

Electron localization in spatially disordered systems

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The homomorphic-cluster coherent-potential approximation is applied to obtain the average Green's function for spatially disordered systems in two and three dimensions, which is described by a tight-binding one-electron Hamiltonian with transfer energy between two $1s$ hydrogenic orbitals. The effective medium to be determined self-consistently is assumed to be an appropriate lattice, and a modified Hertz distribution is used for the random distribution of nearest-neighbor distance. With the use of the $L(E)$ criterion for localization, Anderson's transition is predicted to occur at a critical density $\rho^{1/2}a_B = 0.403$ in two dimensions and $\rho^{1/3}a_B = 0.252$ in three dimensions, where ρ is the number density of atoms and a_B is the effective Bohr radius.

I. INTRODUCTION

In recent years, the question of electron localization in random systems has been extensively studied.¹ While most of the works have been concerned with the cellular disordered systems described by a tight-binding one-electron Hamiltonian, where atomic sites form a regular crystal lattice, a few authors²⁻⁶ have investigated electron localization in spatially disordered systems. Matsubara and Toyozawa² first introduced the following tight-binding Hamiltonian to study electronic properties of spatially disordered systems:

$$H = \sum_{n \neq m} |n\rangle v(r_{nm}) \langle m|, \quad (1.1)$$

where $\text{ket } |n\rangle$ is the Wannier function associated with an atom located at \vec{r}_n and a transfer energy $v(r_{nm})$ is a function of the distance $r_{nm} \equiv |\vec{r}_n - \vec{r}_m|$ between two atoms at \vec{r}_n and \vec{r}_m . They developed a graphical technique to sum up a part of perturbation series of Green's function $(E - H)^{-1}$, E being the energy, when the atoms are distributed uniformly. As an example, they employed the transfer energy between two hydrogenic $1s$ orbitals

$$v(r_{nm}) = -V_0(1 + r_{nm}/a_B)e^{-r_{nm}/a_B}, \quad (1.2)$$

where a_B is an effective Bohr radius of electron under consideration and V_0 is twice the ionization potential of the $1s$ state. They evaluated the density of states and the conductivity as functions of the number density ρ of the atoms. Their approximate method did not show any indication of localization

of eigenstates. The procedure developed by Matsubara and Toyozawa was extended to include a correlation of atomic position by Ishida and Yonezawa.³ They discussed mobility edges by making use of the modified $F(E)$ criterion. Some authors⁴ have utilized more general forms of transfer energy.

The model system introduced by Matsubara and Toyozawa was studied numerically in two dimensions by Kikuchi⁵ and Debney.⁶ Using the sensitivity of eigenenergy to a change of boundary conditions as a criterion of localization, Kikuchi⁵ showed that the mobility edges move inward as the density is reduced, but he did not obtain Anderson's transition. Debney⁶ used the same criterion and predicted that Anderson's transition takes place at $\rho_c^{1/2}a_B = 0.364$ in two dimensions.

The localization of electronic state is well known as a possible mechanism of the metal-insulator transition. As shown by Halperin⁷, a spatially localized eigenstate gives zero dc conductivity. Therefore, if the states near the Fermi energy are spatially localized, we expect that the system is an insulator, and when those states become extended, an insulator-to-metal transition will occur.

Many experiments have been done to observe metal-insulator transition in spatially disordered systems. Expanded liquid metals,⁸ metal-rare-gas mixtures,^{4,9} and doped semiconductors^{4,10} are among the most familiar systems. The mechanism of metal-insulator transition in these systems has been subjected to controversial arguments, i.e., whether it is Mott's transition due to electron correlation or Anderson's transition due to electron

localization. Because the transition density $\rho^{1/3}a_B$ for many cases coincides with the value (0.25) predicted for Mott's transition,¹¹ electron correlation has been supposed to be the dominant mechanism of the transition. However, some authors¹²⁻¹⁴ explained the metal-insulator transition from the percolation viewpoint. The percolation approach is a simplified classical treatment of electron localization. So far, there are no explicit estimation of the critical density of Anderson's transition in spatially disordered systems.

