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Analytical and Numerical Study of the Anderson Localization Length and Residual Resistivity

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An analytical procedure has been developed for calculating the localization length describing the exponential growth of the representative resistance in a one-dimensional disordered system and the associated residual resistance. The present results are compared to numerical simulations performed using a novel set of recurrence relations which provide a rapid and accurate method for computer studies of one-dimensional systems.

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According to Landauer[1] the dimensionless resistance R of a one-dimensional system is given by $R = T^{-1} - 1$, where T is the transmissivity of the linear chain. In a one-dimensional disordered system of length L the resistance exhibits exponential growth in that the average obeys the relation $\ln\langle R\rangle \to \text{const} \times L$ as the length becomes large.[2] Many authors[3,4] have noted that the unrestricted average $\langle R\rangle$ is not representative of the ensemble since it is dominated by the most resistive, and presumably most improbable, samples. A representative average, R_r, characterizing a finite sampling procedure, will generally exhibit a slower rate of growth. We define the localization length L_0 as the parameter characterizing the exponential growth of the representative resistance: $\ln(R_r) \to 2L/L_0$. In this paper we present an expression for L_0 which provides a remarkably accurate description of numerical simulations. In addition, we present a novel method for performing the numerical calculations which provides an efficient way of doing the simulations as well as calculating other properties.[5]

We consider a compositionally disordered system formed from two types of scatterers with concentrations c_1 (called impurities) and $c_2 = 1 - c_1$, respectively. We find an expression for L_0 by performing a restricted average over an ensemble of systems in which the total number N of impurities is precisely specified.[6] In other words, we assert that it is extreme fluctuations in the actual number of impurities that are responsible for the nonrepresentative nature of the unrestricted average. This hypothesis is tested by a comparison of the analytical results with numerical simulations.

An unrestricted average $\langle M_L\rangle$ of the total transfer matrix M_L describing a chain of length L may be expressed in terms of restricted averages $\langle M_L\rangle_N$ (where the subscript N indicates that the number of impurities is fixed) by the formula

$$\langle M_L\rangle = \sum_{N=0}^{L} \binom{L}{N} c_1^N (1-c_1)^{L-N} \langle M_L\rangle_N. \quad (1)$$

It is straightforward to determine the unrestricted average.[7] The overall transfer matrix of the system is

$$M_L = W^{-(L+1)} W\theta_L \cdots W\theta_1 W, \quad (2)$$

where θ_n is the transfer matrix characterizing site n and the matrix W [$W_{11} = \exp(ik)$, $W_{22} = \exp(-ik)$, $W_{12} = W_{21} = 0$] describes propagation between adjacent sites in a lattice of unit spacing. Since the sites are entirely independent the unrestricted average of the transfer matrix is simply Eq. (2) with each transfer matrix replaced by

$c_1\theta^{(1)}+c_2\theta^{(2)}$, where the superscripts denote the species. Making the substitution $z=c_1/(1-c_1)$ we find

$$\sum_{N=0}^{L}\binom{L}{N}z^N\langle M_L\rangle_N = W^{-(L+1)}(zW\theta^{(1)}+W\theta^{(2)})^L W. \quad (3)$$

The averaged transfer matrix in (3) may be written in the form $A\Lambda A^{-1}$, where $\Lambda=\Lambda(z)$ is a diagonal matrix formed from its eigenvalues and $A=A(z)$ is the diagonalizing matrix. Then

$$\sum_{N=0}^{L}\exp(L\sigma_N)z^N\langle M_L\rangle_N = W^{-(L+1)}A\Lambda(z)^L A^{-1}W, \quad (4)$$

in which we have expressed the binomial coefficient in terms of the "entropy" $\sigma_N=-c_N\ln(c_N)-(1-c_N)\ln(1-c_N)$, where $c_N=N/L$. The restricted averages $\langle M_L\rangle_N$ are proportional to the Nth derivatives of the right-hand side of (3). Thus

$$\langle M_L\rangle_N=\exp(-L\sigma_N)W^{-(L+1)}\frac{1}{2\pi i}\oint\frac{A(z)\Lambda(z)^L A^{-1}(z)W}{z^N}\,dz, \quad (5)$$

where the integral is over a contour enclosing the origin and avoiding the singularities of the integrand. L and N are large and the asymptotic behavior may be determined by the steepest-descent method. Since $z^{-N}=\exp(-Lc_N\ln z)$, the stationary points are given by $c_N=d(\ln\lambda)/d(\ln z)$, λ being either one of the eigenvalues of the averaged transfer matrix.

In accordance with the hypothesis that representative values are determined by restricted averages, we equate c_N to c_1, the nominal concentration of impurity scatterers. For each solution and eigenvalue there is a contribution to $\langle M_L\rangle_N$ proportional to $\exp\{L[\ln(\lambda)-c_1\ln(z)-\sigma_N]\}$. In general there are several solutions to the equation for the stationary points; the localization length is given by the root leading to the greatest rate of growth.

