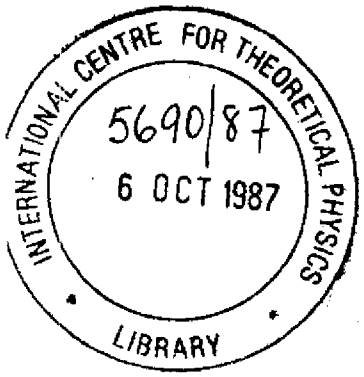

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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

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IN OFF DIAGONALLY DISORDERED CHAINS

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INTERNATIONAL ATOMIC ENERGY AGENCY

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SPECTRAL PROPERTIES AND SCALING RELATIONS IN OFF DIAGONALLY DISORDERED CHAINS *

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ABSTRACT

We obtain the localization length L as a function of the energy E and the disorder width W for an off-diagonally disordered chain. This is done performing numerical simulations involving the continued fraction representations of the transfer matrix. The scaling relation $L = W^s$ is obtained with values of the exponent s in agreement with calculations of other authors. We also obtain the relation $L \sim |E|^\nu$ for $E \to 0$, and use it in the Herbert-Spencer-Thouless formula for L to describe the singularity of the density of states near $E = 0$. We show that the slightest diagonal disorder obliterates this singularity. A practical method is presented to calculate the Green function by exploiting its continued fraction expansion.

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1. INTRODUCTION

The problem of the disordered linear chain has been addressed to by many authors starting, perhaps with the work of Dyson [1]. The continued fraction representation of the transfer matrix (or state ratio, in one dimension) appears in one way or another as the most adequate mathematical frame to describe the model, being useful even for the ordered chain.

The system is represented by the Hamiltonian

$$H = \sum E_n A^+_n A_{n+1} + \sum V_n (A^+_n A_{n+1} + A^+_{n+1} A_n) \quad . \qquad (1)$$

The local (diagonal) Green function can be written in the form

$$G_{nn} = (E - E_n - t_n - q_{n+1})^{-1} \quad , \qquad (2)$$

where the transfer matrices (in this case just the state ratios) t and q satisfy the recursive relations [2]

$$\begin{aligned} t_n &= V^2_n (E - E_{n+1} - t_{n+1})^{-1} \\ q_{n+1} &= V^2_{n+1} (E - E_n - q_n)^{-1} \end{aligned} \qquad (3)$$

The ordered case has $V_n = 1$, $E_n = 0$, $\forall n$. It is well-known that the solution for the ordered case requires the analytical continuation of the continued fraction (Eqs.(3)), which is not well-defined inside the band. Its analytic continuation from the convergence region gives the correct complex values of the transfer matrix. This procedure defines a cut on the real axis of the energy plane and brings about the discontinuity of the imaginary part of the Green function.

In the purely-diagonal-disorder case, $V_n = 1$, $\forall n$, while E_n has a distribution $Q(E_n)$, assumed the same for all n, and independent of the other $\{E_{n'}\}$, $n' \neq n$. The classical example is Anderson's model, where $Q(E)$ is proportional to the characteristic function of the interval $[-D/2, D/2]$ and $D > 0$ is the measure of the disorder. This model, being the simplest realization of disorder, has been the object of rigorous treatment which leads to some general results. Among these, it has been proved that the spectrum is of discrete, pure point nature, under the assumption that the continued fractions in Eqs.(3) converge for a.e. E and that the Lyapunov exponent

$$\gamma(E) = 1/L = - \lim_{N\to\infty} (1/N) \sum_{n=M}^{M+N} \ln |t_n| \qquad (4)$$

is positive for all finite M and a.a. E. L is the localization length [3],[4].

For the purely off-diagonal disordered case we can mention the work of Geda [5] proving that all states are exponentially localized with probability one, with the exception of that for $E = 0$ (centre of the band). The recursion relations for the transfer matrices read in this case

$$\begin{aligned} t_n &= V^2_n (E - t_{n+1})^{-1} \\ q_{n+1} &= V^2_{n+1} (E - q_n)^{-1}. \end{aligned} \qquad (5)$$