The purpose of the present paper is to study electronic properties of systems described by Hamiltonian (1.1) with the transfer energy (1.2) and to provide an estimation of the critical density of Anderson's transition by an analytical method. To this end, we introduce an approximate method to handle spatially disordered systems in Sec. II. We assume that each atom interacts with z neighboring atoms, z being a fixed parameter. Then, we employ a double site version of the homomorphic cluster coherent potential approximation¹⁵ (CPA) by taking a neighboring atomic pair as a disordered unit. The surrounding effective medium to be determined is assumed to have a lattice structure with a coordination number z . The distribution of the distance of neighboring atoms is chosen so as to reflect actual random systems. This procedure is quite general to treat spatially disordered systems. In the present paper, application is specialized to calculate average Green's function and to examine electron localization in systems characterized by Eqs. (1.1) and (1.2) by making use of the $L(E)$ criterion.¹⁶ In Sec. III we study two dimensions and result will be compared with numerical result of Debney. We examine three dimensions in Sec. IV and predict Anderson's transition to occur at $\rho^{1/3}a_B = 0.252$. Finally, a brief discussion will be given in Sec. V.

II. BASIC FORMALISM

Consider a sample of spatially disordered system described by Hamiltonian (1.1). We replace the whole system except for a neighboring atom pair by an effective medium, which is assumed to be a certain crystal lattice with a coordination number z . The effective medium is determined such that the pair of atoms embedded in the medium does not produce further scattering on the average over a distribution of the distance between those two atoms. To ensure the analyticity of the approxima-

tion,¹⁵ we assume that each atom of the pair interact only with z neighboring atoms (one of which is the another atom of the pair and the rest belong to the effective medium) and partition each atom into z subunits, one of which is considered to belong to the random units and others to the effective medium. The situation is schematically shown in Fig. 1. The explicit CPA condition reads as¹⁵

$$\int_0^\infty N(r)\tilde{V}(r)[\tilde{1}-\tilde{G}\tilde{V}(r)]^{-1}dr=0, \quad (2.1)$$

where

$$\tilde{V}(r)=\begin{bmatrix} -\sigma_d/z & v(r)-\sigma_{od} \\ v(r)-\sigma_{od} & -\sigma_d/z \end{bmatrix}, \quad (2.2)$$

$$\tilde{G}=\begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix}, \quad (2.3)$$

and $\tilde{1}$ is the 2×2 unit matrix. Here $v(r)$ is the transfer energy between two neighboring atoms, $N(r)$ is the distribution function of the nearest-neighbor distance, and $G_{11}=G_{22}$ and $G_{12}=G_{21}$, respectively, are the diagonal and next diagonal matrix elements of effective Green's function $(E-\Sigma)^{-1}$, where E is the energy and Σ is the Hamiltonian of the effective medium given by the coherent site energy σ_d and the coherent nearest-neighbor transfer energy σ_{od} . The matrix elements of effective Green's function are expressed as

$$G_{11}(E)=\int_{-\infty}^{\infty} \frac{D(E')}{(E-\sigma_d-\sigma_{od}E'/V)}dE', \quad (2.4)$$

$$G_{12}(E)=[(E-\sigma_d)G_{11}(E)-1]/z\sigma_{od}, \quad (2.5)$$

where $D(E)$ denotes the density of states for a regular lattice of the same structure as the effective medium with the site energy 0 and the nearest-neighbor transfer energy V .

