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NEW NUMERICAL METHOD FOR THE ELECTRONIC PROPERTIES OF DISORDERED SYSTEMS

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Abstract. - We present results of calculations of the localisation length and conductivity of 2 dimensional systems described by the Anderson Hamiltonian. A recently developed method for calculating properties of very long 1D systems is generalised for long strips of varying thickness. We observe scaling behaviour with the thickness but no evidence of an Anderson transition in 2D.

Introduction. - There has been a considerable upsurge of interest in the problem of localisation in disordered systems. This has been due to new experiments on pseudo one, and two dimensional systems [1-5], and to the development of new methods of calculation, both numerical [6-8] and analytical [9-12].

There is some confusion in the results of the theoretical investigations. In the analytical work, where d=2 is found to be the lower critical dimension for the Anderson transition, special models or approximations are chosen, whose consequences are not easily controlled. In the numerical work the system sizes are possibly too small to give conclusive results about the transition between localised and extended states [13]. For instance, although there was analytical evidence that for d=1 all states are localised for any nonzero disorder [14,15] and that the d.c. conductivity is zero [16], it proved difficult to demonstrate this numerically [17]. Only the development of a new numerical method whose storage requirement is independent of the system size made the treatment of macroscopically large systems (10^9 sites) possible and lifted the contradiction between analytical theory and numerical calculation [18].

In this paper we shall generalise this method to higher dimensional systems, and present results for d=2 for both the localisation length and the conductivity.

Method. - The idea of our method is to calculate a physical quantity for a system with N atoms, say A(N), from the same quantity for N-1 atoms, i.e.

\[ A(N) = f \{ A(N-1) \} \]  

For example, the matrix element of the Green's function (resolvent), between the states located at the ends of a chain of N atoms described by the Anderson Hamiltonian with disordered diagonal elements \( \epsilon(i) \), \( <1|G(N)|N> \), is given by

\[ <1|G(N)|N> = <1|G(N-1)|N-1> V <N|G(N)|N> \]  

\[ <N|G(N)|N> = 1/[Z-\epsilon(N)-V^2<N-1|G(N-1)|N-1>] \]

where Z is the (complex) energy, V the (nearest neighbour) off-diagonal element of the Hamiltonian, and \( <N|G(N)|N> \) the diagonal element of the Green's function on the
The localisation length $\lambda$ may then be defined as

$$2\lambda^{-1} = \lim_{N \to \infty} \frac{1}{N-1} \sum_{i=2}^{N} \ln \left( \frac{|<1|G(i-1)|i-1>|^2}{|<1|G(i)|i>|^2} \right)$$

(4)

The same principle can be applied to the conductivity as given by the Kubo-Greenwood formula [18]. The advantage of this recursive method lies not only in the negligible computer storage needed, but also in the fact that the statistical accuracy of the result after $N$ steps may be calculated and used as a criterion for terminating the procedure [13,18].

Thus, we have a method which contains no other restriction on the size of the system than the computer time available, and which allows us to go on increasing the size of the system until a given accuracy of the result is reached. This allows for much more reliable extrapolations than have been possible hitherto. A simple generalisation of the above method to higher dimensions involves replacing the simple basis functions of the one dimensional system with chains ($d=2$) or plains ($d=3$) of atoms giving two or three dimensional systems, which are very long in one direction. The scalar quantities appearing in the recursive relations for $d=1$ then become matrices and all physical properties depend on the thickness $M$ of the system. For example, $|<1|G(i)|i>|^2$ in eq. (4) becomes $\text{Tr} <1|G(i)|i>|^* <i|G(i)|1>$ involving a sum over all combinations of two sites at opposite ends of the system.

Results. - In the results presented in the following we used the rectangular distribution for the site diagonal elements of $H$, i.e.

$$-W/2 < \varepsilon(i) < W/2$$

(5)

The accuracy of our data is $\Delta \lambda = 0.01 \lambda$ for the localisation length, and $\Delta \sigma = 0.1\sigma$ for the conductivity.

