Inverse Anderson Transition Caused by Flatbands

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We propose a new disorder-induced insulator-metal transition of one-electron states, which may be called the "inverse Anderson transition." We first make a highly degenerated localized states by constructing a three-dimensional periodic system possessing only flat dispersion relations. When we introduce a disorder into it, a finite-size scaling of the level statistics shows two clear (localization-delocalization and delocalization-localization) transitions for a wide range of the energy, with increasing the degree of disorder. These transitions are confirmed also by finding the system-size-independent $f(\alpha)$ characteristic of the wave function.

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It is well known that the Anderson transition is a disorder-induced metal-insulator transition of one-electron states [1]. Any periodic system has been believed to be conductive when the Fermi energy is inside of an energy band. When we introduce a disorder into it and the degree of disorder, W, comes to a critical value, the Anderson transition takes place [2–4].

In one dimension it has been proved that the critical value, W_c, vanishes [5–13]. In two dimensions, it has been believed to vanish, while in three dimension, it is positive [14]. The mobility edge in E-W space was calculated theoretically [15] and numerically [15–19]. Level statistics is one of the powerful tools to describe the transition [20]. The $f(\alpha)$ characteristic of wave functions, originally proposed by Hentschel and Procaccia [21], is another tool for describing the mobility edge [19].

However, it is not always true that Bloch waves are conductive. When we find a localized eigenstate in any periodic system, then the shifts of it at equivalent positions are obviously the eigenstates with the same eigenenergy. When the number of the independent eigenstates is equal to that of the unit cell of the crystal, we have a complete set of wave functions to construct a branch of Bloch states forming a flatband (FB). The vanishing of the group velocity of the wave packet and of the off-diagonal elements of the Green's function cause no conduction.

The FB has been studied by Mielke and Tasaki in studying ferromagnetism [22–26]. Recently Nishino, Goda, and Kusakabe proposed a new method of constructing FB by considering a localized eigenstate in any periodic system [27]. The condition of finding a FB usually leads us to a subspace of the parameter space describing the Hamiltonian. When we have a common subspace of all of them, we can find a perfect FB system in which all of the dispersion relations become flat. We cannot say the highly degenerated states of the FB are localized nor extended from a rigorous point of view. If an infinitesimally small periodic perturbation is introduced into the system with a FB to break the degeneracy, Bloch states with an infinite effective mass and an infinitesimally small bandwidth appear. However, when we introduce an infinitesimally small random perturbation into it, localized states appear by the breaking of the symmetry. We can prove in one dimension and numerically observe in two and three dimensions that the decay rate of the wave function (*Lyapunov exponent*) of an impurity state does not vanish for the infinitesimally small local perturbation.

In this Letter, we investigate some disorder-induced transitions of one-electron states in three dimension in the system with only FB's. As a typical example, we prepare a diamond lattice with fourfold-degenerated orbitals on each sites and with only FB's as is shown in Figs. 1 and 2 [28]. Then we introduce a disorder into it. If the weak disorder destroys the phase coherence of the localized eigenstates in a flatband, the localized states may melt into extended states by the disorder.

We describe the disordered system by the following tightly binding Hamiltonian

$$H = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{i,j} t_{i,j} c_i^\dagger c_j,$$

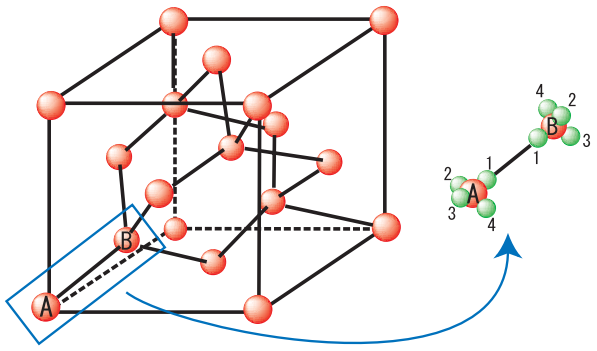

FIG. 1 (color online). Diamond lattice with fourfold-degenerated orbitals on each site. We consider the transfer integrals between orbitals within the nearest-neighbor sites. The two atoms A and B and eight orbits form a unit cell.

