Correlation effect on magnetoconductance in the strongly localized regime with spin-orbit interaction

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Correlation effects are investigated theoretically in the strongly Anderson-localized regime in the presence of spin-orbit (SO) interaction. Based on numerical studies on the Hubbard model with disordered on-site energies, we determine the magnetic-field dependence of the nearest-neighbor hopping conduction. In the absence of the SO interaction the magnetoconductance (MC) is positive through the Zeeman effect. In the presence of the SO effect the MC can be negative in low magnetic fields while it becomes positive in high magnetic fields. The multilevel Hubbard model, which has more than one level at each site, is also examined. The calculated results are qualitatively in good agreement with an experimental result of the nearest-neighbor hopping conduction in a Cu-particle film. We discuss the possibility of observing the proposed MC in other systems, e.g., an array of quantum dots.

I. INTRODUCTION

In the strongly Anderson-localized regime, both the interference effect and the electron-electron interactions play important roles. The interference effect on the variable-range-hopping (VRH) conduction has been studied intensively. It has been investigated by the path integral approach,[1–3] the random matrix theory,[4,5] or other methods.[6] According to these theories, the hopping probability between two sites reflects the interference among the various paths through other sites. The applied magnetic field weakens the interference effect and raises the hopping probability. The positive magnetoconductance (MC) of the VRH observed in some experiments can be explained well by this orbital interference effect.

The effect of the electron-electron interactions is also important in the strongly localized regime. The long-range Coulomb interaction causes a gap of the density of states at the Fermi level, which is called Coulomb gap. It changes the T dependence of the VRH conduction.[7] While the short-range correlation affects the local properties of the impurity states of doped semiconductors in the intermediate concentration regime. The spin-pair approximation has been suggested for the localized electronic structure, in which each spin of the localized electron is paired with its strongest-coupled neighbor.[8] The model and extensions of it, which represent the correlation between electrons of a pair, account for the T dependence of the magnetic properties and the specific heat.[8–11] Later the author and Kamimura investigated the electronic structures from first principles in uncompensated and compensated Si:P.[12,13] The many-body wave functions have been calculated, taking account of all the correlation effect by an exact diagonalization method. It has been shown that the pair-type correlation is the most important in the strongly localized regime, and hence the spin-pair approximation is suitable for representing the local properties in the regime.

In this paper, we investigate the correlation effect of a short range on the nearest-neighbor hopping conduction in a magnetic field. For this purpose, we take, as a model, the Hubbard model with disordered on-site energies and treat the correlation effect in a quantum mechanical way. We have suggested that the correlation effect makes the positive MC through the Zeeman effect in the absence of the spin-orbit (SO) interaction in our previous paper.[14,15] The proposed mechanism is as follows: The orbitals are more localized in the low-spin state than in the high-spin state, reflecting the strong correlation in the former. With increasing magnetic field, the Zeeman effect increases the number of the high-spin states in which the orbitals at the Fermi level are more extended, which causes a positive MC. The proposed MC is independent of the direction of the magnetic field in contrast to the orbital MC mentioned before, in which only the component of H perpendicular to the orbitals is effective. In the first part of the present paper, we give more calculated results and discuss this mechanism of the positive MC in detail. In the second part, we extend the calculation to the case in the presence of the SO interaction.[16] The spin flip processes are taken as random variables.[5,17] We show that the MC can be negative in low magnetic fields, while it becomes positive in high fields. Further, we study the system which has more than one levels per site, since the effect of the intrasite levels cannot be neglected in some real systems. To this end, we examine the multilevel Hubbard model with randomness, showing that the intrasite-level effect weakens the magnetic-field dependence of the hopping conduction.

A motivation of the present work is to explain the MC in the nearest-neighbor hopping conduction, which has been recently observed in a Cu-particle film.[18,19] The film is composed of crystalline Cu particles of about 30 Å in diameter, separated by thin oxide layer. It has been observed in resistive samples that the MC is negative, exhibiting broad minimum, in low magnetic fields, while it can change sign and become positive in high fields. The MC is isotropic, regardless of the orientation of the

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magnetic field being applied parallel or perpendicular to the film plane. The T dependence of the VRH conduction has not been observed in the samples. We will show that our calculated results are qualitatively in good agreement with the experimental results.

Lately, the correlation effect has been studied intensively in the electronic devices fabricated on the submicron scale. Experimentally "Coulomb blockade" oscillations have been observed in systems including a quantum dot,[20] while the Kosterlitz-Thouless-Berezinskii phase transition has been studied for the charge solitons in an array of quantum dots when the long-range Coulomb force is important.[21] We will discuss the condition that the suggested MC can be observed in an array of quantum dots when the interaction is of short-range, due to the screening effect. The existence of several levels in a dot may be a problem for the observation of the MC.

The organization of this paper is as follows. The models and the calculation method are given in the next section (Sec. II). Section III is devoted to the calculated results: In Sec. III A we present the results in the absence of the SO interaction and show the positive MC mechanism of the hopping conduction through the Zeeman effect. In Sec. III B we take account of the SO interaction in the MC. The intrasite-level effect is considered in Sec. III C. The conclusions and discussion are given in the last section (Sec. IV).