Fig. 1. $\lambda(M)/M$ vs. $\lambda(\infty)/M$ for various $W/V$ values and $M = 4, 8, 16, 32$. Insert: $\lambda(\infty)$ vs. $W/V$

The localisation length. - We have calculated the localisation length $\lambda(M)$ of two dimensional systems with $4V \leq W \leq 15V$ for $M = 4, 8, 16, 32$. The data were found to obey a scaling law

$$\lambda(M)/M = f \left\{ \lambda(\infty)/M \right\}$$

(6)

where $\lambda(\infty)$ is the localisation length for $M \to \infty$. They do not fulfil the relationship
found by Pichard and Sarma [19] although their method of calculation is similar to ours. We have seen no evidence of a "phase transition". For $W=5V$ and $W=6V$, $\lambda(M)$ starts linear in $M$, as observed in ref [19] but becomes sublinear for larger $M$. We conclude that the linear range is not indicative of the $M=\infty$ limit.

For this reason, and because we were unable to fit a critical form for $\lambda(\omega, W)$ unambiguously to eq. (6) we attempted to calculate $\lambda(\omega, W)$ without assuming critical behaviour. Since we expect $f(x)$ in eq. (6) to rise monotonically and $f(x) = x$ for small $x$ ($M>>\lambda(\omega)$) we invert eq. (6) and write

$$\lambda(\omega)/M = \lambda(M)/M + g(\lambda(M)/M)$$

where $g(\omega) = g'(\omega) = 0$. Expanding $g(x)$ in some set of functions leads to a system of linear equations for $\lambda(\omega, W)$ and for the expansion coefficients. The resulting scaling function $f(x)$ is shown in fig. 1. $\lambda(\omega, W)$ is shown in the insert. Although $\lambda(\omega, W)$ grows rapidly near $W=5V$ this may not yet be considered evidence for critical behaviour. It does suggest however that, for $W<5V$, $M$ must be very large before $\lambda(M)$ converges.

![Diagram](image)

**Fig. 2.** $\sigma W^2/\nu^2$ vs. $\gamma V/W^2$ for various $\gamma$, $M = 8$ and $W = 1, 2, 4, 5, 6, 8, 10, 12$. Continuous line: Scaling function for $d=1$

The conductivity. - In the case of the dc conductivity it is necessary to study the dependence on the three parameters $M$, $W$, and the imaginary part of the energy, $\gamma$. The latter has proved to be extraordinarily important for $d=1$, where a scaling law

$$W^2\sigma = h(\gamma V/W^2)$$

was found. Fig. 2 shows some data for $M=8$, assuming the above scaling property, together with the scaling function $h(x)$ of $d=1$. The data do not obey relation (8). For large $\gamma V/W^2$ the conductivity is reduced compared with $M=1$, whereas for small $\gamma V/W^2$ it is increased. This increase is clearly a consequence of the larger localisation length. The decrease in the "Drude" part of the curve on the other hand is due to the fact that the important length is now the projection of the "inelastic mean free path" $(1/\gamma)$ onto the axis.

The conductivity is only weakly dependent on $M$ for $W<6V$ and $\gamma>10$ V. Therefore it is difficult to draw any reliable conclusion about the $M=\infty$ limit in this regime.

**Conclusion.** - We have developed a method of computing the localisation length and conductivity of very long thin systems and have applied it to the calculation of
strips of varying thickness in order to study the transition to 2 dimensions. We have seen no evidence of critical behaviour in two dimensional systems. The localisation lengths which we have calculated for $W = 5V$ and $W = 6V$ are however comparable with the thickness of our systems and with the size of systems considered in most simulations up to now. Thus, just as in one dimension, we are forced to conclude that the "Anderson transitions" seen in previous numerical work are due to the localisation length becoming comparable with the system size.

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References.