Numerical study of symmetry effects on localization in two dimensions

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Effects of symmetry on localization on two-dimensional square lattices are studied numerically. The inverse localization length is determined by the system-size dependence of the Thouless number in magnetic fields or in the presence of strong spin-orbit interactions. A finite-size-scaling method is also applied to the case of spin-orbit interactions. Extended states, present in each Landau level in strong magnetic fields or in the case of small randomness, are found to merge together with increasing randomness and disappear beyond a certain critical randomness. In weak magnetic fields, the field tends to reduce the localization near the band center, while the localization is enhanced in the band-tail region. Spin-orbit interactions cause effects similar to, but much stronger than, that due to a weak magnetic field. The critical randomness and exponent for a metal-insulator transition are determined in the presence of strong spin-orbit interactions.

I. INTRODUCTION

In perfect crystals, electron wave functions may be described by Bloch functions extending over the whole crystal. However, actual materials always contain certain randomness, such as impurities, lattice defects, etc. When such randomness is sufficiently large, electrons become confined and localized in a finite region of space.[1] Despite much recent progress, there still remain many unanswered fundamental questions on this Anderson localization problem. Several review articles have already been published on this subject.[2-6] In the localization problem the symmetry as well as the dimensionality of systems are known to play an important role. The purpose of the present paper is to present results of numerical study of symmetry effects on localization in two-dimensional systems.

The localization problem can most easily be understood by a scaling argument.[7,8] Consider a d-dimensional hypercube with characteristic system size L. By combining different hypercubes of the same size, we can construct a hypercube with characteristic system size $2L$. By repeating such a procedure starting with a small system, we can obtain energy levels and wave functions of a system having arbitrary size. Combination of two hypercubes causes mixings of energy levels, especially of those whose energies are closest. Let $V(L)$ be the resonance energy between such levels and $W(L)$ be their energy difference. Whether states are localized or extended is determined by the system-size dependence of the Thouless number $g(L)=V(L)/W(L)$. If states are localized, $g(L)$ decreases with increasing system size L, reflecting how wave function decays with the distance from the localization center. For extended states, $g(L)$ is proportional to the conductance of the hypercube. In the single-parameter scaling theory,[9] we assume that $g(L)$ is only a relevant scaling parameter, i.e., $g(bL)=h(b,g(L))$. This gives the scaling relation $d\ \mathrm{lng}/d\ \mathrm{ln}L=\beta(g)$, which leads to the conclusion that states are all localized for dimensions $d\leq 2$. In $d=1$ this agrees with the well-known fact that states are always localized exponentially however small randomness may be.[10,11]

It has been known that there are essentially three different universality classes for the symmetry of systems, i.e., orthogonal, unitary, and symplectic.[12] The orthogonal case corresponds to systems in the presence of time-reversal symmetry, where the Hamiltonian is represented by a real symmetric matrix and the corresponding wave functions can be chosen as real. Transfer integrals between energy levels of two hypercubes are given by a real number or their "dimensionality" becomes $\omega=1$. When a magnetic field is applied, the time-reversal symmetry is broken, and consequently the wave functions become complex because the Hamiltonian becomes a complex Hermitian matrix. We have now $\omega=2$. If we take into account electron spins, we have another symmetry called symplectic in the presence of spin-orbit interactions. Even in the presence of spin-orbit interactions, each state is always doubly degenerate (the Kramers degeneracy) if the system is invariant under time reversal. In this case interactions are allowed between degenerate levels and $\omega=4$. This ω is the level-repulsion exponent in random-matrix theory.[12]

It is expected that states are less easily localized in systems with large ω. As a matter of fact, there exist some current-carrying extended states giving rise to the quantum Hall effect in each Landau level in strong magnetic fields.[13-15] This is quite in contrast to the system in the absence of fields for which states are believed to be always localized. (See reviews on the quantum Hall effect[16-18] for more details.) There have been some suggestions based on perturbations in weak-localization regime,[19-21] renormalization-group calculations,[22-25] and numerical study[26,27] that a metal-insulator transition is possible in the presence of strong spin-orbit interactions.

Perturbation calculations in weak-localization regime[19-21,28-30] make a very interesting prediction for the behavior of the scaling function $\beta(g)$. In two dimensions for $g\gg 1$, we have $\beta(g)\approx -a/g$ with $a>0$ in the ortho-

gonal case and $a<0$ in the symplectic case. In the unitary case, we have $a=0$ and to the leading order $\beta(g)\approx -a/g^2$ with $a>0$. This predicts that $\beta(g)$ is always negative and states are all localized in the orthogonal and unitary cases. In the symplectic case, however, $\beta(g)$ can be positive for sufficiently large g. In more intuitive terms, this corresponds to a constructive rather than destructive interference in the forward direction due to impurity scattering.[4] Since states are always localized in strong-scattering cases,[31] $\beta(g)$ becomes eventually negative for small g, giving rise to a critical randomness g_c which separates exponentially localized states from those having divergent conductivity. This has naturally led to the expectation that there can be a metal-insulator transition in two dimensions for the symplectic case.

Numerical methods have been used extensively in the localization problem because of the limitations of existing analytical techniques. Various methods have been proposed. Yoshino and Okazaki provided the first numerical evidence for localization by diagonalizing matrix Hamiltonians up to 100×100 sites using Lanczos method.[32] The equation-of-motion method in which the time-dependent Schrödinger equation is integrated numerically has been used to calculate the inverse participation ratio, diffusion constants, and dc conductivity.[33–37] The Thouless-number method, first introduced by Edwards and Thouless,[38] has been used extensively by Licciardello and Thouless[39,40] and it has given the first indication that states are all localized in two dimensions in the orthogonal case. In this method, $g(L)$ is estimated by the energy shift of individual energy levels due to a change in boundary conditions and the localization length is determined by its system-size dependence directly. Various scaling or renormalization-group calculations have been performed,[41–43] and one of the most successful methods has turned out to be the finite-size scaling applied successfully by MacKinnon and Kramer[44,45] and by many others.[46–52] Using this method, we consider systems in the form of a long strip and study the dependence of inverse localization length on the width.

Numerical methods have been applied also to systems belonging to unitary and symplectic universality classes. The localization in strong magnetic fields has been most extensively studied in connection with the quantum Hall effect. In two-dimensional systems in strong magnetic fields, orbital motions are completely quantized and density of states comprises discrete Landau levels. The Thouless-number method has been successful in demonstrating that states are all localized exponentially except at a single energy close to the center of each Landau level.[53] The finite-size-scaling method has also been applied and given the same conclusion.[54,55] Two-dimensional systems on lattices have also been studied in magnetic fields.[56,57] Some have suggested the presence of mobility edge in each Landau level in high magnetic fields.[56] In symplectic cases the investigations based on the finite-size-scaling method by MacKinnon[26] and Evangelou and Ziman[27] have given results consistent with the presence of a metal-insulator transition in two dimensions. However, the maximum width of systems considered has been limited to a very small value and the results are not so conclusive. The symmetry dependence has been studied by other methods also.[58,59]

It is now well known that effects of electron-electron interactions are strongly modified in the presence of randomness and sometimes dominate the transport properties of actual systems at low temperatures. For example, there have been suggestions that the metallic phase in the presence of strong spin-orbit interactions can be destroyed by many-body effects.[60,61] However, the problem on localization of noninteracting-electron systems is still very important and interesting from a fundamental point of view. In this paper, we perform a numerical study to further clarify the roles of different symmetries in the localization problem in two dimensions. We employ both Thouless-number and finite-size-scaling method on square lattices in magnetic fields or in the presence of strong spin-orbit interactions.

The organization of the present paper is as follows. In Sec. II the models are introduced and the numerical methods are briefly reviewed. Results of the Thouless-number study are presented in Sec. III. Extended states present in weak-disorder cases disappear above a certain critical randomness. In weak-magnetic-field regime, the magnetic field always tends to decrease localization for states near the band center, while it tends to enhance localization for states near the band edges. Effects of spin-orbit interactions are similar to those of weak magnetic fields, although effects are much stronger. Results are consistent with the presence of a metal-insulator transition, but cannot give a definite conclusion because of the limitation due to finite system sizes. To obtain more reliable answers on this problem, the finite-size-scaling method is used in the presence of strong spin-orbit couplings in Sec. IV, from which we can obtain the value of critical randomness and exponent. In the appendix a derivation is made of a model Hamiltonian describing spin-orbit couplings in a square lattice. A very preliminary account of a part of this work has been presented elsewhere.[62,63]

II. MODELS AND METHODS

A. Magnetic field

To study effects of magnetic fields, we consider a tight-binding model for the square lattice described by the following Hamiltonian:

$$\mathcal{H}=\sum_i \varepsilon_i c_i^\dagger c_i-\sum_{i,j} V\exp\left[\frac{ie}{2\hbar c}\mathbf{H}\cdot(\mathbf{R}_i\times\mathbf{R}_j)-\frac{ie}{\hbar c}\mathbf{A}\cdot(\mathbf{R}_i-\mathbf{R}_j)\right]c_i^\dagger c_j\ , \tag{2.1}$$

where $\mathbf{R}_i$ denotes the position of the ith site, the site energy ε_i varies at random with distribution width W ($-W/2\le\varepsilon_i\le W/2$), and the magnetic field H perpendicular to the system is included in the form of Peierls' phase factor in the nearest-neighbor transfer integral with $\mathbf{A}=(Hy/2,Hx/2)$. The randomness is character-

ized by the ratio W/V and the magnetic field by the ratio of the flux $\Phi=Ha^2$ within a unit cell of the lattice constant a to the unit flux $\Phi_0=hc/e$. The energy spectrum in the absence of disorder, $W=0$, has been obtained by Hofstadter[64] and comprises p different bands. (Landau levels) when $\Phi/\Phi_0=q/p$ with integers p and q.