II. CALCULATION METHOD

A. Model

We study the Hubbard model with disordered on-site energies in two-dimensional square lattice. The Hamiltonian is

$$H=\sum_{i,\sigma}\left[\varepsilon_i+(-1)^{\sigma}\mu_B H\right]a^{\dagger}_{i,\sigma}a_{i,\sigma} + \sum_{\langle i,j\rangle,\sigma,\sigma'}(T_{ij})_{\sigma,\sigma'}\,a^{\dagger}_{i,\sigma}a_{j,\sigma'}+U\sum_i n_{i,\uparrow}n_{i,\downarrow}, \quad (1)$$

$$-W/2<\varepsilon_i<W/2, \quad (2)$$

where $\langle i,j\rangle$ denotes the nearest-neighbor sites i and j. We take $W,U\gg|t|$ for investigating the large electronic correlation in the strongly Anderson-localized regime. In the absence of the SO interaction, the hopping terms are assumed to be constant, $(T_{ij})_{\sigma,\sigma'}=t\,\delta_{\sigma,\sigma'}$, while in its presence they are written as

$$T_{ij}=\begin{pmatrix}\alpha_{ij} & \beta_{ij}\\ -\beta^{*}_{ij} & \alpha^{*}_{ij}\end{pmatrix}, \quad (3)$$

where α_{ij} and β_{ij} are taken as random variables.[17] As for the electron-electron interactions, we only take into account those of short range by the U terms in Eq. (1). We neglect the long-range part of the Coulomb interaction. In the presence of the magnetic field we only consider the Zeeman effect, neglecting the shrinkage of the Wannier orbitals and the orbital MC mentioned before.[1–6]

We restrict ourselves to 4×4 sites for eight electrons, while we consider larger systems for two electrons.[22] We expect that the finite size effect is not serious because we only consider the strongly localized case in which the localization length is typically from one to two sites. All the calculations are done with free boundary condition. The finite size effect is discussed in the last section.

B. Calculation method

The method we adopt is the unrestricted Hartree-Fock (UHF) method. It is a variational method in which the trial function is a Slater determinant;

$$\Psi=|\psi_1\alpha\psi_2\alpha\cdots\psi'_1\beta\psi'_2\beta\cdots|, \quad (4)$$

in the absence of the SO interaction. Here the orbitals for up-spin electrons, $\{\psi_i\}$, can be different from those for down-spin electrons, $\{\psi'_i\}$, all of which are determined self-consistently to minimize the expectation value of the Hamiltonian. In this procedure not only the mean field but also part of the correlation effect are taken into account. Particularly the largest correlation effect in the strongly localized regime, which is the pair-type correlation,[12,13] is effectively included (see Appendix). Although the eigenstate of the total spin S cannot be obtained by the method, the z component of the total spin, S_z, remains a good quantum number. We calculate all the states with different S_z independently and determine the ground state by comparing their energies.

In the presence of the SO interaction, we extend the UHF method to the spinol space. The trial function is written as a Slater determinant, $\Psi=|\cdots\psi_i\cdots|$, in which each orbital ψ_i includes both components of up and down spins. Then the terms including U are treated as below:

$$\begin{aligned}Un_{i,\uparrow}n_{i,\downarrow}\longrightarrow U[&\langle n_{i,\uparrow}\rangle n_{i,\downarrow}+n_{i,\uparrow}\langle n_{i,\downarrow}\rangle-\langle n_{i,\uparrow}\rangle\langle n_{i,\downarrow}\rangle\\ &-\langle a^{\dagger}_{i,\uparrow}a_{i,\downarrow}\rangle a^{\dagger}_{i,\downarrow}a_{i,\uparrow}-\langle a^{\dagger}_{i,\downarrow}a_{i,\uparrow}\rangle a^{\dagger}_{i,\uparrow}a_{i,\downarrow}\\ &+\langle a^{\dagger}_{i,\uparrow}a_{i,\downarrow}\rangle\langle a^{\dagger}_{i,\downarrow}a_{i,\uparrow}\rangle].\end{aligned}$$

In this case, S_z is no longer a good quantum number, but its average is determined automatically by the self-consistent calculation.

To estimate the degree of localization in the real space, we calculate the participation ratio. It is defined as

$$\langle\psi^4\rangle=\int|\psi(\mathbf{r})|^4d\mathbf{r}=\sum_{i}^{\text{all sites}}|\psi(i)|^4, \quad (5)$$

$$\langle\psi^4\rangle=\sum_{i}^{\text{all sites}}[|\psi_{\uparrow}(i)|^2+|\psi_{\downarrow}(i)|^2]^2, \quad (6)$$

in the absence and presence of the SO interaction, respectively. Here the lattice constant is taken unity. The larger the value is, the more localized the orbital is.

