Eigenfunctions in one-dimensional disordered systems. I. Formalism*

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Within the framework of Anderson's model for disordered lattices, an integral equation for the joint probability distribution of certain quantities directly related to ReG and ImG is obtained: G is the Green's function of the system. The properties of this probability distribution are examined and physically interpreted. Finally convenient expressions for transport-related averages of the type $\langle G^* G \rangle_{av}$ are obtained. $\langle G^* G \rangle$ provides detailed information about the eigenfunctions.

I. INTRODUCTION

The problem of electron or phonon propagation in a one-dimensional (1-D) random potential has been given considerable attention recently in view of the discovery and extensive experimental study of a certain class of organic or metallo-organic materials.[1-4] These materials exhibit strongly anisotropic, quasi-one-dimensional behavior attributed to the fact that they consist of long chains, weakly interacting with each other. In many of those, the presence of random potentials has been proposed in order to explain their behavior.[5]

The 1-D character allows mathematical simplifications which in the case of random systems have permitted the derivation of many exact results.[6-9] In the problem of disordered systems we are studying an ensemble of all possible configurations of the system; to each configuration corresponds a Hamiltonian. We assume that we know the probability of each configuration or equivalently the probability distribution of the matrix elements of the Hamiltonian. Usually the results are derived in the form of statistically averaged quantities (i.e., averaged over all configurations). It is not always possible to calculate such averages directly. In some cases the averages may even diverge or may be deprived of certain very important information. It is then necessary to examine the more difficult problem of determining the full probability distribution of the physical quantity under consideration. This situation arises when one attempts to calculate quantities of the type $\langle G^*(z)G(z)\rangle_{av}$, where $\langle\ \rangle_{av}$ denotes average over all configurations, $G(z) \equiv (z - \hat{H})^{-1}$ is the Green's function of the system, and $\hat{H}$ is the (random) Hamiltonian of the system. Note that quantities of the type $\langle G^*G\rangle_{av}$ are very important physically, because (i) they behave differently depending on whether the eigenstates are localized or extended, and thus can be used to clearly distinguish these two cases, and (ii) they are directly related to transport properties. For these reasons many attempts have been made to calculate quantities like $\langle G^*G\rangle$ directly. The problem has proved considerably more difficult than the calculation of $\langle G\rangle_{av}$. The latter is directly related to the average density of states, but unlike $\langle G^*G\rangle_{av}$, cannot distinguish between extended and localized eigenstates.

In a particular case,[10] $\langle G\rangle_{av}$ can be calculated exactly and directly (without knowledge of the probability distribution of G) not only in the 1-D case but for higher dimensionality as well. In the 1-D case methods have been developed[8,11] for the calculation of the probability distribution of G but very little has been done[9,12] for the calculation of $\langle G^*G\rangle_{av}$. The latter *requires* for its calculation the knowledge of the joint probability distribution of ReG and ImG. In this paper we develop a formalism which gives this joint probability distribution as a solution of an integral equation. Results obtained by solving this integral equation numerically are presented in Paper II of this sequence.

The structure of this paper is as follows: In Sec. II the mathematical properties of the Green's functions of an n-dimensional system ($n = 1, 2, 3$) and their probability distributions are reviewed with particular emphasis on distinguishing the localized or extended character of the eigenstates. In Sec. III we discuss briefly the quantities of physical interest and in Sec. IV we develop a formalism which allows the derivation of an integral equation for the joint probability distribution of certain quantities directly related to ReG and ImG. The mathematical properties of the solution are examined and a physical interpretation is given. Finally, in Sec. V quantities of the type $\langle G^*G\rangle$ are expressed in terms of the solution of the integral equation and a recurrence relation.

II. PROPERTIES OF GREEN'S FUNCTIONS

We consider here a finite N-site system (of one, two, or three dimensions) which is described by a

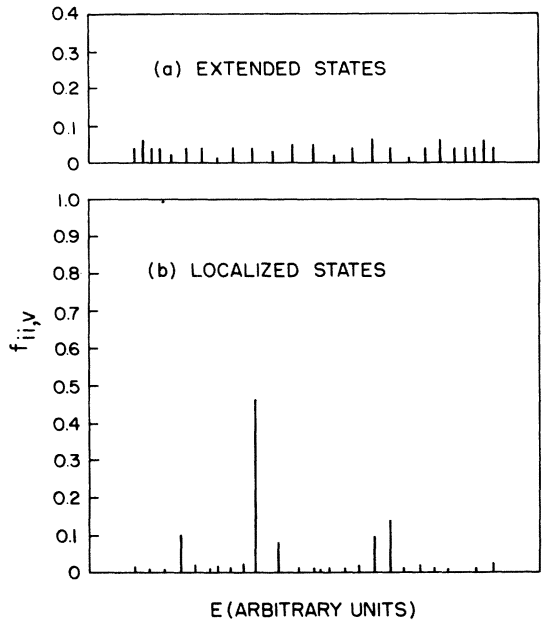

FIG. 1. Position of poles of $G_{ii}(E)$ on the energy axis E and the magnitude of their residues $f_{ii,\nu}$, are shown schematically for (a) extended states and (b) localized states.

complete set of local states $|j\rangle$, $j=1, \ldots, N$, each one associated with a certain site j of the system. In the limit $N\to\infty$ the system becomes infinite. The Hamiltonian of the system $\hat{H}$ is a random operator, i.e., its matrix elements $\langle i|\hat{H}|j\rangle$ are random variables. We examine the Green's function $\hat{G}(z)\equiv(z-\hat{H})^{-1}$ and in particular its matrix elements $G_{ij}(z)$ where

$$G_{ij}(z)\equiv\langle i|(z-\hat{H})^{-1}|j\rangle=\sum_{\nu=1}^{N}\frac{f_{ij,\nu}}{z-E_\nu}\ ; \qquad (2.1)$$

$f_{ij,\nu}=\langle i|\nu\rangle(\nu|j\rangle$ and $|\nu)$ is an eigenstate of $\hat{H}$ with eigenvalue E_ν. $G_{ij}(z)$ is analytic everywhere on the complex z plane, except at the eigenvalues of H where a simple pole behavior is exhibited. The residues at these poles are related with overlap matrix elements, as can be seen from Eq. (2.1). We are actually interested in the limiting case $N\to\infty$. Then the distribution of the poles of $G_{ij}(z)$ becomes dense over certain portions of the real axis which by definition are the energy bands (or energy spectrum) of the system. Note that in the present case the quantities $f_{ij,\nu}$ and E_ν are random variables since they are functions of the random variables $H_{ij}\equiv\langle i|\hat{H}|j\rangle$.

If the eigenstate $|\nu)$ is extended as $N\to\infty$ [i.e., $\langle i|\nu)$ is relatively appreciable for an infinite number of states $|i\rangle$ as $N\to\infty$] then, as $N\to\infty$, $f_{ij,\nu}\to a/N$, where $|a|$ is of the order of or less than 1, owing to the normalization of the eigenfunction. On the other hand, if $|\nu)$ is localized as $N\to\infty$ [i.e., $\langle i|\nu)$ is appreciable for a finite number of states $|i\rangle$ only, as $N\to\infty$] then, when $N\to\infty$, $f_{ij,\nu}\to\bar{f}_{ij,\nu}$, where $\bar{f}_{ij,\nu}$ is independent of N. However, the magnitude of the quantities $\bar{f}_{ij,\nu}$ varies widely depending on where the eigenfunction is localized. If the eigenfunction is localized far away from the states $|i\rangle$ and $|j\rangle$ and decays exponentially away from the region of localization [i.e., as $R\to\infty$, $|\nu)\to$ const. $\exp(-|R|/R_d)$], then

$$|\bar{f}_{ij,\nu}|\sim\exp[-2(|\vec{R}_i-\vec{R}_\nu|+|\vec{R}_j-\vec{R}_\nu|)/R_d]\ .$$

The maximum value of $\bar{f}_{ij,\nu}$ is obtained when $i=j$ and ν is localized in their vicinity; then $\bar{f}_{ij,\nu}$ is of the order of (but less than) 1. In Fig. 1 we schematically show the magnitude of the residues and the position of the poles for the cases of extended and localized eigenstates.