B. Spin-orbit interactions

To study effects of spin-orbit interactions, we consider a system shown in Fig. 1 consisting of s-like and p-like atomic orbitals and concentrate on the band associated with s orbitals. The s orbitals form a square lattice and the effective transfer between the neighboring s orbitals is determined by a second-order perturbation via a transfer integral with the connecting p orbital. The direct transfer integral between s orbitals is neglected. The p orbitals are located on a plane parallel but displaced from the plane of the square lattice formed by s orbitals. Spin-orbit interactions are present only in p atoms whose energy is assumed to lie far from that of s orbitals. The effective Hamiltonian for the s band with spin $\sigma=\uparrow$ or $\downarrow$ is calculated in the Appendix.

We have

$$\mathcal{H}=\sum_i \varepsilon_i c_{i\sigma}^{\dagger}c_{i\sigma}-\sum_{i,j} V(i,\sigma;j,\sigma')c_{i\sigma}^{\dagger}c_{j\sigma'}\ , \tag{2.2}$$

where $V(i,\sigma;j,\sigma')=V_x$ or V_y depending on the direction of the nearest-neighbor site in the x or y direction. We have, in matrix form,

$$V_x=\begin{bmatrix} V_1 & V_2 \\ -V_2 & V_1 \end{bmatrix} \quad \text{and} \quad V_y=\begin{bmatrix} V_1 & -iV_2 \\ -iV_2 & V_1 \end{bmatrix}, \tag{2.3}$$

with

$$|\uparrow\rangle=\begin{bmatrix}1\\0\end{bmatrix} \quad \text{and} \quad |\downarrow\rangle=\begin{bmatrix}0\\1\end{bmatrix}. \tag{2.4}$$

This Hamiltonian is expected to simulate actual two-dimensional systems in n-channel inversion layers on surfaces of III-V compound semiconductors if we consider states with low energies, where the s band corresponds to the conduction band and the p bands correspond to the valence bands.[65] The strength of the spin-orbit interaction is characterized by the parameter $S=V_2/V$ with $V=(V_1^2+V_2^2)^{1/2}$.

Figure 2 compares the energy bands in the presence of strong spin-orbit interactions, i.e., $S=0.5$ with those in its absence ($S=0$). Figure 3 gives the corresponding density of states. Note that the fourfold symmetry is present in spite of apparent breaking in the x and y direction in Eq. (2.2). As a matter of fact, we can change V_x into V_y and vice versa by an appropriate modification of the phase of atomic wave functions at each site. As is well known, the density of states in the square lattice exhibits a steplike increase at the band edge characteristic of two dimensions and a logarithmic singularity at the band center corresponding to a saddle-point dependence of energy on the wave vector in the absence of spin-orbit interactions. Because of the lack of inversion symmetry, the spin-orbit interaction lifts the spin degeneracy except at certain high-symmetry point in the first Brillouin zone (Γ, X, and M in Fig. 2) and gives rise to more singularities in the density of states. These additional logarithmic singularities are not strong and smeared out if randomness is switched on.

The spin splitting in the presence of spin-orbit interactions, which was first pointed out by Ohkawa and Uemura[66] in n-channel inversion layers on narrow-band-gap

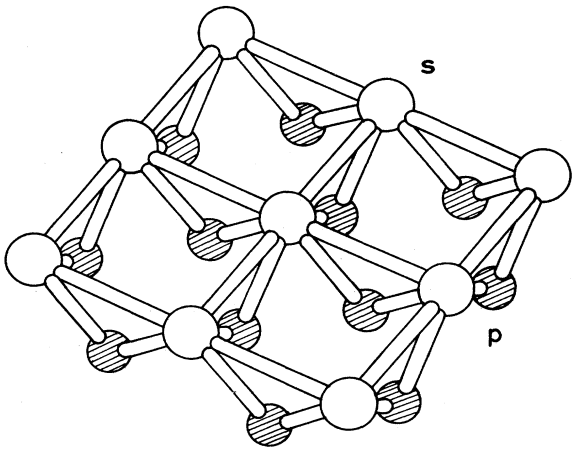

FIG. 1. Schematic illustration of a square-lattice system formed by atoms with s and p orbitals. The open spheres represent s atoms and the shaded spheres p atoms whose atomic plane is displaced by an amount of δ from that of the s atomic plane. The transfer between nearest s orbitals is mediated by transfer through a p atomic orbital lying in between. Spin-orbit interactions are present only in p atomic orbitals.

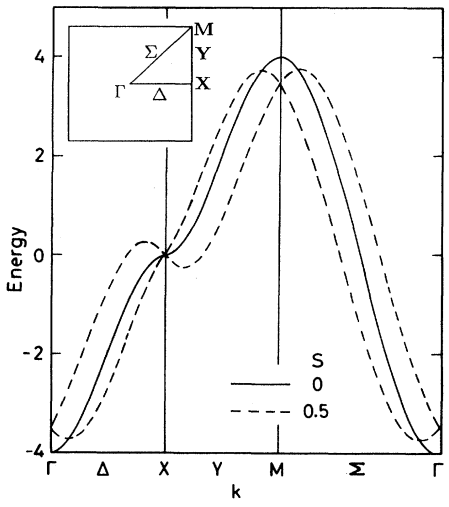

FIG. 2. The energy-band structure of a square lattice. The solid line is that in the absence of spin-orbit interactions and the dashed lines in their presence ($S=0.5$). The energy is measured in units of V and the bandwidth for $S=0$ is 8. The inset shows the two-dimensional Brillouin zone.

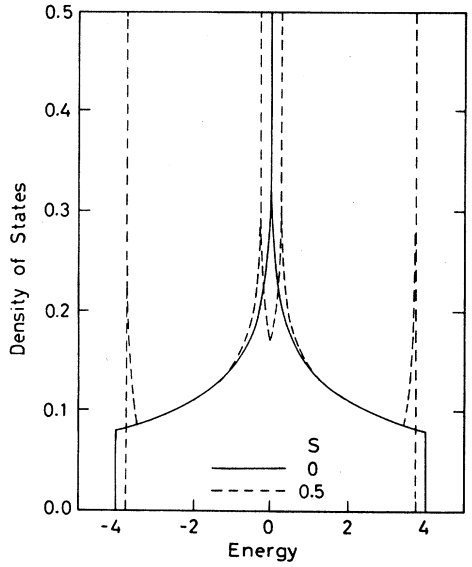

FIG. 3. The density of states of a square lattice without randomness. The solid line is that in the absence of spin-orbit interactions and the dashed lines in their presence ($S=0.5$).

$Hg_{1-x}Cd_xTe$, has been a controversial topic.[65] Note that this spin splitting does not mean the removal of the Kramers degeneracy and that states are always doubly degenerate irrespective of the degree of randomness if we solve Eq. (2.2). Under a magnetic field, this degeneracy is lifted and the symmetry of the system changes from symplectic to unitary and the localization effect is expected to be stronger. As a matter of fact, perturbation calculations in weak-localization regime have predicted positive magnetoresistance meaning stronger localization.[67]

MacKinnon used an anisotropic model with off-diagonal disorder in which in one direction the transfer integrals are constant and connect like spins while in the other direction they have random phases and connect unlike spins equally.[26] Evangelou and Ziman[27] used a model with off-diagonal randomness similar to the local-gauge-invariant model proposed by Wegner.[68] These models are not very realistic although they may retain certain essential aspects of the Hamiltonian which determine its universality class. On the other hand, the present model is more realistic in a sense that it can simulate actual inversion layers or heterostructures in spite of its simplicity.

