

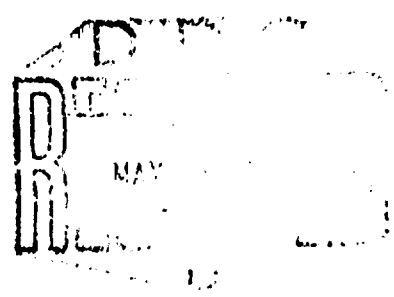
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Spectral Theory for Electron States
In Doped Semiconductors*

Shinzo Haka

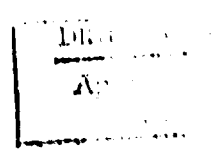
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Energy spectrum of electron states in doped semiconductors is investigated by using spectral theory of random matrices. A part of the content in a previous technical report is repeated in Chapter II for the main part of this report, Chapter III. The comparison with the experimental results is not included, which will be done in the future. It is seen in this approach that the convergence of the Anderson series depends delicately upon the values of random parameters. The condition employed by Meale and Thorpe for amorphous semiconductors may be also examined by the present treatment.

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1. INTRODUCTION

The problem of localization of electrons in amorphous systems has been intensively studied for different disordered materials¹ and discussions have been concentrated on the "effectively" localized states derived by Anderson.² The contribution of these electrons to the conductivity is answered only by analyzing the nature of the electron wavefunctions. Due to mathematical complexity associated with disorder, however, the understanding of electron wavefunctions in disordered systems is still unsatisfactory. We would like to investigate them by a different approach.

We restrict our consideration to an energy spectrum of electron states in doped semiconductors. A high concentration of impurities leads to formation of the impurity band. A spatial distribution of impurity atoms is, however, random. The atomic potential at each impurity site and also the overlap of the electron wavefunction between neighboring impurity atoms vary from one impurity site to another. The effects of this disorder work so as to destroy the coherence of the diffraction that permits delocalization of an electron. Our problem is to study the change in the energy spectrum of the band due to this disorder.

The appearance of localized states in the tails of the impurity band is based on the idea that local fluctuations of potential can produce bound states below the usual conduction band.³ A review on various approaches to this problem has also been given by Ziman.⁴ One of the difficult points in the Green-function approach is that localized states are defined by the convergence of an infinite stochastic series. To take into account the fluctuation, one has to take an average over the values of fluctuating parameters. There is no problem for an exchange of operations, averaging and summing of an infinite series, provided that the series is uniformly convergent with respect to the values of the parameter over a region of variation. This does not always hold as is seen in Chapter III. It seems that there are regions where we can give only statistical answer, and spectral theory⁵ of random matrices would be promising to the present problem.

We will follow an analytical procedure without taking the average. We introduce a simplification that the number of the nearest neighbors of the impurity atom to which an electron hops is two. When the number of the nearest neighbors is larger than two, it is considered that the electron is localized in the region occupied by those impurity atoms and only its most outside orbit is taken account for a hopping action of the electron. Mathematically, this is tridiagonalization of the Permittian matrix, which is a well-known procedure, although complex.⁶ A spectral resolution of the Hamiltonian with random elements is treated. This method enables us to find an asymptotic form of the electron wavefunction. Furthermore, we can study how the states both localized and non-localized are built up in the impurity band. In Chapter II, we formulate the present problem in a matrix form and discuss localized states by using examples in Chapter III.

II. SPECTRAL THEORY

For our subsequent analysis, it is convenient to recapitulate first some well-known results about finite matrices.⁷ Our physical system is characterized by the Hamiltonian which is a Hermitian matrix with random elements. Let H be an $(n \times n)$ Hermitian matrix with distinct eigenvalues, E_1, E_2, \dots, E_n . The Schrodinger equation is written in a matrix form: There exist n non-zero column vectors $\psi_1, \psi_2, \dots, \psi_n$, such that

$$H\psi_\mu = E_\mu \psi_\mu. \quad (1)$$

The corresponding row-vectors, $\phi_\mu \equiv \psi_\mu^\dagger$, are defined by

$$\begin{aligned} \phi_\mu H &= E_\mu \phi_\mu, \\ \phi_\mu &= (c_0^{(\mu)*}, c_1^{(\mu)*}, \dots, c_{n-1}^{(\mu)*}), \end{aligned} \quad (2)$$

where a dagger and an asterisk stand for the Hermitian and the complex conjugate, respectively.

