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LOCALIZATION LENGTHS IN ONE-DIMENSIONAL DISORDERED SYSTEMS*†

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Closed formulae are obtained for the localization length and the density of states in one dimensional tight binding disordered lattice. The results for binary alloy type of randomness exhibit strong structure due to clustering effects.

IT IS generally believed[1,2] that localized eigenstates are associated with various kinds of potential fluctuations, in the sense that the envelope of the eigenstate is appreciable in the region of the potential fluctuation and decays exponentially far away from it. If so, the envelope of the eigenfunction should be characterized by the shape and magnitude of the region where it is appreciable and also by the parameter R_d entering in the exponential factor, e^{-r/R_d}, characterizing the decay of the envelope as the distance $r \to \infty$. Thus *at least* two localization lengths are necessary to describe the localized eigenfunctions: the length R_f being a measure of the magnitude of the region where the eigenfunction is appreciable and the length R_d characterizing its decay at large distances. In general R_f and R_d should be considered as random quantities characterized by distribution functions which depend on the energy of the eigenfunction. It will be demonstrated here that R_d is sharply distributed around a value $R_d(E)$ for a given energy E to which localized eigenstates correspond. On the other hand, probabilistic considerations show that R_f is *not* sharply distributed unless special dynamical correlations are present.[3]

The quantities R_d and R_f are important in order to calculate observable quantities such as the d.c. and a.c. conductivity and their temperature dependence in the case where the Fermi level E_F is well within a region of localized states.[1,4]

Recently one-dimensional disordered conductors were studied[4,5] for which the tight-binding approximation seems to hold. For the time being it is not clear to what extent the properties of these 1-*D* conductors are dominated by disorder or by electron correlation effects.[4,5] It seems that detailed quantitative calculations are needed in order to settle this open question. Such calculations are considerably facilitated due to the one-dimensionality of these systems which allow a number of exact results. Accordingly, we consider here a simple one-dimensional tight binding model

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for a disordered system. The Hamiltonian is

$$< i|H|j > = \epsilon_i \delta_{ij} + V_{ij} \qquad (1)$$

where $|i>$ is the ith atomic orbital centered around the lattice point i, V_{ij} is equal to a constant V for nearest neighbours and zero otherwise, and ϵ_i is a random variable with a given common distribution function $P(\epsilon_i)$. By examining the convergence properties of the renormalized perturbation expansion[6] (RPE) for the self-energy[6] $\Delta_0(E)$ it has recently been shown[7] that all the eigenstates in this model are localized.

By examining the RPE for the off-diagonal matrix element $G_{l0} \equiv <l|(E-H)^{-1}|0>$ we were able to show[8] that the localization length R_d (measured in units of lattice spacing) is sharply distributed around a quantity given by[9]

$$R_d(E) = -[\ln V + <\ln|G^i_{i+1}(E)|>]^{-1}, \qquad (2)$$

where the symbol $<>$ denotes averaging over the random variables $\{\epsilon_j\}$ and the subscript i in (2) means that ϵ_i is taken equal to infinity. Extended states, if any, would correspond to $R_d(E) = \infty$.

There is one particular case for which $R_d(E)$ can be calculated analytically, namely when the distribution function of ϵ_i is a Lorentzian.[8,10] In the general case one can derive[7] an integral equation for the probability distribution of $G^i_{i+1}(E)$. Solving numerically this integral equation and having thus the probability distribution of $G^i_{i+1}(E)$ any average of this quantity can be calculated. Using the integral equation from reference 7 as well as the expressions for the localization length $R_d(E)$ and for the average density of states per atom, $n(E)$, in terms of G^i_{i+1} one obtains after some manipulations

$$n(E) = \frac{1}{V}\int_{-\infty}^{\infty} dt\, f(t;E) f\left(\frac{1}{t};E\right), \qquad (3)$$

$$R_d(E) = -\left[\int_{-\infty}^{\infty} dt\, f(t;E)\ln|t|\right]^{-1}, \qquad (4)$$

where

$$f(t;E) = \frac{1}{t^2}\int P^*\left(\frac{E}{V} - t' - \frac{1}{t}\right) f(t';E)\, dt', \qquad (5)$$

and P^* is the given distribution function of the variable ϵ_i/V.