As $N\to\infty$ the energy bands of the system become lines of singularities for $G_{ij}(z)$ (which means that

$$\lim_{N\to\infty}\left(\lim_{s\to0^{\pm}}G_{ij}(z)\right)$$

does not exist, where $z=E+is$ and E belongs to the energy bands). However, due to the different behavior of $f_{ij,\nu}$ as $N\to\infty$, these lines of singularities are of different nature depending on whether we have localized or extended eigenstates. It is easy to show that these parts of the spectrum associated with extended eigenstates become branch cuts as $N\to\infty$; the limits

$$\lim_{s\to0^{\pm}}\left(\lim_{N\to\infty}G_{ij}(z)\right)$$

exist and, as a matter of fact,

$$\lim_{s\to0^{\pm}}\mathrm{Im}\left(\lim_{N\to\infty}G_{ii}(z)\right)=\mp\pi\rho_i(E)\ ,$$

where $\rho_i(E)$ is the contribution to the density of states from the site i. On the other hand, the parts of the spectrum associated with localized eigenstates become natural boundaries as $N\to\infty$, because even the limits

$$\lim_{s\to0^{\pm}}\left(\lim_{N\to\infty}G_{ij}(z)\right)$$

do not exist. This is due to the fact that the residues $f_{ij,\nu}$ remain finite as $N\to\infty$.

This basic distinction between extended and localized states is wiped out if one averages $G_{ij}(z)$ over all configurations. Then

$$\langle G_{ij}(z)\rangle_{\mathrm{av}}=\sum_{\nu=1}^{N}\left\langle\frac{f_{ij,\nu}}{z-E_\nu}\right\rangle_{\mathrm{av}}\ , \qquad (2.2)$$

where the average in $\langle f_{ij,\nu}/(z-E_\nu)\rangle$ is over the random variables $f_{ij,\nu}$ and E_ν. Assuming that the probability distribution of E_ν is a smooth function, it follows that $\langle f_{ij,\nu}/(z-E_\nu)\rangle_{\mathrm{av}}$ will exhibit branch cuts coinciding with the energy bands of the sys-

tem. Consequently $\langle G_{ij}(z)\rangle_{av}$ will show a branch cut for both extended and localized states. Taking the limit $N\to\infty$ will not change this analytic behavior of $\langle G_{ij}(z)\rangle_{av}$.

If, instead of taking the average of $G_{ij}(z)$, we consider its probability distribution, the distinction between localized and extended states is retained. We examine first the diagonal matrix element $G_{ii}(z)$. Each term $f_{ii,\nu}/(z-E_\nu)$ in Eq. (2.1) is important as $z\to E$, where E belongs to the spectrum, only if $|E-E_\nu|\lesssim f_{ii,\nu}$, i.e., if $E\in P_\nu$, where P_ν is the interval $[E_\nu-f_{ii,\nu}, E_\nu+f_{ii,\nu}]$. Then the contribution of all the terms with $\nu>\nu_0$ is important only if E belongs to the union Π_{ν_0} of P_ν with $\nu>\nu_0$.

The sum in Eq. (2.1) can always be arranged in order of decreasing $f_{ii,\nu}$. Then, for localized eigenstates, the number of regions P_ν ($\nu>\nu_0$) increases linearly with N, as $N\to\infty$, while the extent of each region decreases exponentially with N, as $N\to\infty$ (since the extent is proportional to $f_{ii,\nu}$). Thus the extent of the union Π_{ν_0} approaches zero as $\nu_0\to\infty$. Consequently the probability of E belonging to Π_{ν_0} is vanishingly small for $\nu_0\to\infty$. This simply means that the terms of high ν ($\nu>\nu_0$) make a vanishingly small contribution to the probability distribution of $G_{ii}(E)$, when E is associated with localized eigenstates.

We can conclude that the probability distribution of $G_{ii}(E)$ is dominated by the few largest terms of the right-hand side of Eq. (2.1) if E belongs to a spectrum of localized eigenstates. As a matter of fact, under certain conditions[13] the probability distribution of $G_{ii}(E)$ is equal to the probability distribution of the largest single term in Eq. (2.1). Certainly the probability distribution of the largest single term behaves in a qualitatively similar way to the probability distribution of $G_{ii}(z)$. We shall use this property to examine certain qualitative features of the probability distribution of $G_{ii}(z)$. In the case of the off-diagonal matrix elements $G_{ij}(z)$ there is a complicating factor; for large values of $|\vec{R}_i-\vec{R}_j|$ there are many $f_{ij,\nu}$ of about equal magnitude but of different signs. Thus there is a natural tendency for cancellation. This feature is demonstrated in calculations of $\langle G_{ij}(E)\rangle_{av}$ where[14] $G_{ij}(E)$ is not dominated by the largest single term in Eq. (2.1) but by the largest term $f_{ij,\nu}/(E-E_\nu)$ with E_ν lying in the *immediate vicinity* of E. It seems that only when $E\cong E_\nu$ the signs of $f_{ij,\nu}$ do not create complete cancellations of terms. Here we avoid the problem of finding the probability distribution of $G_{ij}(z)$ by expressing $G_{ij}(z)$ in terms of the diagonal matrix element $G_{ii}(z)$, as will be seen in Sec. V.

Let $f_\nu/(z-E_\nu)$ be the largest term in the right-hand side of Eq. (2.1) for $i=j$. We argue that at least the qualitative features of the probability distribution of $G_{ii}(z)$ are the same[15] as the probability distribution of $f_\nu/(z-E_\nu)$. Let $z=E+is$ and

$$X_s\equiv \mathrm{Re}\,\frac{f_\nu}{z-E_\nu}=\frac{(E-E_\nu)f_\nu}{(E-E_\nu)^2+s^2}\,, \tag{2.3a}$$

$$Y_s\equiv \mathrm{Im}\,\frac{f_\nu}{z-E_\nu}=\frac{-sf_\nu}{(E-E_\nu)^2+s^2}\,, \tag{2.3b}$$

$$Y'_s\equiv\frac{-Y_s}{s}=\frac{f_\nu}{(E-E_\nu)^2+s^2}\,. \tag{2.3c}$$

Let $P_{1s}(X_s, Y'_s)$ be the probability distribution of X_s, Y'_s and $P_2(E_\nu, f_\nu)$ the probability distribution of E_ν, f_ν. Then, using Eqs. (2.3a)–(2.3c), we obtain

$$P_{1s}(X_s, Y'_s)=\int dE_\nu\, df_\nu\, P_2(E_\nu, f_\nu)\times\delta\left(X_s-\frac{(E-E_\nu)f_\nu}{(E-E_\nu)^2+s^2}\right)\times\delta\left(Y'_s-\frac{f_\nu}{(E-E_\nu)^2+s^2}\right)\,. \tag{2.4}$$

One can easily show that $\lim_{s\to 0}P_{1s}(X_s, Y'_s)=P_1(X, Y')$ exists. After some algebraic manipulation we obtain

$$P_1(X, Y')=X^2P_2(E-X/Y', X^2/Y')/Y'^3=f_\nu P_2(E-f_\nu/X, f_\nu)/Y'^2\,, \tag{2.5}$$

where $f_\nu=X^2/Y'$ is the residue of the largest term on the right-hand side of Eq. (2.1) for $i=j$. Note that $0\le f_\nu\le 1$. By integrating $P_1(X, Y')$ over Y' or X one can obtain the probability distribution of X or Y', $P_X(X)$ or $P_{Y'}(Y')$, which for large values behave like X^{-2} and $Y'^{-3/2}$, respectively. These long tails are consequences of the simple pole in $X[X\sim(E-E_\nu)^{-1}]$ and the second-order pole in Y' $[Y'\sim(E-E_\nu)^{-2}]$. A consequence of the long tails in P_X, $P_{Y'}$ (or equivalently the poles in X and Y') is that $\langle X\rangle_{av}$ and $\langle Y'\rangle_{av}$ do not exist. Of course $\langle X_s\rangle_{av}$ and $\langle Y'_s\rangle_{av}$ exist for $s\neq 0$ (the tails in P_{X_s}, $P_{Y'_s}$ disappear for $s\neq 0$ since the poles in X_s, Y'_s disappear), but

$$\lim_{s\to 0}\langle X_s\rangle_{av}=\infty\,,\qquad \lim_{s\to 0}\langle Y'_s\rangle_{av}\to A(E)/|s|\to+\infty$$

as $s\to 0$, where $A(E)$ is a function of E. Note that

$$\lim_{s\to 0^\pm}\langle -sY'_s\rangle_{av}\equiv\lim_{s\to 0^\pm}\langle \mathrm{Im}[f_\nu/(z-E_\nu)]\rangle_{av}=\mp A(E),$$

as expected from the function $\langle f_\nu/(z-E_\nu)\rangle_{av}$ which, as was explained before, exhibits branch cuts.