Since the eigenvectors that correspond to distinct eigenvalues are linearly independent, matrices defined by

$$U = (\psi_1, \psi_2, \dots, \psi_n)$$

and U^\dagger are non-singular. The orthogonality of eigenfunctions is written as

$$\phi_\mu \psi_\nu \equiv \psi_\mu^\dagger \psi_\nu = \delta_{\mu\nu},$$

and the eigenfunctions are normalized by multiplying $(\delta_{\mu\mu})^{-1/2}$. For the normalized wavefunctions, the matrix U is unitary. The Hamiltonian H is diagonalized with the use of this unitary matrix; $U^\dagger H U = \Gamma$, where Γ is a diagonal matrix with diagonal elements, E_1, E_2, \dots, E_n , respectively. Hence, we obtain

$$H = U \Gamma U^\dagger = \sum_{\mu=1}^n E_\mu J_{\mu\mu}, \quad (3)$$

where J_μ are matrices given by $\Psi_\mu \phi_\mu$. These matrices have the property that $J_\mu^2 = J_\mu$, $J_\mu J_\nu = 0$ for $\mu \neq \nu$, and are called the orthogonal idempotents of H . The system of idempotents is complete in the sense that $J_1 + J_2 + \dots + J_n = I$, where I is the n -dimensional unit matrix. The equation (3) is referred to as the spectral resolution of H .

Now, we formulate hopping actions of an electron in an aperiodic lattice. Let $V_{mn} = V(|R_m - R_n|)$ be the energy integral for the transfer of an electron from the n -th site to the m -th site of impurity atoms and the Hamiltonian of the system is given by

$$H = \sum_{\{m\}} \epsilon_m a_m^\dagger a_m + \sum_{\{m\}} \sum_{\{n\}} V_{mn} a_m^\dagger a_n.$$

Here, the diagonal elements V_{mm} are assumed to be zero, and a_m^\dagger and a_m are creation and annihilation operators of an electron at the m -th site, respectively; $[a_m, a_n^\dagger]_+ = \delta_{mn}$. We assume impurity atoms with a single bound state. The impurity sites of the summation in (4) are distributed at random in the lattice. A fluctuating field at one site to another is taken into account by assigning random negative values to ϵ_m . We introduce an indispensable simplification to our analysis; that is, an impurity electron can hop only between the nearest impurity neighbors, the number of which is two. Randomly distributed impurity sites are then relabeled in such a way that the nearest neighbors may have their indices different by one. The disorder in location is now included in the hopping distance, $R_m, m \pm 1$, and random complex values are assigned to the matrix elements, $V_m, m \pm 1$. The Hamiltonian (4) is thus rewritten as

$$H = \sum_m \sum_n (\epsilon_m \delta_{mn} + V_{mn}) a_m^\dagger a_n,$$

$$V_{m, m+1} = \beta_m, \quad V_{m, m-1} = \beta_m^*$$

and $V_{m, n} = 0$ for $n = m$ and $n \neq m \pm 1$.