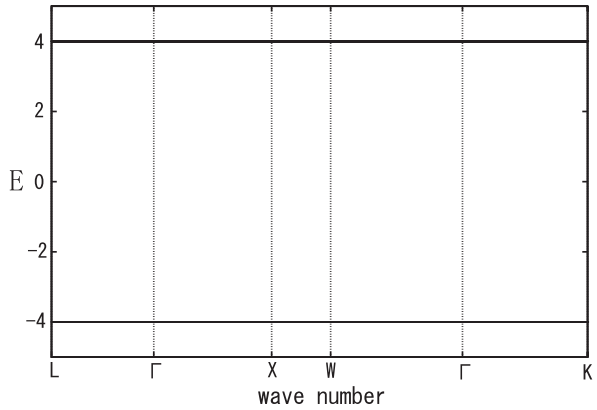

FIG. 2. Dispersion relations of the flatband model. The matrix elements of the Hamiltonian are selected as $t_{A1,A2} = 0.0$, $t_{A1,B1} = -1.0$, $t_{A1,B2} = 1.0$, $t_{A2,B4} = -1.0$, $t_{A2,B3} = -1.0$, as in Ref. [28], so that the entire dispersion relations become flat and fourfold degenerated. Cf. the indices of orbitals in Fig. 1.

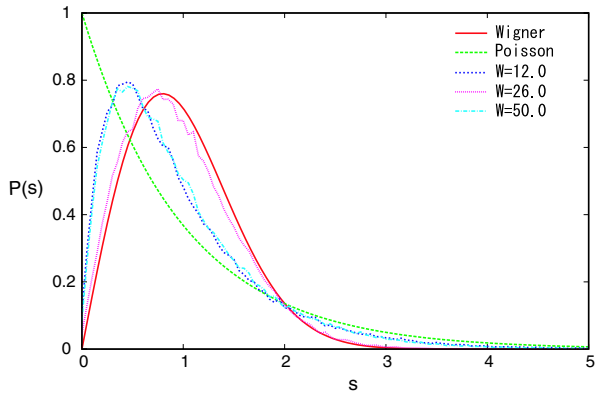

FIG. 3 (color online). Nearest-neighbor level-spacing distribution function $P(s)$ for different degrees of disorder; $W = 12$, $W = 26$, and $W = 50$, at $E = 0$ for the case of $N = 7$. Wigner (solid line) and Poisson (dotted line) functions are also shown for comparison.

where $c_i^\dagger$ and c_i are the electron creation and annihilation operators of an orbital ϕ_i, ε_i is the random on-site energy of ϕ_i, and $t_{i,j}$ is the off-diagonal matrix element between ϕ_i and ϕ_j. The values of the off-diagonal matrix elements $\{t_{i,j}\}$ have been selected as Fig. 21 of Ref. [28] so that this system has only FB's in the regular system with $\varepsilon_i = 0$ as is shown in Fig. 2. Then we introduce a disorder into all ε's so that the value of each mutually independent random variable ε_i is uniformly distributed over the range from $-W/2$ to $W/2$.

We firstly study the transition of the wave functions by the finite-size scaling of the level statistics by Shklovskii *et al.* [20]. The eigenvalues and eigenfunctions are calculated by QR algorithm with the accuracy of double precision. For extended states, the probability density $P(s)$ of the normalized nearest-neighbor level spacing s is close to the Wigner surmise $P_W(s)$, while for localized states, it is close to the Poisson distribution $P_P(s)$. They calculated numerically a parameter $\gamma(W, N)$ to measure a distance of the distribution P from P_W toward P_P, defined as

$$\gamma(W, N) \equiv \frac{A - A_W}{A_P - A_W}, \qquad A \equiv \int_2^\infty P(s)ds,$$

where A_P and A_W have been made, respectively, by P_P and P_W. The deviation $\gamma(W, N)$ from Wigner surmise ($\gamma = 0$) toward Poisson distribution ($\gamma = 1$) usually increases with increasing W for all N's, and they intersect at a particular point of W. This point gives a transition point W_c.