Equation (2.5) is very useful because it expresses the probability distribution $P_1(X, Y')$ {which is essentially the probability distribution of $\mathrm{Re}G_{ii}(E)$ and $(-1/s)\lim_{s\to 0}[\mathrm{Im}G_{ii}(E+is)]$} in terms of $P_2(E_\nu, f_\nu)$, the probability distribution of the pole and residue of the largest term on the right-hand side of Eq. (2.1). Because $0\le f_\nu\le 1$ and E_ν be-

long to the spectrum, certain features of P_2 are known, which in turn provide information about the behavior of $P_1(X, Y')$.

III. QUANTITIES OF INTEREST

A quantity of great physical importance is the average density of states per site $\langle \rho_{ii}(E)\rangle_{\rm av}$ which is equal to

$$\mp (1/\pi)\,\mathrm{Im}\lim_{s\to 0^{\pm}}\langle G_{ii}(E+is)\rangle_{\rm av} \ .$$

The latter requires for its calculation the knowledge of the probability distribution of

$$-\lim_{s\to 0^{\pm}}[(1/s)\,\mathrm{Im}G_{ii}(E+is)] = -\frac{\partial}{\partial E}\lim_{s\to 0}\mathrm{Re}G_{ii}(E+is) \ .$$

In a 1-D case this problem has been solved by calculating the probability distribution[8] of a quantity which is directly related with either $\mathrm{Im}G_{ii}$ or $\mathrm{Re}G_{ii}$.

Here we are interested in quantities of the type

$$\langle \zeta_{ij}(E)\rangle_{\rm av} = \lim_{s\to 0}\langle (s/\pi)G_{ij}(E+is)G_{ji}(E-is)\rangle_{\rm av} \ , \tag{3.1}$$

which in contrast to $\langle G_{ij}(E+is)\rangle_{\rm av}$ are directly related to transport properties[16] and thus can clearly distinguish between localized and extended eigenstates. The calculation of $\langle \zeta_{ij}(E)\rangle_{\rm av}$ requires the knowledge of the joint probability distribution of both $\mathrm{Re}G_{ij}$ and $\mathrm{Im}G_{ij}$. Since $\mathrm{Re}G_{ij}$ and $\mathrm{Im}G_{ij}$ are not statistically independent the calculation of this joint probability distribution is a much more complicated problem than finding the probability distribution of each one separately.

Using Eq. (2.1) we can rewrite (3.1) as

$$\langle \zeta_{ij}(E)\rangle_{\rm av} = \sum_{\nu}\langle |f_{ij,\nu}|^2\delta(E-E_\nu)\rangle_{\rm av} \ . \tag{3.2}$$

By integrating Eq. (3.2) over E we obtain

$$P_{ij} \equiv \int_{-\infty}^{\infty} dE\langle \zeta_{ij}(E)\rangle_{\rm av} = \sum_{\nu}\langle |f_{ij,\nu}|^2\rangle_{\rm av} \ . \tag{3.3}$$

One can easily show[13] that $\sum_\nu\langle |f_{ij,\nu}|^2\rangle_{\rm av}$ is the (time-averaged) probability of finding a particle in the state $|j\rangle$ as $t\to\infty$, if initially ($t=0$) the particle was in the state $|i\rangle$. In particular p_{ii} gives the probability of rediscovering after an infinite time lapse a particle at the initial state $|i\rangle$. It is obvious that extended eigenstates do not contribute to p_{ij} since for them $|f_{ij,\nu}|^2 \sim 1/N^2$ as $N\to\infty$. On the other hand, localized eigenstates make a nonzero contribution to p_{ij}. Thus $\langle \zeta_{ij}(E)\rangle_{\rm av}$ does or does not vanish when the eigenstates at E are extended or localized, respectively.

Let us write $j=i+l$ and then sum Eq. (3.2) over i:

$$\sum_i \langle \zeta_{i,i+l}(E)\rangle_{\rm av} = \sum_\nu \langle \delta(E-E_\nu)\sum_i |f_{i,i+l,\nu}|^2\rangle_{\rm av} \ . \tag{3.4}$$

The quantity $\sum_i |f_{i,i+l,\nu}|^2$ depends only on E_ν; consequently we can write

$$\sum_\nu \left\langle \delta(E-E_\nu)\sum_i \left| f_{i,i+l,\nu}\right|^2\right\rangle_{\rm av}$$

$$= \int dE'\,\rho(E')\delta(E-E')\sum_i \langle |f_{i,i+l}(E')|^2\rangle_{\rm av}$$

$$= \rho(E)\sum_i \langle |f_{i,i+l}(E)|^2\rangle_{\rm av} \ , \tag{3.5}$$

where $\rho(E) = N\langle \rho_{ii}(E)\rangle_{\rm av}$ is the total density of states. Note also that $\langle \zeta_{i,i+l}(E)\rangle_{\rm av}$ depends only on l and as a result $\sum_i \langle \zeta_{i,i+l}(E)\rangle_{\rm av} = N\langle \zeta_{0l}(E)\rangle_{\rm av}$. Thus substituting in Eq. (3.4) we obtain

$$\sum_i \langle |f_{i,i+l}(E)|^2\rangle_{\rm av} = \frac{\langle \zeta_{0l}(E)\rangle_{\rm av}}{\langle \rho_{00}(E)\rangle_{\rm av}} \ . \tag{3.6}$$

In particular, for $l=0$ we obtain

$$\sum_i \langle |f_{ii}(E)|^2\rangle_{\rm av} = \frac{\langle \zeta_{00}(E)\rangle_{\rm av}}{\langle \rho_{00}(E)\rangle_{\rm av}} \ . \tag{3.7}$$

The quantity $\sum_i f_{ii}^2(E)$ is a measure of the total extent of the eigenfunction $|\nu\rangle$ with $E_\nu = E$. To see this, consider the fictitious case of an eigenfunction occupying equally L^* sites; then on these sites $f_{ii} = 1/L^*$, since $\sum_i f_{ii} = L^* f_{ii} = 1$. Hence $\sum_i f_{ii}^2 = 1/L^*$. Thus the quantity

$$L^*(E) \equiv \left(\sum_i f_{ii}^2(E)\right)^{-1} \tag{3.8}$$

provides a reasonable definition of the number of sites L^* participating in the eigenstate $|\nu\rangle$ with $E_\nu = E$, even when the eigenfunction is not uniform. In the theory of lattice vibrations[17] an essentially identical definition is used to characterize the extent of the eigenmodes. The so-called participation ratio $p(E)$ is introduced and defined as the number of sites participating in the eigenmode $|E\rangle$ divided by the total number of sites N. Thus

$$p(E) \equiv L^*(E)/N \ . \tag{3.9}$$

$L^*(E)$ is defined as in Eq. (3.8). Using Eqs. (3.7) and (3.8) we obtain

$$\left\langle \frac{1}{L^*(E)}\right\rangle_{\rm av} = \frac{\langle \zeta_{00}(E)\rangle_{\rm av}}{\langle \rho_{00}(E)\rangle_{\rm av}} \ . \tag{3.10}$$

We define the quantity $L_{\rm eff}$ by the relation

$$L_{\rm eff}(E) = \left\langle \frac{1}{L^*(E)}\right\rangle_{\rm av}^{-1} = \frac{\langle \rho_{00}(E)\rangle_{\rm av}}{\langle \zeta_{00}(E)\rangle_{\rm av}} \ . \tag{3.11}$$

