Extended states in a one-dimensional system with off-diagonal disorder*

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We prove for a one-dimensional tight-binding Hamiltonian with only off-diagonal randomness that the state at the middle of the band is extended, regardless of the probability distribution of the hopping matrix elements and also derive a sum rule for the density of states. In particular, for the case where the probability distribution of the hopping matrix elements is a generalized Poisson distribution, we derive an expression for the localization length near the middle of the band. We also calculate the localization length for a chain of potential wells with randomly fluctuating depths, separated by regions of zero potential, the length of the latter being also random.

One of the points of interest in the study of one-dimensional disordered systems is the nature of the eigenstates, i.e., localized or extended. Mott and Twose[1] were the first to suggest that all the electronic eigenstates in one-dimensional (1-D) disordered systems are localized. Borland[2] was the first to give a rather general proof of this statement. His proof was done for the case in which electrons are moving in the field of a 1-D infinite chain of identical potentials separated by regions of zero potential, the length of these regions being a random variable. Borland's proof breaks down only at certain isolated energies, for certain special potentials.[3] This can be understood as follows[4]: The transmission coefficient, for some particular forms of the central potential in Borland's model and for certain values of energy, can be equal to unity (Ramsauer effect). In that case an electron will propagate freely throughout the chain, and these particular states are extended.

Economou and Cohen[5] examined the problem of localization in the 1-D tight-binding model. Their method was based on the convergence of a perturbation expansion of the self-energy, and they also concluded that all states are localized in the case where only nearest-neighbor interaction is considered. However for the case where only off-diagonal disorder is present their perturbation expansion of the self-energy is not valid for the energy at the middle of the band because the denominators of the unrenormalized expansion become zero. Therefore the character of the state (i.e., extended or localized) at the middle of the band remains unresolved for off-diagonal disorder only. In this paper we present proof that this state is an extended one, independent of the probability distribution of off-diagonal disorder, and give the energy dependence of the localization length for a special class of distributions of off-diagonal randomness for which the density of states can be evaluated analytically.

We consider a tight-binding Hamiltonian with nearest-neighbor interaction only and with constant diagonal and random off-diagonal matrix elements. Shifting the origin of energy we can eliminate the diagonal matrix elements so that the Hamiltonian of the system is given by

$$H=\sum_n V_{n,n+1}(|n\rangle\langle n+1| + |n+1\rangle\langle n|), \tag{1}$$

with the $\{V_{n,n+1}\}$ statistically independent and having the same probability distribution. The Schrödinger equation of the system can be written

$$V_{n,n+1}a_{n+1} + V_{n,n-1}a_{n-1} = E\,a_n \ , \tag{2}$$

with a_n the amplitudes for the eigenstate with energy E. For zero energy Eq. (2) gives the recurrence relation $a_{n+1} = -(V_{n,n-1}/V_{n,n+1})\,a_{n-1}$. Successive applications of this relation give

$$\frac{a_{2n+1}}{a_1} = \left(-\frac{V_{2n,2n-1}}{V_{2n,2n+1}}\right)\left(-\frac{V_{2n-2,2n-3}}{V_{2n-2,2n-1}}\right)\cdots\left(-\frac{V_{2,1}}{V_{2,3}}\right) . \tag{3}$$

Defining the localization length by the expression

$$\frac{1}{L(E=0)} = -\lim_{n\to\infty}\frac{1}{2n}\ln\left|\frac{a_{2n+1}}{a_1}\right| , \tag{4}$$

and applying the central-limit theorem we obtain

$$1/L(E=0) = 0. \tag{5}$$

Therefore the state with zero energy is extended regardless of the probability distribution of $\{V_{n,n+1}\}$, except when the total probability for $V=0$ is finite $[P(V) = c\delta(V) + P_1(V)]$, in which case the chain is broken. A similar conclusion was reached for more restricted classes of distributions by Herbert and Jones[6] and by Bush.[7] Equation (5.10) of Ref. 6 on which the conclusion of Herbert and Jones was based is, however, incorrect. Bush restricted his considerations to distributions of V limited to positive values only. However, his

argument remains correct when extended to arbitrary distributions.