We verify our predictions for the localization length by comparing them with the results of computer simulations. The calculations were done for a lattice of δ-function potentials,

$$V(x)=\sum V_n\delta(x-x_n), \quad (6)$$

where the coefficients V_n may have either of two values $V^{(1)}$ or $V^{(2)}$. For $x_{n-1}<x<x_n$ the wave function may be written

$$\psi(x)=A\exp(\tfrac{1}{2}G_n)\cos[k(x-x_{n-1})-\tfrac{1}{2}\varphi_n], \quad (7)$$

where A is arbitrary and the quantities G_n and φ_n may be obtained in terms of the initial values $G_1=0$ and an arbitrary initial phase φ_1 by straightforward application of the transfer matrices appropriate to the δ-function potentials. Using a series of algebraic transformations[5] we have developed a recursion relation for the quantities $X_n=\tan(\frac{1}{2}\varphi_n+\frac{1}{4}\pi+h_{n-1})$, where $\tanh_n=V_n/2k$, which yields the exponent G_n directly (cf. Peres and co-workers[7]) and thus is very suitable for a situation in which the wave function grows exponentially with the length of the chain. We find the result[5]

$$G_L=\sum_{n=0}^{L}\ln\frac{1+X_n^2}{\omega_{n-1}+X_n^2/\omega_{n-1}}, \quad (8)$$

in which $X_n=\omega_{n-1}(X_{n-1}-r_{n-1})/(1+X_{n-1}r_{n-1})$, $\omega_n=\tan^2(\frac{1}{2}h_n+\frac{1}{4}\pi)$, and $r_n=\tan[k-(h_n+h_{n-1})/2]$. Two independent solutions are obtained by choosing $\varphi_1=0$ and $\varphi_1=\pi$. These may be combined to form an eigenfunction having only an outgoing wave at one end of the chain, from which we derive[5] the expression for the resistance:

$$R=(\exp G+\exp G'-2)/4, \quad (9)$$

where G and G' are the values of G_L for the two particular solutions just mentioned.

We determine L_0 by calculating G and G' for a particular sequence of length L and employing the relation $L_0=2L/\ln R$. [Strictly speaking L_0 should be defined in terms of an average with respect to independently chosen sequences. While some of the data presented are of this form, it is rarely necessary to generate more than one sequence since according to Eq. (8) G_L is the sum of independent quantities (provided $L\gg L_0$) and thus will exhibit only conventional $(L_0/L)^{1/2}$ fluctuations.]

Evaluation of the analytic results for the δ-function model is straightforward but tedious.[5] In terms of the variable $y=c_1c_2(z+1)/(c_2z-c_1)$ the equation for the stationary points of the integrand in (5) is

$$y^3+2(c_2-c_1)y^2+[(c_1-c_2)^2-2c_1c_2-a^2-b]y+2c_1c_2[(c_1-c_2)-a-d]=0, \quad (10)$$

where $a=V/U$, $b=4k(V\cot k-k)/U^2$, $d=2k\cot k/U$, $V=c_1V^{(1)}+c_2V^{(2)}$, and $U=V^{(1)}-V^{(2)}$. In terms of the

solution to the cubic equation,

$$1/L_0 = \mathrm{Re}[iq - c_1 \ln(1 + c_2/y) - c_2 \ln(1 - c_1/y)],$$

where

$$\cos(q) = \cos(k) + [\sin(k)/2k](V + c_1 c_2 U/y).$$

Figure 1 shows our results for the case $V_1 = -1$, $V_2 = 0$, and for several values of k, the square root of the dimensionless energy.[8] In all cases L_0 diverges as c_1^{-1} for $c_1 \to 0$ since the system becomes ordered and states of all energies are extended. In the important case of long wavelengths, this regime begins when $c_1 < k$ at which point the distance between the impurities exceeds the wavelength and the localization is due to individual scattering events. For long wavelengths L_0 increases when $c_1 \gg k$; for $c_1 \to 1$ the system is nearly ordered (and the energy is not in a band gap) and $L_0 \sim c_2^{-1}$, analogous to the low-concentration regime, while for intermediate concentrations $L_0 \sim c_1^{1/2}$ corresponding to a situation in which the state is averaging over the impurities and the localization is due to relative fluctuations in the potential. (The averaging is responsible for the increase in L_0 at a remarkably small concentration.) This is the only regime in which there is some discrepancy between the analytic and numerical results (impurity fluctuations rather than their concentrations are important). For intermediate energies (as illustrated by the case $k = 1.5$) $L_0^{-1} \sim c_1 c_2$ throughout the entire concentration range. For $\pi - k \ll 1$ L_0 decreases continuously with increasing c_1 since the increase which occurs for small k does not happen if the energy belongs to a band gap of the ordered lattice of impurities. We find $L_0 \sim c_1^{-1}$ for $c_1 \ll \pi - k$ while $L_0 \sim c_1^{-1/2}$ for $c_1 > (\pi - k)^{1/2}$. The rapid change in L_0 (by a factor of 40) as c_1 changes from 1.5% to 6.5% is remarkable.