The analytic theory of continued fractions provides us with some general results applicable to this case. Let us highlight Worpitzky's theorem and a theorem by Stieltjes relating the Jacobi type continued fractions (Eqs.(3) and (5)) to the kind of generalised integrals carrying his name [6]. Worpitzky proves that the continued fraction

$$1 + za_1/1 + za_2/1 + \ldots \qquad (6)$$

converges for $|za_{p+1}| \leq 1/4$; $p = 1,2,\ldots$. It can also be proved that for bounded $\{a_p\}$ the continued fraction represents an analytic function of z, which can be defined as the Stieltjes integral [6]

$$s = \int \frac{dv(u)}{z-u} \quad . \qquad (7)$$

It can be shown that these theorems apply to the continued fraction obtained by iterating Eqs.(3) and (5) when the sets $\{E_n\}$ and $\{V_n\}$ are bounded; the integral above represents then t_n or q_n for complex $E = z$. Worpitzky's theorem gives only a sufficient condition for convergence, but not a necessary one. However, if the $\{a_p\}$ in Eq.(6) or the $\{V_n\}$ in Eq.(5) tend to a limit, that is

$$\lim_{n\to\infty} V_n = V < \infty$$

then it is well-known that Worpitzky's condition is necessary and sufficient and that when $|V/4| < 1/2$ the continued fraction diverges. In that range

of E the integral representation [7], which is absolutely general for Jacobi type continued fractions, has a branch cut in the complex E plane. When, as in the case in hand, the sequence $\{V_n\}$ has no limit, one must resort to probability arguments.

In order to make rigorous calculations we should study the probability distribution of t, $W(t)$, in the complex t plane, maintaining a small imaginary part for the energy $e = \mathrm{Im}(E)$, which together with the number of trials N, must satisfy the condition $N \to \infty$, $e \to 0$ and $Ne \to \infty$ in order to obtain a meaningful and correct result in the thermodynamic limit [6],[8].

This implies that for small $|E|$, since obviously one needs $e \ll |E|$, very large values of N are required. This approach was found to be too exacting in terms of numerical computations and so we resorted to a direct approach, described in Sec.2, which allows to calculate the Green function and the localization length directly, by making use of the continued fractions recurrence relations for purely off-diagonal disorder.

2. METHOD OF CALCULATION

The random $\{V_n\}$ were generated with a distribution $P(V_n) = 1/2W$ for $1-W < V_n < 1+W$ and zero otherwise. For real E we determine the localization length $L(E)$ by the two following methods:

a) by recursively constructing the successive finite approximants [6]

$$t_p = A_p/B_p \quad . \qquad (8)$$

In order that $|t_p - t_{p+1}| < e$ it is necessary to reach the order $p \simeq N(e,E,W)$. For a given e, N was determined as a function of E and W. Then we assumed [9] that L is proportional to N, the constant of proportionality being obviously a function of e, so that, to within an additive constant

$$\ell n \gamma(E) = -\ell n L = -\ell n N \quad . \qquad (9)$$

The dependence on e was found not to alter the scaling exponents s and ν defined below.

b) We also obtain the Lyapunov exponent $\gamma = 1/L$ directly from the definition

$$\gamma = - < (1/N) \sum_{k=M}^{M+N} \ell n|t_k| > \quad . \qquad (10)$$

After M steps, with $M \simeq 500$, we used t_M as the starting value t_1 and we generated $t_2 \ldots t_N$.

3. RESULTS FOR LOCALIZATION LENGTH

Our results for the relation $L = W^s$ obtained by both methods are shown in Fig.1 They can be summarized as follows. For energies inside the band and far from the band edges we find two regimes:

$$\text{for } W < W_c(E) \qquad s = -2.0 \pm 0.3$$

$$\text{for } W > W_c(E) \qquad s = -8.5 \pm 1.0 \quad , \qquad (11)$$

where $W_c(E)$ as found by Roman and Wiecko (RW) [10] is $\simeq 10\,E$, that is the change of regime occurs for $E \simeq W/10$. Krey [11] and RW [10] remark that $s = -2$ indicates the applicability of second order (small W) perturbation theory, in which case the imaginary part of the self-energy of a Bloch state would be $\Gamma \propto W^2$ and then $L \propto W^{-2}$. The regime $W > W_c$ for which one obtains $s = -8/5$ obviously would correspond to the failure of low order perturbation theory. On the other hand, near the band edges the exponent s has a different value as can be seen in Fig.1, with Krey [11] and RW [10] reporting $s \approx -2/3$.