Dyson[8] in a pioneering work studied the problem of a disordered linear chain of harmonic oscillators. Smith[9] pointed out that Dyson's model for the case where the chain consists of identical atoms and random XY model. Because the random XY model is equivalent to that of spinless fermions[10] described by Eq. (1), we can apply Dyson's solution to our problem. We shall concentrate on the special case for which the probability distribution of the hopping matrix elements is a generalized Poisson distribution given by

$$P_n\frac{V}{V_0}=\frac{2n^n}{(n-1)!}\left(\left|\frac{V}{V_0}\right|\right)^{2n-1}\exp\frac{-nV^2}{V_0^2},\quad n=1,2,\ldots, \tag{6}$$

because for this case Dyson's model has an analytic solution for the frequency spectrum, which in our case represents the electronic density of states. Thus the symmetric density of states for Hamiltonian (1) is given by

$$D_n(\epsilon)=D_n(-\epsilon)=\frac{dM_n(\epsilon^2)}{d\epsilon}, \tag{7}$$

with $\epsilon = E/V_0$ and $M_n(\epsilon^2)$, the integrated density of states, given by

$$M_n(\epsilon^2)=\frac{1}{2}+\frac{1}{2}\,\frac{G_1^2(\epsilon^2)-F_2(\epsilon^2)G_2(\epsilon^2)e^{-n\epsilon^2}+[F_0(\epsilon^2)-F_1^2(\epsilon^2)+(\frac{1}{6}\pi^2-t_{n-1})F_0^2(\epsilon^2)]e^{-2n\epsilon^2}}{(G_1^2(\epsilon^2)+\{F_1(\epsilon^2)-[\ln(n\epsilon^2)+s_{n-1}+\gamma]F_0(\epsilon^2)\}e^{-n\epsilon^2})^2+\pi^2F_0^2(\epsilon^2)e^{-2n\epsilon^2}}, \tag{8}$$

with

$$s_j=\sum_{l=1}^{j}l^{-1},\quad t_j=\sum_{l=1}^{j}l^{-2},\quad s_0=t_0=0,$$

and γ Euler's constant. The analytic expressions for F_0, F_1, F_2, G_1, G_2 can be found in Dyson's paper [Eqs. (64)–(69)]. The density of states is shown for $n=1$, 3, 5 in Fig. 1. For $|\epsilon| \ll 1$ D_n has the asymptotic behavior

$$D_n(\epsilon)\simeq 2(\tfrac{1}{6}\pi^2-t_{n-1})/|\epsilon|\,[-\ln(n\epsilon^2)]^3. \tag{9}$$

That is, the density of states has a singularity at the middle of the band.

There is an indication that the presence of a singularity in the middle of the band is characteristic of the 1-D tight-binding Hamiltonian with off-diagonal disorder only and not of the special form of the probability distribution used here. Numerical calculations done by Weissman and Cohan[11] for a square probability distribution indicate the presence of a peak at the middle of the band. However, since their numerical method does not work for $E \to 0$ they did not manage to give any conclusive evidence of the existence of the singularity. It is interesting to note that calculations[12,13] done for the 1-D tight-binding Hamiltonian with diagonal disorder only do not reveal the existence of any singularity in the density of states. In the general case, where both diagonal and off-diagonal disorder are present, all states are localized as proven by Economou and Cohen,[5] and thus the density of states, which is proportional to the volume accessible to an electron, is finite. From the above argument we conclude that the introduction into Eq. (1) of even a small amount of diagonal disorder destroys the singularity in the density of states.