The distribution function $N(r)$ of nearest-

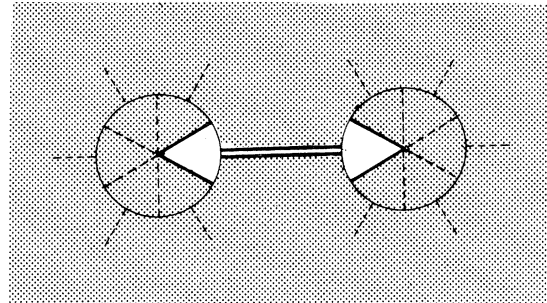


FIG. 1. Schematic illustration of the homomorphic cluster CPA. Dotted region denotes the effective medium and undotted part is a random unit.

neighbor distance is given by a modified Hertz distribution,

$$N(r) = \rho S(r) g(r) \exp \left[- \int_0^r \rho S(r') g(r') dr' \right], \quad (2.6)$$

where ρ and $g(r)$ are the number density of atoms and the pair correlation function, respectively. The surface area $S(r)$ of one of z equivalent parts of d -dimensional sphere with radius r , i.e., d -dimensional cone is written as

$$S(r) = \begin{cases} (2\pi)^{d/2} r^{d-1} / z(d-2)!! & (d = \text{even}) \\ 2(2\pi)^{(d-1)/2} r^{d-1} / z(d-2)!! & (d = \text{odd}) \end{cases} \quad (2.7)$$

where

$$n!! = \begin{cases} n(n-2)\cdots 3\cdot 1 & (n = \text{odd}) \\ n(n-2)\cdots 4\cdot 2 & (n = \text{even}) \end{cases} \quad (2.8)$$

The factor $1/z$ in Eq. (2.7) takes account of the fact that the atoms in the random unit interact with z neighbors. In each d -dimensional cone we pick up the nearest-neighbor atom from the vertex of the cone lying in the spherical shell between r and $r + dr$.

In the following sections, we employ the $L(E)$ criterion¹⁶ to obtain mobility edges. Explicitly, $L(E)$ is defined by

$$L(E) = K \tilde{V} |G_{11} - G_{12} G_{21} / G_{11}|, \quad (2.9)$$

where K , the connectivity constant of the system, is chosen to be the corresponding value of the regular lattice and

$$\ln \tilde{V} = \int_0^\infty N(r) \ln |v(r)| dr. \quad (2.10)$$

Mobility edges will be determined by $L(E) = 1$.

In the present paper, we consider a uniform distribution of atoms so that $g(r)$ in Eq. (2.6) is set to be unity. In a forthcoming paper, we will study

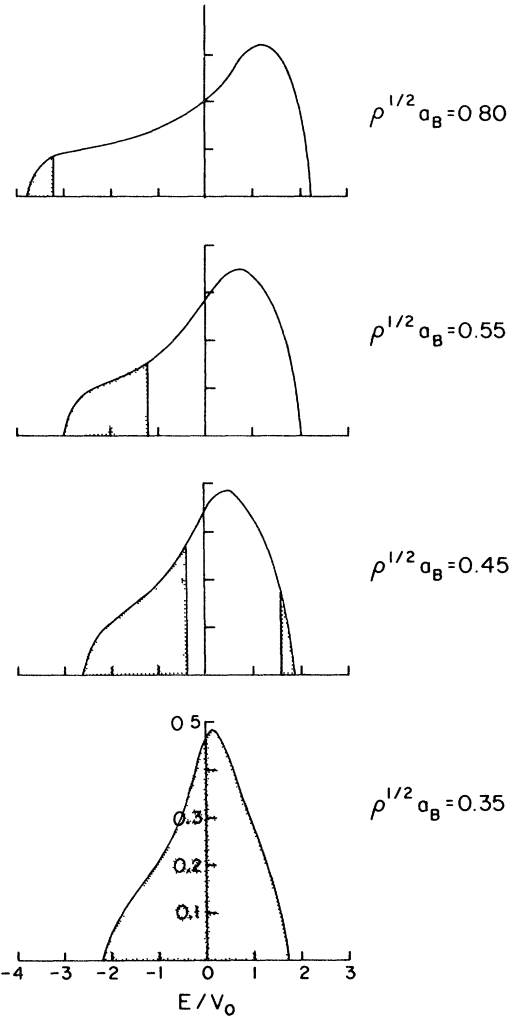


FIG. 2. Density of states and mobility edges for a two-dimensional system determined by the effective medium with triangular lattice ($z=6$). Eigenstates in the shaded region are localized.

the effect of the short-range order by using a functional form for $g(r)$.