We exemplify in Fig. 3 $P(s)$ of the disordered FB model of size N^3 for three different values of W, at $E = 0$ for the case of $N = 7$, where N is the number of the primitive unit cells in one direction. A unit cell contains two atoms and eight orbits. Cyclic boundary condition is adopted to obtain the eigenvalues and eigenfunctions. We consider an extremely narrow window of energy containing about a few % of the total energy levels around $E = 0$ so that 10^5 levels are used to define the density, and take sample average of P to get $P(s)$. Looking at the tails of the distributions, we can see that the function $P(s)$ corresponds to the Poisson function for small W, to the Wigner function for medium W and again to the Poisson function for large W.

To compare the $P(s)$'s for different system size, we evaluate $\gamma(W, N)$ for $N = 5, 6, 7, 8$ and for $W = 12 \sim 50$. The results are shown in Fig. 4. Surprisingly, the deviation $\gamma(W, N)$ is not a monotonously increasing function with increasing W. It once drops off rapidly to a very small value and then recovers gradually with increasing W. Further, the curves intersect at $W = W_{c1} \approx 13.5$ and $W = W_{c2} \approx 37.0$, which we identify as the transition points. The transition at W_{c2} is understood as the well-known Anderson transition. On the other hand, the transition at W_{c1} is caused by the change from localized states to extended states with increasing W. It is an unknown and new transition. We calculated $\gamma(W, N)$ in a two-dimensional flatband model, and obtained again concave functions with respect to W, but these functions did not

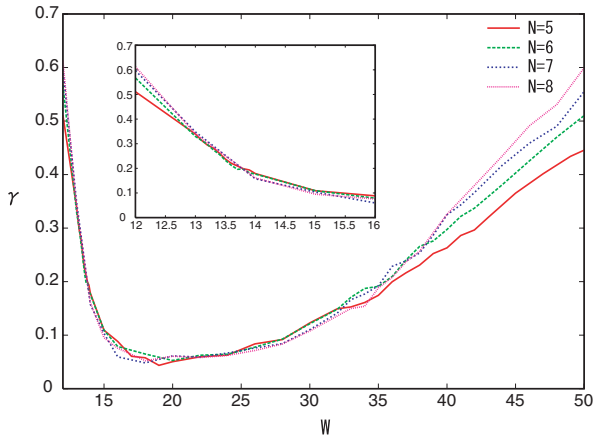

FIG. 4 (color online). The parameter γ as a function of W at $E = 0$ for different system sizes. We can find two intersecting points at which the system-size-invariant $P(s)$ appears.

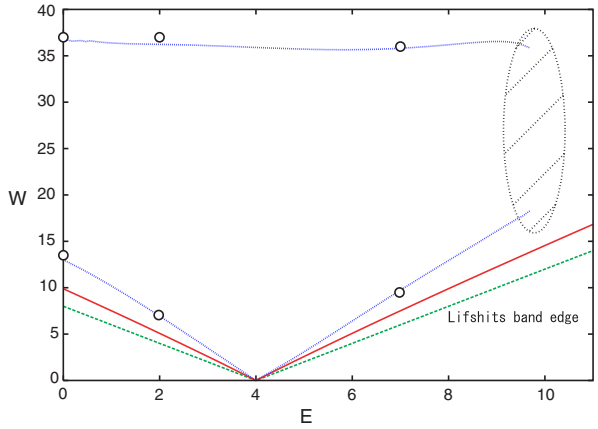

FIG. 5 (color online). The mobility-edge trajectory of the flatband model derived by the system-size-independent level statistics. There are two transition points over the entire range of energy. The mesh is the energy area in which we cannot estimate two transition points accurately. The marks ○ show the points on which the system-size-independent $f(\alpha)$ characteristics are confirmed.

intersect at any particular point. That is, we could not find disorder-induced localization-delocalization-localization transition in two dimension.