C. Thouless-number method

The inverse localization length $\alpha(E)$ is determined by the study of the system-size dependence of the Thouless number $g(L)$, i.e., $g(L)\propto\exp(-\alpha L)$. The Thouless number is defined as the ratio of the shifts ΔE of the individual energy levels due to a change in boundary conditions to the level separation $L^{-2}[D(E)]^{-1}$, where $D(E)$ is the density of states. The calculation of the density of states is straightforward. The number of eigenvalues is counted in each energy interval and the results are accumulated for all the samples of a given size. As the density of states is insensitive to the system size L, the final density of states is obtained by further averaging of those systems with different sizes. The energy shifts are calculated by replacing periodic boundary conditions by antiperiodic conditions in the y direction. The geometric mean ΔE of energy shifts ΔE_i is defined as $\ln\Delta E=\langle\ln|\Delta E_i|\rangle$, where $\langle\cdots\rangle$ denotes an average over levels and samples for a given energy interval. In actual numerical calculations we take averages over a large number of samples, the size of which is in the range $5<L/a<32$.

D. Finite-size-scaling method

Consider a system with width L_y and length L_x. If L_x is much larger than L_y, the system is essentially one dimensional and states are all localized exponentially in the x direction. Let $\alpha(L_y)$ be the inverse localization length of a system with width L_y. Then, we can determine the inverse localization length α in two dimensions by a study of the L_y dependence of $\alpha(L_y)$. Conventionally, we plot $\alpha(L_y)L_y$ as a function of L_y in logarithmic scales and seek the following scaling relation:

$$\alpha(L_y,E,W/V,H,S)L_y=f(\alpha(E,W/V,H,S)L_y)\ . \tag{2.5}$$

The inverse localization length $\alpha(L_y)$ can be calculated within a desired accuracy using the well-known technique of Green's function. We first separate the system into cells in such a way that the cell k consists of the L_y sites (k,l) $(l=1,2,\ldots,L_y)$. The Hamiltonian is written as

$$\mathcal{H}=\sum_{k=1}^{L_x}|k)\mathcal{H}_k(k|+\sum_{k=1}^{L_x-1}[|k)\mathcal{H}_{k,k+1}(k+1|+\text{H.c.}]\ , \tag{2.6}$$

where $|k)$ is the set of L_y ket vectors belonging to the kth cell and $\mathcal{H}_k=\mathcal{H}_{k,k}$. We define the diagonal and off-diagonal Green's functions, respectively, by

$$g(j)=(j|(E-\mathcal{H}^{(j)})^{-1}|j)\ , \tag{2.7a}$$

$$G(j)=(1|(E-\mathcal{H}^{(j)})^{-1}|j)\ , \tag{2.7b}$$

where $\mathcal{H}^{(j)}$ is the total Hamiltonian for the strip comprising the first to jth cells excluding the intercell Hamiltonian $\mathcal{H}_{j,j+1}$ and $\mathcal{H}_{j+1,j}$. These Green's functions for long strips can be obtained by a set of recursion formulas in matrix form,

$$G(j+1)=G(j)\mathcal{H}_{j,j+1}g(j+1)\ , \tag{2.8a}$$

$$g(j+1)=[E-\mathcal{H}_{j+1}-\mathcal{H}_{j+1,j}g(j)\mathcal{H}_{j,j+1}]^{-1}\ . \tag{2.8b}$$

We can thus calculate $G(j)$ for arbitrary j by iteration starting form $G(1)=g(1)=(E-\mathcal{H}_1)^{-1}$ with numerical procedure limited only by the availability of computation time. The inverse localization length can be obtained from G as

$$\alpha(L_y)=-\lim_{j\to\infty}[2(j-1)]^{-1}\ln[\mathrm{Tr}G^{+}(j)G(j)]\ . \tag{2.9}$$

In magnetic fields, elements of Green's function appearing in the above recursion formula are complex. In the presence of spin-orbit interactions each element is given by a quaternion number. A quaternion z is generally written as

$$z = z_0\tau_0 + z_1\tau_1 + z_2\tau_2 + z_3\tau_3 , \tag{2.10}$$

where $\tau_0\tau_u = \tau_u\tau_0 = \tau_u$, $\tau_p^2 = -\tau_0$, and $\tau_p\tau_q = -\tau_q\tau_p = \tau_r$ with $u = 0,1,2,3$ and (p,q,r) an even permutation of (1,2,3). Explicitly, we have

$$\tau_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \tau_1 = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad \tau_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

and (2.11)

$$\tau_3 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}.$$

There can be several ways of performing actual numerical calculations in the presence of spin-orbit interactions. The method employed in this paper is to express each matrix element in terms of a quaternion number [a set of four real numbers z_j $(j = 0,1,2,3)$] and explicitly use its multiplication table. It is also possible to express each number in terms of a (2×2) matrix and perform usual matrix calculations. However, the latter method has turned out to require more computational time than the former. Further, it leads to a numerical instability, in which each element of Green's function is no longer expressed by Eq. (2.10) after many times of iterations.

III. THOULESS-NUMBER STUDY

The Thouless-number method has been used extensively by Licciardello and Thouless.[39,40] At first they tried to confirm the presence of the minimum metallic conductivity and its universality in two dimensions suggested originally by Mott.[69] Numerical calculations for smaller systems have shown that there really exists a minimum metallic conductivity independent of randomness and lattice structures.[39] The critical randomness has been suggested to be $(W/V)_c \sim 6$ for square lattices. However, later investigations for larger systems ($L \sim 30$) have revealed that states are always localized in two dimensions.[40]

We first apply the method to square lattices ($L_x = L_y = L$) with $L = 8$, 16, 24, and 32 in units of the lattice constant a in the absence of a magnetic field and

TABLE I. Sample numbers used in the Thouless-number study. Actual sample numbers are twice those shown below because of the symmetry about the band center.

W/V:	3	4	5	6	7	8	10	15	20
				$H = S = 0$					
$L = 8$	1200	1200	1200	1200		1200	1200	1180	1200
$L = 16$	300	300	300	300		300	300	234	436
$L = 24$	130	130	130	130		130	130	130	130
$L = 32$	75	75	75	75		75	75	0	0
				$Ha^2/\Phi_0 = \frac{1}{4}$					
$L = 8$	720	2240	2240	2240	2240	720	720		
$L = 16$	180	600	600	600	600	180	180		
$L = 24$	80	270	270	270	280	90	90		
$L = 32$	48	158	257	158	160	50	50		
				$Ha^2/\Phi_0 = \frac{1}{8}$					
$L = 8$	720	2240	2240	2240	2240	720	720	990	1020
$L = 16$	180	600	600	600	600	180	180	234	237
$L = 24$	90	280	280	280	280	90	90	112	113
$L = 32$	50	160	160	160	160	50	50	0	0
				$Ha^2/\Phi_0 = \frac{1}{5}$					
$L = 10$	486	486	486	486	486	486	486		
$L = 15$	216	216	216	216	216	216	216		
$L = 20$	121	121	121	90	90	121	121		
$L = 25$	77	77	77	77	77	77	77		
$L = 30$	54	54	54	54	54	54	54		
				$S = 0.5$					
$L = 5$		2415	2415	2415	2415	2415	2415	2415	
$L = 10$		600	600	537	600	600	600	600	
$L = 15$		265	265	265	265	265	265	265	
$L = 20$		150	150	150	150	150	150	150	
$L = 25$		95	95	95	95	95	95	0	

spin-orbit interaction. The numbers of samples used in the calculation are listed in Table I. Figure 4 gives the density of states and Fig. 5 gives an example of the system-size dependence of the Thouless number for randomness $W/V=6$, which shows that the Thouless number decreases with increasing system size L exponentially at all energies indicating that states are all localized exponentially. Although not shown explicitly, the same conclusion can be obtained also for $W/V=5$. For randomness smaller than $W/V\sim 4$, the localization length becomes much larger than the maximum system size $L=32$ and we can no longer deduce any definite conclusions.

A. Magnetic fields

Sample numbers used in the Thouless-number study in magnetic fields are also listed in Table I. Figure 6 shows the density of states in the magnetic field $H\alpha^2/\Phi_0=\frac{1}{4}$ as a function of energy for different degrees of disorder. In this magnetic field, the density of states is split into four Landau levels symmetric about the band center ($E=0$) for sufficiently small randomness. With increasing randomness the density of states of adjacent levels overlaps with each other.