III. TWO-DIMENSIONAL SYSTEM

Let us consider a two-dimensional system where atoms are distributed uniformly. We first employ a triangular lattice for the structure of the effective medium. The density of states of the regular triangular lattice with site energy 0 and nearest-neighbor transfer energy -1 is given by

$$D(E) = \begin{cases} 3F(\arcsin \phi, k) / 2\pi^2 (3-E)^{1/4} & \text{if } -6 \leq E \leq 2 \\ 6F(\arcsin(1/\phi), 1/k) / \pi^2 [12 - E^2 + 8(3-E)^{1/2}]^{1/2} & \text{if } 2 \leq E \leq 3, \\ 0 & \text{otherwise} \end{cases} \quad (3.1)$$

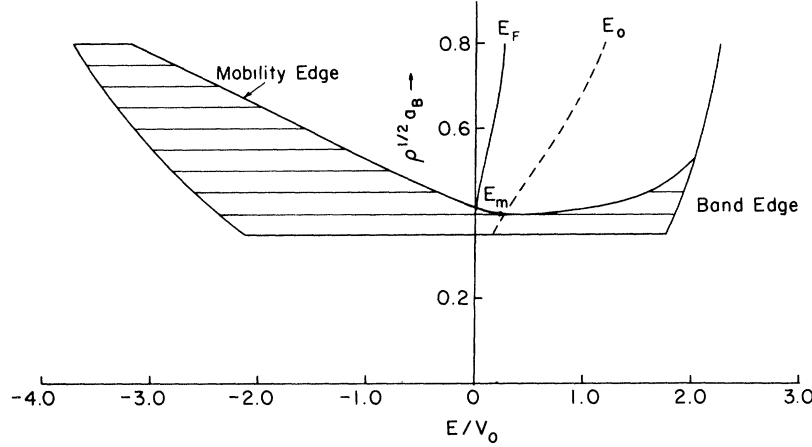


FIG. 3. Dependence of band edges (BE), mobility edges (ME), band center E_0 , and Fermi energy E_F on $\rho^{1/2}a_B$ for a two-dimensional system determined by the effective medium with triangular lattice. Eigenstates in the shaded region are localized.

where

$$\phi = 2/[1 + (3 - E)^{1/2}], \quad (3.2)$$

$$k = [12 - E^2 + 8(3 - E)^{1/2}]^{1/2} / 4(3 - E)^{1/4}, \quad (3.3)$$

and $F(\phi, k)$ is elliptic integral of the first kind. The simultaneous equations (2.1)–(2.3), with (1.2), (2.4)–(2.6), and (3.1) have been solved numerically to find as yet unknown coherent site energy σ_d and coherent transfer energy σ_{0d} . Figure 2 shows the density of states which is given by $-(1/\pi)\text{Im}G_{11}$ and mobility edges by the $L(E)$ criterion for various values of ρ . All eigenstates are localized in the shaded region. Band edges and mobility edges are plotted as functions of $\rho^{1/2}a_B$ in Fig. 3. According to the $L(E)$ criterion, Anderson's transition takes place at $\rho_c^{1/2}a_B = 0.403$.

In Fig. 3, also are plotted two characteristic energies as functions of $\rho^{1/2}a_B$: E_0 is the energy at which the density of states takes the maximum value and E_F is the energy which will be the Fermi energy if the energy band is half filled. A careful analysis shows that two mobility edges meet at an energy E_m which is very close to E_0 larger than E_F . In the present numerical accuracy, the difference $(E_m - E_F)/V_0$ is 0.2.

