Degree of Localization for the Eigenstates in One-Dimensional Random Systems

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(Received December 13, 1971; revised manuscript received May 14, 1973)

By solving integral equations, approximate stationary probability densities of some random variables associated with two kinds of random processes are obtained. The degrees of localization $L(E)$ and $L(\omega)$ are calculated therefrom analytically over almost whole range of energy or frequency for several models of the one-dimensional random system. It is found that $L(E)$ and $L(\omega)$ are always positive as was proved most generally by Matsuda and Ishii and that they are proportional to the variance of the random variables characterizing the random system.

§ 1. Introduction

Upon the basis of Anderson's conclusion concerning the absence of diffusion in certain random lattices, Mott, Twose and Mott conjectured that all the eigenstates for an electron in an infinitely long disordered chain are localized entirely, while those in the three-dimensional random system are localized only for energies in the neighborhood of the band edge. Furthermore Mott argued that the d.c. conductivity should vanish at $0^\circ$K if all the eigenstates are localized in space. Borland defined a quantity named the degree of localization $L(E)$ for one-dimensional disordered systems. If $L(E)$ is positive, the amplitude of a real solution of the Schrödinger equation increases on an average with the distance from one end where the boundary conditions are imposed. Borland supposed that two solutions, each of which satisfies the boundary condition imposed at one of the ends match smoothly when $E$ corresponds to an eigenenergy or eigenfrequency and therefore all the eigenstates are localized spatially if $L(E)$ is positive. Using Furstenberg's work on the asymptotic behavior of the products of the random matrices, Matsuda and Ishii showed that $L$ is always positive, so that the localized solution in the infinite system would have tails with a decay constant $L$. In a previous paper, we calculated the degree of localization $L$ exactly and analytically for a certain disordered electronic system. It turned out that $L$ is always positive except for the energies corresponding to the band edges of the periodical system where $L = 0$.

In this paper we calculate $L(E)$ or $L(\omega)$ approximately for more general cases of the distribution of the random variable. In § 2, approximate solutions of the integral equations associated with two typical random processes are obtained.
In § 3, the degrees of localization are calculated for some models, upon the basis of these solutions. These models are (A) two kinds of random Kronig-Penney model, one of which consists of equi-distant δ-function potentials with random intensities and the other consists of δ-function potentials with random spacings, (B) the one-dimensional Anderson model and (C) the isotopically disordered harmonic chain.

§ 2. Solutions of functional equations

Consider the random processes which are described by the following equations:

1) \[ y_{n+1} = \alpha_n - \frac{1}{y_n}, \quad (2·1) \]

2) \[ \tan \varphi_{n+1} = -v + \tan (\varphi_n + \lambda_n), \quad (2·2) \]

where \( y_n(\varphi_n) \) and \( y_{n+1}(\varphi_{n+1}) \) are the random variables defined respectively for the \( n \)-th and \( (n+1) \)-th lattice sites; the \( \alpha_n 's(\lambda_n 's) \) are the independent random variables, each of which generates \( y_{n+1}(\varphi_{n+1}) \) from \( y_n(\varphi_n) \), and \( v \) is a constant. If \( Z_n = \tan \varphi_n \) and \( \beta_n = \tan \lambda_n \) are used, (2·2) can be written as

\[ Z_{n+1} = -v + \frac{Z_n + \beta_n}{1 - \beta_n Z_n}. \quad (2·3) \]

In a previous paper, we obtained the exact stationary probability density of \( y_n \)'s for the random process of type 1) for the case in which each \( \alpha_n \) is an independent random variable with the Lorentz distribution. The degree of localization \( L(E) \) was then calculated analytically over the whole range of energy. In this paper we shall study more general cases and find approximate stationary probability densities for the above two random processes, to the lowest order of the deviation of \( \alpha_n 's(\lambda_n 's) \) from their average values.

