Off-diagonal disorder in one-dimensional systems

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We examine the nature of the zero-energy state in a one-dimensional tight-binding system with only nearest-neighbor off-diagonal disorder. We find that, although the localization length diverges at this energy, the state must nevertheless be considered as localized because the mean values of the transmission coefficient (which is directly related with the dc conductance) approach zero as the size of the system L goes to infinity. In particular, we find that the geometric and harmonic mean values of the transmission coefficient behave as $\exp(-\gamma\sqrt{L})$, while the arithmetic mean value follows the power law $L^{-\delta}$ with $\delta \simeq 0.50$. This is in contrast with the usual case of only diagonal disorder, where all three means behave as $\exp(-\lambda L)$.

The question of the localization of the eigenstates in one-dimensional (1D) disordered systems has been extensively studied both numerically[1] and analytically.[1] The Anderson model for a disordered lattice defined by the tight-binding Hamiltonian $H = \Sigma_n \epsilon_n | n \rangle\langle n | + \Sigma'_{n,m} V_{nm} | n \rangle\langle m |$, where the sites n form a regular lattice, is employed in most of the studies. Disorder has been introduced by assuming that the diagonal matrix elements ϵ_n are random variables. Although some questions[2] have been raised recently regarding the localization of states in 1D random systems, it seems that the questions have been answered[3,4] satisfactorily and thus all eigenstates in a disordered (diagonal disorder only) 1D system are always localized. The rôle of randomness in the off-diagonal matrix elements V_{nm} has not been studied until recently,[5,6] the underlying assumption being that the off-diagonal disorder is somehow similar to the diagonal one. A first indication that this may not be so was provided by Theodorou and Cohen,[5] who suggested that in a 1D system the eigenstate at the middle of the band remains extended in the presence of pure off-diagonal disorder. They based their argument on the fact that the usual definition of the localization length diverges on the band center and so they argued that the state is extended. Their claim was questioned by Fleishman and Licciardello[7] who found that, although the localization length diverges at this energy, the state is nevertheless localized due to fluctuations.

An unambiguous way of deciding whether or not an infinite localization length does imply localization is to study the transmission coefficient T of the system at this energy ($E = 0$). The transmission coefficient is a very important physical quantity in its own right in deciding about the extended or localized nature of an eigenstate and most significantly since it is directly related[8,9] to the dc conductance G of the system, which determines whether or not the states are localized.

In this paper we present results for the transmission coefficient of a 1D disordered system with only off-diagonal disorder at the center of the band. We find that this state is a localized one (although the localization length is infinite), independently of the probability distribution of off-diagonal disorder, because the mean values of the transmission coefficient approach zero as $L \to \infty$.

We consider here a tight-binding Hamiltonian with nearest-neighbor interaction only, with constant diagonal and random off-diagonal matrix elements. Shifting the origin of energy to eliminate the constant diagonal matrix elements we have that the Schrödinger equation in the site representation is

$$V_{n,n+1}c_{n+1} + V_{n,n-1}c_{n-1} = Ec_n \quad , \tag{1}$$

where c_n are the amplitudes of the states at energy E and each $V_{n,m}$ is a random variable characterized by a probability distribution. (The specific form of the distribution will be given below.) When $E = 0$, iterating Eq. (1) we obtain

$$\frac{c_{2n}}{c_0} \equiv x = (-1)^n \left[\frac{V_{2n-1,2n-2}}{V_{2n,2n-1}}\right] \times \left[\frac{V_{2n-3,2n-4}}{V_{2n-2,2n-3}}\right] \cdots \left[\frac{V_{1,0}}{V_{2,1}}\right] \quad . \tag{2}$$