Diagonalization of this Hamiltonian into the form, $\sum_\mu \epsilon_\mu \Lambda_\mu^\dagger \Lambda_\mu$ is performed by a transformation,

$$a_m = \sum_\mu C_m^{(\mu)} \Lambda_\mu,$$

where $[A_{\nu}, A_{\nu}^+]_{+} = \delta_{\mu\nu}$. The quantities $c_{\mu}^{(\mu)}$ are determined by the Schrodinger equation (1) with

$$H = \begin{pmatrix} \epsilon_0 & \beta_0 & 0 & \cdot & \cdot & \cdot & 0 & 0 & 0 \\ \beta_0^* & \epsilon_1 & \beta_1 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ 0 & \beta_1^* & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \beta_{n-3} & \cdot & 0 \\ 0 & \cdot & \cdot & \cdot & \cdot & \beta_{n-3}^* & \epsilon_{n-2} & \beta_{n-2} & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & 0 & \beta_{n-2}^* & \epsilon_{n-1} & \cdot \end{pmatrix}$$

or by

$$\beta_{m-1}^* c_{m-1} + (\epsilon_m - E) c_m + \beta_m c_{m+1} = 0, \quad (5)$$

$$(m = 0, 1, \dots, n-1; c_{-1} = c_n \equiv 0),$$

where the superscript μ is suppressed for simplicity. In order that the simultaneous equations (5) may be solved, the determinant of the coefficients, designated by $P_n(E)$, should vanish. On expanding it with respect to the last row or column, one gets

$$P_n(E) - (E - \epsilon_{n-1}) P_{n-1}(E) + |\beta_{n-2}|^2 P_{n-2}(E) = 0, \quad (6)$$

which is valid for $n \geq 2$ if we define

$$P_0(E) = 1, \quad P_1(E) = E - \epsilon_0.$$

The roots of $P_n(E)$ are all distinct and negative, and separated by the roots of $P_{n-1}(E) = 0$, provided that $P_n(0) > 0$. Let us first examine the inequality of $P_n(0)$. Define λ_j and μ_j by

$$-\varepsilon_0 = \lambda_0, \quad \mu_0 = 0,$$

$$-\varepsilon_i = \lambda_i + \mu_i, \quad |\beta_i - 1|^2 = \lambda_i - 1\mu_i, \quad (i \geq 1),$$

and one successively obtains

$$\lambda_i = -\varepsilon_i(1 - b_i X_i), \quad \mu_i = -\varepsilon_i b_i X_i, \quad (i \geq 1),$$

where $b_i = |\beta_i - 1|^2 / \varepsilon_i \varepsilon_{i-1}$ and

$$X_i = \frac{1}{1 - \frac{b_{i-1}}{1 - \frac{b_{i-2}}{\dots \frac{b_2}{1 - \frac{b_1}{1 - b_0}}}}}$$

We assume that $b_0 = 0$, $X_1 = 1$ and $X_0 = 0$. The quantity X_n , as n tends to infinity, is a continued fraction. It follows from equation (6) that

$$P_n(0) = \lambda_0 \lambda_1 \dots \lambda_{n-2} \lambda_{n-1}, \quad (n \geq 1).$$

If all the partial numerators satisfy⁸

$$|b_i| \leq \frac{1}{4}, \quad (7)$$

the continued fraction X_n uniformly converges and the value of it and its approximants are in the domain $|X - (4/3)| \leq 2/3$, (Poincaré's theorem). Under the condition (7), all λ 's are positive and hence $P_n(0) > 0$.

The only one root of $P_i(E) = 0$ is $E_i^{(1)} (= \varepsilon_0)$, which is negative. It follows from (6) that

$$P_2(-\infty) > 0, \quad P_2(E_1^{(1)}) < 0, \quad P_2(0) > 0, \quad P_2(\infty) > 0.$$