$L_{\rm eff}$ is a measure of the average number of sites over which an eigenfunction (of eigenenergy E) is spread. Note that the quantity $L^*(E)$ is expected not to have so sharp a probability distribution and consequently $L_{\rm eff}(E) \neq \langle L^*(E)\rangle_{\rm av}$. In most cases we expect $L_{\rm eff}(E) < \langle L^*(E)\rangle_{\rm av}$. The quantity $L_{\rm eff}(E)$ should not be confused with the decay localization length $R_d(E)$ defined from the exponential decay of

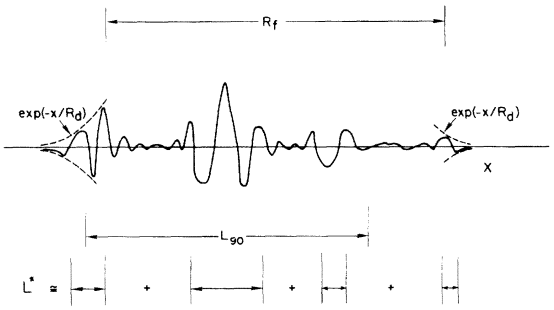

FIG. 2. In a one-dimensional disordered system every eigenfunction is exponentially localized with a decay length R_d outside a region of fluctuations of length R_f. In the eigenfunction shown above, four regions contribute mainly to the length L^*, which characterizes its total extent. The length L_{90}, within which 90% of the squared modulus of the eigenfunction lies, is also shown schematically.

the eigenfunction $|\nu)$ (with $E_\nu = E$) far away from the region where the eigenfunction is appreciable, i.e.,

$$|\langle i|\nu)|_{R_i \to \infty} \exp[-R_i/R_d(E_\nu)] . \tag{3.12}$$

The quantity $R_d(E)$ is no more difficult to calculate in 1-D systems than the average density of states. It can be calculated either from the probability distribution[8,14] of $\mathrm{Re}G_{ii}(E)$ or from numerical solutions of Schrödinger's equation in random samples.[18] Both approaches give identical results. Thus the values of $R_d(E)$ are well established. Although we are not primarily interested in $R_d(E)$ here, we calculate this quantity (as well as the average density of states) for completeness.

One can easily convince himself that

$$\sum_{i,l} |f_{i,i+l}(E)|^2 = \sum_l \frac{\zeta_{0l}(E)}{\rho_{00}(E)} = 1 . \tag{3.13}$$

The above relation allows the definition of yet another characteristic length L_p such that within L_p consecutive sites, $p\%$ of the squared modulus of the eigenfunction $|E)$ is located, i.e.,

$$\sum_i \sum_{l=-L_p/2}^{L_p/2} \langle |f_{i,i+l}(E)|^2 \rangle_{\mathrm{av}} = \sum_{l=-L_p/2}^{L_p/2} \frac{\langle \zeta_{0l}(E) \rangle_{\mathrm{av}}}{\langle \rho_{00}(E) \rangle_{\mathrm{av}}} \equiv \frac{p}{100} . \tag{3.14}$$

Since the eigenfunction $|E)$ is localized, every set of L_p consecutive sites centered around a site i will cover different percentages of an eigenstate depending on its position relative to the site i. To avoid this difficulty in the defining Eq. (3.14) we have summed the quantity

$$\sum_{l=-L_p/2}^{L_p/2} |(E|\, i+l\rangle|^2$$

over all sites i, weighting each contribution according to $|(E|\, i\rangle|^2$.

In the practical calculations we have arbitrarily chosen $p\% = 90\%$, defining thus the length L_{90}. One should clearly distinguish between L_p and L_{eff}. L_p gives the number of consecutive sites where most of the eigenstate lies; L_{eff} counts only those sites at which the eigenfunction is appreciable. If between sites where the eigenfunction is appreciable there are many sites where the eigenfunction is almost zero, then we expect that $L_{90} \gg L_{\mathrm{eff}}$.

In Fig. 2 we present schematically an eigenfunction in a 1-D disordered system; we denote explicitly the various characteristic lengths. Outside a region of fluctuation[7] of length R_f, it decays exponentially with the decay length R_d. Inside the region of fluctuation the behavior of the eigenfunction varies widely, depending on the details of this region. There is no reason to expect that in general the eigenfunction will be smooth within the region R_f. As a matter of fact, the eigenfunction may look as in Fig. 2. In this case the total extent L^* will receive contributions mainly from the four regions shown in Fig. 2. We expect that the quantities R_f, L^*, and L_{90} are not sharply distributed and that the lengths L_{90}, L^*, R_f, and R_d are not simply related. We have already discussed the question of calculating R_d, L_{90}, and $\langle 1/L^* \rangle_{\mathrm{av}}$. One can obtain what should be essentially $\langle R_f \rangle_{\mathrm{av}}$ by considering the quantity

$$\sum_i \langle |f_{i,i+l}(E)|^2 \rangle_{\mathrm{av}}$$

as a function of l for a given E. When l is considerably larger than $\langle R_f \rangle_{\mathrm{av}}$, the quantity

$$\sum_i \langle |f_{i,i+l}(E)|^2 \rangle_{\mathrm{av}}$$

should behave as e^{-2l/R_d}. The reason is that $|f_{i,i+l}(E)|^2$ is equal to the squares of the amplitudes of the eigenfunction $|\nu)$ $(E_\nu = E)$ at two sites a distance l apart. If $l \gg R_f$ both sites will essentially sample the exponential tails of the eigenfunction, thus giving the exponential decay e^{-2l/R_d}. In general the quantity

$$\sum_i \langle |f_{i,i+l}(E)|^2 \rangle_{\mathrm{av}}$$

studied as a function of l provides information about the shape of the eigenfunction.

IV. DERIVATION AND PROPERTIES OF THE INTEGRAL EQUATION

From now on we restrict ourselves to a 1-D Anderson model described by a Hamiltonian of the form

$$\langle l|\, H\, |m\rangle = \epsilon_l \delta_{lm} + V(\delta_{m,l+1} + \delta_{m,l-1}) , \tag{4.1}$$

where $|l\rangle$ is an atomiclike orbital centered around the lattice point l ($l=0, \pm1, \pm2, \ldots$), ϵ_l are independent random variables each of which has a common probability distribution $P_0(\epsilon_l)$, and V is a positive constant. The Green's function $G_{00}(z) = \langle 0|(z-H)^{-1}|0\rangle$ can be written

$$G_{00}(z) = [z - \epsilon_0 - \Delta_0(z)]^{-1} , \tag{4.2}$$

where $\Delta_0(z)$ is the so-called self-energy at site 0. Using the renormalized perturbation expansion[13] we can write[11] for $\Delta_0(z)$

$$\Delta_0(z) = t_0^+(z) + t_0^-(z) , \tag{4.3}$$

where

$$t_0^{\pm}(z) = V^2 G^0_{\pm1,\pm1}(z) . \tag{4.4}$$

The superscript zero indicates that the system has been broken at the site 0 (i.e., $\epsilon_0 = \infty$) so that $G^0_{\pm1,\pm1}(z)$ is the Green's function for a semi-infinite system starting from the site 1 (-1) and extending to the right (left) of it. $G^0_{\pm1,\pm1}$ can then be expressed in terms of $t_1^{\pm}(z)$ which in turn can be expressed in terms of $G^{\pm1}_{\pm2,\pm2}(z)$ and so on. Thus recurrence relations of the type

$$t^{\pm}_{i-1}(z) = V^2 G^{\pm i\mp1}_{\pm i,\pm i}(z) = V^2/[z - \epsilon_{\pm i} - t_i^{\pm}(z)], \tag{4.5}$$

are obtained where $i = 1, 2, \ldots$. Thus the diagonal matrix elements of $G(z)$ can be expressed in terms of the quantities $t_i^{\pm}(z)$ which are Green's functions for a semi-infinite system (starting from $\pm i \pm 1$) and satisfy the recurrence relation (4.5). It turns out that the off-diagonal matrix elements of $G(z)$ can also be expressed[13] in terms of $t_i^{\pm}(z)$ as follows:

$$G_{i+l,i}(z) = G_{ii}(z)\,\frac{1}{V^l}\prod_{j=i}^{i+l-1} t_j^+(z) , \quad l \geq 1 , \tag{4.6}$$

with a similar expression for $l \leq -1$. Since both $t_i^{\pm}(z)$ satisfy similar equations we consider the quantities $t_i^+(z)$ and we drop the superscript + except in cases where confusion may arise. Since $t_i(z)$ is a diagonal matrix element of a Green's function (apart from a V^2 factor), it has all the general properties of $G_{ii}(z)$ discussed in Sec. II. In particular,

$$t_i(E+is) = \tau_i(E) - is\theta_i(E) \tag{4.7}$$

to first order in s, where $\tau_i(E)$ is real and $\theta_i(E)$ is positive definite. The joint probability distribution of τ_i, θ_i should have the qualitative features of $P_1(X, Y')$, τ_i being analogous to X and θ_i to Y'.