Considering the quantity

$$y = \ln|x| = \sum_{j=1}^{n} y_j \ ,$$

where

$$y_j = \ln|V_{2j-1,2j-2}/V_{2j,2j-1}| \ ,$$

one has that the y_i's are independent variables with mean 0 and standard deviation σ. For large n we use the central limit theorem to obtain the probability distribution of y,

$$P(y)dy = (2\pi n\sigma^2)^{-1/2}\exp(-y^2/2n\sigma^2)dy \ . \quad (3)$$

Defining the localization the usual way, $1/l_c(E=0) = -\lim_{n\to\infty} y/2n$, where $y = \ln|c_{2n}/c_0|$, we obtain from Eq. (3) that $1/l_c(E=0)=0$. Therefore Theodorou and Cohen[5] argue that this state is extended regardless of the probability distribution of V_{nm}, except when the probability for $V=0$ is finite, in which case the chain is broken and of course the state is localized. Fleishman and Licciardello[7] questioned this claim and argued that fluctuations, previously ignored, localized the $E=0$ state, and that the envelope of the wave function has the asymptotic behavior $\exp(-\lambda_2\sqrt{n})$.

An unambiguous way to decide whether or not the $E=0$ state with infinite localization length is localized is by studying the transmission coefficient T of the system. At $E=0$, the transmission coefficient T is given by

$$T = \frac{4}{|x + 1/x|^2} \ . \quad (4)$$

Using the normal probability distribution [Eq. (3)] for the random variable y we have that the probability of y not being in the interval $[-\epsilon\sigma\sqrt{n}, \epsilon\sigma\sqrt{n}]$ is equal to $1-\epsilon(2/\pi)^{1/2}$ when $\epsilon\to 0$ and $n\to\infty$. Therefore for the random variable x, which is equal to $\exp(y)$, we have that

$$\Pr[x > \exp(+\epsilon\sigma\sqrt{n}) \text{ or } x < \exp(-\epsilon\sigma\sqrt{n})] \underset{\substack{\epsilon\to 0\\ n\to\infty}}{\longrightarrow} 1-\epsilon(2/\pi)^{1/2} \ , \quad (5)$$

where Pr is the probability; i.e., the quantity $x = c_{2n}/c_0$, which is a measure of the exponential growth or decay of the envelope of the wave function, is almost certainly either very big or very small for large n. But in either case the transmission coefficient T [Eq. (4)], due to its specific form, is small, which implies that the $E=0$ state is always localized. In particular we can say that

$$\Pr[T < 4\exp(-2\epsilon\sigma\sqrt{n})] \underset{\substack{\epsilon\to 0\\ n\to\infty}}{\longrightarrow} 1-\epsilon(2/n)^{1/2} \ . \quad (6)$$

It is worthwhile to note that while it is correct to discuss probabilities with the help of the normal distribution derived by the central-limit theorem, one cannot in general use the normal distribution to obtain the various moments.

In order to further check the above analysis and in order to calculate the different mean values of T we have numerically calculated the transmission coefficient T of our system for $E=0$ as a function of the length L of the system for different distributions of V_{nm}.

Our numerical results show, in agreement with our previous results[9] for only diagonal disorder, that the random variables T and $1/T$ are not normally distributed. In fact their probability distributions have very long tails which completely dominate the behavior of their means. Only the random variable $\ln T$ seems to follow a normal distribution.

Results for the geometric mean. In Fig. 1(a) we plot the results for the $-\langle \ln T\rangle$ as a function of $\sqrt{L}$ for different off-diagonal disorder. We employed, in our numerical work, the rectangular probability distribution $P(V_{nm})$ defined by

$$P(V_{nm}) = \begin{cases} 1/2W & \text{if } |V_{nm}-W_0| \le W \\ 0 & \text{otherwise} \ . \end{cases} \quad (7)$$