Each of the intervals, $(-\infty, E_1^{(1)})$ and $(E_1^{(1)}, 0)$, thus contains a root of $P_2(E) = 0$; $0 > E_1^{(2)} > E_1^{(1)} > E_2^{(2)}$. This becomes a basis of induction. Assume now for any $s \geq 3$,

$$0 > E_1^{(s)} > E_1^{(s-1)} > E_{s-1}^{(s)} > E_{s-1}^{(s-1)} > E_s^{(s)}, \quad (7)$$

and we deduce that the sign of $P_{s-1}(E_r^{(s)})$ is given by $(-1)^{r-1}$, where r runs from 1 to s . On putting $E = E_r^{(s)}$ and $n = s+1$ in (7), we obtain

$$P_{s+1}(E_r^{(s)}) = -|\beta_{s-1}|^2 P_{s-1}(E_r^{(s)}),$$

whence the sign of $P_{s+1}(E_r^{(s)})$ is $(-1)^r$. Since the sign of $P_{s+1}(-\infty)$ is equal to $(-1)^{s+1}$, it follows that each of the intervals,

$$(-\infty, E_s^{(s)}), \quad (E_{s-1}^{(s)}, E_{s-2}^{(s)}), \quad \dots, \quad (E_1^{(s)}, 0)$$

contains a root of $P_{s+1}(E) = 0$. This completes the proof of (8) for $s \rightarrow s+1$.

It is also shown that the smallest root $E_n^{(n)}$ of $P_n(E) = 0$ remains finite as n goes to infinity, provided that all $(-E)$'s and $|\beta|$'s are finite. We can always find a number α , $0 < \alpha < 1$ in

$$\frac{P_{n-2}(E_n^{(n)})}{P_{n-1}(E_n^{(n)})} = \frac{n-2 \prod_{i=1}^{n-2} (E_n^{(n)} - E_i^{(n-2)})}{n-1 \prod_{i=1}^{n-1} (E_n^{(n)} - E_i^{(n-1)})} = \frac{(\alpha^2)^{n-2}}{E_n^{(n)} - E_{n-1}^{(n-1)}}$$

Combining this with $P_{n-1}(E_n^{(n)})/P_{n-1}(E_{n-1}^{(n)}) = [E_n^{(n)} - E_{n-1}^{(n-1)}]/[E_{n-2}^{(n-2)} - E_{n-1}^{(n-1)}]^2$ obtained from (7), we can derive

$$E_n^{(n)} \geq \min. (E_{n-1}^{(n-1)}, E_{n-1}^{(n-1)}) - \alpha^{n-2} |E_{n-2}^{(n-2)}|,$$

where the first term on the right hand side stands for a smaller quantity of the two. Thus, infinitely many states appear within a finite region

of the negative energy, as n goes to infinity.

It is now quite natural to ask the nature of the energy spectrum, whether it is continuous or discrete. To investigate it, we have to define a spectral function. Let us first consider a simple example, in which $\epsilon_n (= v < 0)$ and $|c_n|^2 (= |v|^2)$ are both constant and independent upon n . The recurrence relation (6) is then satisfied by the Tschobycheff polynomials of the second kind. Defining $\cos \omega = (E - v)2|v|^{-1}$, we obtain

$$P_n(E) = |v|^n \frac{\sin[(n+1)\omega]}{\sin \omega}. \quad (9)$$

The eigenvalues are therefore given by

$$\omega_\mu^{(n)} = \mu\pi/(n+1), \quad (\mu = 1, 2, \dots, n).$$

It follows from (5) that the eigenfunction corresponding to the eigenvalue

$$E_\mu^{(n)} = v + 2|v| \cos[\mu\pi/(n+1)] \quad (10)$$

is

$$\psi_\mu = \{c_\mu^{(n)}\}^{-1/2} \begin{pmatrix} P_0(E_\mu^{(n)}) \\ P_1(E_\mu^{(n)})/v \\ \cdot \\ \cdot \\ \cdot \\ P_{n-1}(E_\mu^{(n)})/v^{n-1} \end{pmatrix}. \quad (11)$$