The energy dependence of L_0 is illustrated in Fig. 2. The localization length increases by an order of magnitude with increasing energy, falls precipitously for a narrow range (depending upon concentration) within the forbidden band of the ordered lattice of impurities, and then diverges[9] as $k \to \pi$, corresponding to the energy for which states are always extended.[10] (An effect of this type may explain recent experiments in Bi.[11]) The explicit dependence[8] near the "mobility point"[9] $k = \pi$ is $L_0 \sim (\pi - k)^{-1/2}$ for $\pi > k$, and $L_0 \sim (k - \pi)^{-1}$ for $k > \pi$, in agreement with Kantor and Kapitulnik.[12]

Andereck and Abrahams[13] have provided an exact solution for a quantity L_0^* describing the growth of the average resistance $\langle R \rangle \sim \exp(4L/L_0^*)$. Since necessarily $\langle R \rangle \geq R_r$ there is the exact result that $L_0^* \leq 2L_0$. On the other hand, Anderson *et al.*[3] speculate, and Andereck and

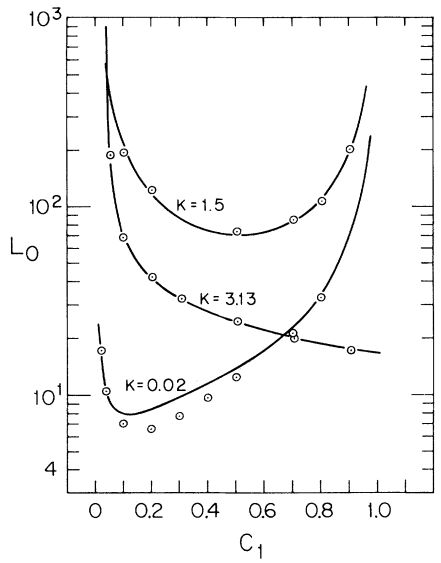

FIG. 1. L_0 (in units of the lattice constant) as a function of concentration for several energies. The solid curves show our analytical results while the "data" points indicate the results of computer calculations.

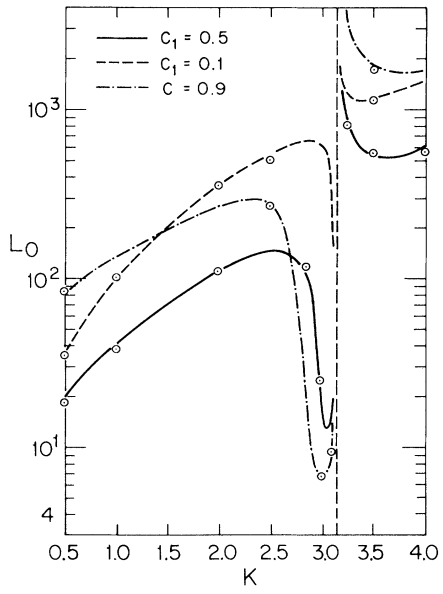

FIG. 2. L_0 (in units of the lattice constant) as a function of energy for several concentrations. The solid curves show our analytical results while the "data" points indicate the results of computer calculations.

Abrahams[13] seem to confirm, that $\langle R\rangle \approx R_r^2$, which would imply $L_0^* \approx L_0$. We find that this last relation is valid except (a) in the fluctuation regime illustrated in Fig. 2 by the values $k = 0.02$ and $c_1 \approx 0.2$ where L_0^* is $\approx 20\%$ greater than L_0, and (b) in the "forbidden band" regime (as defined by the mean crystal) in which $L_0^* \approx 2L_0$ or $\langle R\rangle \approx R_r$. While the near equality between the representative and average resistance is fairly obvious when the localization length is very small it is interesting that it holds exactly even in the regime $k \to \pi - 0$ where $L_0 \to \infty$.

The resistance depends linearly upon the length when $L \ll L_0$.[14] Thus, using (9), the Ohmic resistivity ρ_0 is

$$\rho_0 = \lim_{L\to 0} R_r/L = (4L)^{-1}[\langle G\rangle + \langle G'\rangle], \qquad (11)$$

where the averages are with respect to systems satisfying $L \ll L_0$. We find that in the middle of the "allowed" band $\rho_0 \approx 1/L_0$ and thus $\ln R_r \approx 2\rho_0 L$ (cf. Ref. 3) while near the edges of the band ρ_0 and $1/L_0$ may differ by several orders of magnitude and thus the inverse localization length is not simply related to the Ohmic (classical) resistivity. According to our results one may expect quite a bizarre behavior as a function of impurity concentration.

In summary, we have developed a quantitatively accurate theory of the localization length in a one-dimensional random system. In addition, we have presented a useful technique for computer studies of localization in one dimension and have compared the "experimental" results obtained with that technique to the analytical results.

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