C. Multilevel Hubbard model

We consider the case in which there are more levels than one at each site in Sec. III. We perform numerical studies on the disordered Hubbard model having M intrasite levels. The SO interaction is neglected. The Hamiltonian is written as

$$H = \sum_{i,\lambda,\sigma} [\varepsilon_{i\lambda} + (-1)^{\sigma}\mu_B H]\, a^{\dagger}_{i\lambda,\sigma} a_{i\lambda,\sigma} + t \sum_{\langle i,j\rangle,\lambda,\mu,\sigma} a^{\dagger}_{i\lambda,\sigma} a_{j\mu,\sigma} + U_0 \sum_{i,\lambda} n_{i\lambda,\uparrow} n_{i\lambda,\downarrow} + U_1 \sum_{i,\lambda\neq\mu} n_{i\lambda,\uparrow} n_{i\mu,\downarrow} + U_2 \sum_{i,\lambda<\mu} [n_{i\lambda,\uparrow} n_{i\mu,\uparrow} + n_{i\lambda,\downarrow} n_{i\mu,\downarrow}], \quad (7)$$

where suffices, $\lambda, \mu = 1, \ldots, M$, indicate the intrasite levels. There appear three kinds of on-site Coulomb energies; U_0 for intralevel, U_1 for interlevel with the different spins, and U_2 for interlevel with the same spins. The energy level is taken as, $\varepsilon_{i\lambda} = \varepsilon_{i1} + (\lambda - 1)D$, where the level spacing D is fixed, while the lowest intrasite level ε_{i1} is randomly distributed in $-W/2 < \varepsilon_{i1} < W/2$. The transfer integral between the nearest-neighbor sites, t, is assumed to be independent of the intrasite levels.

In the UHF calculation, the contribution from U_0 and U_1 terms is the same as before, while the U_2 terms cause a new effect:

$$\begin{aligned} U_2 n_{i\lambda,\uparrow} n_{i\mu,\uparrow} \longrightarrow\ & U_2[\langle n_{i\lambda,\uparrow}\rangle n_{i\mu,\uparrow} + n_{i\lambda,\uparrow}\langle n_{i\mu,\uparrow}\rangle \\ & - \langle n_{i\lambda,\uparrow}\rangle\langle n_{i\mu,\uparrow}\rangle - \langle a^{\dagger}_{i\lambda,\uparrow} a_{i\mu,\uparrow}\rangle a^{\dagger}_{i\mu,\uparrow} a_{i\lambda,\uparrow} \\ & - \langle a^{\dagger}_{i\mu,\uparrow} a_{i\lambda,\uparrow}\rangle a^{\dagger}_{i\lambda,\uparrow} a_{i\mu,\uparrow} \\ & + \langle a^{\dagger}_{i\lambda,\uparrow} a_{i\mu,\uparrow}\rangle\langle a^{\dagger}_{i\mu,\uparrow} a_{i\lambda,\uparrow}\rangle], \end{aligned}$$

in which the exchange terms appear as well as the Coulomb terms. The former terms lower the energy of the high-spin states. In consequence, there are two competing effects on the spin states: (1) A wave function can be extended through more levels per site to lessen the kinetic energy, by which the low-spin state is more favorable. (2) The exchange interaction decreases the energy of the high-spin state.

We define the participation ratio as

$$\langle \psi^4 \rangle = \sum_{i}^{\text{all sites}} \left[\sum_{\lambda=1}^{M} |\psi(i,\lambda)|^2 \right]^2, \quad (8)$$

for estimating how many sites a wave function is extended over.

We only treat the case of $M = 2$, as schematically shown in Fig. 1, and $U_0 = U_1 = U_2 \equiv U$, in the present paper.

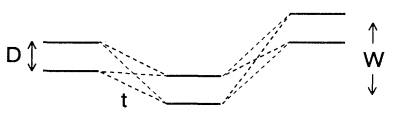

FIG. 1. Schematic drawing of the multi-intrasite-level model with randomness W and the level spacing D. Each site has two levels. The transfer of the electrons is denoted by broken lines with the common transfer integral t.

III. CALCULATED RESULTS

A. Absence of SO interaction

First of all, we present an example to indicate that the one-electron orbitals can be changed when the spin state is changed owing to the correlation effect, in the absence of the SO interaction. Figure 2 shows the one-electron orbitals in a 8×8 square lattice with two electrons. The parameters are $W = 10|t|$ and $U = 20|t|$ ($t < 0$). The orbitals in the low-spin state ($S_z = 0$) are shown in Fig. 2(a)$_1$ and (a)$_2$, while those in the high-spin state ($S_z = 1$) are shown in (b)$_1$ and (b)$_2$. The former orbitals are more localized than the latter ones, although they have almost the same shape around the localization center. The participation ratio is larger for the spin-antiparallel electrons [(a)$_1$ 0.200, (a)$_2$ 0.324] than for the spin-parallel electrons [(b)$_1$ 0.176, (b)$_2$ 0.289].