The normalization factor is evaluated as

$$c_\mu^{(n)} = (n+1)/2 \sin^2[\omega_\mu^{(n)}]. \quad (12)$$

A spectral function $\rho^{(n)}(E)$ is defined as a non-decreasing step-function

for $-\infty < E < \infty$ with discontinuities $1/\theta_{\mu}^{(n)}$ at $E = E_{\mu}^{(n)}$:

$$\rho^{(n)}(E) = \begin{cases} 0, & E \geq E_1^{(n)} \\ \cdot & \cdot \\ \cdot & \cdot \\ - \sum_{i=1}^r \{ \theta_i^{(n)} \}^{-1}, & E_{r+1}^{(n)} \leq E < E_r^{(n)}, \\ \cdot & \cdot \\ \cdot & \cdot \\ - \sum_{i=1}^n \{ \theta_i^{(n)} \}^{-1}, & E < E_n^{(n)}. \end{cases} \quad (13)$$

Upon writing $\Delta\omega = \pi/(n+1)$, we see from

$$\{ \theta_{\mu}^{(n)} \}^{-1} = (2/\pi) \Delta\omega \sin^2 [(\mu+1)\omega] \quad (14)$$

that by a formal limiting process $n \rightarrow \infty$, the level density becomes

$$\begin{aligned} d\rho(E) &= -(2/\pi) \sin^2 \omega \, d\omega, \\ D(E) &= \frac{d\rho(E)}{dE} = \frac{1}{\pi|\beta|} \left[1 - \left(\frac{E-\alpha}{2|\beta|} \right)^2 \right]^{\frac{1}{2}}. \end{aligned} \quad (15)$$

The discontinuities (14) of the spectral function disappear as n goes to infinity. The spectrum becomes continuous and extends over the interval $\alpha - 2|\beta| \leq E \leq \alpha + 2|\beta|$. The completeness relation of the orthogonal idempotents,

$$\delta_{\mu\nu} = (2/\pi) \int_0^{\pi} \sin [(\mu+1)\omega] \sin [(\nu+1)\omega] \, d\omega,$$

is nothing but the orthonormality of Tscheycheff polynomials with the weight function (15).

The other example that is exactly soluble is given by assuming

$$\begin{aligned} \epsilon_{n-1} &= -2nK \quad (K > 0), \quad (n \geq 1), \\ |\epsilon_{n-2}|^2 &= K^2 n(n-1) \quad (n \geq 2), \end{aligned}$$

where we assume that β 's are all real for simplicity. Although this example is physically not interesting, it is instructive to observe how the continuous spectrum arises. The recurrence relation (7) is satisfied by the associated Laguerre polynomials,

$$P_n(E) = K^n n! L_n^{(1)}(-E/K).$$

The wavefunction corresponding to the eigenvalue $E_\mu^{(n)}$ of $L_n^{(1)}(-E_\mu^{(n)}/K) = 0$, is calculated as

$$\Psi_\mu = \{ \theta_\mu^{(n)} \}^{-\frac{1}{2}} \begin{pmatrix} L_0^{(1)}(-E_\mu^{(n)}/K) \\ L_1^{(1)}(-E_\mu^{(n)}/K)/\sqrt{2} \\ \cdot \\ \cdot \\ \cdot \\ L_{n-1}^{(1)}(-E_\mu^{(n)}/K)/\sqrt{n} \end{pmatrix}$$

The polynomial $L_n^{(1)}(x)$ has n positive zero-points and, hence, the energy eigenvalues are all negative. They are not confined to the finite region in the limit of $n \rightarrow \infty$. As a result of this limit, the energy spectrum becomes continuous over the range, $0 > E > -\infty$, which is seen from the orthonormality of the associated Laguerre polynomials. Comparing

$$\int_0^\infty e^{-x} x^\alpha L_i^{(\alpha)}(x) L_j^{(\alpha)}(x) dx = \{(i + \alpha)! / i!\} \delta_{ij},$$