Substituting (4.7) in Eqs. (4.3) and (4.2) we obtain

$$G_{00}(E+is) = \frac{E - \epsilon_0 - \tau_0^+ - \tau_0^-}{(E - \epsilon_0 - \tau_0^+ - \tau_0^-)^2 + s^2(1+\theta_0^+ + \theta_0^-)^2} - i\,\frac{s(1+\theta_0^+ + \theta_0^-)}{(E - \epsilon_0 - \tau_0^+ - \tau_0^-)^2 + s^2(1+\theta_0^+ + \theta_0^-)^2} . \tag{4.8}$$

Thus

$$\lim_{s\to0^{\pm}} \mathrm{Im} G_{00}(E+is) = \mp\pi\,\delta(E - \epsilon_0 - \tau_0^+ - \tau_0^-) \tag{4.9}$$

and

$$\begin{aligned}\zeta_{00}(E) &= \lim_{s\to0}(s/\pi)\,|G_{00}(E+is)|^2 \\ &= \lim_{s\to0}(1/\pi)s/[(E - \epsilon_0 - \tau_0^+ - \tau_0^-)^2 + s^2(1+\theta_0^+ + \theta_0^-)^2] \\ &= \delta(E - \epsilon_0 - \tau_0^+ - \tau_0^-)/(1+\theta_0^+ + \theta_0^-) .\end{aligned} \tag{4.10}$$

We see from (4.9) that the calculation of

$$\lim_{s\to0^{\pm}} \mathrm{Im}\langle G_{00}(E+is)\rangle_{\mathrm{av}}$$

requires the knowledge of the probability distribution of τ_0. The quantities τ_0^+, τ_0^- are independent statistically, since τ_0^+ depends on $\{\epsilon_i\}$ for $i \geq 1$ and τ_0^- depends on $\{\epsilon_i\}$ for $i \leq 1$, as can be seen from Eq. (4.5). Since all ϵ_i have the same probability distribution, the probability distributions of τ_0^+ and τ_0^- are identical. Equation (4.10) shows that for the calculation of $\langle\zeta_{00}(E)\rangle_{\mathrm{av}}$ we need the joint probability distribution of τ_0 and θ_0.

In the rest of this section we derive and discuss an integral equation obeyed by the joint probability distribution of τ_i, θ_i. Substituting (4.7) in (4.5) we obtain

$$\tau_i - is\theta_i = V^2[E + is - \epsilon_{i+1} - (\tau_{i+1} - is\theta_{i+1})]^{-1} , \tag{4.11}$$

or by taking real and imaginary parts,

$$\tau_i = V^2\,\frac{E - \epsilon_{i+1} - \tau_{i+1}}{(E - \epsilon_{i+1} - \tau_{i+1})^2 + s^2(1+\theta_{i+1})^2} , \tag{4.12a}$$

$$\theta_i = V^2\,\frac{1+\theta_{i+1}}{(E - \epsilon_{i+1} - \tau_{i+1})^2 + s^2(1+\theta_{i+1})^2} . \tag{4.12b}$$

Allowing $s \to 0^{\pm}$ we have

$$\tau_i = V^2(E - \epsilon_{i+1} - \tau_{i+1})^{-1} , \tag{4.13a}$$

$$\theta_i = (\tau_i/V)^2(1+\theta_{i+1}) . \tag{4.13b}$$

The last relation shows that θ_i is obeying

$$\theta_i \geq (\tau_i/V)^2 . \tag{4.14}$$

Applying standard mathematical techniques we can use (4.13a) to express the probability distribution $f(\tau_i; E)$ in terms of $P_0(\epsilon_i)$ as

$$f(\tau_i; E) = \left(\frac{V}{\tau_i}\right)^2 \int_{-\infty}^{+\infty} P_0\left(E - X - \frac{V^2}{\tau_i}\right) f(X; E)\,dX , \tag{4.15}$$

and therefore the variables τ_i obey the same integral equation as the variable t_i in Ref. 8 [Eq. (3.5)]. Applying the same mathematical techniques, one can use Eq. (4.13) to express the joint probability distribution $P(\tau_i, \theta_i; E)$ in the form

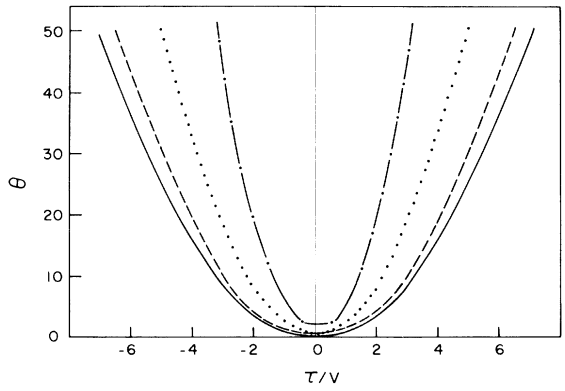

FIG. 3. The solution $P(\tau, \theta; E)$ of the integral equation (4.17) (see text) is nonzero inside the parabola $\theta = \tau^2/V^2$ (solid line) and exhibits appreciable values around a parabola $\theta = k_0\tau^2/V^2$ (dotted line) for τ not close to zero. For terminating distribution $P_0(\epsilon_i)$, $P(\tau, \theta; E)$ is nonzero between the parabolas $\theta = k_{\min}\tau^2/V^2$, $k_{\min} > 1$ (dashed line), and $\theta = k_{\max}\tau^2/V^2$ (dashed-dotted line) for τ not close to zero. For τ around zero these parabolas are deformed so that $P(0, \theta; E)$ is nonzero in a region between a minimum and a maximum value of θ.

$$P_i(\tau_i, \theta_i; E)$$
$$= \int_{-\infty}^{+\infty} \delta\left(\tau_i - \frac{V^2}{E - \epsilon_{i+1} - \tau_{i+1}}\right)\delta\left(\theta_i - \left(\frac{\tau_i}{V}\right)^2(1 + \theta_{i+1})\right)$$
$$\times \mathcal{P}(\epsilon_{i+1}, \tau_{i+1}, \theta_{i+1}; E)\, d\epsilon_{i+1}\, d\tau_{i+1}\, d\theta_{i+1} , \qquad (4.16)$$

$\mathcal{P}(\epsilon_{i+1}, \tau_{i+1}, \theta_{i+1}; E)$ represents the joint probability distribution of $\epsilon_{i+1}, \tau_{i+1}, \theta_{i+1}$. From (4.13a) and (4.13b) we observe that ϵ_i is uncorrelated to τ_i, θ_i; the same holds for $\epsilon_{i+1}, \tau_{i+1}, \theta_{i+1}$. Therefore

$$\mathcal{P}(\epsilon_{i+1}, \tau_{i+1}, \theta_{i+1}) = P_0(\epsilon_{i+1})P_{i+1}(\tau_{i+1}, \theta_{i+1}; E) .$$

Since all the sites ϵ_i have the same probability distribution we can conclude that $P_i(\tau, \theta; E) = P_{i+1}(\tau, \theta; E) = P(\tau, \theta; E)$, meaning that the functional form of $P(\tau, \theta; E)$ is independent of the site; we thus omit the indices. Performing the integrations in (4.16) we obtain the basic integral equation satisfied by $P(\tau, \theta; E)$

$$P(\tau, \theta; E) = \left(\frac{V}{\tau}\right)^4 \int_{-V[\theta(V/\tau)^2-1]^{1/2}}^{V[\theta(V/\tau)^2-1]^{1/2}} P_0\left(E - X - \frac{V^2}{\tau}\right)$$
$$\times P\left(X, \left[\theta\left(\frac{V}{\tau}\right)^2 - 1\right]; E\right) dX . \qquad (4.17)$$

The limits of integration are such as to satisfy (4.14) that requires $P(X, y; E) = 0$ for $(X/V)^2 > y$. The above equation (4.17) is consistent with the relation

$$\int_{(\tau/V)^2}^{\infty} P(\tau, \theta; E)\, d\theta = f(\tau; E) , \qquad (4.18)$$

where $f(\tau; E)$ is the solution of Eq. (4.15). We observe that relations (4.17) and (4.18) hold both for (τ^+, θ^+) and (τ^-, θ^-).