The reason is as follows. The electrons with antiparallel spins are interacting with each other through the U terms in the Hamiltonian (1), while the electrons having parallel spins do not interact. Thus spin-antiparallel electrons tend to be apart from each other, that is, the correlation effect is strong between them. As a result, in the low-total-spin state the orbitals are more localized, due to the correlation. (See Ref. 14 for the detailed results for two-electron systems.)

When the magnetic field is applied, the electron spins tend to be parallel to the direction of the field owing to the Zeeman effect and hence be parallel to each other. The calculated result described above, therefore, implies that the orbitals are more extended in the presence of the magnetic field H. To investigate the H dependence of the localization length, we study the system of eight electrons in a 4×4 square lattice, without SO interaction. We calculate the total energy including the Zeeman energy for all the states of $S_z = 0, 1, 2, 3, 4$ and determine the ground state as a function of H. Then we calculate the participation ratio of the orbital at the Fermi level, E_F,

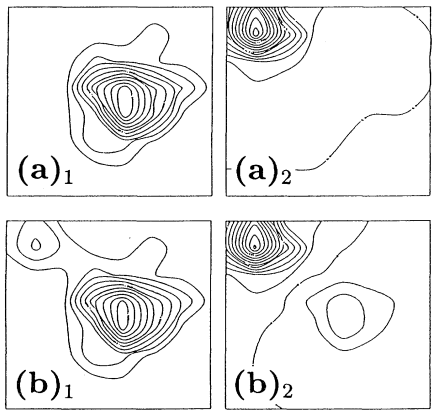

FIG. 2. The one-electron orbitals for a two-electron system of 8×8 sites; (a)$_1$ and (a)$_2$ in the spin-antiparallel state ($S_z = 0$), while (b)$_1$ and (b)$_2$ in the spin-parallel state ($S_z = 1$). $W = 10|t|$, $U = 20|t|$, and the SO interaction is neglected. The contour lines are drawn every 0.05.

(the highest occupied orbital) in the ground state.

Before discussing the H dependence of the physical quantities, we present the relation between the participation ratio and S_z in Fig. 3. The participation ratio of the orbitals at E_F is averaged over 200 samples for each U and W ($t < 0$). The quantity is plotted in such a manner that it is reduced along the vertical axis; the wave function is more extended when it is plotted upward. The figure shows that the orbitals at E_F are more extended in the higher-spin states. As for the W dependence, the orbitals for larger randomness W are more localized. When W is fixed, the relation between the participation ratio and S_z seems almost independent of U, except in the case of $U = 10|t|$ and $W = 15|t|$, in which U is smaller than W.

The H dependence of the averaged S_z (magnetization per eight electrons) is shown for $U/|t| = 10, 15, 20$ and $W = 10|t|$ in Fig. 4. An ensemble average is taken over 400 samples for each parameter. The number of the high-spin states increases with the magnetic field, reflecting the Zeeman effect. The high-spin states can appear more easily when the correlation effect U is larger. This is because the correlation effect raises the energy of the low-spin states more, compared to the high-spin states. The magnetization is almost H linear although it is not zero at $H = 0$.[23]

In Fig. 5 we show the H dependence of the participation ratio of the orbitals at E_F, which is averaged over 400 samples. With increasing magnetic field, the participation ratio is reduced and thus the orbitals are more extended, reflecting the increased number of the high-spin states. The H dependence of the localization length seems to be almost linear. When the value of U is larger, the extension of the orbitals with H is more remarkable.

Since the orbitals around E_F mainly contribute to the hopping conduction at low temperatures, this result indicates the positive MC. The MC is due to the Zeeman effect, which is independent of the direction of the magnetic field. This is contrast to the orbital MC in which only the component of H perpendicular to the orbitals is effective.[1–6] Thus the two mechanisms can be distinguished in experiments.

Finally, we show the calculated results for the different W ($W/|t| = 5, 10, 15$) when the value of U is fixed at $15|t|$ in Fig. 6. As the randomness W increases, the role of the kinetic energy becomes more important. Accordingly, the correlation effect relatively declines. Hence, the H dependence of the localization length is weaker for larger W.

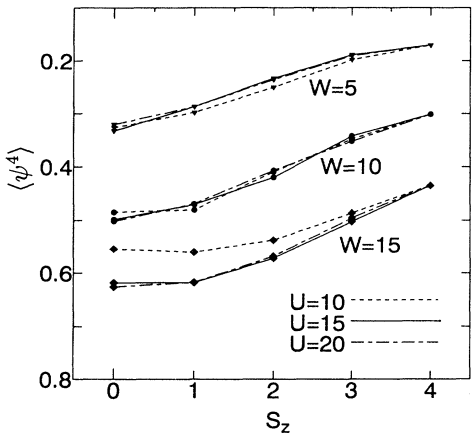

FIG. 3. The relation between the participation ratio at the Fermi level, $\langle\psi^4\rangle$, and the z component of the total spin, S_z, in the absence of the SO interaction. The participation ratio is averaged over 200 samples for each parameter. It is plotted in such a way that it becomes smaller along the vertical direction. The unit of W and U is $|t|$.

