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LOCALIZATION LENGTH AND FRACTAL DIMENSION OF BAND CENTRE STATES
FOR 1-d OFF-DIAGONAL DISORDERED SYSTEMS *

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ABSTRACT

We study and characterize the eigenstates near the centre of the band of a 1-d tight binding model with off-diagonal disorder W_T . We find a new exponent for the localization length λ on an energy-dependent range of disorder W_m . We correlate this feature with a change of structure of the wave-function displayed by the behaviour of its fractal dimensionality.

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Eigenstates near the band centre of an off-diagonal disordered model have been extensively studied in the past because of their controversial character (Soukoulis and Economou 1981 and references therein). In particular the $E = 0$ state has an infinite localization length and presents a transmission coefficient that approaches zero as $\exp(-\sqrt{L})$, L being the size of the system. It has been defined therefore as localized.

In this letter we want to point out the existence of a new exponent for the localization length λ in a range of the disorder W_T for energies close to the band centre. This change of exponent shows up in a different structure of the wave-function as depicted in its "fractal dimensionality" (to be defined below).

Our model is the Anderson tight-binding Hamiltonian:

$$H = \sum_n \epsilon |n\rangle\langle n| + \sum_n (t_{n,n+1} |n\rangle\langle n+1| + t_{n-1,n} |n-1\rangle\langle n|) \quad (1)$$

with the hopping terms being random variables distributed uniformly as:

$$t - \frac{W_T}{2} < t_{n,j} < t + \frac{W_T}{2} \quad (2)$$

The mean value $\langle t_{n,j} \rangle = t$ determines the unit of energy. The lattice spacing determines the unit of length. We calculate λ from the asymptotic behaviour of the wave-function from:

$$\lambda = \lim_{m \rightarrow \infty} \left\langle \frac{m}{\ln |a_m|} \right\rangle \quad (3)$$

where a_n is the coefficient in the equation for the wave-function ψ_n :

$$t_{0,1} \psi_0 + a_n \psi_n + b_m \psi_{n+1} = 0 \quad (4)$$

obtained from the recursion relations:

$$\begin{aligned} a_m &= -(\epsilon/t_{n-1,m}) a_{m-1} + b_{m-1} \\ b_m &= -(t_{m,m+1}/t_{m-1,m}) a_{m-1} ; m \geq 1 \end{aligned} \quad (5)$$

where $\epsilon \equiv c - E$, E being the eigenvalue and for initial values $a_0 = -t_{0,1}$ and $b_0 = 0$. A relation analogous to (4) is obtained to the left. With this procedure we can attain a precision of about 2%. Similar iteration procedures are being currently used (MacKinnon and Kramer 1983). The full wave-function is obtained by imposing periodic boundary conditions at the ends of the system and by adjusting appropriately the eigenvalue (Roman and Wiecko 1985).

In Fig.(1) we show the dependence of λ on W_T for different energies. An initial exponent $s = -2$ in $\lambda \sim W_T^{-s}$ is obtained for energies close to the band centre and $s = -2/3$ is obtained for $E = 2$ in agreement with previous work (Krey 1983). However for very small energies ($E \leq 0.001$) an exponent $s \approx -8/5$ is obtained for an energy dependent range of disorder above a crossover into $s = -2$ regime.

The "fractal dimensionality" D as introduced by Soukoulis and Economou (1984) is defined from

$$A(L) = \text{const } L^D \quad (6)$$

where $A(L)$ is the density correlation function:

$$A(L) = \int d\tau |\Psi(\tau)|^2 \int_0^L d\tau' |\Psi(\tau+\tau')|^2 \quad (7)$$

In Fig.(2a) we show the wave-function (ψ^2) for disorder $W_T = 0.1$ and E corresponding to $s = -2$. The fractal dimensionality shown in Fig.(2b) is unique and well defined for $L < \lambda$. This is analogous to what happens for the case of diagonal disorder (Soukoulis and Economou 1984; Roman and Wiecko 1985). In Fig.(3a) we show the wave function for the same

W_T as above but for a lower energy corresponding to the regime with $s \approx -8/5$. The structure of the wave-function is now more similar to "connected packets" (Wiecko and Roman 1984) which, as shown up in Fig.(3b) means that at least two different fractal dimensionalities appear for $L < \lambda$. The appearance of several D at different length scales has also been observed by us at higher W_T (Roman and Wiecko 1985) whereas a unique D is found for purely diagonal disorder W_E and for mixed disorder where W_E predominates over W_T . This suggests that the diagonal disorder (alloy) models are different from the off-diagonal (amorphous) models at least as far as amplitude fluctuations of the wave-functions over different length scales are concerned.

The lower the energy, the lower the value of W_T at which the transition occurs from a regime with exponent $s = -2$ to $s = -8/5$. We can expect therefore that the controversial state at $E = 0$ (Soukoulis and Economou 1981 and references therein) would directly start with exponent $s \approx -8/5$. Therefore, it will not present a unique D , having however, an infinite λ . This situation is also being found by us studying incommensurate models at critical values of the parameters (Aubry 1980). We therefore suggest that the $E = 0$ state can be an example of a singular continuous state in disordered systems.