It should be noted that expressions similar to equations (3) and (5) have been obtained by Borland[11] and Halperin[12] in connection with other one-dimensional disordered systems. Halperin[12] has also obtained an expression similar to equations (4) and (5) for the average rate of increase of the solutions of Schrodinger's equation (which in general do not coincide with the eigenfunctions, since they do not satisfy the boundary conditions). In contrast to these different approaches, the present method calculates directly the decay rate of the envelope of the eigenfunctions.[13]

The integral equation (5) has been solved numerically by iteration for different distribution functions P^*, after an appropriate transformation of the variable t. Details of the numerical method will be discussed elsewhere.[13]

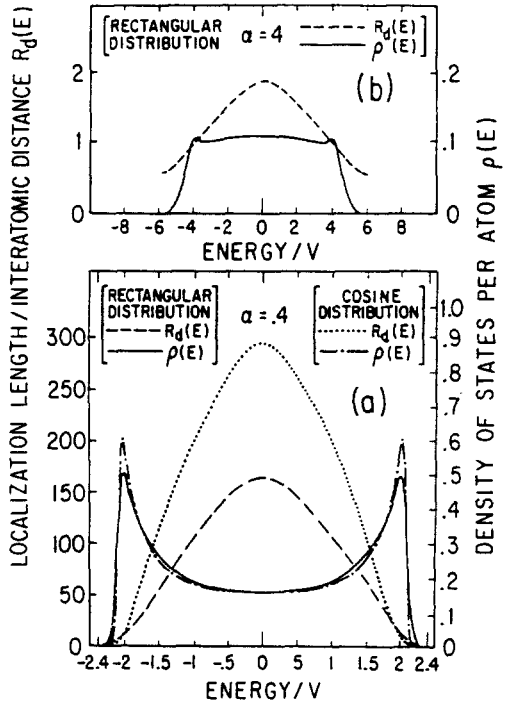

FIG. 1. Average density of states and localization length for a tight binding one-dimensional random system. The probability distribution of the site energies is a cosine (see text) or a rectangular with width taken as $\alpha = 0.4$ (a) or 4 (b).

In Fig. 1(a) we present the results for the case of a cosine distribution where $P^*(x) = (\pi/4\alpha)\cos(\pi x/2\alpha)$ for $|x| \leqslant \alpha$ and zero otherwise. It is worthwhile to note that while the rigorous band edge is at $E/V = 2.4$ the density of states is very close to zero already $E/V \approx 2.18$. This is a rather common feature in disordered systems: the density of states at the deep tail is very close to zero. One should keep this in mind when theoretical predictions for the positions of the band edge are compared with experiments.

In Fig. 1(a) and 1(b) we present the results for Anderson's case where P^* is a rectangular distribution $P^*(x) = 1/2\,\alpha^{-1}$ for $|x| < \alpha$ and zero otherwise. As one goes from the cosine to the rectangular case a further reduction of the localization length is observed together with an increased broadening of the band; both effects are due to the enhanced probabilities for large fluctuations in the rectangular case in comparison with the cos case. When $\alpha = 4$ (this value of α would give an Anderson transition[6,2] in the 3-dimensional case) the localization length R_d becomes of the order one throughout the whole band and the density of states approaches that of the probability distribution of ϵ_i.

The binary alloy case where $P^*(\epsilon) = (1 - x)\delta(\epsilon - \epsilon_A) + x\delta(\epsilon - \epsilon_B)$ is presented in Fig. 2(a). x is the concentration of the B atoms and $\epsilon_A(\epsilon_B)$ is the center of the band for the pure $A(B)$ lattice. The main peaks [Fig. 2(a)] in the density of states and the localization length for the impurity subband ($E/V = 1.763$, 2, 2.1667) are due to the eigenstates bound around clusters of the form B, BB, BBB embedded in an environment of A atoms. Dean[14] was the first to demonstrate the existence of these peaks using his numerical method. The present method not only verifies this important property but shows that the peaks are much sharper than has been previously anticipated.[15] There is also additional structure in the host subband not previously identified. It is seen also that the structure in the density of states is reflected in the localization length and vice versa, which is to be expected since the density of states is roughly proportional to the volume available to the wavefunction at