An example of the system-size dependence of the Thouless number is shown in Fig. 7. By fitting the results

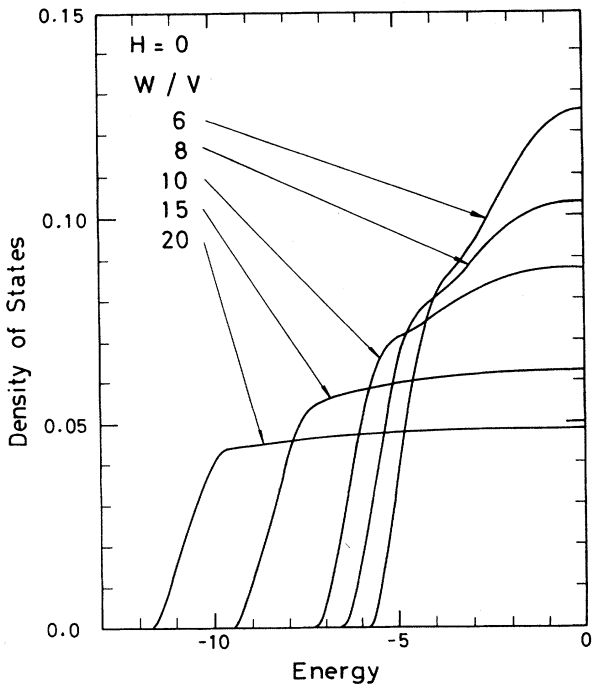

FIG. 4. The density of states of a square lattice for different values of the randomness W/V in the absence of magnetic fields and spin-orbit interactions. Only the low-energy part is shown because of the symmetry about the band center ($E=0$). For large randomness such as $W/V\gtrsim 8$ the density of states is not affected by spin-orbit interactions ($S=0.5$) and weak magnetic fields ($Ha^2/\Phi_0=\frac{1}{8}$).

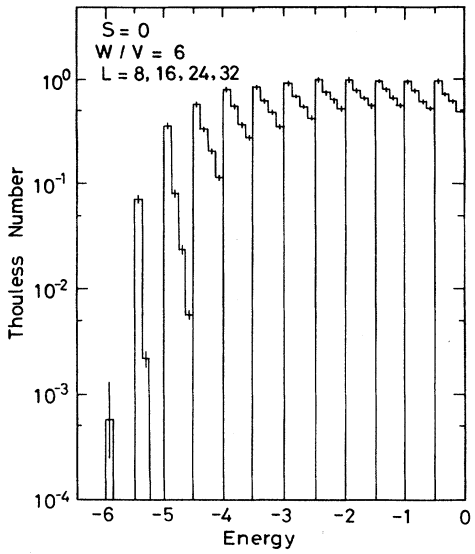

FIG. 5. An example of system-size dependence of the Thouless numbers in the absence of magnetic fields and spin-orbit interactions. Within each energy interval with width 0.5 (in units of V), $g(L)$'s for $L=8$, 16, 24, and 32 are plotted. All states are localized exponentially.

to $g(L)=g_0\exp[-\alpha(E)L]$, we can determine the inverse localization length $\alpha(E)$. The results are shown in Fig. 8. For small randomness, the inverse localization length becomes extremely small at a certain energy within each Landau level. Although it is difficult to give definite con-

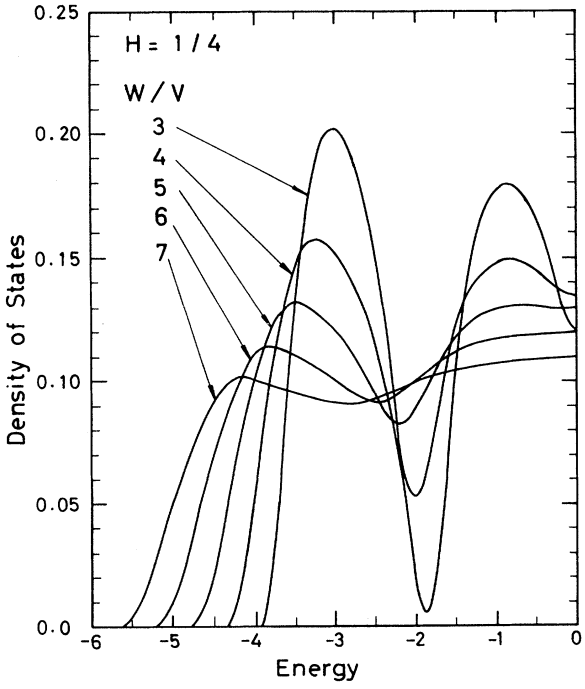

FIG. 6. Calculated density of states of a square lattice in the magnetic field $Ha^2/\Phi_0=\frac{1}{4}$. Only the low-energy half is shown because of the symmetry about the band center $E=0$.

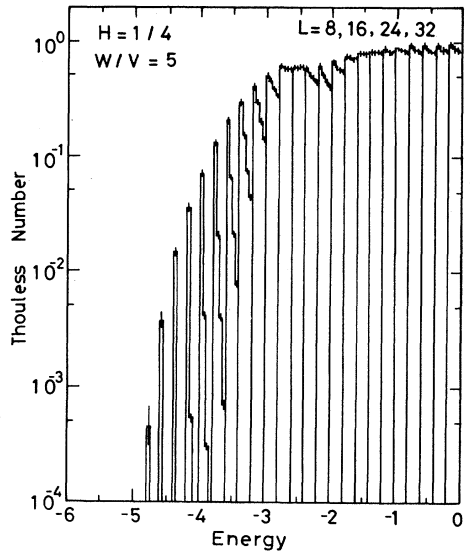

FIG. 7. An example of system-size dependence of the Thouless numbers in a magnetic field $Ha^2/\Phi_0=\frac{1}{4}$ for $W/V=5$. Within each energy interval with width 0.2 (in untis of V), $g(L)$'s for $L=8$, 16, 24, and 32 are plotted.

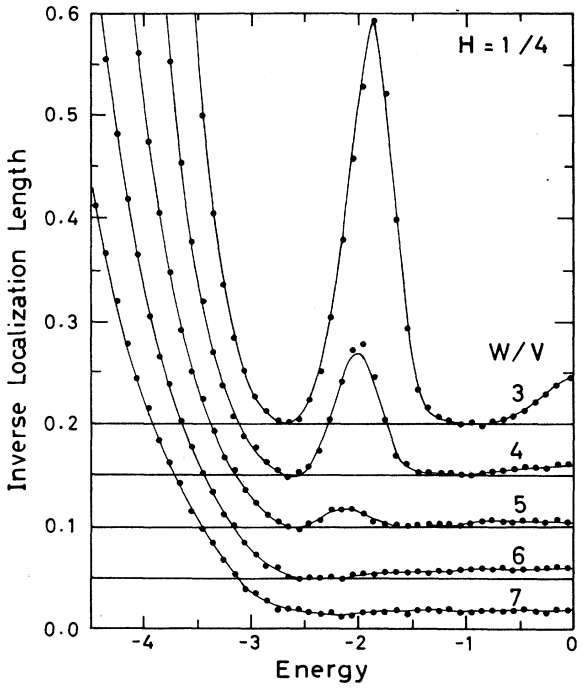

FIG. 8. Calculated inverse localization length of a square lattice as a function of energy in the magnetic field $Ha^2/\Phi_0=\frac{1}{4}$. There seem to exist two extended states for randomness $W/V<6$. The energies of the two extended states approach each other with increasing W/V and merge together around $W/V=6$. Above this randomness the inverse localization length is everywhere positive, meaning that states are localized exponentially.

clusions, we can expect that there exist extended states at a single energy in each Landau level. This is in agreement with the conclusion obtained in planar two-dimensional systems in high magnetic fields. In the limit of high magnetic fields, the argument based on the Hall conductivity has shown the presence of current-carrying extended states in each Landau level.[13–15] Previous calculations[53–55] have given a power-law dependence of α on energy in the vicinity of extended states, $\alpha(E)\propto|E|^s$ with $s\sim 2$ for the lowest and $s\lesssim 4$ for the first excited Landau level.[70]

The energy of extended states for the lowest Landau level is shifted toward the higher-energy side from that of the peak of the density of states. This is due to strong mixings with higher Landau levels and again agrees qualitatively with the result obtained in systems without lattices.[53] The two extended states below the band center (the two above the band center, because of the symmetry) merge together with increasing randomness and disappear above a certain randomness of the order of $(W/V)_c\approx 6$.

Similar results are obtained for $Ha^2/\Phi_0=\frac{1}{8}$, where the band splits into eight Landau levels (four below and four above the band center) as is shown in Fig. 9. The corresponding inverse localization length is given in Fig. 10. Unfortunately, the maximum system size is still too small and statistical fluctuations are too large to give a definite answer in this magnetic field. Again, extended states disappear above a similar critical randomness, where ex-

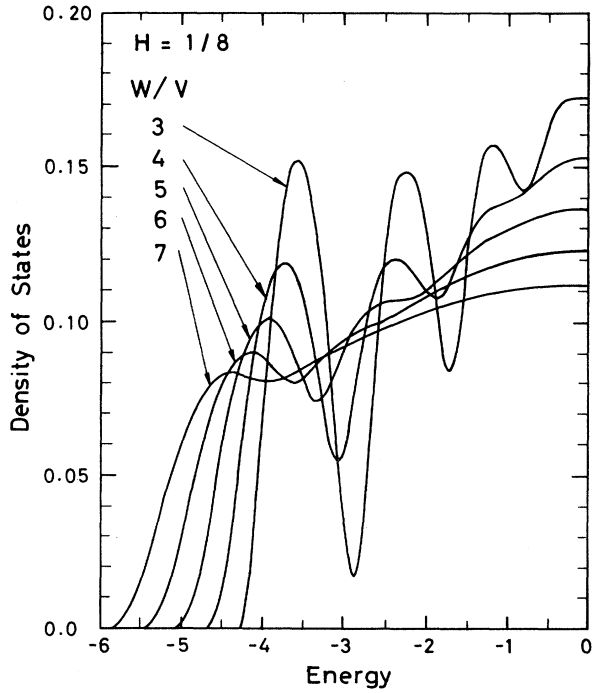

FIG. 9. Calculated density of states of a square lattice in the magnetic field $Ha^2/\Phi_0=\frac{1}{8}$. Only the low-energy half is shown because of the symmetry about the band center $E=0$.