Upon finishing this work we were informed that the off-diagonal model is also being studied (Ure and Majlis 1985) through convergence properties of the coefficients of the continuous fraction expansion of the propagator. There seems to be qualitative agreement with our results for λ .

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REFERENCES

- Aubry S. 1980 in Bifurcation Phenomena in Mathematical Physics and Related Topics, Eds. C. Bardos and C. Bersis (Reidel, New York) pp. 163-184.
- Krey U. 1983, Z. Phys. B 54, 1.
- MacKinnon A. and Kramer E. 1983, Z. Phys. B 59, 385.
- Roman E. and Wiecko C. 1985, preprint sent to Z. Phys. B.
- Soukoulis C.M. and Economou E.N. 1981, Phys. Rev. B 24, 5698.
- Soukoulis C.M. and Economou E.N. 1984, Phys. Rev. Lett. 52, 565.
- Ure J.E. and Majlis N. 1985, preprint Neteroi, Brasil 1985.
- Wiecko C. and E. Roman 1984, Phys. Rev. B 30, 1603.

FIGURE CAPTIONS

- Fig. 1 Initial dependence of λ on W_T for different energies. The scale for $E = 2$ is different as marked on the figure.
- Fig. 2 a) The wave function squared for $W_T = 0.1$ and $E = 0.00475$ (regime $s = 2$) as function of position.
 b) $\ln A(L)$ as function of $\ln(X)$ where $\lambda = 2.300$ indicates the mean squared dispersion and the slope means D .
- Fig. 3 Idem as in Fig. 2 for the same W_T and $E = 0.000047$ (regime $s = 1.61$). $\lambda = 5.200$ and two different slopes are observed as indicated.