Since, as we proved before, the state at $E=0$ is extended, our model has a singularity in the density of states at the point of transition from localized to extended states. On the other hand Lloyd's model,[14] the only exactly soluble model in three dimensions with diagonal disorder only, gives no singularity in the density of states at the transition point. Edwards and Thouless[15] tried to extend this result to the case of a square probability distribution of width W. They proved that for $W > \pi ZV$, with Z the coordination number, the density of states is analytic at the middle of the band. However, the latest estimates[16] of the critical disorder required for an Anderson

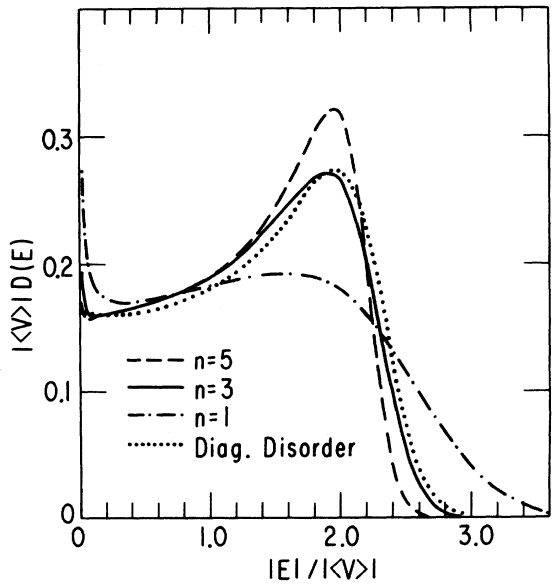

FIG. 1. Density of states for off-diagonal randomness with generalized Poisson distribution, Eq. (6), with n = 1, 3, 5 and for diagonal randomness with Gaussian distribution and rms $\sigma = 0.57\,|\nu|$ (dotted line).

transition give $W_c < \pi ZV$ for square, diamond and simple cubic lattices. Therefore Edward's and Thouless's result does not give any information as to what happens at the transition point.

The localization length for a one-dimensional random system expressed in terms of the density of states is given by[6,17]

$$L^{-1}(E) = \int D(E') \ln|E - E'| \, dE' - \langle \ln|V| \rangle, \qquad (10)$$

where V is the hopping matrix element. The localization length is shown in Fig. 2 for the case where $D(E)$ is given by Eq. (7). Combining Eqs. (10) and (5) we conclude that the density of states for a tight-binding Hamiltonian with off-diagonal randomness only and arbitrary distribution satisfies the sum rule

$$\int D(E) \ln|E| \, dE = \langle \ln|V| \rangle. \qquad (11)$$

We can prove that the singularity of $\ln|E - E'|$ at E in the integrand of Eq. (10) does not give an important contribution to the integral. Therefore separating the integral into two parts, one for the integration in region $|E'| \leq |E|$ and the other for integration in region $|E'| > |E|$, and making the approximation $\ln|E - E'| \simeq \ln|E|$ in the first region and $\ln|E - E'| \simeq \ln|E'|$ in the second one we obtain with the use of Eq. (11) that for a symmetric density of states the localization length is given by

$$L^{-1}(E) \simeq \int_0^{|E|} (\ln E^2 - \ln E'^2) D(E') \, dE'. \qquad (12)$$

The behavior of the localization length near the middle of the band in the case where the probability distribution of hopping matrix elements is given by (6) can be found by utilizing the asymptotic form for the density of states given by Eq. (9). We found that in that case the localization length near the middle of the band is given by the expression

$$L_n(E/V_0) \simeq -2 \ln(nE^2/V_0^2)/(\tfrac{1}{6}\pi^2 - t_{n-1}). \qquad (13)$$

In Fig. 3 we compare Eq. (13) to our numerical results and show that Eq. (13) gives an asymptotic representation of $L(E)$ for $n = 1$.

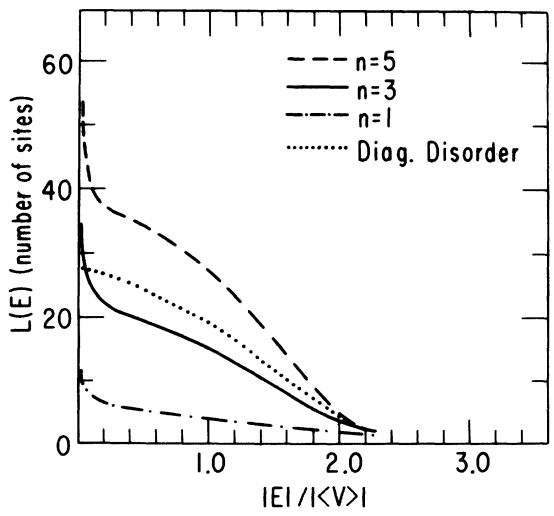

FIG. 2. Localization length for off-diagonal randomness with generalized Poisson distribution, Eq. (6), with $n = 1$, 3, 5 and for diagonal randomness with Gaussian distribution and rms $\sigma = 0.57|V|$ (dotted line).