To observe the sensitivity of the critical density on the lattice structure used as the effective medium, we have also considered the effective medium to be a square lattice, where the density of states is given by

$$D(E) = \begin{cases} F(\pi/2, (1 - E^2/16)^{1/2}) / 2\pi^2 & \text{if } |E| \leq 4 \\ 0 & \text{otherwise.} \end{cases} \quad (3.4)$$

Figure 4 shows the dependence of the density of states and mobility edges on ρ . The critical density for the Anderson transition reads as $\rho^{1/2}a_B = 0.375$.

IV. THREE-DIMENSIONAL SYSTEM

We assume the effective medium to be a lattice which has a semielliptic unperturbed density of states (Hubbard density of state)

$$D(E) = (z^2 - E^2)^{1/2} / (2/\pi z^2). \quad (4.1)$$

We set $z = 6$ corresponding to a simple cubic lattice.

The simultaneous equations, (2.1)–(2.3), with (1.2), (2.4)–(2.6), and (4.1) have been solved numerically and yielded the density of states shown in Fig. 5. Figure 6 shows the dependence of mobility edges determined by the $L(E)$ criterion and band edges on the reduced density $\rho^{1/3}a_B$. Both mobility edges meet at $\rho^{1/3}a_B = 0.252$, which indicates that Anderson's transition occurs at this density.

V. DISCUSSION

In this paper we have introduced an approximate method based on the homomorphic cluster CPA to handle spatially disordered systems and applied it to obtain mobility edges of the systems described by Hamiltonian (1.1) with transfer energy (1.2). A

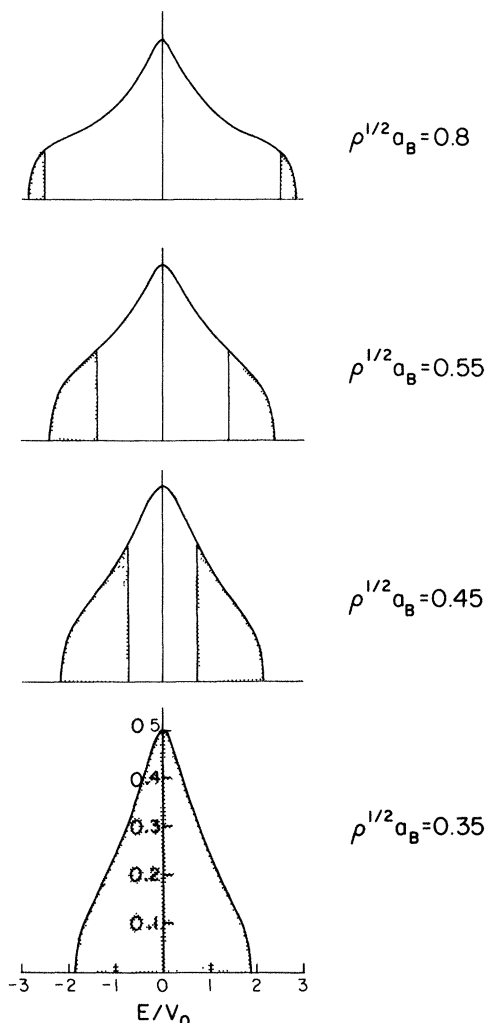


FIG. 4. Density of states and mobility edges for a two-dimensional system determined by the effective medium with square lattice ($z=4$). Eigenstates in the shaded region are localized.

similar application of the CPA has been considered by Djordjevic *et al.*¹⁷ A crucial difference of the present method from theirs is to use the modified Hertz distribution (2.6) for the nearest-neighbor distance, which describes spatial randomness adequately. The same distribution has been successfully used to examine an impurity conduction in doped-semiconductors by Odagaki and Lax.¹⁸

In the present method, an effective medium to be determined has been assumed to have a regular lattice structure. This assumption has been made in order that one can have a definite relation between diagonal and next-diagonal elements of Green's function and coherent site energy and coherent transfer energy such as Eqs. (2.4) and (2.5). Therefore, if Eqs. (2.4) and (2.5) hold, the unperturbed