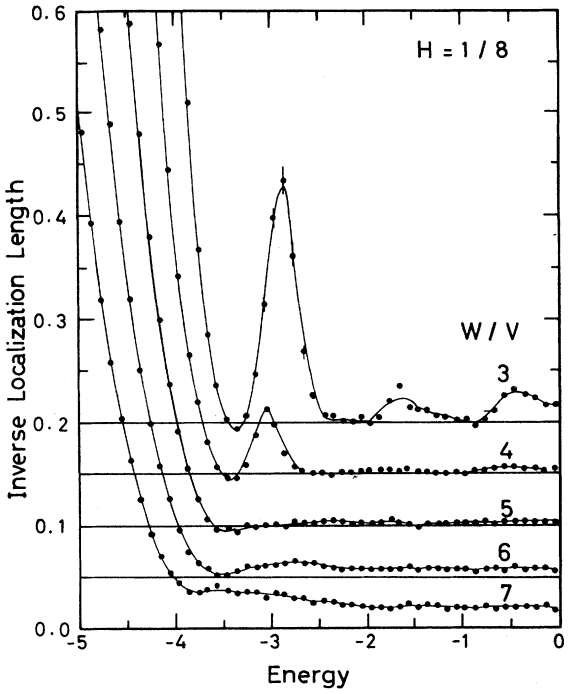

FIG. 10. Calculated inverse localization length of a square lattice as a function of energy in the magnetic field $Ha^2/\Phi_0=\frac{1}{8}$. There seem to exist extended states for each Landau level except that closest to the band center. Above $W/V\sim 6$ the inverse localization length is everywhere positive, meaning that states are all localized exponentially.

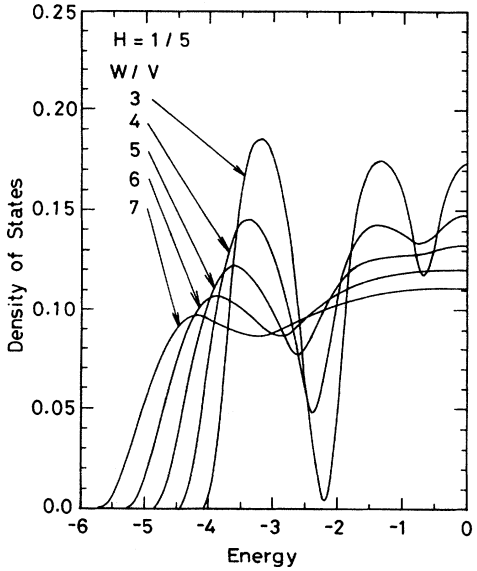

FIG. 11. Calculated density of states of a square lattice in the magnetic field $Ha^2/\Phi_0=\frac{1}{5}$. Only the low-energy half is shown because of the symmetry about the band center $E=0$.

tended states of the lowest two Landau levels seem to merge.

Figure 11 shows the density of states in the field $Ha^2/\Phi_0=\frac{1}{5}$, for which the density of states is split into five Landau levels. There exists a Landau level (with large broadening even in the absence of randomness) just at the band center in this case. The inverse localization length is shown in Fig. 12. The two lowest Landau levels below the band center are quite similar to those for $Ha^2/\Phi_0=\frac{1}{4}$, i.e., they merge with increasing randomness and disappear above a certain randomness of the order of $(W/V)_c\approx 6$. At the band center the inverse localization length is small for sufficiently small randomness and becomes definitely positive for $W/V\gtrsim 6$.

When the randomness is sufficiently large, i.e., in weak-magnetic-field regime, states are always localized exponentially. Figure 13 compares the inverse localization length $\alpha(E)$ in the presence and absence of a magnetic field. The magnetic field tends to reduce the localization for states close to the band center, i.e., the negative magnetoresistance, while it enhances the localization for states in the region of the band tails, i.e., the positive magnetoresistance. The decrease of the localization effect around the band center is consistent with the results of perturbation calculations in weak-localization regime[19–21] and also with other numerical works.[58] Note here that the density of states for such large randomness is not influenced by a magnetic field at all ($W/V\gtrsim 8$). This increase of the localization effect at band tails due to magnetic fields can easily be understood by the analogy with a hydrogen atom, in which, as is well known, the magnetic field tends to enhance the binding energy and

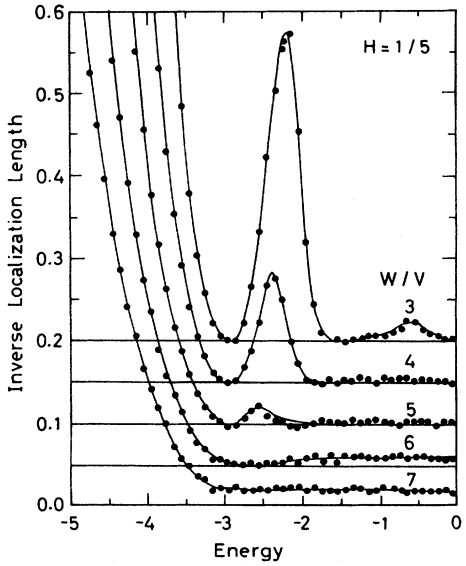

FIG. 12. Calculated inverse localization length of a square lattice as a function of energy in the magnetic field $Ha^2/\Phi_0=\frac{1}{5}$. There seem to exist extended states for each Landau level. Above $W/V\sim 6$ the inverse localization length is everywhere positive, meaning that states are all localized exponentially.

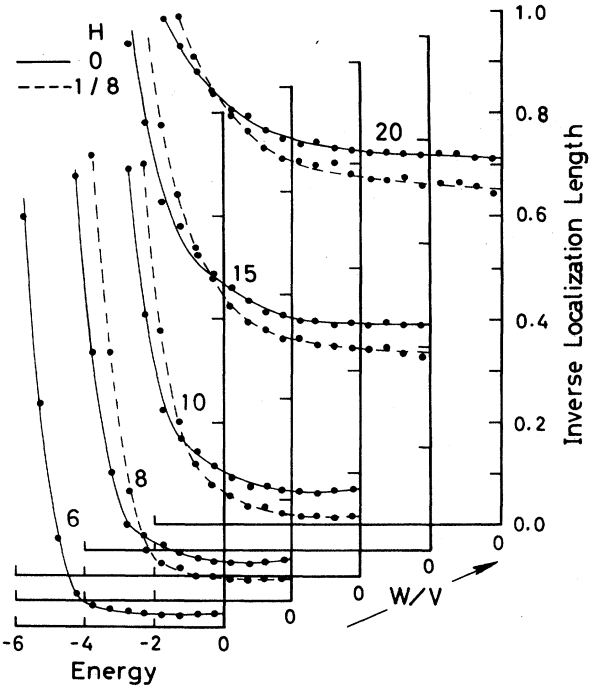

FIG. 13. Calculated inverse localization length of a square lattice. Only the low-energy part is shown because of the symmetry about the band center ($E=0$). The solid lines represent results in the absence of magnetic fields and spin-orbit interactions, and the dashed lines those in the magnetic field $Ha^2/\Phi_0=\frac{1}{8}$. The numbers appearing in the figure show W/V. Statistical errors are within the size of circles.