We select $W_0=1$ as the unit of energy. Note that, for all the strengths W of the off-diagonal disorder, $\langle \ln T\rangle$ behaves, within our numerical uncertainties, as $-\gamma_1\sqrt{L}$. The coefficient γ_1 as a function of the width W is also shown in the insert of Fig. 1(a). Note that γ_1 initially increases as W increases, reaches a maximum, and later saturates. This indicates that as W is increased beyond a certain value it does not introduce more disorder. Why this is so can be seen by considering the limit $W >> W_0$, where W_0 can be taken as zero. In this case W is the only energy scale in our problem and its further increase does not produce any physical effect since it can be compensated for completely by changing the unit of energy.[10] Therefore the width W of the rectangular probability distribution for V_{nm} is not a good measure of the disorder, because after some disorder $W \gtrsim W_0$ it really reproduces the same physical situation. We therefore used another probability distribution which gives more weight to small values of V_{nm} as disorder increases. A logical choice is to use a rectangular probability distribution not for the V_{nm} but for the $\ln(V_{nm})$.[11] We use

$$P(\ln V_{nm}) = \begin{cases} 1/2V_0 & \text{if } |\ln V_{nm}| \le V_0 \\ 0 & \text{otherwise} \end{cases} \quad (8)$$

With this choice, we can easily see that V_{nm} is restricted to positive values, with the small values of V_{nm} weighted by higher probability as V_0 increases. The numerical results for the $\langle \ln T \rangle$ for the probability distribution given by Eq. (8) are shown in Fig. 1(b). Note that within our numerical uncertainties $\langle \ln T \rangle = -\gamma_1 \sqrt{L}$. The coefficient γ_1 as a function of the width V_0 of the off-diagonal disorder is shown in insert of Fig. 1(b) and it follows a straight line. To a good approximation $\gamma_1 = 0.9V_0 = 1.56\sigma_{\ln V}$, where $\sigma_{\ln V}$ is the standard deviation of the $\ln V_{nm}$. This very simple relation between γ_1 and V_0 suggests that a good way of measuring the size of the off-diagonal disorder is probably the standard deviation $\sigma_{\ln V}$ of the probability distribution. For the probability distribution given by Eq. (8) we have that $\sigma_{\ln V} = V_0/\sqrt{3}$. To check if $\sigma_{\ln V}$ is a good measure of the off-diagonal disorder for the distribution given by Eq. (7) we first calculate the $\sigma_{\ln V}$ for this case. After some algebra we get that

$$\sigma_{\ln V}^2 = 1 + 0.25(1 - 1/W^2) \times \{\ln[(1+W)/(1-W)]\}^2 \ . \quad (9)$$

In Fig. 2 we plot $\sigma_{\ln V}$ given by Eq. (9) as a function of W. Note that $\sigma_{\ln V}$ follows pretty well the coefficient γ_1 of Fig. 1(a), in fact as $W \to \infty$, $\sigma_{\ln V} \to 1$. Furthermore, if we replot the coefficient γ_1 of Fig. 1(a) not a function of W but a function of $\sigma_{\ln V}$ we get the points exactly *on* the curve in the insert of Fig. 1(b) [see $\times$'s in the insert of Fig. 1(b)]. So it seems very tempting to suggest that a universal quantity of measuring the degree of the off-diagonal disorder is the standard deviation $\sigma_{\ln V}$ of the $\ln V_{nm}$, independently of the probability distribution of the random variables V_{nm}.

Results for the harmonic mean. As we mentioned above the probability distributions for T and $1/T$ are not normally distributed. In addition, due to the long tails in the probability distributions we expect large fluctuations in the average values of $\ln\langle T \rangle$ and $\ln\langle 1/T \rangle$. In fact, that was the case for the harmonic mean where $\ln\langle 1/T \rangle \simeq \gamma_2 \sqrt{L}$ for all widths V_0 of the off-diagonal disorder. The relation between γ_2 and V_0 is again linear, in particular $\gamma_2 \simeq 4V_0$ but with some larger errors due to fluctuations in the value of $1/T$. Note that the harmonic mean $\ln\langle 1/T \rangle$ also follows the $\sqrt{L}$ dependence and correctly gives that the coefficient γ_2 is almost four times larger than the geometric one, because in the harmonic case the mean value $\langle 1/T \rangle$ is dom-