We examine now the behavior of the solutions of (4.17). For simplicity we write $P(\tau, \theta)$ for $P(\tau, \theta; E)$ leaving the energy dependence implicit in $P(\tau, \theta)$. First we observe that $P(\tau, \theta) = 0$ for $\theta < (\tau/V)^2$ since, as discussed above, (θ, τ) should obey relation (4.14). This means that the nonzero values of $P(\tau, \theta)$ (see Fig. 3) should be inside the parabola $\theta = (\tau/V)^2$. Let us then investigate the values of $P(\tau, \theta)$ along a line $\theta = k(\tau/V)^2$, where k is a certain constant larger than 1. Equation (4.17) then becomes

$$P(\tau, \theta)$$
$$= \left(\frac{V}{\tau}\right)^4 \int_{-V(k-1)^{1/2}}^{V(k-1)^{1/2}} P_0\left(E - X - \frac{V^2}{\tau}\right) P(X, k-1)\, dX . \qquad (4.19)$$

The last form is convenient for the study of $P(\tau, \theta)$ both at the limit $\tau \to 0$, $\theta \to 0$ and the limit $\tau \to \infty$, $\theta \to \infty$ along the line $\theta = k(\tau/V)^2$. For the first limit we observe that

$$P_0(E - X - V^2/\tau) \to P_0(V^2/\tau) \quad \text{as } \tau \to 0 \qquad (4.20)$$

because $|x| < V(k-1)^{1/2}$ from the limits of integration in (4.19). Then from (4.19) we obtain

$$P(\tau, \theta) \to \left(\frac{V}{\tau}\right)^4 P_0\left(-\frac{V^2}{\tau}\right) \int_{-V(k-1)^{1/2}}^{V(k-1)^{1/2}} P(x, k-1)\, dx \qquad (4.21)$$

as $\tau \to 0$. The τ dependence of the last form is $\tau^{-4}P_0(-V^2/\tau)$. Assuming $P_0(\epsilon) \to |\epsilon|^{-a}$ as $\epsilon \to \infty$, we see that

$$P(\tau, \theta) \sim |\tau|^{a-4} \to 0 \quad \text{as } \tau \to 0, \quad \text{for } a > 4 , \qquad (4.22)$$

and since (4.22) holds along the line $\theta = k(\tau/V)^2$, $\tau \to 0$ means $\theta \to 0$ and thus, assuming continuity of $P(\tau, \theta)$ around $(0, 0)$, we get the result

$$P(0, 0) = 0 \qquad (4.23)$$

for probability distributions $P_0(\epsilon)$ that fall off at infinity faster than $|\epsilon|^{-4}$. This is a very wide class of distributions $P_0(\epsilon)$ including the Gaussian and all terminated distributions [i.e., $P_0(\epsilon) = 0$ for $|\epsilon| > |\epsilon_0|$]. We will restrict our analysis to the latter class of distributions because among the well-known distributions only the Lorentzian $P_0(\epsilon) = (1/\pi)[\Gamma/(\epsilon^2 + \Gamma^2)]$ produces a $P(\tau, \theta)$ that diverges at $(\tau = 0, \theta = 0)$. For the limit $\tau \to \infty$ we observe that

$$P_0\left(E - x - \frac{V^2}{\tau}\right) \to P_0(E - x) \quad \text{as } \tau \to \infty \qquad (4.24)$$

and (4.19) becomes

$$P(\tau, \theta) \to \tau^{-4}V^4 \int_{-V(k-1)^{1/2}}^{V(k-1)^{1/2}} P_0(E - x)P(x, k-1)\, dx$$

as $\tau \to \infty$, or for constant k

$$P(\tau, \theta) \to V^4\sigma(E, k)\tau^{-4} = k^2\sigma(E, k)\theta^{-2} , \qquad (4.25)$$

as $\tau \to \infty$, where $\sigma(E, k)$ is a function of E and k. We can also take the limit $k \to 1$ in (4.19) to show that [since $P(0,0)=0$]

$$P(\tau, \theta) \to 0 \quad \text{as } V^2\theta \to \tau^2 , \tag{4.26}$$

which is expected since the line $\theta = (\tau/V)^2$ defines the region of nonzero values of $P(\tau, \theta)$. Finally, we investigate the limiting behavior of

$$f(\tau; E) = \int_{(\tau/V)^2}^{\infty} P(\tau, \theta; E)\, d\theta \tag{4.27}$$

and

$$P(\theta; E) = \int_{-V\theta^{1/2}}^{V\theta^{1/2}} P(\tau, \theta; E)\, d\tau \tag{4.28}$$

for $\tau \to \infty$ and $\theta \to \infty$, respectively. Using Eqs. (4.15) and (4.20) we see that

$$f(\tau; E) \to \tau^{-2} S(E) \quad \text{as } \tau \to \infty , \tag{4.29}$$

where $S(E)$ is a function of E. For $P(\theta; E)$ we use (4.17) to express (4.28) in the form

$$P(\theta; E) = \int_{-V\theta^{1/2}}^{V\theta^{1/2}} d\tau \left(\frac{V}{\tau}\right)^4 \int_{-V[\theta(V/\tau)^2-1]^{1/2}}^{V[\theta(V/\tau)^2-1]^{1/2}} P_0\left(E - x - \frac{V^2}{\tau}\right) \times P\left(x, \theta\left(\frac{V}{\tau}\right)^2 - 1\right) dx .$$

In the limit $\theta \to \infty$ we can ignore the unit in front of $\theta(V/\tau)^2$ to simplify the form

$$P(\theta; E) \to \int_{-V\theta^{1/2}}^{V\theta^{1/2}} d\tau \left(\frac{V}{\tau}\right)^2 \int_{-V^2\theta^{1/2}/|\tau|}^{V^2\theta^{1/2}/|\tau|} P_0\left(E - x - \frac{V^2}{\tau}\right) \times P\left(x, \theta\left(\frac{V}{\tau}\right)^2\right) dx \tag{4.30}$$

as $\theta \to \infty$. Then changing variables $k = V\theta^{1/2}/\tau$ we have

$$P(\theta; E) \to \theta^{-3/2} V \int_1^{\infty} k^2\, dk \int_{-V|k|}^{V|k|} \left[P_0\left(E - x - \frac{Vk}{\theta}\right) + P_0\left(E - x + \frac{Vk}{\theta}\right)\right] P(x, k^2)\, dx \tag{4.31}$$

as $\theta \to \infty$. The double integral goes to a θ-independent limit as $\theta \to \infty$. We can see this by carrying the integration over k up to a very large number M; then $Vk/\theta^{1/2} \to 0$ as $\theta \to \infty$ and therefore is independent of θ. As for the remaining part of the integral (from M to ∞) one can easily show that it is of order $1/M$ and is negligible comparing to the first part of the integral.

Therefore we obtain

$$P(\theta; E) \to \theta^{-3/2} C(E) \quad \text{as } \theta \to \infty , \tag{4.32}$$

where $C(E)$ is a function of E.