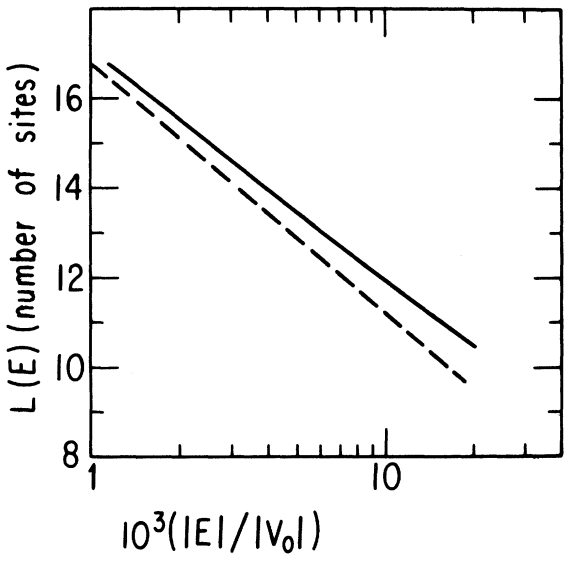

FIG. 3. Localization length for $n = 1$ as given by Eq. (10) (solid line), and by Eq. (13) (broken line).

We consider now the case of a 1-D chain of potential wells separated by regions of zero potential. The width of the wells is equal to a, while the depth U fluctuates from site to site according to the relation $U = U_0 + \delta$, with U_0 constant and δ a random variable with probability distribution given by

$$P(\delta) = \begin{cases} 1/\Delta & \text{for } |\delta| \leq \Delta, \\ 0 & \text{otherwise.} \end{cases} \qquad (14)$$

The length of the regions of zero potential is a random variable. The fluctuations in U correspond to diagonal disorder in the tight-binding Hamiltonian, while fluctuations in the length of zero potential regions correspond to off-diagonal disorder.

Let $T(E, \delta)$ be the transmission coefficient of the potential well for given δ at $E > 0$. As a zero-order approximation to the transmission coefficient of the chain, we could compute the transmission coefficient of each well and multiply them

together.[18] This approximation ignores all multiple reflections and interference effects. This is a good approximation only if the following conditions are met: (a) The potential wells have resonance energies E_r $[T(E_r)=1]$ and we take into consideration only energies close to the resonance energies so that the reflection coefficient is small, and (b) off-diagonal randomness is present so that the contributions from multiple reflections and transmissions add randomly and are expected to give a small contribution. In this approximation we have

$$|\psi_N|^2 = \prod_i T_i(E,\delta_i)\,|\psi_0|^2, \tag{15}$$

where ψ_N is the wave function at site N, corresponding to a plane wave incident on site 0 with amplitude $|\psi_0|$. The localization length is given by

$$1/L = -(1/N)\ln|\psi_N/\psi_0|. \tag{16}$$

Combining Eqs. (15) and (16) we obtain

$$L \simeq -2/\langle \ln T(E,\delta)\rangle, \tag{17}$$

where $\langle\ \rangle$ denotes an average over δ. The transmission coefficient for the square wells is given by the expression

$$T(E,\delta) = \left(1+\frac{(U_0+\delta)^2}{4E(E+U_0+\delta)}\sin^2(ka)\right)^{-1}, \tag{18}$$

where $k=[2m(E+U_0+\delta)]^{1/2}/\hbar$. The resonance energies are given by

$$E_n = \frac{\hbar^2\pi^2n^2}{2ma} - U_0 - \delta = E_n^0 - \delta, \tag{19}$$

and they too are random variables. We consider the case for which E_n is close to E_n^0, so that $\Delta \ll \hbar^2\pi^2/2ma^2$. For $E\simeq E_n^0$, $\ln T(E,\delta)$ can be approximated by

$$\ln T(E,\delta) \simeq \frac{U_0^2ma^2}{8\hbar^2E_n^0(E_n^0+U_0)^2}\ (E_n^0+\delta-E)^2.$$