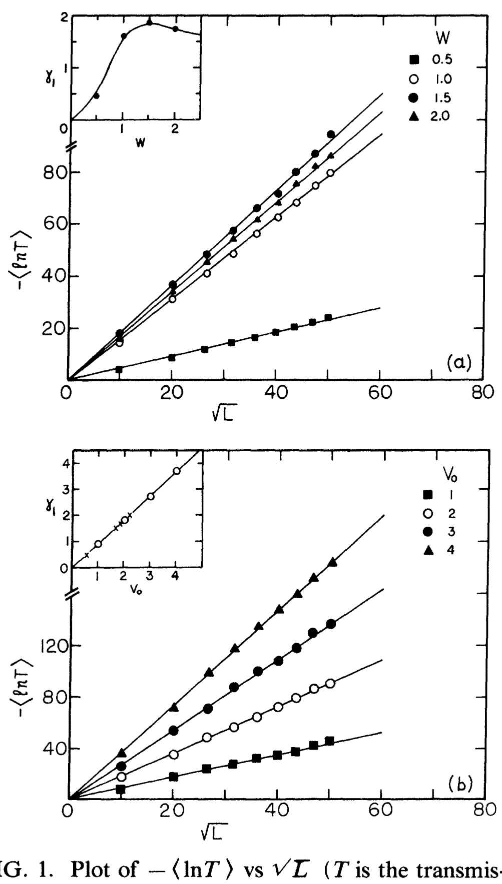

FIG. 1. Plot of $-\langle \ln T \rangle$ vs $\sqrt{L}$ (T is the transmission coefficient of the 1D disordered system of length L) for (a) a rectangular probability distribution for V_{nm} with mean $W_0 = 1$ and width $2W$ and (b) a rectangular probability distribution for $\ln V_{nm}$ with mean 0 and width $2V_0$. Results are for different values of W and V_0. The inserts plot the coefficient γ_1 as a function of W and V_0, respectively.

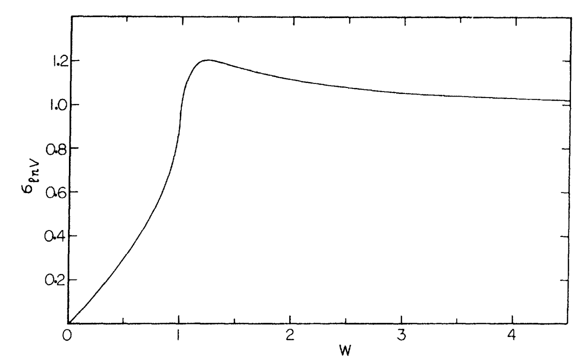

FIG. 2. Plot of the standard deviation $\sigma_{\ln V}$ of a rectangular probability distribution for V_{nm} as a function the half-width W.