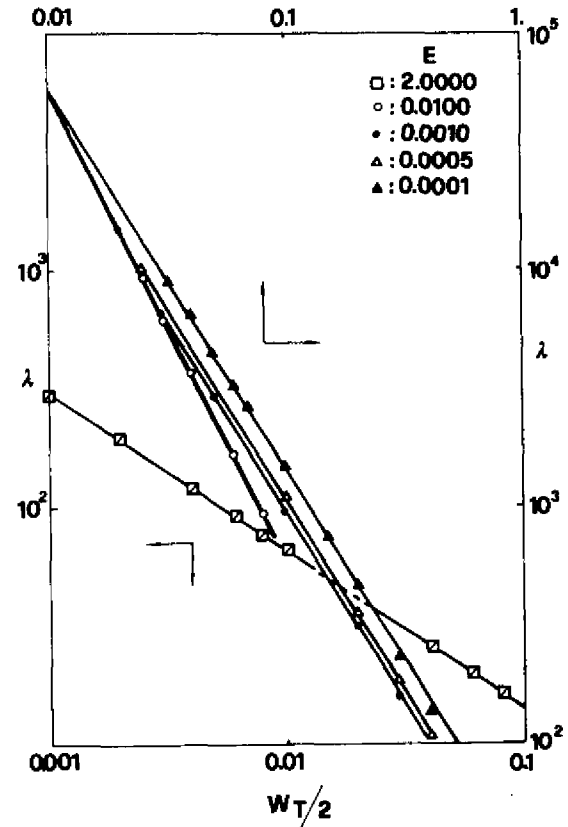


Fig.1

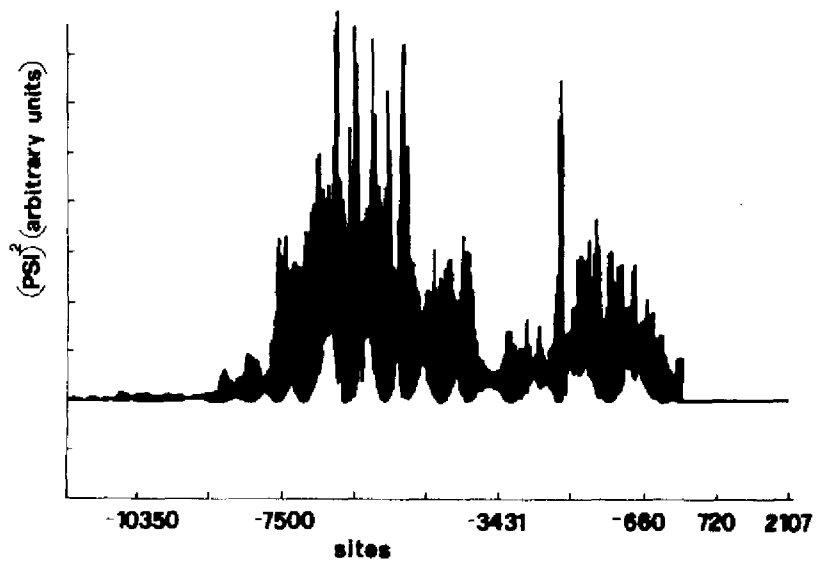


Fig.2a

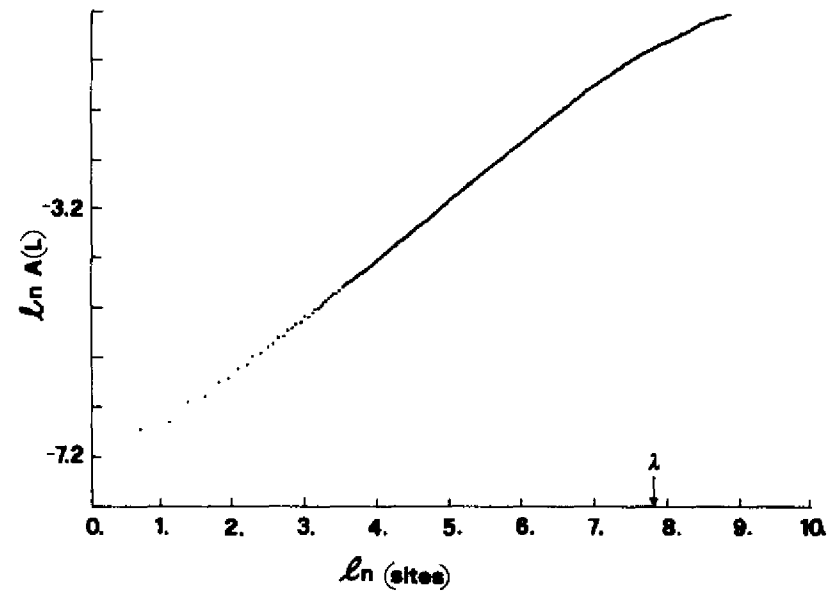


Fig.2b

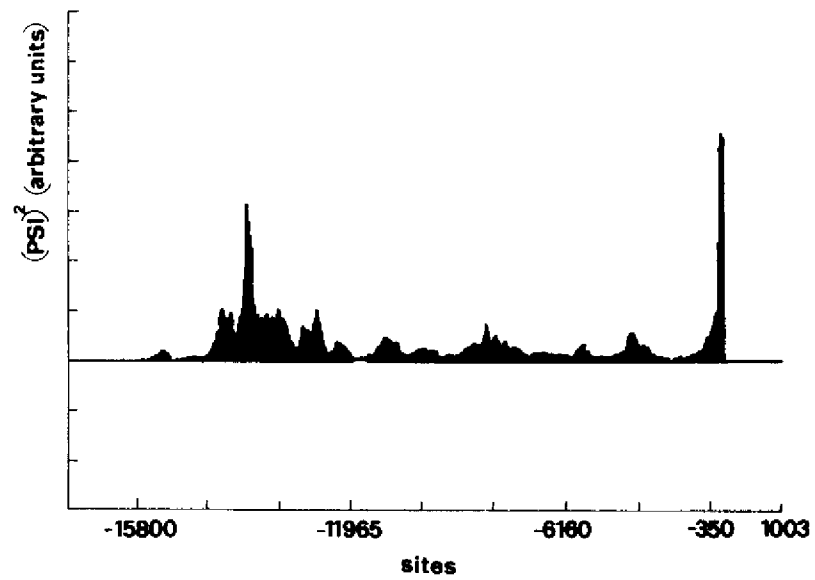


Fig. 3a

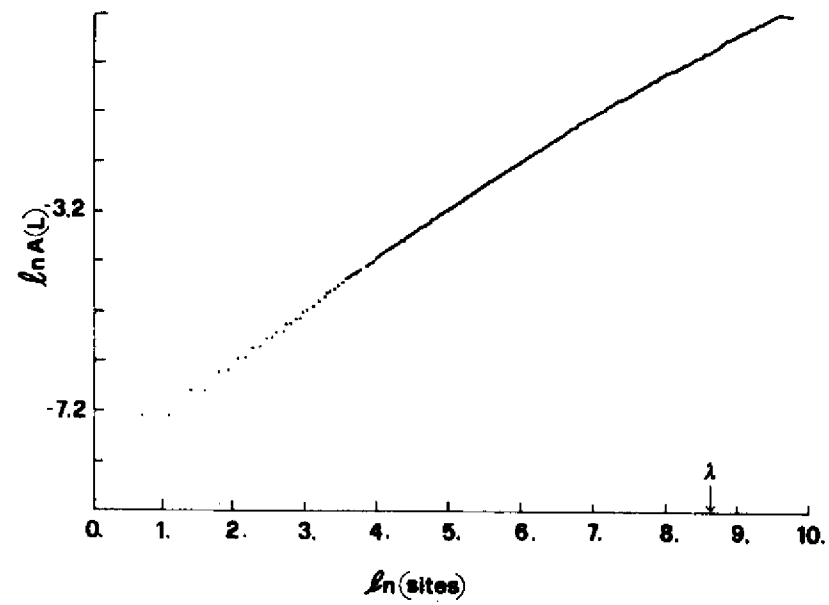


Fig. 3b