Let us remark that both non-perturbative regions occur for values of E where the density of states has peaked features, the one at $E = 0$ being a singularity [5],[12]-[16], thereby inducing an anomalous behaviour of L. We describe below the singularity at the centre of the band. We also looked for a scaling relation

$$L(E) \propto |E|^{\nu}$$

determining the divergence of the localization length at constant W, when $|E| \to 0$. The result, shown in Fig.2, is

$$\nu \approx -0.20 \pm 0.02$$

for $W < 0.1$. This scaling relation was not considered in the previous works already alluded to. We shall relate below the value obtained for ν to a closed formula for the density of states near $|E| = 0$.

The average of Eq.(10) is shown in Fig.3, where we plot $t = \exp(-\gamma)$ vs. W. There we see that t is < 1, tending to 1 both as $E \to 0$ or, for $|E| < 2$, as $W \to 0$; while for $|E| > 2$, t is always < 1. One will be tempted to consider the states with L larger than several thousands times a lattice constant, as quasi-extended states, especially in the presence of some perturbation which can introduce a mean free path shorter than the localization length [17].

4. RESULTS FOR THE DENSITY OF STATES

In order to obtain the configuration average of the Green function defined by Eq.(2) we can use the probability measure $W(t)$, of the transfer matrix t, over the complex t plane. We define

$$< G(E) > = \int d^2t \int d^2q \cdot W(t)\, W(q)(E-t-q)^{-1} \quad . \qquad (12)$$

Such a formula was given originally for the special case of imaginary E t and q by Bernasconi et al. [14]. Since we do not know $W(t)$ we used instead the recurrent definition of t_n and q_n (Eq.(5)) for complex E to generate a sampling of the variables in the complex plane. This sampling proved statistically stable upon varying the configurations. Two different random sequences $\{t_n\}$ and $\{q_n\}$ are generated. The average density of states per atom

$$n(E) = -\frac{1}{\pi} \operatorname{Im} < G_n(E) > = -\frac{1}{\pi} \operatorname{Im}\left\{(1/N) \sum_{n=1}^{N} (E - t_n - q_n)^{-1}\right\} \qquad (13)$$

calculated with $\operatorname{Im}\{E\} = 0.01$ and $N = 90000$ is shown in Fig.4 together with a histogram obtained using the method of negative eigenvalue counting [18]. The very good agreement between the two methods can be explained by the fact that the sparse large values of t_n (or q_n) are not significant to the average and therefore the requirements on $\operatorname{Im}(E)$ and N are not so strict.

Besides the peak at $E = 0$ there is another peak near the band edge of the ordered chain which is a reminiscence of the Van Hove singularity [12],[13]. It can be observed that, though our approximation with complex E has a rounding off effect, the tail of the band is very smooth and without a band edge, confirming the presence of a Lifschits tail.

5. DISCUSSION

From the knowledge of the exponent ν we can get information on the density of states near $E = 0$. To this end, let us apply the relation [19]

$$\gamma(E) = \int \ell n|E-E'|\, n(E')\, dE' - \langle \ell n|V| \rangle \quad , \tag{14}$$

where $n(E)$ is the average density of states. Let us assume that the density of states near $E = 0$, for the pure off-diagonal disorder, takes the form

$$n(E)_{off} \sim |E|^{-b}/\ell n|E| \tag{15}$$

and approximately,

$$\gamma(E) \sim \int_0^{W/2} dE' \cdot \ell n|(E\,E')/E'|\; |E'|^{-b}/|\ell n|E'|| \quad . \tag{16}$$

Then we must have, since $\gamma \sim |E|^{-\nu}$ for off-diagonal disorder,

$$1 - b = -\nu \simeq 0.20 \tag{17}$$

so that for the purely off-diagonal disorder near the centre of the band

$$n(E)_{off} \sim |E|^{-0.80}/\ell n|E| \tag{18}$$

this equation has the general features of another proposed form for $n(E)$ [15],[13] and fits within 2% the $n(E)$ calculated by Weissmann and Cohan [12],[20] for $0.1 < |E| < 0.3$ and $W = 0.9$. It is not possible to extend the comparison to lower values of $|E|$ since their method did not allow to reach them. It is known that, however, for systems with mixed or purely diagonal disorder, there is no sign of singularities near the centre of the band [13]. We shall give an argument that may provide a clue to this striking difference betwen the two kinds of systems. We shall make use, to this end, of the extension of Eq.(16) to the case of mixed disorder

$$n(E) = \mathrm{Im}\,\frac{1}{\pi} \int du\, Q(u) \int d^2t \int d^2q W(t) w(q) (E-u-t-q)^{-1} \tag{19}$$