Calculating $\langle \ln T(E,\delta)\rangle$ and inserting it in (17) we obtain

$$L(E,\Delta) \simeq \frac{8\hbar^2E_n^0(E_n^0+U_0)^2/U_0^2ma^2}{(E-E_n^0)^2+(\Delta/\sqrt{3})^2}\ . \tag{20}$$

Therefore the localization length for $E\simeq E_n^0$ has a Lorentzian form with width $\Delta/\sqrt{3}$. For $\Delta=0$, which corresponds to the absence of diagonal disorder, Eq. (20) reduces to

$$L(E) \propto 1/(E-E_n)^2. \tag{21}$$

In that case $L(E_n)=\infty$, and the state at this energy is extended. Equation (20) implies that the introduction of an infinitesimal amount of diagonal disorder has the effect of localizing all states.

We note that numerical calculations by Tong and Wong[19] of $\ln|\psi_N/\psi_0|$ for identical square wells indicated that $\ln|\psi_N/\psi_0| \propto (E-E_r)^2$, in agreement with Eq. (21). Also from (13) and (21) it is apparent that the energy dependence of the localization length near an isolated extended state will depend on the detailed form of the Hamiltonian.

It is well known that introduction of disorder with rms σ in the matrix elements of the tight-binding Hamiltonian will have as an effect the broadening of the band by 2σ, if the introduction takes place in the diagonal elements, and by 4σ if it takes place in the off-diagonal ones. For the sake of comparison we included in Fig. 1 the density of states for the tight-binding Hamiltonian with diagonal disorder $\sigma = 0.57\ |V|$ and Gaussian distribution of the single site energies. Thus from Fig. 1 it can be seen that an amount $\sigma = 0.294\ |\langle V\rangle|$ ($n=3$ case) of off-diagonal disorder has the same effect as that of $\sigma = 0.57\ |V|$ of diagonal disorder. A similar conclusion can be drawn from Fig. 2 as regards the localization length.

Finally let us examine the case in which the off-diagonal disorder has the probability distribution

$$P(V) = c\delta(V-V_0) + (1-c)\delta(V+V_0), \tag{22}$$

with $0\le c\le 1$ and $\delta(x)$ the δ function. Making a transformation of phases we can prove that this problem has the same density of states as the periodic case. Therefore, using (10) we get that the localization length is the same as that for the periodic potentials $P(V)=\delta(V\pm V_0)$, $L(E)=\infty$, where $n(E)\neq 0$. Consequently we have a form of off-diagonal randomness for which all states are extended.

In applying these considerations to real quasi-one-dimensional materials one must be careful to examine cases in which the presence of off-diagonal disorder does not automatically imply substantial diagonal disorder as well. One possible case is that of dilute substitutional alloys which possess a well separated impurity band. A related case is that of Frenkel excitons in dilute substitutional alloys. Finally, in considering the response of electrons to time-varying external fields of frequencies higher than phonon frequencies, the electron-phonon interaction can be regarded as producing static disorder.[20,21] When intramolecular modes can be ignored or are absent, we have a case of pure off-diagonal disorder. It would thus be of considerable interest to extend the considerations of the present paper to the frequency-dependent conductivity.

Economou and Antoniou[22] have generalized the contents of the present paper to two and three dimensions. They have shown that instead of having one extended state at the center of the band for off-diagonal randomness, there is a finite

range of states which remain extended. Thus no Anderson transition occurs in the absence of diagonal randomness. Such results are of primary importance for the interpretation of data such as that reported on excitation propagation by Koo *et al.*[23] for ruby.

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