It is worthwhile to compare the above conclusions based on examination of the integral equation for $P(\tau, \theta)$ to those reached about the behavior of $P_1(X, Y')$, remembering that $X \to \tau/V^2$, $Y' \to \theta/V^2$, $P_1 \to V^4 P$, and $f_\nu \to \tau^2/V^2\theta \equiv 1/k$. First, by glancing at Eqs. (2.5) and (4.19) we see, since $\theta/k = (\tau/V)^2$, the following correspondence:

$$P_2(E - f_\nu/X, f_\nu) \to k^3 \int_{-V(k-1)^{1/2}}^{V(k-1)^{1/2}} P_0\left(E - x - \frac{1}{\tau}\right) \times P(x, k-1)\, dx . \tag{4.33}$$

The behavior of $P(\tau, \theta)$ as $\tau, \theta \to \infty$, or $\tau, \theta \to 0$, with $k = \text{const}$, can be deduced directly from Eq. (2.5) for $f_\nu = \text{const}$. The asymptotic expressions for the probability distribution of either τ or θ are in agreement with those obtained for X and Y', respectively, by using Eq. (2.5). Since $0 \le f_\nu \le 1$, $P_2(E_i, f_\nu)$ is equal to zero for f_ν outside the interval $[0, 1]$. The behavior of $P_2(E_i, f_\nu)$ near the boundary $f_\nu \to 1$ is controlled by the behavior of $P_0(\epsilon_i)$ as $\epsilon_i \to \infty$. This follows from (4.33) and the fact that $P(X, \theta)$ for $X, \theta \to 0$ depends on the behavior $P_0(\epsilon_i)$ as $\epsilon_i \to \infty$. Thus we expect for a terminating $P_0(\epsilon_i)$ that $f_\nu \le f_{\max} < 1$. The behavior of $P_2(E_i, f_\nu)$ as $f_\nu \to 0^+$ is probably controlled again by the behavior of $P_0(\epsilon_i)$ as $\epsilon_i \to \infty$. The reason is that f_ν, being the residue of the Green's function $G_{ii}^{i-1}(z)$, equals the overlap of an appropriate eigenstate $|\nu)$ with the site i. This overlap can approach zero only if $\epsilon_i \to \infty$, because the product $\epsilon_i f_\nu$ cannot become zero. The reason for the last statement is that all the eigenfunctions contributing to $G_{ii}^{i-1}(z)$ have zero overlap with the site $i-1$ (since by definition $\epsilon_{i-1} = \infty$) and thus if $\epsilon_i f_\nu$ were zero the eigenfunctions being solutions of Schrödinger's equation would be zero everywhere. According to the previous argument one expects, for a terminating probability distribution, that $0 < f_{\min} \le f_\nu$. Hence for a terminating distribution $P_0(\epsilon_i)$, $0 < f_{\min} \le f_\nu \le f_{\max} < 1$ or, equivalently, $1 < k_{\min} = 1/f_{\max} \le k \le k_{\max} = 1/f_{\min} < \infty$. This double inequality implies that the function $P(\tau, \theta)$ is nonzero essentially[19] between the parabolas $\theta = k_{\max}\tau^2/V^2$ and $\theta = k_{\min}\tau^2/V^2$ and exhibits appreciable values around a parabola $\theta = k_0\tau^2/V^2$ for $\theta > 0$, where k_0^{-1} is the most probable value of f_ν. These boundaries are modified around $\tau = \theta = 0$ where there is an additional region inside of which $P(\tau, \theta)$ is zero. This modification comes from the factor V^2/τ inside P_0 in Eq. (4.19). The behavior described above is shown in Fig. 3. For a nonterminating $P_0(\epsilon_i)$ but without long tails, $P(\tau, \theta)$ will still be appreciable inside the two parabolas shown in dashed lines in Fig. 3, with a local maximum around the parabola $\theta = k_0\tau^2/V^2$. $P(\tau, \theta)$ will fall quickly as one moves away from the region just described. It should be noted that the numerical solution of the integral equation is in agreement with the qualitative behavior deduced from the integral equation (4.17) and the general discussion in Sec. II.

V. CALCULATIONS OF THE QUANTITIES $\langle \zeta_{0l}(E)\rangle_{\rm av}$

As we have discussed before, the quantities of interest here are $\langle \zeta_{0l}(E)\rangle_{\rm av} = \langle \zeta_{l0}(E)\rangle_{\rm av}$ where

$$\zeta_{0l}(E) = \lim_{s\to 0}(s/\pi) G_{0l}(E+is) G_{l0}(E-is) \ . \qquad (5.1)$$

Using the property $G_{0l}(E+is) = [G_{l0}(E-is)]^*$ [which follows from Eq. (2.1)] and Eq. (4.6) for $i=0$, we obtain

$$\zeta_{0l}(E) = \lim_{s\to 0}(s/\pi)\left|G_{00}(E+is)\right|^2 \times \frac{1}{V^{2l}} \prod_{j=0}^{l-1} t_j^+(E+is) t_j^+(E-is) \ . \qquad (5.2)$$

From Eqs. (4.7) and (4.10) it follows that

$$\zeta_{0l}(E) = \frac{\delta(E-\epsilon_0-\tau_0^+-\tau_0^-)}{1+\theta_0^+ +\theta_0^-}\left(\frac{\tau_0^+}{V}\right)^2 \cdots \left(\frac{\tau_{l-1}^+}{V}\right)^2, \qquad l=1,2,\ldots . \qquad (5.3)$$

We have already derived that

$$\zeta_{00}(E) = \delta(E-\epsilon_0-\tau_0^+-\tau_0^-)/(1+\theta_0^+ +\theta_0^-) \ . \qquad (5.4)$$

Equations (5.3) and (5.4) express the general quantity $\zeta_{0l}(E)$ ($l=0,1,\ldots$) in terms of the quantities $\tau_0^{\pm}$, $\theta_0^{\pm}$, τ_i^+ which have been examined in previous sections. We are interested, of course, in the average of $\zeta_{0l}(E)$, i.e., $\langle \zeta_{0l}(E)\rangle_{\rm av}$. For this purpose we need the joint probability distribution of the quantities $\tau_0^{\pm}$, $\theta_0^{\pm}$, ϵ_0, τ_i^+ ($i=1,\ldots l-1$). By repeated application of the basic iteration relation (4.5), one can easily convince oneself that the quantity $t_i^+(z)$ (and hence the pair τ_i^+, θ_i^+) depends only on the random variables ϵ_{i+j}, $j=1,2,\ldots$, to the right-hand side of the site i; similarly $t_i^-(z)$ (and consequently the pair τ_i^-, θ_i^-) depends only on ϵ_{-i-j}, $j=1,2,\ldots$, i.e., the random variables to the left-hand side of the site $-i$. Thus the total number of random variables entering in Eq. (5.3) can be separated into the following groups, each group being statistically independent from the rest: ϵ_0; θ_0^-, τ_0^-; θ_0^+, τ_i^+, $i=0,1,\ldots$. We can then write

$$\langle \zeta_{00}(E)\rangle_{\rm av} = \int_{-\infty}^{\infty} \frac{\delta(E-\epsilon_0-\tau_0^+-\tau_0^-)}{1+\theta_0^+ +\theta_0^-} \times P_0(\epsilon_0) P(\tau_0^+,\theta_0^+) P(\tau_0^-,\theta_0^-)\, d\epsilon_0\, d\tau_0^+ d\theta_0^+ d\tau_0^- d\theta_0^- \ . \qquad (5.5)$$