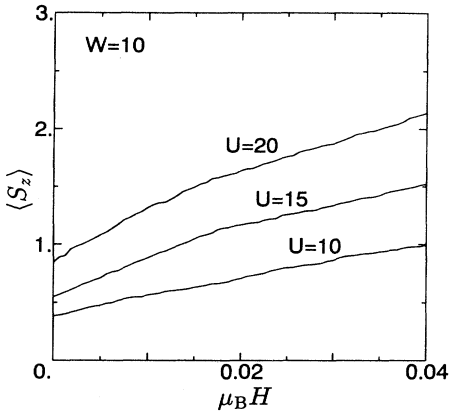

FIG. 4. The magnetic-field (H) dependence of the averaged S_z (magnetization per eight electrons) without SO interaction. The ensemble average is taken over 400 samples for each parameter. The unit of W, U, and $\mu_B H$ is $|t|$.

B. Presence of SO interaction

For spin flip processes, we take a model of Ref. 5: α_{ij} and β_{ij} in Eq. (3) are randomly distributed under the condition

$$\det(T_{ij}) = |\alpha_{ij}|^2 + |\beta_{ij}|^2 = |\tilde{t}|^2, \tag{9}$$

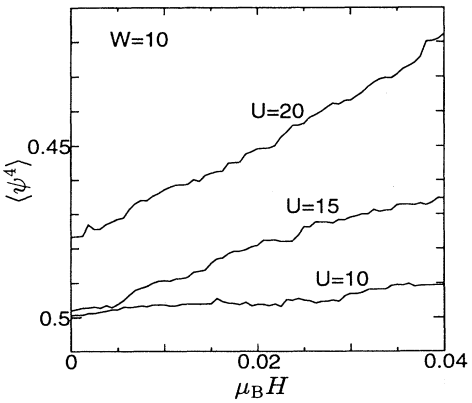

FIG. 5. The magnetic-field (H) dependence of the averaged participation ratio at the Fermi level, $\langle\psi^4\rangle$, without SO interaction. The ensemble average is taken over 400 samples for each parameter. The unit of W, U, and $\mu_B H$ is $|t|$.

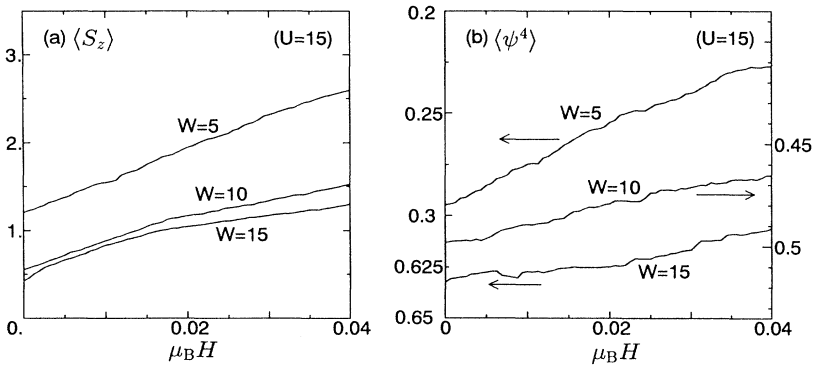

FIG. 6. The magnetic-field (H) dependence of the averaged S_z (a), and participation ratio at the Fermi level, $\langle\psi^4\rangle$ (b), in the absence of the SO interaction. The degree of randomness W is changed, while U is fixed at $15|t|$. The ensemble average is taken over 400 samples for each W. The unit of W and $\mu_B H$ is $|t|$.

where $|\tilde{t}|$ is fixed. The SO disorder is assumed to be independent of the site disorder. We consider eight electrons in a 4×4 square lattice with $W = 10|\tilde{t}|$ and $U = 20|\tilde{t}|$. The ensemble average is taken over 200 samples.

The calculated results are indicated by broken lines in Fig. 7. The results in the absence of the SO interaction ($W = 10|t|$, $U = 20|t|$) are shown by solid lines for comparison. Although the H dependence of the magnetization is almost the same in both the cases [Fig. 7(a)], that of the averaged participation ratio at E_F is very much changed by the SO interaction, as seen in Fig. 7(b); (i) its absolute value gets smaller, (ii) the H dependence becomes weaker, and (iii) it increases first and then it decreases as the magnetic field grows larger.

These properties are due to the interplay between the SO interaction and the correlation effect. The SO interaction brings the transfer from spin-up states to spin-down states, and vice versa, and in consequence, the wave functions can be more extended to reduce the kinetic energy, compared to the SO-interaction-free case. Under the magnetic field, there are two different effects. First, with increasing magnetic field, the spin flip processes are suppressed since the Zeeman effect expands the separation between the levels of the up and down spin. This gives the negative MC in low magnetic fields. Second, as the magnetic field increases, the number of the high-spin states increases in which the orbitals are more extended due to the smaller correlation effect, as discussed in the previous subsection. In high magnetic fields, the second effect becomes dominant, resulting in the positive MC. The calculated result is in good agreement with the experimental result of the nearest-neighbor hopping conduction in a Cu-particle film.[18,19]

C. Multi-intrasite-level effect

Now we examine the multilevel Hubbard model which has two levels per site. The system consists of 4×4 sites and includes eight electrons. With $W = 10|t|$ and $U = 20|t|$ ($t < 0$), we change the intrasite-level spacing; $D/|t| = 5$, 10, and 15. The SO interaction is neglected. The ensemble average is taken over 400 samples for each value of D.