First consider the random process of type 1). From (2·1), it follows that the stationary probability density \( w(y) \) of the variable \( y \) satisfies an integral equation

\[ w(y) = \int w\left( \frac{1}{\alpha - y} \right) \frac{f(\alpha)}{(\alpha - y)^2} d\alpha, \quad (2·4) \]

where \( f(\alpha) \) is the probability density of \( \alpha \). Here let us assume that \( f(\alpha) \) has a sharp maximum at the mean value \( \alpha_0 \) and expand \( w\left( \frac{1}{\alpha - y} \right)/ (\alpha - y)^2 \) around \( 1/\alpha_0 - y \). Then the integral equation (2·4) can be transformed into a kind of functional differential equation

\[ w(y) = w\left( \frac{1}{\alpha_0 - y} \right) \left( \frac{1}{\alpha_0 - y} \right)^3 + \frac{\sigma^2}{2} \frac{d^2}{dy^2} \left\{ w\left( \frac{1}{\alpha_0 - y} \right) \left( \frac{1}{(\alpha_0 - y)^3} \right) \right\}, \quad (2·5) \]
where the terms including the higher order moments of $\alpha - \alpha_0$ than the second have been neglected and $\sigma^2$ is the variance $(\alpha - \alpha_0)^2$ of the random variable $\alpha$. Now we seek a solution of (2·5), under the conditions that
\[
\int_{-\infty}^{\infty} w(y) dy = 1, \quad w(y) \geq 0. \tag{2.6}
\]
When $\sigma^2 \ll \alpha_0^2$, we assume the solution in the following form:
\[
w(y) = w_0(y) + \frac{\sigma^2}{2} w_1(y), \tag{2.7}
\]
where $w_0(y)$ is the solution of (2·5) with $\sigma^2 = 0$:
\[
w_0(y) = \frac{\sqrt{1 - \alpha_0^2/4}}{\pi} \frac{1}{y^2 - \alpha_0 y + 1}. \tag{2.8}
\]
$w_1(y)$ may be written as
\[
w_1(y) = \frac{ay^3 + by^2 + cy + d}{(y^2 - \alpha_0 y + 1)^3}. \tag{2.9}
\]
Inserting (2·8), (2·9) into (2·5) and equating the terms proportional to $\sigma^2$, we obtain
\[
a = -c = 2\sqrt{1 - \alpha_0^2/4} \pi \alpha_0, \quad b = d = 0. \tag{2.10}
\]
Note that the solution is valid only for $1 - (\alpha_0^2/4) > 0$.

Next consider the random process of type 2) governed by (2·2). It follows that the stationary probability density $P(\varphi)$ of $\varphi$ satisfies
\[
P(\varphi) = \int P(-\lambda + \tan^{-1}(v + \tan \varphi)) \frac{\sec^2 \varphi}{1 + (v + \tan \varphi)^2} g(\lambda) d\lambda, \tag{2.11}
\]
where $g(\lambda)$ is the probability density function of the random variable $\lambda$ with the mean value $\lambda_0$. Expanding $P(-\lambda + \tan^{-1}(v + \tan \varphi))$ around $-\lambda_0 + \tan^{-1}(v + \tan \varphi)$ in the same way as for the random process of type 1), we obtain
\[
P(\varphi) = P(-\lambda_0 + \tan^{-1}(v + \tan \varphi)) \frac{\sec^2 \varphi}{1 + (v + \tan \varphi)^2}
+ \frac{\sigma^2}{2} \frac{d^2 P(-\lambda_0 + \tan^{-1}(v + \tan \varphi))}{d(-\lambda_0 + \tan^{-1}(v + \tan \varphi)^2} \tag{2.12}
\]
where all the terms including the higher order moments of $\lambda - \lambda_0$ than the second have been neglected. $\sigma^2$ is the variance $(\lambda - \lambda_0)^2$ of the random variable $\lambda$. We seek a solution of the functional differential equation (2·12) under the conditions
\[
\int_{-(\pi/2)}^{\pi/2} P(\varphi) d\varphi = 1, \quad P(\varphi) > 0. \tag{2.13}
\]
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Let the probability density of $Z = \tan \varphi$ be $R(Z)$. Then the equation (2·12) can be rewritten as

\begin{equation}
R(Z) = R\left(\frac{Z + v - \beta_0}{1 + \beta_0(Z + v)}\right) \frac{1 + \beta_0^2}{(1 + \beta_0(Z + v))^2} + \frac{\varepsilon^2}{2} \frac{d}{dZ} \left[ (1 + (Z + v)^2) \frac{d}{dZ} \left\{ R\left(\frac{Z + v - \beta_0}{1 + \beta_0(Z + v)}\right) \left(1 + \beta_0^2 \right) (1 + (Z + v)^2) \right\} \right],
\end{equation}