with the completeness relation of the orthogonal idempotents,

$$\{(i + 1)(j + 1)\}^{-1} \int_{-\infty}^0 L_i^{(1)}(-E/K) L_j^{(1)}(-E/K) d\rho(-E/K) = \delta_{ij},$$

we find that

$$d\rho(x) = e^{-x} dx = -d\{e^{-x}(x + 1)\}.$$

In summary, the behavior of an electron over random impurity sites is described by the wavefunction in a form of a column vector. A position variable in this wavefunction is a row suffix, and is discrete. If the recurrence relation (6) is that of the well-known orthogonal polynomial, the region within which the polynomial is defined gives a region of variation of the energy eigenvalues. The weight function for the orthonormality of the polynomials is associated with the energy level density.

III. LOCALIZED STATES

The eigenvalue problem of a special matrix has been discussed using examples in which the structure of energy spectra is comparatively simple. It is necessary to inquire a little more closely into the nature of the spectral function for the problems of our interest. The spectral function (13) has discontinuities of the amount $1/\theta_{\mu}^{(n)}$ at $E = E_{\mu}^{(n)}$. If all $\theta_{\mu}^{(n)}$'s diverge as n goes to infinity, discontinuities disappear, while if any of them is finite in the limit, there remains a discontinuity at the point in the energy spectrum. By looking at the behavior of the wavefunction with the position variable, we can examine whether the state is localized.

The random parameters, $(\epsilon_1$ and $\beta_1)$, cannot be easily related to the spectrum function and nothing can be said about the energy spectrum unless any restriction is put on the random parameters. We first assume that

$$|\beta_1| = V, \quad \epsilon' \leq \epsilon_1 \leq \epsilon'', \quad (16)$$

where $\epsilon'' < 0$ and V is constant. It is not necessary to assume that $|\beta_1| =$ constant, and it will be removed later. The suffix μ of $E_{\mu}^{(n)}$ remains unaltered through the present analysis and the letter x is used instead of $E_{\mu}^{(n)}$.

By defining a quantity

$$Z_s(E) = P_s(E)/VP_{s-1}(E), \quad (17)$$

we have from (6) a recurrence relation

$$Z_{s-1}^{-1}(E) = V^{-1}(E - \epsilon_{s-1}) - Z_s(E). \quad (18)$$

Suppose that x is one of the eigenvalues of the n -th section of the Hamiltonian; $Z_n(x) = 0$. It follows then that

$$Z_{n-1}^{-1}(x) = V^{-1}(x - \epsilon_{n-1}).$$

Let us restrict our consideration to a region where $x - \epsilon'' > 0$ or $\epsilon' - x > 0$. As the both cases are analyzed similarly and the result is symmetrical with respect to the middle point $(\epsilon' + \epsilon'')/2$, we treat the first case only. Assume that

$$x - \epsilon'' = 2V \cosh \omega, \quad (\omega > 0),$$

and we have an inequality, $Z_{n-s+1} \leq \sinh \omega / \sinh (2\omega)$. With this as a basis we use an inductive argument. Assuming

$$Z_{n-s+1} \leq \sinh [(s-1)\omega] / \sinh (s\omega)$$

for $n > s > 2$, one obtains from (18)

$$Z_{n-s}^{-1} \geq \left\{ 2 \cosh \omega - \frac{\sinh [(s-1)\omega]}{\sinh (s\omega)} \right\} = \frac{\sinh [(s+1)\omega]}{\sinh (s\omega)}.$$

Hence, one has the result

$$Z_{n-s} \leq \frac{\sinh (s\omega)}{\sinh [(s+1)\omega]}, \quad n > s > 1. \quad (19)$$