In Fig. 8 and Fig. 9 we present the H dependence of the averaged S_z (magnetization) and the participation ratio of the orbitals at E_F, respectively. The results of the single-intrasite-level systems with the same W and U, are shown by broken lines in the figures.

Figure 8 shows that the averaged S_z is reduced by the intrasite-level effect; it becomes smaller with the decrease of the level spacing D. As seen in Fig. 9, the wave functions are more extended at $H = 0$ for smaller D. This is because the wave functions can be more extended through two levels a site to reduce the kinetic energy. As a result, the correlation effect is attenuated by the screening and hence the low-spin states can have lower energies. The exchange terms by which the high-spin state is favorable do not seem important.

As regards the H dependence, Fig. 9 shows that the participation ratio of the orbitals at E_F decreases with increasing H though its H dependence becomes weaker as D is reduced. This is also due to the smaller cor-

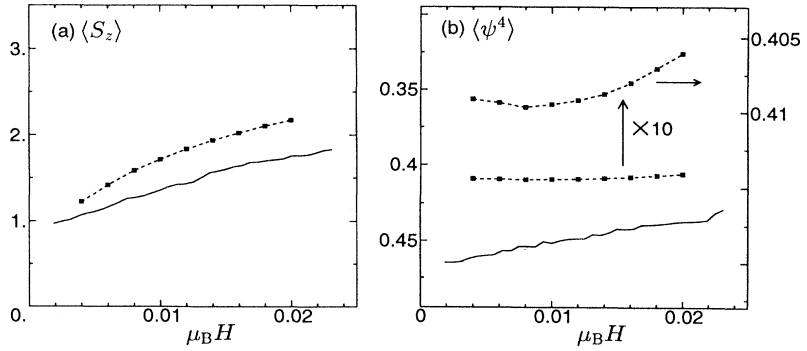

FIG. 7. The magnetic-field (H) dependence of the averaged S_z (magnetization) per system (a), and of the participation ratio at the Fermi level, $\langle\psi^4\rangle$ (b), in the SO-interacting systems with $W = 10|\tilde{t}|$ and $U = 20|\tilde{t}|$ (broken lines). The ensemble average is taken over 200 samples. The results without SO interaction ($W = 10|t|$, $U = 20|t|$) are also indicated by solid lines. The unit of $\mu_B H$ is $|\tilde{t}|$ ($|t|$).

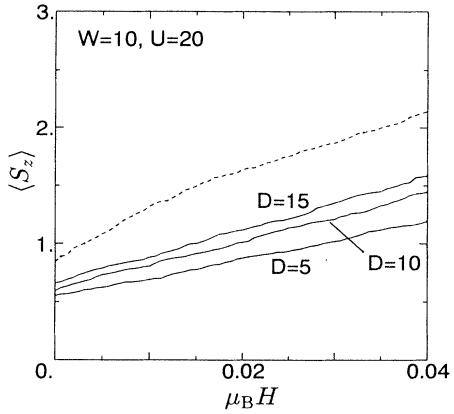

FIG. 8. The magnetic-field (H) dependence of the averaged S_z (magnetization per eight electrons) in the multilevel Hubbard model. The intrasite-level spacing D is changed when $W = 10|t|$ and $U = 20|t|$. The ensemble average is taken over 400 samples for each D. The unit of D and $\mu_B H$ is $|t|$. A broken line indicates the result of the single intrasite-level system with the same W and U.

relation effect. The positive MC can still be expected when $D \approx W$, which is the case in a Cu-particle film, as discussed later. However, the MC is difficult to observe when $D \ll W, U$. This may be a serious condition for the case of an array of quantum dots.

IV. CONCLUSIONS AND DISCUSSION

In this paper, we have studied the correlation effect on the magnetoconductance (MC) in the strongly localized regime. Based on the numerical studies on the Hubbard model with disordered on-site energies, we have investigated the magnetic-field dependence of the nearest-neighbor hopping conduction through the Zeeman effect. (1) In the absence of the SO interaction a new mechanism of the positive MC is proposed; the Zeeman effect increases the number of the high-spin states in which the orbitals at E_F are more extended owing to the weaker correlation than in the low-spin states. The MC is independent of the direction of the magnetic field and hence it is distinguishable from the orbital MC.[1–6] (2) It is well known that the SO interaction weakens the localization of electrons in the weakly localized regime.[24] The tendency seems to be the same in the strongly localized regime. It extends the wave functions and diminishes the correlation effect on the MC. However, the interplay of the SO interaction and the correlation effect makes the interesting character of the hopping conduction. The MC can be negative in low magnetic fields, while it becomes positive in high magnetic fields. (3) The system which has more than one level per site is also examined. Although the intrasite-level effect weakens the H dependence, the positive MC can be still observable when the intrasite-level spacing D is larger than the randomness W and the on-site Coulomb energy U, or comparable to those.