(2·14)

where $\beta_0 = \tan \lambda_0$. When $\varepsilon^2 \ll \lambda_0^2$, we can obtain the solution in the form

\begin{equation}
R(Z) = R_0(Z) + \frac{\varepsilon^2}{2} R_1(Z),
\end{equation}

(2·15)

where $R_0(Z)$ is a solution of (2·14) with $\varepsilon^2 = 0$, which is given by

\begin{equation}
R_0(Z) = \frac{\sqrt{1 - (v/\beta_0)^2 - (v^2/4)}}{\pi} \frac{1}{Z^2 + vZ + 1 - (v/\beta_0)^2}.
\end{equation}

(2·16)

$R_1(Z)$ may be written as

\begin{equation}
R_1(Z) = \frac{\sqrt{1 - (v/\beta_0)^2 - (v^2/4)}}{\pi} \frac{eZ^4 + fZ^3 + gZ^2 + hZ + i}{(Z^2 + vZ + 1 - (v/\beta_0)^2)^3}.
\end{equation}

(2·17)

This function contains five undetermined coefficients in the numerator. Substituting (2·15) into (2·14) and equating the terms proportional to $\varepsilon^2$, we get

\begin{equation}
R_1(Z) = R_1\left(\frac{Z + v - \beta_0}{1 + \beta_0(Z + v)}\right) \frac{1 + \beta_0^2}{(1 + \beta_0(Z + v))^2} + \frac{d}{dZ} \left[ (1 + (Z + v)^2) \frac{d}{dZ} \{R_0(Z) \left(1 + (Z + v)^2\right)\} \right].
\end{equation}

(2·18)

If we rearrange (2·18) by substituting (2·16) and (2·17), we can completely determine five parameters $e, f, g, h$ and $i$. However, for simplicity, let us confine ourselves to three extreme cases for $v$ and $\beta_0$, where the five parameters can be evaluated respectively as follows:

(I), $|v| \ll 1, \left|\frac{v}{\beta_0}\right| \ll 1$

\begin{equation}
e = 0, f = -\frac{2(1 + \beta_0^2)}{\pi \beta_0^2} v, g = 0, h = -\frac{2(1 + \beta_0^2)}{\pi \beta_0^2} v, i = 0.
\end{equation}

(2·19)

(II), $|\beta_0| \gg 1, \left|\frac{v}{\beta_0}\right| \ll 1$

\begin{equation}e = f = g = 0, h = -\frac{4v\sqrt{1 - (v^2/4)}}{\pi}, i = -\frac{2v^3\sqrt{1 - (v^2/4)}}{\pi}.
\end{equation}

(2·20)
Note that the solution (2·17) is not valid for the values of \( \beta_0 \) lying in the intervals \( 1 - (v/\beta_0) - (v^2/4) < 0 \). Finally, we should like to note that an analogous solution was obtained by Schlup. 8

\[ e = O\left( \frac{1}{\beta_0^2 \pi} \right), \quad f = g = h = O\left( \frac{1}{\beta_0^3 \pi} \right), \quad i = \sqrt{1 - (v/\beta_0) - (v^2/4)} \quad \frac{v(11v^2 + 4)}{8\beta_0^8} \]

(2·21)

\section{Calculations of \( L(E) \) and \( L(\omega) \)}

In this section we shall obtain the approximate expressions for \( L(E) \) and \( L(\omega) \) for three models.

\textit{Model A.} Disordered Kronig-Penney model with potential \( V(x) = \sum_n V_n \delta(x - x_n) \).

If we write the wave function in the interval between \( x_n \) and \( x_{n+1} \) as

\[ \psi(x) = A_n \cos \{ k(x - x_n) + \varphi_n \}, \quad x_n < x < x_{n+1}, \quad (3·1) \]

it follows, from the continuity conditions for \( \psi(x) \) and \( d\psi/dx \) at \( x = x_{n+1} \), that

\[ \tan \varphi_{n+1} = -v_n + \tan(\varphi_n + \lambda_n), \quad (3·2) \]

where \( \lambda_n = k(x_{n+1} - x_n), \) \( v_n = V_n/k \) and \( k = \sqrt{2mE/\hbar} \). If we put \( Z_n = \tan \varphi_n \), (3·2) becomes

\[ Z_{n+1} = -v_n + \frac{Z_n + \tan \lambda_n}{1 - Z_n \tan \lambda_n}. \quad (3·3) \]