In order to express the joint probability distribution of τ_0^+, τ_1^+, $\ldots$, τ_{l-1}^+, θ_0^+ in terms of known functions we introduce the function $\tilde{P}_l(\tau_0^+,\theta_0^+;\ \tau_1^+,\theta_1^+;\ldots;\ \tau_{l-1}^+,\theta_{l-1}^+)$, which is the joint probability distribution of the variables τ_i^+, θ_i^+, $i=0,1,\ldots,l-1$. Then we can write

$$\langle \zeta_{0l}(E)\rangle_{\rm av} = \int_{-\infty}^{\infty} \frac{\delta(E-\epsilon_0-\tau_0^+-\tau_0^-)}{1+\theta_0^+ +\theta_0^-}\left(\frac{\tau_0^+}{V}\right)^2 \cdots \left(\frac{\tau_{l-1}^+}{V}\right)^2 \times P_0(\epsilon_0) P(\tau_0^-,\theta_0^-) \tilde{P}_l(\tau_0^+,\theta_0^+;\cdots;\tau_{l-1}^+,\theta_{l-1}^+) \times d\epsilon_0\, d\tau_0^- d\theta_0^- d\tau_0^+ d\theta_0^+ \cdots d\tau_{l-1}^+ d\theta_{l-1}^+ , \qquad l=1,2\ldots . \qquad (5.6)$$

The function $\tilde{P}_l$ can be expressed in terms of known functions. For this purpose we first show that

$$\mathcal{P}_c(\tau_i^+,\theta_i^+/\tau_{i+1}^+,\theta_{i+1}^+,\tau_{i+2}^+,\theta_{i+2}^+,\cdots) = \mathcal{P}_c(\tau_i^+,\theta_i^+/\tau_{i+1}^+,\theta_{i+1}^+) \ , \qquad (5.7)$$

where the symbol $\mathcal{P}_c(\{x_j\}/\{y_i\})$ denotes the probabilty distribution of the quantities $\{x_j\}$ under the condition that the variables $\{y_i\}$ are kept constant. Using Eqs. (4.13a) and (4.13b) we can write

$$\mathcal{P}_c(\tau_i^+,\theta_i^+/\tau_{i+1}^+,\theta_{i+1}^+,\tau_{i+2}^+,\theta_{i+2}^+,\cdots) = \int \delta\left(\tau_i^+ - \frac{V^2}{E-\epsilon_{i+1}-\tau_{i+1}}\right)\delta\left(\theta_i^+ - \left(\frac{\tau_i^+}{V}\right)^2(1+\theta_{i+1}^+)\right) \times \mathcal{P}_c(\epsilon_{i+1}/\tau_{i+1}^+,\theta_{i+1}^+,\cdots)\, d\epsilon_{i+1} \ . \qquad (5.7a)$$

We have already shown that the quantities τ_{i+1}^+, θ_{i+1}^+, ... depend only on ϵ_{i+2}, ϵ_{i+3}, ... Consequently, since the variables ϵ_j have been assumed independent, we have

$$\mathcal{P}_c(\epsilon_{i+1}/\tau_{i+1}^+,\theta_{i+1}^+,\cdots) \equiv P_0(\epsilon_{i+1}) \ . \qquad (5.8)$$

Combining Eqs. (5.7), (5.7a), and (5.8) we obtain

$$\mathcal{P}_c(\tau_i^+,\theta_i^+/\tau_{i+1}^+,\theta_{i+1}^+) = \delta\left(\theta_i^+ - \left(\frac{\tau_i^+}{V}\right)^2(1+\theta_{i+1}^+)\right)\left(\frac{V}{\tau_i^+}\right)^2 \times P_0\left(E-\tau_{i+1}^+ - \frac{V^2}{\tau_i^+}\right) . \qquad (5.9)$$

The joint probability distribution $\tilde{P}_l$ can now be expressed as

$$\tilde{P}_l(\tau_0^+,\theta_0^+,\tau_1^+,\theta_1^+,\cdots,\tau_{l-1}^+,\theta_{l-1}^+) = P(\tau_{l-1}^+,\theta_{l-1}^+) \times \mathcal{P}_c(\tau_{l-2}^+,\theta_{l-2}^+/\tau_{l-1}^+,\theta_{l-1}^+)\cdots\mathcal{P}_c(\tau_0^+,\theta_0^+/\tau_1^+,\theta_1^+) \ , \qquad (5.10)$$

with each $\mathcal{P}_c(\tau_i^+,\theta_i^+/\tau_{i+1}^+,\theta_{i+1}^+)$ given by (5.9). In obtaining (5.10) we have used Eq. (5.7). Substituting Eq. (5.10) in (5.6) we obtain

$$\langle \zeta_{0l}(E)\rangle = \int \frac{\delta(E-\epsilon_0-\tau_0^+-\tau_0^-)}{1+\theta_0^+ +\theta_0^-}\left(\frac{\tau_0^+}{V}\right)^2 \cdots \left(\frac{\tau_{l-1}^+}{V}\right)^2 P_0(\epsilon_0) P(\tau_0^-,\theta_0^-)\mathcal{P}_c(\tau_0^+,\theta_0^+/\tau_1^+,\theta_1^+) \cdots \mathcal{P}_c(\tau_{l-2}^+,\theta_{l-2}^+/\tau_{l-1}^+,\theta_{l-1}^+) P(\tau_{l-1}^+,\theta_{l-1}^+)\, d\epsilon_0\, d\tau_0^- d\theta_0^- d\tau_0^+ d\theta_0^+ \cdots d\tau_{l-1}^+ d\theta_{l-1}^+, \qquad l \geq 1 \ , \qquad (5.11)$$

where always $\mathcal{P}_c$ is given by (5.9). We observe that a simple algorithm permits the calculation of successive $\langle \zeta_{0l}(E)\rangle_{\rm av}$. One can easily verify that (5.11) is equivalent to the following set of relations for $l \geqq 1$;

$$Z_1(\tau, \theta; E) = \int \frac{\delta(E - \epsilon_0 - \tau_0^- - \tau)}{1 + \theta_0^- + \theta} \times P_0(\epsilon_0) P(\tau_0^-, \theta_0^-)\, d\epsilon_0\, d\tau_0^-\, d\theta_0^- , \quad (5.12)$$

$$Z_l(\tau, \theta; E) = \int Z_{l-1}\left(x, \left(\frac{x}{V}\right)^2 (1+\theta); E\right) \times P_0\left(E - \tau - \frac{V^2}{x}\right) dx , \quad (5.13)$$

$$\langle \zeta_{0l}(E)\rangle_{\rm av} = \int Z_l(\tau, \theta; E) \left(\frac{\tau}{V}\right)^2 P(\tau, \theta)\, d\tau\, d\theta . \quad (5.14)$$

Equations (5.5) and (5.12)–(5.14) show that the only functions required for the evaluation of the $\langle \zeta_{0l}(E)\rangle_{\rm av}$ are $P_0(\epsilon)$, the probability distribution of the independent random-site energies that define the degree and type of randomness in the disordered (1-D) system under consideration, and $P(\tau, \theta)$, which is the solution of the integral equation (4.17) discussed in Sec. IV.

In Paper II the integral equation (4.17) will be solved numerically and several quantities of physical importance will be obtained and discussed.

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[15]Note that

$$\lim_{s\to 0} \mathrm{Re}\, G_{ii}(E + is)$$

passes through zero between any two successive poles while

$$-\lim_{s\to 0^{\pm}} \mathrm{Im} G_{ii}(E + is)/s$$

remains positive there. This means that the joint probability distribution of $\mathrm{Re}G_{ii}(E)$ and

$$-\lim_{s\to 0^{\pm}} \mathrm{Im} G_{ii}(E + is)/s$$

is nonzero for $\mathrm{Re}G_{ii}(E)$ around zero and values of

$$-\lim_{s\to 0^{\pm}} \mathrm{Im} G_{ii}(E + is)/s$$

around a positive number depending on the probability distribution of ϵ_n. It is clear that such a behavior *cannot* be described by a single-pole approximation which allows only $\mathrm{Re}G_{ii}(E)$ and

$$-\lim_{s\to 0^{\pm}} \mathrm{Im} G_{ii}(E + is)/s$$

to go together to zero as $E \to \infty$. At least two poles are needed to qualitatively describe this aspect of the behavior of G_{ii}.

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[19]$P(\tau, \theta)$ is also nonzero for $\tau \cong 0$ and $\theta > 0$ and inside some finite range. These nonzero values appear because τ becomes zero between its poles, while θ remains finite at these points. Such a behavior cannot be described by a single-pole approximation as was pointed out before.