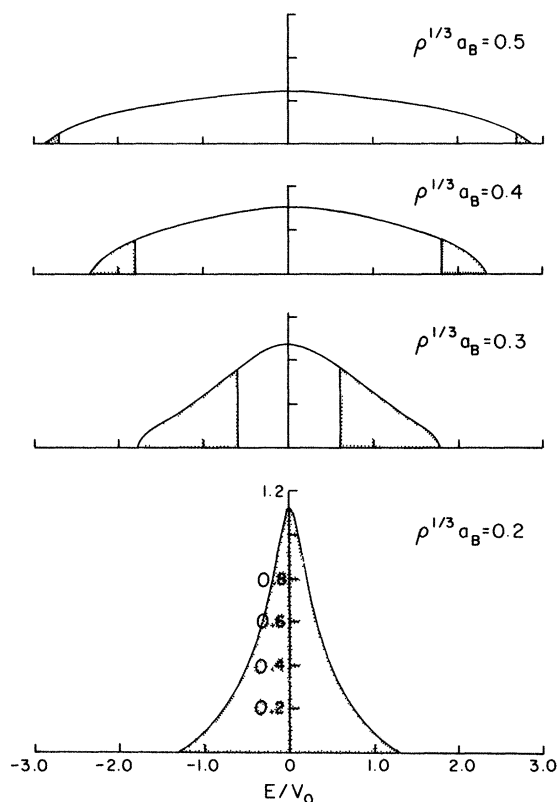


FIG. 5. Density of states and mobility edges for a three-dimensional system determined by the effective medium with Hubbard density of state ($z=6$). Eigenstates in the shaded region are localized.

density of states can be of any form, for example, one of a regular crystal as we used in Sec. III or one of a pseudolattice as we used in Sec. IV. The

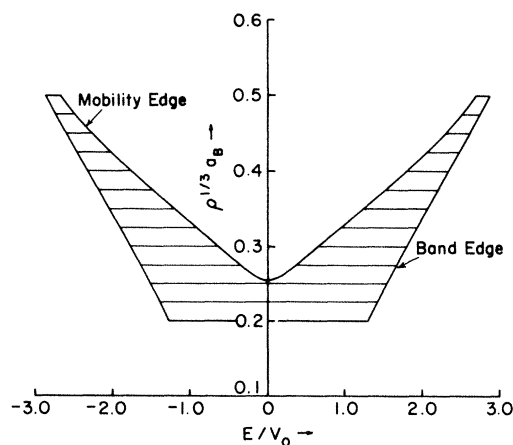


FIG. 6. Dependence of band edges (BE) and mobility edges (ME) on $\rho^{1/3}a_B$ for a three-dimensional system determined by the effective medium with Hubbard density of state. Eigenstates in the shaded region are localized.

unperturbed density of states should be also chosen so as to reflect actual spatial randomness. In this sense, an asymmetric function will be preferable as the unperturbed density of states. As for the question of the electron localization, however, the choice of the unperturbed density of states will be less important, partly because the Anderson's transition occurs at a rather low density where the average density of states look alike regardless of the choice and partly because we are concerned with the properties of eigenstates in the vicinity of the center of the energy band. Actually, the critical density at which Anderson's transition is predicted to occur in two dimensions differed 5% for different choice of the unperturbed density of states (3.1) or (3.4). These values are somewhat larger than the value $\rho_c^{1/2} a_B = 0.364$ obtained by Debney.

For three dimensions we estimated the critical density of Anderson's transition in spatially disordered systems. Our estimation $\rho_c^{1/3} a_B = 0.252$ is very close to the value predicted for Mott's transition and observed in various metal-insulator transition. A simplified model system also gave a similar value.¹⁹ This fact suggests that the density it-

self is not a relevant quantity to judge the mechanism of metal-insulator transition in spatially disordered systems.

After we completed the present work, we have learned Fertis *et al.*²⁰ used a method similar to the present one to observe localization. However, they used different forms for $N(r)$ and $V(r)$ and they have considered Bethe lattice as their effective medium. Their critical value $\rho_c^{1/3} a_B = 0.162$ for three dimensions is 36% smaller than our value.

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