Let us consider two cases:

\textbf{Case (I)} \( (v_n \) is random but \( \lambda_n \) is constant \( (= \lambda_0) \).) \ If we write \( y_n = -Z_n \sin \lambda_0 + \cos \lambda_0 \), (3·3) becomes

\[ y_{n+1} = \alpha_n - \frac{1}{y_n}, \quad (3·4) \]

where

\[ \alpha_n = 2 \left( \cos \lambda_0 + \frac{v_n}{2} \sin \lambda_0 \right). \quad (3·5) \]

This is the random process of type 1). Therefore the degree of localization \( L(E) \) can be calculated by using the stationary probability density given by (2·7), (2·8) and (2·9):

\[ L(E) = \frac{1}{2} \lim_{n \to \infty} \left\langle \ln \left| A_{n+1} \right|^2 \right\rangle = \frac{1}{2} \lim_{n \to \infty} \left\langle \ln \left\{ \frac{Z_{n+1} + 1}{Z_n + 1} \right\} \right\rangle \]

\[ = \frac{1}{2} \int_{-\infty}^{\infty} w(y) \ln y^2 dy = \frac{\sigma^2}{8} \frac{1}{1 - (\alpha_0^2/4)} \]
It is apparent from (3·6), that \( L(E) \) is proportional to the variance of the random variable \( V_n \). Furthermore, we find that \( L(E) \) becomes zero as \( \lambda = k \ell \) tends to \( n \pi (n: \text{integer}) \). This can be understood also from the fact that the variance \( \sigma^2 \) vanishes at \( \lambda = n \pi \) and the solution is then reduced to that of the periodical system with \( \sigma^2 = 0 \). This corresponds to the extended state at the band edge of the periodical system. It is believed that an eigenstate near the band edge in the three-dimensional random system is localized in space. However, our result suggests that, if we consider the three-dimensional electronic state in the field of periodically distributed muffin-tin potentials of infinitely small radius, whose intensities are the random variables, then we would have some extended states at the energy value corresponding to the band edges of the periodical system in a fashion similar to that for the one-dimensional case. Besides, it is found from (3·6) that \( L(E) \) becomes zero for the high energy limit \( k^2 \to \infty \).

Case (II) \( (\lambda_n \text{ is random but } v_n \text{ is constant } (= v).) \) In this case, we have the random process of type 2). Therefore for the degree of localization

\[
L(E) = \frac{1}{2} \lim_{n \to \infty} \langle \ln \left| \frac{A_{n+1}}{A_n} \right| \rangle = \frac{1}{2} \lim_{n \to \infty} \langle \ln \left\{ \frac{Z_{n+1}}{(Z_n + v)^2 + 1} \right\} \rangle, \quad (3.7)
\]

we obtain, by using the stationary probability densities given by (2·15), (2·16), (2·17), (2·19), (2·20) and (2·21)

(I) \( |v| < 1, \quad \left| \frac{v}{\beta} \right| < 1 \)

\[
L(E) = \frac{v^2 (1 + \beta^2) e^2}{\pi \beta^2} \int_{-\infty}^{\infty} Z^2 dZ + O(v^3) = \frac{V^2 (I^2 - I I)}{8 \sin^2 k \ell} + O(V^3). \quad (3.8)
\]

(II) \( |\beta| \to \infty, \quad \left| \frac{v}{\beta} \right| \to 0 \)

\[
L(E) = -2 \sqrt{1 - \left( \frac{v^2}{4} \right)} \frac{ve^2}{\pi} \int_{-\infty}^{\infty} \ln \left\{ \frac{Z^2 + 1}{(Z + v)^2 + 1} \right\} (Z + v) dZ
\]

\[
= \frac{ve^2}{4 (1 - \left( \frac{v^2}{4} \right))} = \frac{V^2 (I^2 - I I)}{4 \left( 1 - \left( \frac{V^2}{4k^2} \right) \right)} \quad (1 - \frac{V^2}{4k^2} > 0). \quad (3.9)
\]

(III) \( |\beta| \to 0, \quad -\frac{v}{\beta} \to \infty \)
\[ L(E) = O(\beta_0^{1/2}), \quad (3\cdot10) \]

where \( \bar{t} \) is the average spacing between neighboring lattice sites. We note that the solution \((2\cdot15)\) becomes useless for the high energy limit \(E \rightarrow \infty (k \rightarrow \infty)\) because the variance \( \sigma^2 \) is proportional to \( k^2 \). Therefore our result \((3\cdot8)\) cannot be compared with that \(^{(a)}\) obtained by Borland in the limit \(E \rightarrow \infty \).