Since

$$P_s(x) = V^s Z_s Z_{s-1} \cdots Z_2 Z_1, \quad (s \geq 1)$$

$$P_0(x) = 1,$$

Inequalities for $s \leq (n-1)$,

$$P_s(x) \leq V^s \sinh [(n-s)\omega] / \sinh (n\omega),$$

are obtained. From the eigenfunction corresponding to the eigenvalue x ,

$$\{\psi_\mu\}^+ = \{0_\mu^{(n)}\}^{-1/2} (P_0(x), P_1(x)/V, \dots, P_{n-1}(x)/V^{n-1}),$$

the normalization constant is proved to satisfy

$$\theta_{\mu}^{(n)} \leq \frac{\cosh[(n+1)\omega]}{2 \sinh \omega \sinh(n\omega)} - \frac{n}{2 \sinh^2(n\omega)} \quad (20)$$

In the limit, $n \rightarrow \infty$, the right hand side is finite for $\omega \neq 0$. The limit of $1/\theta_{\mu}^{(n)}$ does not vanish and the discontinuity exists at $E = \lim_{\mu} E_{\mu}^{(n)}$ in the energy spectrum. Looking at the wavefunction, one finds that

$$\lim_{n \rightarrow \infty} P_{n-1}(x)/V^{n-1} < e^{2\omega} \lim_{n \rightarrow \infty} \exp(-n\omega).$$

As the wavefunction vanishes exponentially with respect to the position variable n , the state is localized.

To remove the restriction that all $|\beta_j|$'s are constant, we have to redefine $Z_s(E)$ with the assumption $|\beta|' \leq |\beta_j| \leq |\beta|''$, by

$$Z_s(E) = P_s(E) / |\beta_{s-1}| \cdot P_{s-1}(E)$$

and obtain the recurrence relation

$$Z_{s-1}^{-1}(E) = \frac{E - \epsilon_{s-1}}{|\beta_{s-2}|} - \frac{|\beta_{s-1}|}{|\beta_{s-2}|} Z_s(E).$$

As $Z_n(x) = 0$, we successively find

$$Z_{n-1}(x) = |\beta_{n-2}| / (x - \epsilon_{n-1}),$$

$$Z_{n-s}(x) = |\beta_{n-s-1}| \cdot J_{n-s} / (x - \epsilon_{n-s}), \quad (2 \leq s < n),$$

$$J_{n-s} = \frac{1}{1 - \frac{|\beta_{n-s}|^2 / (x - \epsilon_{n-s})(x - \epsilon_{n-s+1})}{1 - \frac{|\beta_{n-s+1}|^2 / (x - \epsilon_{n-s+1})(x - \epsilon_{n-s+2})}}$$

1 -

$$1 - \frac{|\beta_{n-2}|^2 / (x - \epsilon_{n-2})(x - \epsilon_{n-1})}{1}$$

If for any i ,

$$|\beta_i|^2 / |(x - \epsilon_i)(x - \epsilon_{i+1})| \leq \frac{1}{4},$$

all J_i , as n goes to infinity, are in the domain $|J - (4/3)| \leq 2/3$. The continued fraction converges uniformly under the above condition, which may be replaced by the stronger condition

$$|\beta''| / (x - \epsilon'') \leq \frac{1}{2} \quad \text{or} \quad |\beta''| / (\epsilon' - x) \leq \frac{1}{2}, \quad (21)$$

for $x > (\epsilon' + \epsilon'')/2$ or $x < (\epsilon' + \epsilon'')/2$, respectively. Since $P_s =$

$(|\beta_0| \cdots |\beta_{s-1}|)(z_s z_{s-1} - 1) + (|\beta_0| \cdots |\beta_{s-1}|)(z_s z_{s-1} - 1 \cdots z_1)$
and the wavefunction is

$$\psi_\mu^+ = \{O_\mu^{(n)}\}^{-\frac{1}{2}} (P_0(E_\mu^{(n)}), P_1(E_\mu^{(n)})/\beta_0^*, \dots, P_{n-1}(E_\mu^{(n)})/\beta_0^* \cdots \beta_{n-2}^*), \quad (22)$$

It is easily shown that $O_\mu^{(n)}$ converges under the sufficient condition (21) corresponding to Anderson's condition.