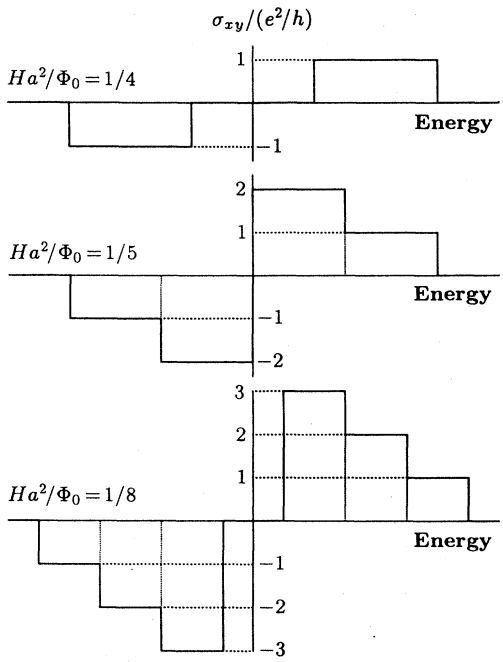

FIG. 14. A schematic illustration of the Hall conductivity in a square lattice in magnetic fields in the absence of randomness. The top figure corresponds to the magnetic field $Ha^2/\Phi_0=\frac{1}{4}$ with four Landau levels, the middle to $Ha^2/\Phi_0=\frac{1}{5}$ with five Landau levels, and the bottom to $Ha^2/\Phi_0=\frac{1}{8}$ with eight Landau levels. The Hall conductivity in the spectral gap is always quantized into an integer multiple of e^2/h.

shrink the ground-state wave function. Figure 13 shows that the inverse localization length remains almost independent of energy away from the center $E=0$ and then starts to grow rapidly below a certain energy. The energy which separates the positive and negative magnetoresistance corresponds to such a crossover energy.

For $W/V=6$, 8, and 10, the inverse localization length takes a local maximum at the band center in the absence of a magnetic field. This is in qualitative agreement with the results of Zdetsis *et al.*,[48] who employed the finite-size-scaling method in calculating the inverse localization length away from the band center. This has been ascribed to effects of the logarithmic singularity of the density of states at the band center. The present results in the absence of a field are also quantitatively in agreement with those of the finite-size-scaling method: We have, for example, $\alpha\approx 0.027$ for $W/V=6$ and $\alpha\approx 0.44$ for $W/V=15$ at the band center. The corresponding results of MacKinnon and Kramer[45] are $\alpha\approx 0.027$ for $W/V=6$ and $\alpha\approx 0.45$ for $W/V=15$.

The way in which extended states disappear with increasing randomness is closely related to the Hall conductivity σ_{xy}, which is always quantized into integer multiples of e^2/h whenever energy is in spectral gaps. The integers have been obtained by Thouless *et al.* for arbitrary magnetic fields given by $Ha^2/\Phi_0=p/q$ with p and q integers in the absence of randomness.[71] Figure 14 gives a schematic illustration of σ_{xy} as a function of energy in magnetic fields $Ha^2/\Phi_0=\frac{1}{4}$, $\frac{1}{5}$, and $\frac{1}{8}$. The Hall conductivity in the present system is antisymmetric with respect to the band center, i.e., $\sigma_{xy}(-E)=-\sigma_{xy}(E)$.

In magnetic field $Ha^2/\Phi_0=\frac{1}{4}$, σ_{xy} becomes $-e^2/h$ when the Fermi energy lies between the lowest two Landau levels. There must be two extended states below the band center and they should disappear together at $(W/V)_c$, which is consistent with the present result that the two extended states associated with the two Landau levels merge and disappear. In magnetic field $Ha^2/\Phi_0=\frac{1}{5}$, σ_{xy} changes from $-2e^2/h$ to $2e^2/h$ when the Fermi energy moves from the spectral gap lying below the Landau level at the band center to the gap lying above. The present result shows that the two extended states associated with the lowest two Landau levels merge and disappear at a critical randomness. It is not possible to determine whether the extended states at the band center disappear faster than these two or not. (It is even likely that states at the band center become localized immediately in the presence of randomness.) If the extended states just at the band center disappear faster than the two below and above, σ_{xy} just below the band center should change suddenly from $-2e^2/h$ to 0. In the opposite case, σ_{xy} should become identically zero as soon as the extended states associated with the lowest two Landau levels disappear.

Because of insufficient system sizes in magnetic field $Ha^2/\Phi_0=\frac{1}{8}$, we cannot determine whether four extended states below the band center merge and disappear at the same time or separately. However, there should exist at least two different extended states just below the critical randomness at which all extended states disappear, and they should disappear at the same time. In any case, it would be very interesting if we could calculate the Hall conductivity in the present system. There have been attempts to calculate σ_{xy} in finite-size systems numerically.[72] However, exact determination of the quantized value of σ_{xy} is quite difficult, because σ_{xy} depends strongly on boundary conditions and only its average over different boundary conditions is quantized into integer multiple of e^2/h.

B. Spin-orbit interactions

To study effects of strong spin-orbit interactions, we consider systems with size $L=5$, 10, 15, 20, and 25. Sample parameters are listed in Table I and Fig. 15 gives calculated system-size dependence of the Thouless number. Systems with size $L=5$ exhibit behavior quite different from other larger systems, which is presumably due to their too-small size. In the following analysis we shall neglect data for $L=5$ completely.

Figure 16 shows the inverse localization length $\alpha(E)$ as a function of energy for $S=0.5$ and 0. It is clear that the spin-orbit interaction tends to reduce the localization effect for states near the band center. For $W/V=6$ the inverse localization length at the center almost vanishes in the presence of spin-orbit interaction, while states already exhibit clear exponential localization in its absence. From the present results, however, it is not possible to conclude the presence of extended states, i.e., the position of the mobility edge E_c, for sufficiently small randomness. Even if there is a mobility edge, the critical exponent s defined by $\alpha(E)\propto|E-E_c|^s$ is much larger than unity, which makes it improbable to determine E_c.

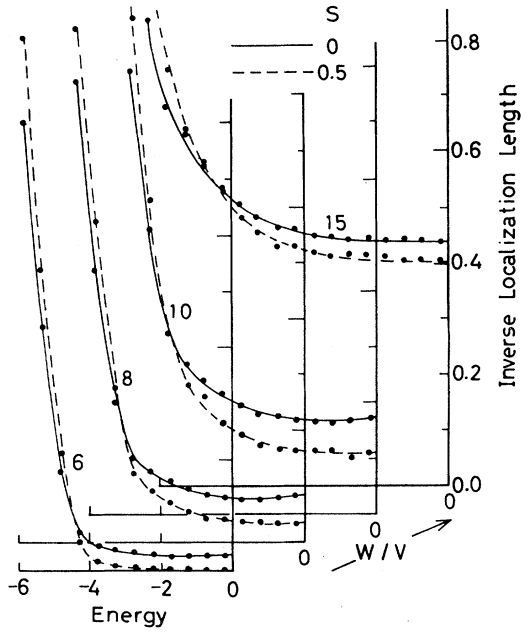

FIG. 16. Calculated inverse localization length of a square lattice. Only the low-energy part is shown because of the symmetry about the band center ($E=0$). The solid lines represent results in the absence of spin-orbit interactions ($S=0$) and the dashed lines those in their presence ($S=0.5$). The numbers appearing in the figure show W/V. Statistical errors are within the size of circles.

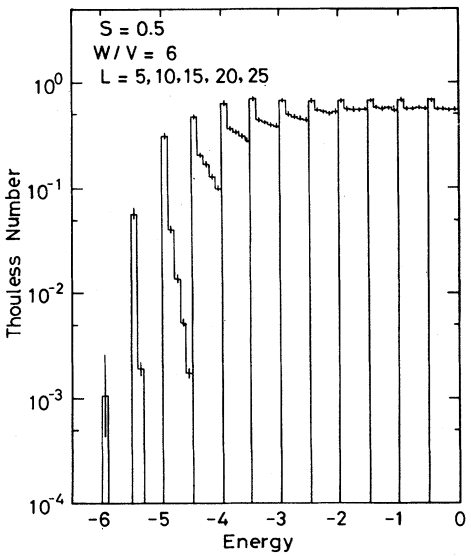

FIG. 15. An example of system-size dependence of the Thouless numbers in the presence of strong spin-orbit interactions ($S=0.5$). Within each energy interval with width 0.5 (in units of V), $g(L)$'s for $L=5$, 10, 15, 20, and 25 are plotted. The system with size $L=5$ exhibits results quite different from those with large sizes and the results for $L=5$ are discarded in the analysis.

In the energy region corresponding to the band tails, the spin-orbit interaction enhances the localization effect. This is exactly the same as the weak-magnetic-field case discussed in the previous section and can also be understood by the analogy with a hydrogen atom in the presence of the spin-orbit interaction. The spin-orbit interaction lowers the energy of the ground state in the second order, thus decreasing the spatial extent of the wave function. Note, however, that the density of states for randomness larger than $W/V\sim4$ is not influenced by nonzero S if the energy is measured in units of V.

IV. FINITE-SIZE-SCALING STUDY

In order to determine whether a metal-insulator transition is possible in the presence of strong spin-orbit interactions, the finite-size-scaling method is applied to states at the band center. The inverse localization length $\alpha(L_y)$ is calculated for systems with width $L_y=4$, 8, 16, 32, and 64 by the iteration technique given in Sec. II. The maximum length of samples is typically $L_x\sim4\times10^5$,

which gives $\alpha(L_y)$ within a statistical error of the order of a few percent. We employ periodic boundary conditions in the y direction, i.e., we consider the geometry of long cylinders. The inverse localization length $\alpha(L_y)$ can depend on these boundary conditions in the y direction. This dependence has already been examined by MacKinnon and Kramer in the orthogonal case and been shown to be unimportant except in the case of very small L_y's and weak randomness.[44] We can expect that the same is applicable to the present case.