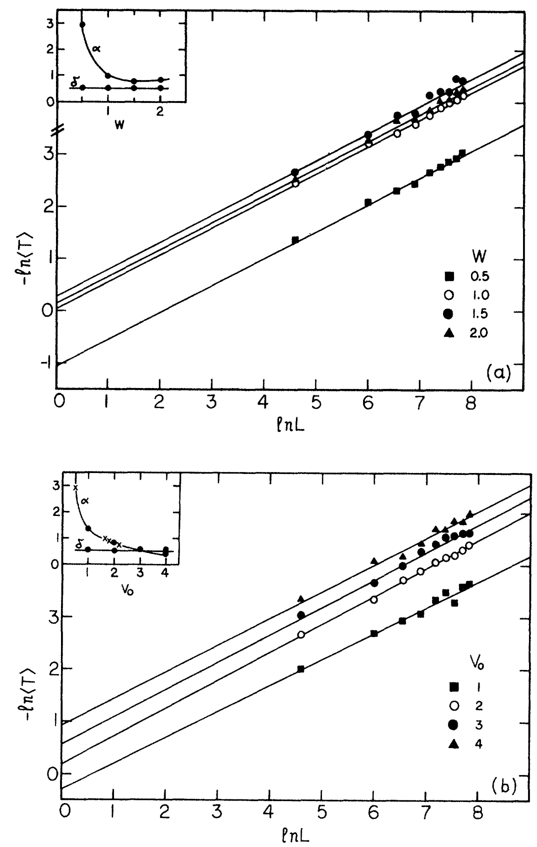

FIG. 3. Plot of $-\ln\langle T\rangle$ vs $\ln L$ for different values of off-diagonal disorder. With (a) a rectangular probability distribution for V_{nm} with mean $W_0 = 1$ and width $2W$ and (b) a rectangular probability distribution for $\ln V_{nm}$ with mean 0 and width $2V_0$. The inserts plot α and δ as functions of W and V_0, respectively. $\langle T\rangle = \alpha L^{-\delta}$.

inated by the small values of T, owing to the long tails of the distributions for T and $1/T$. We want to point out that the $\exp(-\gamma\sqrt{L})$ dependence of the harmonic and geometric mean values of T of a 1D disordered system with off-diagonal disorder is in contrast to the case of only diagonal disorder where all the three means behave as $\exp(-\lambda L)$, of course with a different coefficient λ for every case.

Results for the arithmetic mean. Our numerical results for the arithmetic mean $\langle T\rangle$ show that $\langle T\rangle$ does not follow either an $\exp(-\lambda\sqrt{L})$ dependence but a power-law behavior as a function of L. In fact we find that $\langle T\rangle \sim L^{-\delta}$ with $\delta \simeq 0.50$. In Figs. 3(a) and 3(b) we plot $-\ln\langle T\rangle$ as a function of $\ln L$ for different disorders W and V_0, respectively. Note that in spite of the fluctuations, $-\ln\langle T\rangle$ vs $\ln L$ can be approximated by a straight line. Therefore $\langle T\rangle = \alpha L^{-\delta}$. In the insert of Fig. 3(a) we plot α and δ as a function of disorder W. Note that $\delta \simeq 0.53 \pm 0.03$, while α decreases as W increases in the beginning but finally saturates. On the other hand, for the distribution given by Eq. (8) again $\delta = 0.50 \pm 0.01$ while α decreases as V_0 increases [see insert of Fig. 3(b)]. If we replot α for the distribution given by Eq. (7) not as a function of W but as a function of $\sigma_{\ln V}$, the curve of the insert of Fig. 3(a) coincides pretty well with that of the insert of Fig. 3(b) [see $\times$'s in the insert of Fig. 3(b)]. This again suggests that $\sigma_{\ln V}$ is a very good way of measuring off-diagonal disorder independently of the probability distribution of V_{nm}.

In conclusion we have investigated the localization character of the $E = 0$ eigenstate of a 1D tight-binding Hamiltonian by studying the transmission coefficient T of the system when only off-diagonal disorder is present. It is found that diagonal and off-diagonal disorder have qualitatively different behavior for the length dependence of the eigenstates. From our previous[9] analysis, for the case of only diagonal disorder all three means of the transmission coefficient behave as $\exp(-\lambda L)$ and therefore approach zero as $L \to \infty$, which of course implies localization of the eigenstates. In the off-diagonal case we find that the $E = 0$ state is again localized, in spite of the infinite localization length. In contrast to the diagonal disorder case we find that the geometric and harmonic mean values of T behave as $\exp(-\gamma\sqrt{L})$, while the arithmetic average $\langle T\rangle \sim L^{-\delta}$ with $\delta \simeq 0.50$. Finally our study for the two probability distributions of V_{nm} seems to suggest that $\sigma_{\ln V}$ is a universal quantity for measuring the strength of the off-diagonal disorder.

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