We calculated $\gamma(W, N)$ for the entire energy region to determine the mobility-edge trajectory which is shown in Fig. 5 only for positive energy. It is symmetrical around the origin of the energy axis. The solid line represents the band edge determined numerically and the dashed line does Lifshitz band edge. We cannot estimate the mobility-edge trajectory for $9 < |E| < 11$ accurately because two transition points come nearer to each other. We also avoid to describe it for $|E \pm 4| \lesssim 0.04$ $(W < 0.01)$ to keep the numerical accuracy safely enough for the quasidegenerated eigenvalues.

We secondly verify the two transitions by investigating the system-size dependence of the $f(\alpha)$ characteristic of the electronic wave functions [29]. The function $f(\alpha)$ describes the fractal dimension of the subset of space on which the strength of singularity of the probability measures $\mu_k(L) = \sum_{n_k=1}^{L^3} |\psi(n_k, E)|^2$ $(k = 1, 2, \ldots, N^3/L^3)$ of the wave function $\psi(n, E)$ takes a value of α, where L and N are the linear sizes of a box and the total system, respectively, and $\mu_k(L) = l^\alpha$ for a small decreasing parameter $l \equiv L/N$.

To obtain $f(\alpha)$ numerically, by the standard box counting method [21,29,30], we define $\mu_k(q, L) = \mu_k^q(L)/\sum_{k'} \mu_{k'}^q(L)$ and calculate the strength of singularity

$$\alpha(q) = \lim_{l \to 0} \sum_k \mu_k(q, L) \ln \mu_k(1, L) / \ln l,$$

as well as the corresponding fractal dimension

$$f(q) = \lim_{l \to 0} \sum_k \mu_k(q, L) \ln \mu_k(q, L) / \ln l,$$

for various values of q on the range $[-5, 5]$. The symbol $\lim_{l \to 0} \sum$ describes the asymptotic behavior of $\sum$ for decreasing L down to 1 for a fixed N.

It is well known that the $f(\alpha)$ characteristic at the transition points is system-size independent [31]. The $f(\alpha)$ characteristics of the FB model for the particular values of W, $W = 14.0$, and $W = 37.0$ at $E = 0$ are shown in Fig. 6. We can see that the $f(\alpha)$ characteristics for the two particular values of disorder are size independent. Of course, $f(\alpha)$ characteristics for $W < 14.0$ and for $W > 37.0$ both exhibit localization behavior, while for $14.0 < W < 37.0$ does delocalization one. And hence, the two values of W show us two transition points. The new $f(\alpha)$ characteristic for the localization-delocalization transition at W_{c1} seems slightly different from that of the ordinary Anderson transition at W_{c2}. However, the error bars are too big for insisting the difference.

Some studies on Anderson transition in a three-dimensional simple cubic lattice reported an existence of two transition points near the band edge [17,19]. But the level statistics in the present study have not been able to find the two transition points in it [32]. The level statistics need an amount of level density even near the band edge. But the localized states near the Lifshitz band have a very low density of states and they are usually on or outside of the numerically estimated band edge for systems with a tractable size. The level statistics for systems with a numerically tractable size can find only the well-known Anderson transition in the ordinary disordered systems.

To summarize, we have shown a new disorder-induced localization-delocalization transition starting from a perfect FB system by a finite-size scaling of level statistics and $f(\alpha)$ characteristic. The localization for $W < W_{c1}$ is not due to the strength of disorder but to the characteristic of localization in FB which persists under a weak random perturbation. Therefore, the localized states for $W < W_{c1}$ are expected to be of new type and the insulator-metal