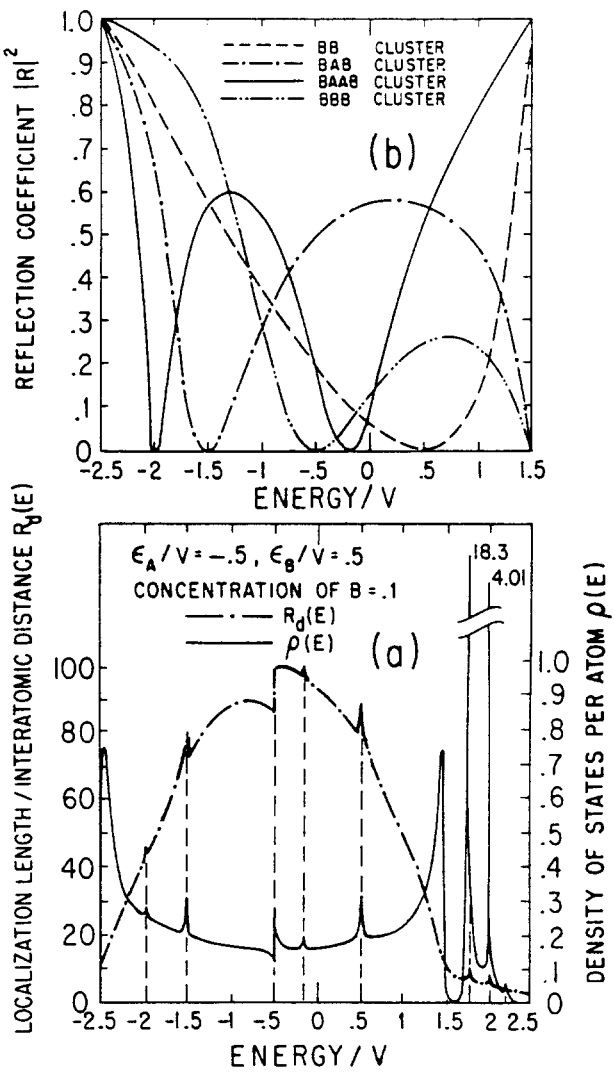

FIG. 2. (a) Average density of states and localization length for a tight binding one dimensional random alloy $A_{1-x}B_x$.
(b) Reflection coefficients from different clusters embedded in an environment of A atoms.

this energy. To understand the structure in the host subband one should examine the behavior of the reflection coefficient in an environment of A atoms. This behavior is shown in Fig. 2(b) for some of the most probable configurations. The absence of reflection from each cluster at certain energies explains the longer localization length and higher density of states there. Thus $BAAB$ clusters are responsible for the peaks at

$E/V = -1.9812, -0.1889$. At $E/V = -1.5, -0.5, 0.5$ sharper peaks appear because at each of those energies a whole group of clusters is non-reflecting.[13] The jump in the localization length at $E/V = -0.5$ (center of the host band) is due to properly weighted contributions from all clusters of the form $BA \ldots AB$ and seems to be a characteristic of binary alloys at low concentration.[13] More structure certainly exists in both subbands, but it is very weak as the probability for the occurrence of the clusters responsible for it is very small.[13]

We would like to emphasize here that these exact results obtained in the present simple one dimensional model are of importance because they provide the conceptual framework for understanding realistic cases for which quantitative calculations are beyond our present ability. The case of the strong structure in the localization length at $\epsilon = -0.5$ revealed by the present calculation is of such importance: it has been hypothesized[16] that clustering effects are responsible for the metal-semiconductor transition observed in certain liquid and amorphous semiconductors. The present calculation lends support to this hypothesis since it shows quantitatively that clusters can be responsible for significant changes in the localization length accompanied by corresponding changes in the density of states. Moreover, extension of the present method to include short range correlations can be used for a quantitative study of a model system exhibiting metal-semiconductors transition.[17]

The present method can also directly apply to the important problem of vibrations in linear chains replacing Dean's numerical method.[14]

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9. In a recent preprint FUJITA and HORI, following a different technique, obtained a formula for $R_d(E)$ identical to the one given by equation (2). They have also attempted to generalize the method to the 3-dimensional case. THOULESS D., also obtained a formula for the localization length in terms of the average density of states.
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15. The present method computes the density of states directly and not through its integral as in Dean's method. Consequently our results are much more accurate close to sharp peaks.

16. COHEN M.H. and SAK J., to be published in the *J. Non-Crystalline Solids*. We are indebted to COHEN M.H. for pointing out to us the relevance of our results to the problem of metal–semiconductor transition in certain alloys.

17. PAPATRIANTAFILLOU C., EGGARTER T. and COHEN M.H., unpublished.

Für die Lokalisierungslänge und die Zustandsdichte von eindimensionalen, stark gebundenen, ungeordneten Gittern werden geschlossene Formeln angegeben. Die Resultate für Verteilungen vom binären Legierungstyp zeigen starke Abhängigkeit von Clustereffekten.