The results are given in Fig. 17. Using these results, we can calculate the scaling function, which is shown in Fig. 18. This scaling function is quite similar to those obtained for three-dimensional systems in the absence of spin-orbit interactions and shows the presence of a metal-insulator transition around $W/V \sim 6$ in agreement with the result obtained by the Thouless-number study discussed in the previous section. To determine the absolute magnitude of the inverse localization length, we use the result of the Thouless-number study. In particular we use α for $W/V=15$ for which the Thouless-number method can give α in good accuracy. The resulting inverse localization lengths are plotted as a function of the randomness W/V in Fig. 19 together with the results of the Thouless-number study. The two different methods give results in good agreement with each other. The inverse localization length approaches zero very gradually with decreasing randomness.

To determine the critical randomness $(W/V)_c$ and the critical exponent ν, defined by $\alpha \propto |(W/V)-(W/V)_c|^{\nu}$, we plot $\ln\alpha$ as a function of $\ln|(W/V)-(W/V)_c|$ for different values of $(W/V)_c$ and seek $(W/V)_c$ which makes the result closest to a straight line. The obtained result is given in Fig. 20, from which we can estimate $(W/V)_c=5.875\pm0.010$ and $\nu=2.05\pm0.08$. As has been pointed out by MacKinnon and Kramer,[45] this method

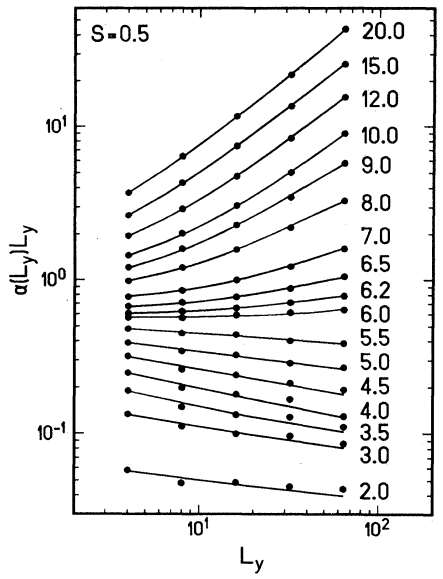

FIG. 17. Calculated inverse localization length of long strips multiplied by width L_y at the band center as a function of L_y in the presence of strong spin-orbit interactions ($S=0.5$). Lines are just guide to the eye. Error bars due to statistical fluctuations are much smaller than the circles size for $W/V \gtrsim 5$ but are of the same order or slightly larger for smaller randomness.

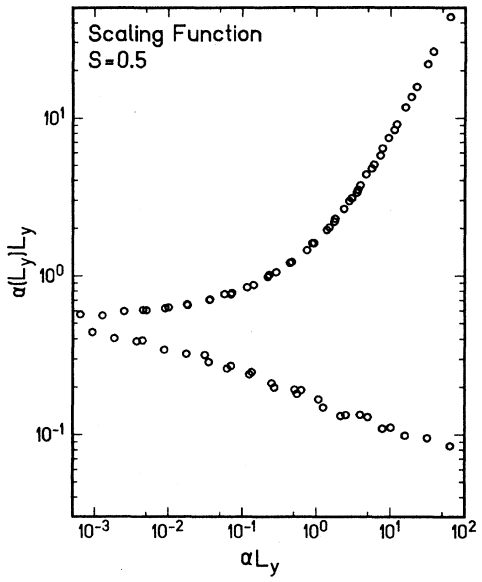

FIG. 18. Scaling function in the presence of strong spin-orbit interactions ($S=0.5$) determined from the data given in the previous figure.

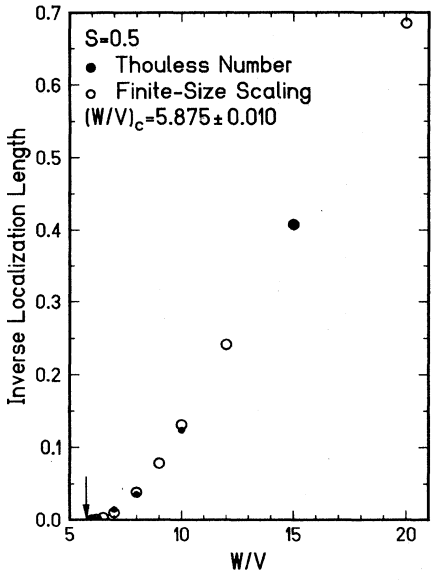

FIG. 19. Calculated inverse localization length vs randomness W/V in the presence of strong spin-orbit interactions ($S=0.5$). Open circles represent results calculated by the finite-size-scaling method and solid circles by the Thouless-number method. The absolute value of α in the finite-size-scaling method is set equal to that of the Thouless-number method at $W/V=15$. The arrow indicates the position of the critical randomness at which a transition to metallic conduction occurs (see next figure).

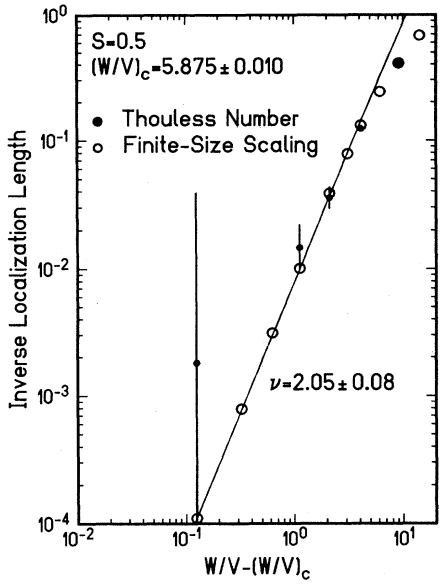

FIG. 20. Inverse localization length vs randomness measured from the critical values $(W/V)_c=5.875$ in the presence of strong spin-orbit interactions ($S=0.5$). Open circles represent results calculated by the finite-size-scaling method and closed by the Thouless-number method. From the straight line the critical exponent is estimated as $\nu=2.05\pm0.08$.

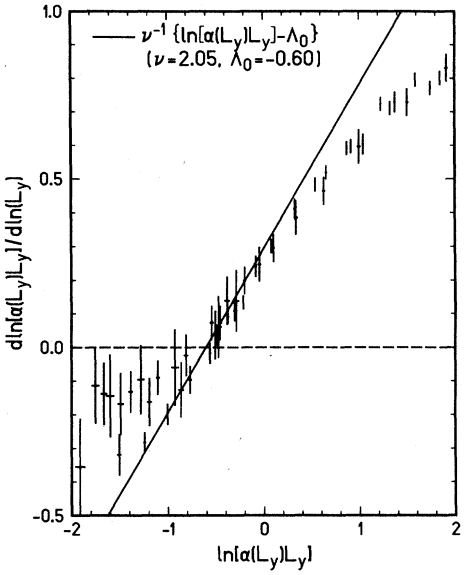

FIG. 21. Calculated logarithmic derivative $d\ln[\alpha(L_y)L_y]/d\ln L_y$ as a function of $\ln[\alpha(L_y)L_y]$ in the presence of strong spin-orbit interactions. The derivatives, estimated by taking differences of the results given in Fig. 18, are plotted only for $W/V\geq4$. The solid straight lines corresponds to $\nu=2.05$.

may possibly give rise to a systematic error in the critical exponent ν. Another way of calculating ν is to plot the logarithmic derivative $d\ln[\alpha(L_y)L_y]/d\ln L_y$ as a function of $\ln[\alpha(L_y)L_y]$ and calculate the gradient χ at the point where the logarithmic derivative vanishes. The critical exponent ν is related to χ through $\nu=1/\chi$. The logarithmic derivatives can be estimated by corresponding differences, which are plotted in Fig. 21. Unfortunately, the results are noisy because of large statistical errors originating from taking differences and can hardly give a definite value of χ. It is clear, however, that they are consistent with $\nu=2.05$ obtained above.

MacKinnon[26] has performed a finite-size-scaling calculation based on his model of anisotropic off-diagonal randomness up to width $L_y=16$ in contrast to the present maximum width $L_y=64$. Evangelou and Ziman[27] have reported similar calculations within a model with off-diagonal randomness again up to width $L_y=16$. Both of these works have given scaling functions qualitatively similar to that given in Fig. 19 with a different critical value of randomness. MacKinnon has given $(W/V)_c\sim4$ and Evangelou and Ziman $(W/V)_c\sim7$. This difference originates presumably from the difference in the model. Because of insufficiencies in the width of systems, the critical exponent has not been obtained in these works.