To continue our analytical procedure into the inside region excluded by (21), it is necessary to specify the n -dependences of ϵ_n and $|\beta_n|$ in detail. We cannot carry out an analytical procedure, though physically interesting, for a random assignment of value to those parameters out of uniformly distributed values within certain ranges. On the other hand, when we take an example in which $|\beta_s| = V$, $\epsilon_s = \epsilon' + [s(\epsilon'' - \epsilon')/n]$, ($s = 0, 1, \dots, n-1; n \rightarrow \infty$), we cannot expect localized states in the inside region. Because, the values of Z 's oscillate around zero infinitely many times, as n goes to infinity. Localized states arise in the following example:

$$\epsilon_s = \frac{\epsilon' + \epsilon''}{2} = \begin{cases} \frac{\epsilon'' - \epsilon'}{2(m+1)}, & (s = 2m), \\ -\frac{\epsilon'' - \epsilon'}{2(m+1)}, & (s = 2m+1), \end{cases} \quad (23)$$

where s runs from 0 to infinity. Let us consider a region where $|x - (\epsilon' + \epsilon'')/2| > 2V$, where $Z_n(x) = 0$. Since the eigenvalues x are

distributed symmetrically with respect to the middle point $(\epsilon' + \epsilon'')/2$, we will treat only the case, $[x - (\epsilon' + \epsilon'')/2] > 2V$ and assume that n is even. We choose an integer S for fixed x , such that

$$\frac{\epsilon'' - \epsilon'}{2S} > x - \frac{\epsilon'}{2} - \frac{\epsilon''}{2} - 2V > \frac{\epsilon'' - \epsilon'}{2(S+1)},$$

and define $\omega(>0)$ for even n , ($Z_n(x) = 0$), by

$$x - \frac{\epsilon' + \epsilon''}{2} - \frac{\epsilon'' - \epsilon'}{2(S+1)} = \dots \cosh \omega.$$

We then obtain from (18)

$$Z_{2m-1} = \frac{V}{x - \epsilon_{2m-1}} < \frac{\sinh \omega}{\sinh(2\omega)}.$$

Taking this as a basis of induction, we use again an inductive argument for a finite sequence

$$Z_{2m-2}, Z_{2m-3}, \dots, Z_{2S+1}, Z_{2S}.$$

The verification goes in the same way as before and the result is

$$Z_{2S} < \frac{\sinh[2(m-S)\omega]}{\sinh\{[2(m-S)+1]\omega\}}.$$

By repeated use of (10), we can further evaluate $Z_{2S-1}, Z_{2S-2}, \dots, Z_1$. They are finite but change signs frequently as the suffix decreases, and cannot be specified in a simple way. One easily finds for $2m-1 \geq s \geq 2S$,

$$|P_s(x)| < V^s C(2S-1) \frac{\sinh[(2m-s)\omega]}{\sinh\{[2(m-s)+1]\omega\}},$$

where a finite constant $C(2S-1)$ is given by

$$C(2S-1) = |Z_{2S-1}| \cdot |Z_{2S-2}| \cdot \dots \cdot |Z_1|.$$

We are thus led to the result

$$\theta_{\mu}^{(n)} < \frac{(C(2S - 1))^2}{\sinh^2[(n - 2S + 1)\omega]} \sum_{k=1}^{n-2S} \sinh^2(k\omega) + C, \quad (24)$$

and C is a finite constant given by

$$C = \sum_{l=0}^{2S-1} |P_l(x)|^2 / (V^2)^l.$$

By taking a limit $n \rightarrow \infty$, the right hand side of (24) is finite. It therefore turns out that the states existing in the regions between $(\epsilon' + \epsilon'')/2 + 2V$ and $\epsilon'' + 2V$, and between $(\epsilon' + \epsilon'')/2 - 2V$ and $\epsilon' - 2V$ are localized states.

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