where the distribution $Q(u)$ of the diagonal terms in the Hamiltonian (Eq.(1)) must also be integrated over to obtain the configuration average. Let us assume that

$$n(E) \sim \int Q(u) \cdot n_{off}(E-u)\, du \quad . \tag{20}$$

If $Q(u)$ is the uniform distribution in the interval $[-D/2, D/2]$, then

$$n|E| \sim \int_{-D/2}^{D/2} du\, |E-u|^{-b}/\ell n|E-u| \tag{21}$$

calling

$$I(x) \sim \int_0^x du |u|^{-b}/\ell n|u| \quad , \quad b < 1 \tag{22}$$

$$n(E) \sim 2I(D/2) + (E^2/2)I''(D/2) \tag{23}$$

qualitatively coincident with a simple application of Dean's method of negative eigenvalue counting, which shows that the singularity becomes a peak with a width of the same order of magnitude as the diagonal disorder. According to Eqs.(14) and (23), γ remains finite for mixed (or diagonal) disorder, at $E \to 0$.

The results described for the off-diagonal disorder suggest the consideration of interactions which might lead to mean free paths shorter than the localization length for quasi-extended states. Hopping conduction at low temperature in a quasi-one-dimensional amorphous system with a nearly half-filled conduction band, should produce anomalous conductivity at low frequencies. Phonon induced delocalization has already been considered in amorphous semiconductors [17].

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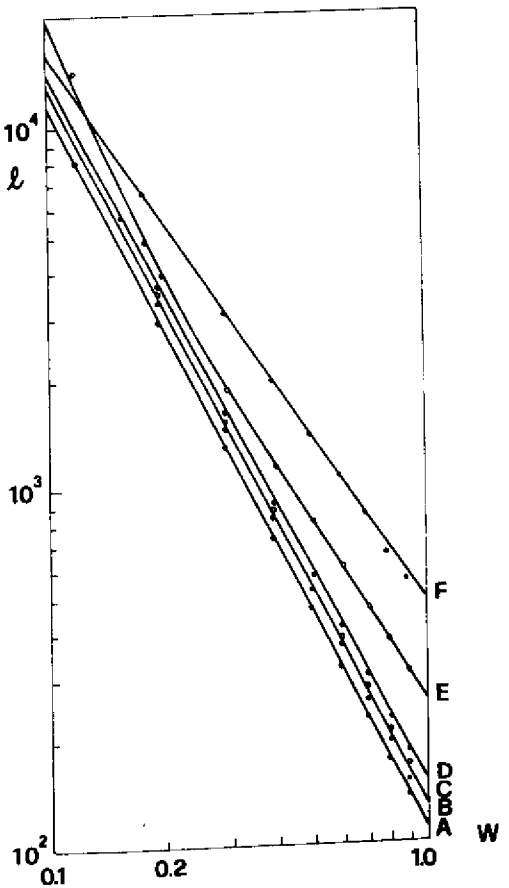
FIGURE CAPTIONS

Fig.1 Localization length L defined in Sec.2a) as a function of disorder W. The letters correspond to different energies E = 0.8 (A), 0.6 (B), 0.4 (C), 0.2 (D), 0.02 (E) and 0.002 (F).

Fig.2 Localization length L, defined in Sec.2a) as a function of energy E for different values of disorder W = 0.8 (A), 0.2 (B), 0.9 (C), 0.4 (D) and 0.6 (E). The logarithmic scale for curves A and C translated in one order of magnitude to smaller values of L, as indicated on the right of the graph. The average exponent in the relation $L = \text{const.} \, |E|^{-\bar{\nu}}$ is $\bar{\nu} = 0.20 \pm 0.2$.

Fig.3 $t = e^{-\gamma}$ with γ equal to the average defined in Eq.(15), as a function of disorder W. γ was obtained for complex t_n and E. The value of E is indicated on each curve.