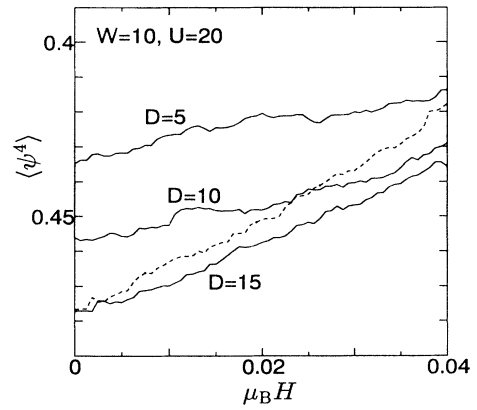

FIG. 9. The magnetic-field (H) dependence of the averaged participation ratio at the Fermi level, $\langle \psi^4 \rangle$, in the multilevel Hubbard model. The intrasite-level spacing D is changed when $W = 10|t|$ and $U = 20|t|$. The ensemble average is taken over 400 samples for each D. The unit of D and $\mu_B H$ is $|t|$. A broken line indicates the result of the single intrasite-level system with the same W and U.

The calculated result with the SO interaction is qualitatively in accordance with an experimental result of the nearest-neighbor hopping conduction in a Cu-particle film.[18,19] In this system, the energy spacing between one-electron levels in a particle is as large as 70 K. The intraparticle Coulomb energy, U, is estimated to be larger than that.[18] Thus, we expect that our model with $W = D = 70$ K represents such a system. The model having only two intrasite levels does not seem serious for the phenomena below a few K. Now we give a rough estimation of the positive MC for the nearest-neighbor hopping conduction.[14] The participation ratio is $\langle \psi^4 \rangle \sim 1/l^2$, where l is the localization length. Hence at $W = 10|t|$, $U = 20|t|$,

$$\frac{1}{l^2} \sim 0.45,$$

$$\delta\langle \psi^4 \rangle \sim -2\frac{1}{l^3}\delta l \sim -0.025, \quad \text{at} \quad \mu_B H = 0.02|t|.$$

The resistance, $R \propto \exp(a/l)$, where the hopping length a is unity now, and thus

$$\frac{R(H = 0.02|t|/\mu_B) - R(0)}{R(0)} \sim -\frac{a}{l}\frac{\delta l}{l} \sim -1.9\%.$$

The similar calculation gives the magnetoresistance of -0.4% for a SO-interacting case ($W = 10|\tilde{t}|$, $U = 20|\tilde{t}|$), and -0.7% for a multi-intrasite-level case ($W = 10|t|$, $U = 20|t|$, $D = 10|t|$). These values are the same in order as the experimental result[18,19] though the uncertainties are left in the values of U and t ($\tilde{t}$). If W is 70 K, the above-mentioned magnetic field ($\mu_B H = 0.02|t|$) corresponds to 0.2 T. It should be noted, however, that the energy of the low-spin state tends to be overestimated, compared with that of the high-spin state in the UHF approximation. Consequently, the value of the magnetic field is underestimated, e.g., it should be doubled for the two-site model (Appendix). Although we only consider

the quarter-filled case (eight electrons per 16 sites) in the present paper, the electron configuration can change the MC in a quantitative way.[14]

We should comment on the finite size effect here. We only consider the strongly localized regime in which the localization length is from one to two sites, so that the finite size effect is not expected to be serious. For checking it, we have performed the calculations with the periodic boundary condition when $U = 20|t|$ and $W = 10|t|$. We got qualitatively the same result although the value of the MC is somewhat smaller.

Another mechanism of the positive MC, due to the Zeeman effect was suggested by Fukuyama and Yosida[25] in the VRH conduction. Their theory is based on the one-electron picture and applicable to the vicinity of the metal-insulator transition, where E_F is close to the mobility edge (intermediate concentration region). We simulate their mechanism in our model without the correlation U. We find out that the positive MC can occur when the magnetic field is greater by two order than that in Fig. 5. The MC due to the correlation, therefore, is much larger than that of the one-particle theory in the strongly localized regime, although the latter mechanism becomes important in the region of small $W/|t|$, where the electronic correlation is not large owing to the screening effect. In the region there can also be a negative MC mechanism.[9,26,27]

Lastly, we discuss the possibility of the observation of this mechanism in other experiments. It may be observed in the nearest-neighbor hopping conduction among impurities doped in semiconductors. To observe the mechanism of the MC in an array of artificial quantum dots, the following conditions should be necessary: (i) the strong enough interaction U ($\sim e^2$/Capacitance); (ii) the coherent transfer interaction between the dots, or not too small $|t|$. (iii) In addition, the level spacing in a dot should be small. Anyway, it is interesting to study the proposed MC in experiments, because we can observe the correlation effect on the localized states by that.