**Model B.** One-dimensional Anderson model with independently distributed site-energies \( \delta_n \), which is described by the Schrödinger equation

\[ (E - \delta_n) a_n = J (a_{n-1} + a_{n+1}), \quad (3\cdot11) \]

where \( J \) is the transfer energy which is nonzero only for nearest neighboring sites and \( a_n \) is the probability amplitude of an electron at the site \( n \).

If we put \( y_n = (a_n/a_{n-1}) \), \((3\cdot11)\) can be transformed as

\[ y_{n+1} = \alpha_n - \frac{1}{y_n} \quad (3\cdot12) \]

where

\[ \alpha_n = \frac{E - \delta_n}{J}. \quad (3\cdot13) \]

Thus we have the random process of type 1). Therefore, \( L(E) \) becomes

\[
L(E) = \frac{1}{2} \lim_{n \to \infty} \langle \ln \frac{a_n}{a_{n-1}} \rangle = \frac{1}{2} \int_{-\infty}^{\infty} w(y) \ln y^2 dy \\
= \frac{\sigma^2}{8} \frac{1}{1-(\alpha_0^2/4)} = \frac{\delta^2 - \langle \delta \rangle^2}{8J^2} \frac{1}{1-(E^2/4J^2)}, \quad 1 - \frac{E^2}{4J^2} > 0, \quad (3\cdot14)
\]

which shows a tendency that \( L(E) \) increases as \( E \) becomes close to the band edges from the inside of the band of the periodical system.

**Model C.** Isotopically disordered harmonic chain of infinite length, which is described by the time-independent equation of motion

\[ -M_n \omega^2 x_n = K (x_{n+1} + x_{n-1} - 2x_n), \quad (3\cdot15) \]

where \( M_n \) and \( x_n \) are the mass and the displacement from its equilibrium position of the \( n \)-th atom and \( K \) is the strength of the springs between nearest atoms.

The masses \( M_n \) are assumed to be independent random variables.

If we put \( y_n = (x_n/x_{n-1}) \), \((3\cdot15)\) becomes

\[ y_{n+1} = \alpha_n - \frac{1}{y_n} \quad (3\cdot16) \]

where

\[ \alpha_n = 2 - \frac{M_n \omega^2}{K}. \quad (3\cdot17) \]
Thus we again have a random process of type 1), so that $L(\omega)$ is given by

$$L(\omega) = \frac{1}{2} \lim_{n \to \infty} \left( \ln \frac{x_{n+1}}{x_n} \right)^2 = \frac{1}{2} \int_{-\infty}^{\infty} w(y) \ln y^2 dy$$

$$= \frac{\sigma^2}{8} \frac{1}{1 - (\alpha \omega^2/4)} = \frac{(M^2 - \bar{M} \bar{M}) \omega^2}{8MK(1 - (M/4K) \omega^2)} \cdot \left( 1 - \frac{\bar{M}}{4K} \omega^2 > 0 \right) (3.18)$$

For the low frequency limit $\omega \to 0$, our result is reduced to that obtained by Matsuda and Ishii:

$$L(\omega) = \frac{M^2 - \bar{M} \bar{M}}{8MK} \omega^2. \quad (3.19)$$

§ 4. Conclusions

The expressions for $L(E)$ and $L(\omega)$ obtained above suggest that an eigenstate of the one-dimensional random system tends to be strongly localized as the energy or frequency approaches the edge of the energy band from its inside, except at $k\ell = n\pi (n = 1, 2, \ldots)$ in the case of the disordered Kronig-Penney model with equidistant $\delta$-function potentials.

Acknowledgments

The author wishes to thank Dr. J. Hori and Dr. T. Asahi for their helpful suggestions and encouragement. The author also wishes to express his gratitude to Dr. H. Matsuda and Dr. K. Ishii for valuable discussions.

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