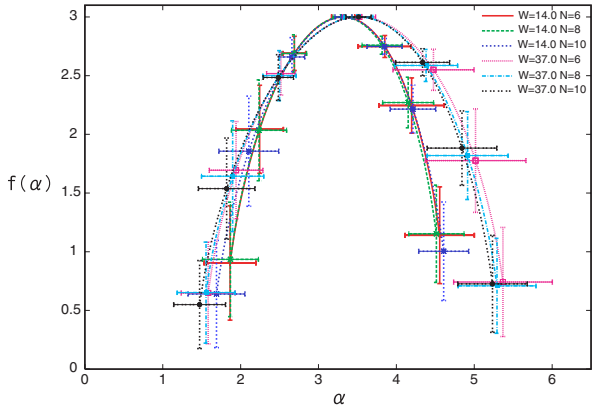

FIG. 6 (color online). The $f(\alpha)$ characteristics of the wave functions for $W = 14.0$ and $W = 37.0$ at $E = 0$. Error bars are made by using 100 samples and are indicated on f and α for $q = -5, -2, -1, 0, 1, 2, 5$ for the case $N = 6, 8, 10$.

transition at $W = W_{c1}$ is also expected to be of new one. Further studies will be made on these issues.

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[1] P. W. Anderson, Phys. Rev. **109**, 1492 (1958).
[2] See a review by B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993), and references therein.
[3] See a review by I. M. Lifshitz, S. A. Gredeskul, and A. Pastur, *Introduction to the Theory of Disordered Systems* (Wiley, New York, 1988), and references therein.
[4] See a review by C. M. Soukoulis and E. N. Economou, Waves Random Media **9**, 255 (1999), and references therein.
[5] R. Landauer, Philos. Mag. **21**, 863 (1970).
[6] K. Ishii, Prog. Theor. Phys. Suppl. **53**, 77 (1973).
[7] I. Y. Goldsheid, S. A. Molchanov, and S. A. Pastur, Funct. Anal. Appl. **11**, 1 (1977).
[8] M. Goda, Prog. Theor. Phys. **62**, 608 (1979).
[9] M. Goda, Prog. Theor. Phys. Suppl. **72**, 232 (1982).
[10] E. Abrahams and M. J. Stephen, J. Phys. C **13**, L377 (1980).
[11] B. Anderech and E. Abrahams, J. Phys. C **13**, L383 (1980).
[12] H. Kunz and B. Souillard, Commun. Math. Phys. **75**, 179 (1980).
[13] F. Deylon, H. Kunz, and B. Souillard, J. Phys. A **16**, 25 (1983).
[14] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).
[15] A. D. Zdetsis, C. M. Soukoulis, E. N. Economou, and G. S. Grest, Phys. Rev. B **32**, 7811 (1985).
[16] A. MacKinnon and B. Kramer, Z. Phys. B **53**, 1 (1983).
[17] B. Bulka, B. Kramer, and A. MacKinnon, Z. Phys. B **60**, 13 (1985).
[18] M. Schreiber, Phys. Rev. B **31**, R6146 (1985).
[19] H. Grussbach and M. Schreiber, Phys. Rev. B **51**, R663 (1995).
[20] B. I. Shklovskii, B. Shapiro, B. R. Sears, P. Lambrianides, and H. B. Shore, Phys. Rev. B **47**, 11 487 (1993).
[21] H. G. E. Hentschel and I. Procaccia, Physica (Amsterdam) **8D**, 435 (1983).
[22] A. Mielke, J. Phys. A **24**, 3311 (1991).
[23] A. Mielke, J. Phys. A **25**, 4335 (1992).
[24] A. Mielke, Phys. Lett. A **174**, 443 (1993).
[25] H. Tasaki, Phys. Rev. Lett. **69**, 1608 (1992).
[26] A. Mielke and H. Tasaki, Commun. Math. Phys. **158**, 341 (1993).
[27] S. Nishino, M. Goda, and K. Kusakabe, J. Phys. Soc. Jpn. **72**, 2015 (2003).
[28] S. Nishino and M. Goda, J. Phys. Soc. Jpn. **74**, 393 (2005).
[29] A. Chhabra and R. V. Jensen, Phys. Rev. Lett. **62**, 1327 (1989).
[30] J. Feder, *Fractals* (Plenum, New York, 1992).
[31] M. Schreiber and H. Grussbach, Phys. Rev. Lett. **67**, 607 (1991).
[32] E. Hofstetter and M. Schreiber, Phys. Rev. B **48**, 16 979 (1993).