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APPENDIX: SPIN-PAIR MODEL BY THE UHF APPROXIMATION

Our calculation method, the unrestricted Hartree-Fock (UHF), is a variational method. The trial function is a Slater determinant, Eq. (4), in the absence of the SO interaction. Since the orbitals for up-spin electrons can be different from those for down-spin electrons, some part of the correlation effect can be taken into account as well as the mean field part, that is, Coulomb and exchange terms.

In the strongly Anderson-localized regime the most important type of the correlation effect is a pair-type correlation,[12,13] which is included effectively by the method. To demonstrate it, we show the result of two-site Hubbard model without randomness nor SO interaction.[15] The number of electrons is assumed to be two. The Hamiltonian is

$$H = -|t| \sum_{\sigma=\uparrow,\downarrow} (a^\dagger_{R,\sigma} a_{L,\sigma} + a^\dagger_{L,\sigma} a_{R,\sigma}) + U \sum_{i=L,R} n_{i,\uparrow} n_{i,\downarrow}. \tag{A1}$$

For the state of $S_z = 0$, the UHF wave function can be written as $\Psi = |\psi_1 \uparrow \psi_2 \downarrow|$, where $\psi_1 = (x a^\dagger_{L,\uparrow} + y a^\dagger_{R,\uparrow})|0\rangle$ and $\psi_2 = (y a^\dagger_{L,\downarrow} + x a^\dagger_{R,\downarrow})|0\rangle$ owing to the symmetry.

The self-consistent solution is as follows.

(i) When $U < 2|t|$, then $x = y = 1/\sqrt{2}$ with the total energy, $E_{\rm tot} = -2|t| + U/2$. In this case, the solution is the same as that by the usual HF method.

(ii) When $U > 2|t|$, then $x, y = \frac{1}{\sqrt{2}}[1 \pm \sqrt{1 - 4(t/U)^2}]^{1/2}$ with $E_{\rm tot} = -2t^2/U$. A schematic drawing for the orbitals is given in Fig. 10(b), which shows that two electrons are localized to reduce the repulsive interaction between them. The spin-pair approximation, which has been suggested by several authors,[8–11] represents this type of the correlation between two electrons in a pair.

We present the total energy in Fig. 10(a) as a func-

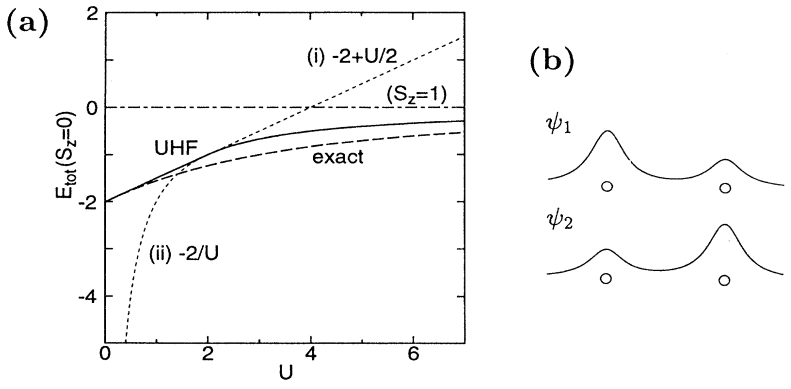

FIG. 10. Results of the UHF calculation for a two-site Hubbard model without randomness nor SO interaction. Two electrons exist in it. (a) The total energy of the $S_z = 0$ state, as a function of U. The unit of the energy is $|t|$. (b) Schematic drawing of the orbitals in the $S_z = 0$ state when $U > 2|t|$.

tion of $U/|t|$. A broken line indicates the exact solution, $E_{\rm tot} = \frac{1}{2}[U - \sqrt{U^2 + 16t^2}]$, of the spin-singlet state. The state of $S_z = 1$ has the total energy, $E_{\rm tot} = 0$, in this approximation, which coincides with the exact solution. Generally, the energy of the low-spin state is overestimated, compared to that of the high-spin state in this approximation.

In the presence of the magnetic field, the transition occurs from the $S_z = 0$ state to the $S_z = 1$ state when

$$E_{\rm tot}(S_z = 1) - E_{\rm tot}(S_z = 0) = 2\mu_B H_c. \quad \text{(A2)}$$

Hence, $\mu_B H_c = t^2/U$ by the UHF method in the case of $U > 2|t|$, while $\mu_B H_c \approx 2t^2/U$ in the exact solution when $U \gg |t|$. Since we are considering the case of the strong correlation in the present paper, the magnetic field H_c is underestimated to be half of the exact value.

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[22] We find a technical problem for larger systems (5×5 sites). There are so many local minimal solutions that we cannot obtain a reliable result. For 4×4 system, we can perform the calculations beginning with enough initial conditions to get the solution of the minimal energy.

[23] Some samples have the high-spin ground state even in the absence of H. The existence of the high-spin states has been pointed out in the intermediate concentration regime of the doped semiconductors by Kamimura *et al.* (Ref. 9) although the number of the high-spin states is overestimated in the UHF approximation.

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