Grempel[24] and Kawabata[25] have independently suggested that the single-parameter scaling is inadequate and the spin-relaxation time is required as an additional relevant scaling parameter. In particular, Kawabata has obtained a phase diagram in which for a fixed strength of spin-orbit scatterings the system undergoes a transition from insulator to metal (having infinite conductivity) with decreasing randomness. Although the present calculation is consistent with the single-parameter scaling, it may not have enough accuracy to rule out the possibility suggested by them. Kawabata has shown that the phase diagram is quite insensitive to the strength of spin-orbit interactions over the wide range, suggesting that the deviation from the single-parameter scaling can be very small.

MacKinnon and Kramer[44,45] calculated the scaling function $\beta(g)$ appearing in the single-parameter scaling function using Landauer's conductance formula in one dimension,[73] $g=(e^2/\pi\hbar)T/(1-T)$, and setting the transmission coefficient $T=\exp[-2\alpha(L_y)L_y]$. This is based on the assumption that the long strip is made up of blocks of size L_y and that the resultant one-dimensional system of blocks has the inverse localization length $\alpha(L_y)$. It is certainly possible to calculate $\beta(g)$ in the present case under the same assumptions. The resulting $\beta(g)$ changes from negative to positive at sufficiently large g, which is quite similar to that obtained by MacKinnon and Kramer in three dimensions in the orthogonal case except in the case of very large g. (We cannot give any reliable results for very large g or in weak-localization regime because of the insufficient system width.) This is obvious because the scaling function $f(\alpha L_y)$ itself looks similar. Note, however, that replacement of the system by the one-dimensional system of blocks may not be straightforwardly justified in the present case. As a matter of fact, in one dimension, spin-orbit interactions disappear and the system belongs to orthogonal universality class.

V. SUMMARY AND CONCLUSION

In this paper, a numerical study has been made of the effect of different symmetries on localization in two-dimensional systems. We have considered magnetic-field effects as an example of systems belonging to the unitary universality class and effects of spin-orbit interactions belonging to the symplectic universality class. Effects of magnetic fields have been included as a Peierls' phase factor of transfer integrals in square lattices. As the model of systems with strong spin-orbit interactions, we have considered the band consisting of s atomic orbitals with transfer integrals mediated by a p atomic orbital lying in between. A strong spin-orbit splitting of degenerate p orbitals give rise to direction-dependent spin off-diagonal transfers among s orbitals.

The Thouless-number method has been applied to study effects of magnetic fields. The results strongly suggest that there exist extended states (at a single energy) in each Landau level for sufficiently small randomness and disappear above a certain critical randomness. The critical randomness is given by $(W/V)_c \sim 6$ almost independent of magnetic-field strength within the field range studied ($Ha^2/\Phi_0 = \frac{1}{4}, \frac{1}{5}$, and $\frac{1}{8}$). At $(W/V)_c$, at least two extended states merge and disappear together. This agrees with the prediction obtained from discussions of the quantization of the Hall conductivity. In case of large randomness or in weak magnetic fields (in the sense that $\omega_c \tau \ll 1$ with $\hbar\omega_c$ the energy separation of Landau levels and $\hbar/\tau$ broadening due to scattering from randomness), the magnetic field always tends to reduce localization effects at the band center, whereas it tends to enhance localization effects at band tails.

Effects of spin-orbit interactions have also been studied in the Thouless-number method. It has been shown that spin-orbit interactions give effects qualitatively similar to magnetic fields in the weak-field regime, i.e., they reduce localization effects around the band center but enhance localization at band tails. Even in the presence of strong spin-orbit interactions, states are all localized exponentially for randomness larger than $W/V \sim 6$. For smaller randomness, they may be extended states but the limitation of system sizes prevents any definite conclusions. We have applied a finite-size-scaling method to systems with strong spin-orbit interactions, in which the maximum width reaches up to $L_y = 64$. The results have turned out to be consistent with the presence of extended states for small randomness and given the critical randomness $(W/V)_c = 5.875 \pm 0.010$ with exponent $\nu = 2.05 \pm 0.08$.

It may be worthwhile to give a warning on the well-known limitation of the numerical study: The maximum size of systems treated is limited by the current ability of computers and more importantly conclusions are strongly influenced by various assumptions made in the analysis of results of calculations. In the present study, the crucial assumptions are $g(L) = \exp(-\alpha L)$ in the Thouless-number method and the scaling hypothesis $\alpha(L_y)L_y = f(\alpha L_y)$ in the finite-size-scaling method. The results should always be taken with some reservation, which certainly applies to the present study.

ACKNOWLEDGMENTS

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APPENDIX: SPIN-ORBIT INTERACTIONS

Let E_s and E_p be the energy of s and p atomic orbitals, respectively, where $E_s > E_p$. In the presence of spin-orbit interactions the degenerate p levels consisting of the $|x)$, $|y)$, and $|z)$ orbitals split into the two sets $J = \frac{3}{2}$ and $J = \frac{1}{2}$ with J the total angular momentum. The states $J = \frac{3}{2}$ have energy $E_p + \Delta/3$ and those with $J = \frac{1}{2}$ have $E_p - 2\Delta/3$. The parameter Δ characterizing the strength of spin-orbit interactions is defined as

$$\Delta = i\frac{3\hbar}{4m^2c^2}\left[x\left|\frac{\partial U}{\partial x}p_y - \frac{\partial U}{\partial y}p_x\right|y\right], \tag{A1}$$

where U is the atomic potential for p-like orbitals. The eigenfunctions for states $J = \frac{3}{2}$ are as follows:

$$|+\tfrac{3}{2}) = +\frac{1}{\sqrt{2}}|(x - iy)\uparrow), \tag{A2a}$$

$$|+\tfrac{1}{2}) = +\frac{i}{\sqrt{6}}|(x + iy)\downarrow) - i\sqrt{\tfrac{2}{3}}|z\uparrow), \tag{A2b}$$

$$|-\tfrac{1}{2}) = +\frac{1}{\sqrt{6}}|(x - iy)\uparrow) + \sqrt{\tfrac{2}{3}}|z\downarrow), \tag{A2c}$$

$$|-\tfrac{3}{2}) = +\frac{i}{\sqrt{2}}|(x - iy)\downarrow), \tag{A2d}$$

and those for $J = \frac{1}{2}$ are

$$|+\tfrac{1}{2}) = +\frac{1}{\sqrt{3}}|(x - iy)\downarrow) + \frac{1}{\sqrt{3}}|z\uparrow), \tag{A3a}$$

$$|-\tfrac{1}{2}) = -\frac{i}{\sqrt{3}}|(x - iy)\uparrow) + \frac{i}{\sqrt{3}}|z\downarrow). \tag{A3b}$$

Consider the configuration in which s-like orbitals form a lattice with lattice points $(i_x a, i_y a, 0)$, where i_x and i_y are an integer. We assume, as is shown in Fig. 1, that a p-like orbital connecting s-like orbitals at $(i_x a, i_y a, 0)$ and $((i_x + 1)a, i_y a, 0)$ is at $((i_x + \frac{1}{2})a, i_y a, -\delta)$ and a p-like orbital connecting s-like orbitals at $(i_x a, i_y a, 0)$ and $(i_x a, (i_y + 1)a, 0)$ is at $(i_x a, (i_y + \frac{1}{2})a, -\delta)$. Define further $E_g = E_s - E_p - \Delta/3$. By simple second-order perturbation theory, we can easily get

$$V_x \equiv V(i_x, i_y; i_x + 1, i_y) = \begin{bmatrix} V_1 & V_2 \\ -V_2 & V_1 \end{bmatrix}, \tag{A4a}$$

$$V_y \equiv V(i_x, i_y, ; i_x, i_y + 1) = \begin{bmatrix} V_1 & -iV_2 \\ -iV_2 & V_1 \end{bmatrix}, \tag{A4b}$$

with

$$V_1=\frac{3E_g+2\Delta}{3E_g(E_g+\Delta)}(V_{sp}^{\sigma})^2\cos(2\theta)\ , \tag{A5a}$$

$$V_2=-\frac{\Delta}{3E_g(E_g+\Delta)}(V_{sp}^{\sigma})^2\sin(2\theta)\ , \tag{A5b}$$

where $\tan\theta=2\delta/a$ and V_{sp}^{σ} is the transfer integral between an s atomic orbital and a p orbital.

When the atomic plane of p orbitals is the same as that of s orbitals ($\delta=0$ or $\theta=0$), the matrix element between different spins vanishes and the spin splitting disappears. This is in agreement with the well-known theorem that the bands are always doubly degenerate even in the presence of spin-orbit interactions if the system has an inversion symmetry. In this limit, however, the Hamiltonian belongs to the orthogonal university class. In the present model we can choose any values for the ratio of V_1 and V_2 by varying θ as long as the spin-orbit parameter Δ is nonzero.

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