Fig.4 Density of states vs energy in units of $\bar{V}_n$. Dots are present calculations. The histogram corresponds to a calculation with Dean's method.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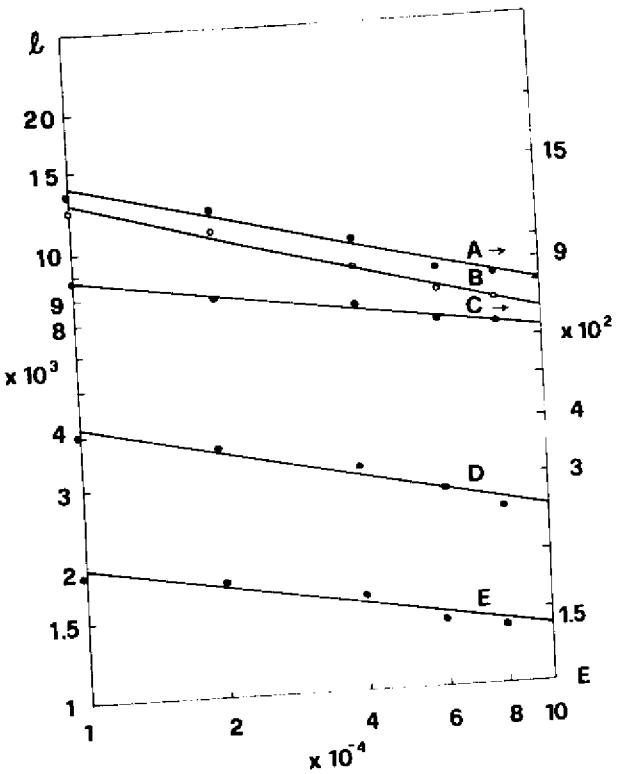
0.2
1.0
W
F
E
D
C
B
A

Fig.1


ℓ
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15
10
9
8
x 10^3
4
3
2
1.5
1
15
9
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B
C →
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1
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8
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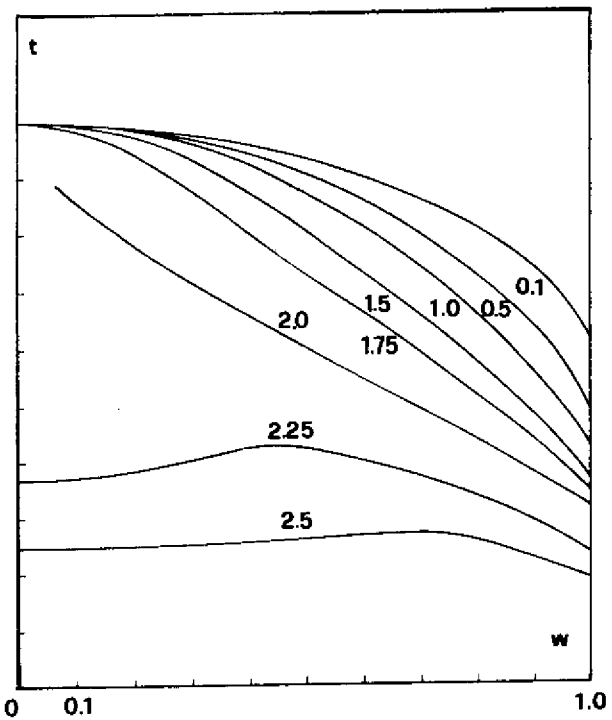
x 10^{-4}

Fig.2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w
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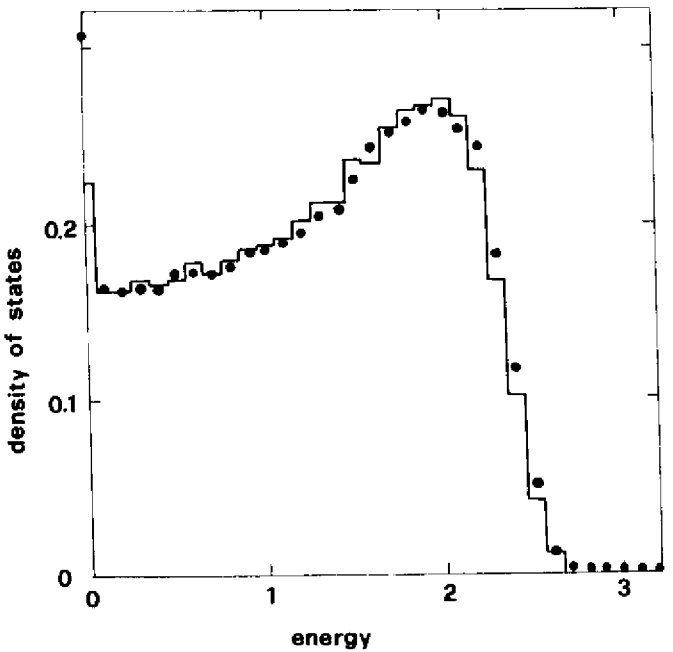
0.1
1.0

Fig.3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0.2
0
1
2
3
energy

Fig.4