get $\beta_d(g) = \mp 1$ for $d=1$ and 3, respectively, because $f_1(x)=x$ and $f_3(x) \sim x^{-1}$ as $x \to 0$, in the conducting regime. In 2D our data are consistent with $f_2(x) \sim \ln x$ as $x \to \infty$. This implies $\beta(g) \sim 1/g$, as predicted analytically.[2,14] Since the behavior of our numerically determined β function depends crucially on the scaling functions for the localization length, which were derived *without any a priori assumption about* the

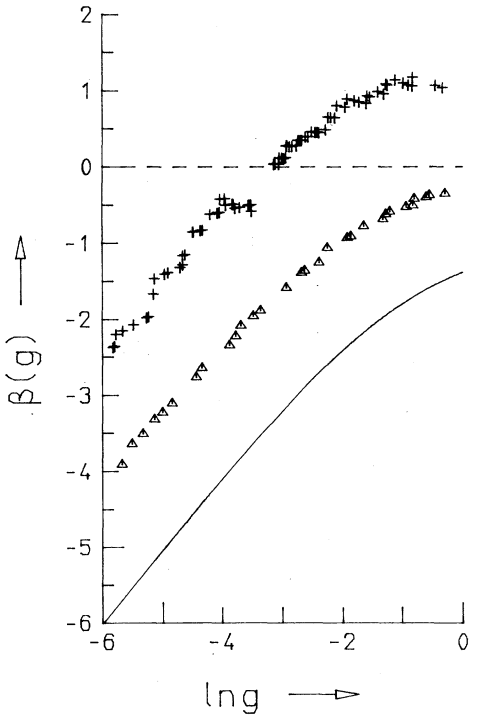

FIG. 2. Scaling function $\beta(g)$ for the conductance g. Full line is for $d=1$. Triangles and plusses are for $d=2$ and $d=3$, respectively, as calculated from the data in Fig. 1.

shapes of f_d purely from the numerical data, we may consider the present results as an *a posteriori* justification of the assumptions of continuity and monotonicity of $\beta(g)$ in Ref. 2 and as supporting the existence of a single scaling variable. Since the conductivity of a macroscopically large system is a meaningful quantity, and the analysis of Eqs. (4) to (7) does not depend on the *assumption* of only one dominant channel, the number of contributing channels must not depend on M for a very large square or cube; i.e., the number of channels for which $\lambda(W, M) \sim M^2$ must become independent of M when $M \to \infty$. This strongly supports the assumption of only one dominant channel and therefore the use of the Landauer formula for G also in the case of a multichannel system.[15]

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[1]F. Wegner, Z. Phys. B 25, 327 (1976).
[2]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).
[3]P. Lee, Phys. Rev. Lett. 42, 1492 (1979).
[4]J. Stein and U. Krey, Z. Phys. B 37, 13 (1980).
[5]B. Kramer, A. MacKinnon, and D. Weaire, Phys. Rev. B 23, 6357 (1981).
[6]J. L. Pichard and G. Sarma, J. Phys. C 14, L127 (1981).
[7]P. A. Lee and D. S. Fisher, Phys. Rev. Lett. 47, 882 (1981).
[8]A. MacKinnon, J. Phys. C 13, L1031 (1980).
[9]D. J. Thouless and S. Kirkpatrick, J. Phys. C 14, 235 (1981).
[10]J. Sak and B. Kramer, Phys. Rev. B 24, 1761 (1981).
[11]G. Czycholl, B. Kramer, and A. MacKinnon, Z. Phys. B 43, 5 (1981).
[12]R. Landauer, Philos. Mag. 21, 863 (1970).
[13]P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B 22, 3519 (1980).
[14]D. Vollhardt and P. Wölfle, to be published.
[15]P. W. Anderson, Phys. Rev. B 23, 4828 (1981).

Anomalous Frequency-Dependent Conductivity of Polyacetylene

A. J. Epstein, H. Rommelmann, M. Abkowitz, and H. W. Gibson
Xerox Webster Research Center, Webster, New York 14580
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The frequency (f) and temperature (T) dependent conductivity (σ) is reported for *cis*-$(CH)_x$, *trans*-$(CH)_x$, and ammonia-compensated $(CH)_x$. A strongly T-dependent dc σ together with a weakly T-dependent ac σ were observed for predominantly *cis*-$(CH)_x$ and for NH_3-compensated samples, similar to $\sigma(f,t)$ of many semiconductors. The *trans*-$(CH)_x$ has a larger "weakly" T-dependent dc σ and anomalous strongly T-dependent ac σ. The latter results are in good agreement with Kivelson's theory of charge transport via intersoliton electron hopping.

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Recently, considerable experimental[1,2] and theoretical[3,4] interest has focused on the two isomers of polyacetylene,[5] *trans*-$(CH)_x$ and *cis*-$(CH)_x$. According to the soliton model,[3,4] undoped $(CH)_x$ is a semiconductor due to a commensurate Peierls distortion. For the *trans* isomer, the two possible phases of the dimerization are degenerate in energy, and a soliton is the boundary between regions of the two phases. The energy level associated with the soliton is at midgap. When singly occupied the soliton is neutral with spin $\frac{1}{2}$. If the state is doubly occupied or empty the soliton is charged and spinless. For the *cis*-$(CH)_x$ the two possible phases of dimerization (*cis-transoid* and *trans-cisoid*) are not degenerate in energy. Hence the formation of solitons is not favored energetically in *cis*-$(CH)_x$. Magnetic,[6-8] infrared,[9] luminescence,[10] and photoconductivity[11] studies have been intepreted as evidence for the presence of solitons in the *trans* isomer and their absence in the *cis* isomer.

In this Letter we report the results of an exten-

