Hubbard-gap tunneling in disordered quantum-dot chains

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In a Hubbard chain under an overall confining potential, electron tunneling through a Hubbard gap in the center of the chain can be expected even when disorder is introduced into the chain. Two kinds of randomness, in on-site single-particle energy and in on-site electron-electron interaction, are considered not only separately, but simultaneously. Because of the randomness in on-site single-particle energy, the variance of the tunneling amplitude has a peak when the degree of randomness changes. This peak is caused by the interplay between single-electron tunneling and Hubbard-gap tunneling in the chain where the Fermi statistics of electrons are important. On the other hand, the effect of randomness in on-site electron-electron interaction is similar to that in the potential barrier of single-electron tunneling. These effects of randomness on Hubbard-gap tunneling are important in determining the electronic structures of tunneling-coupled quantum dots.
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I. INTRODUCTION

The nature of correlated electrons in low-number dimension structures with disorder has been an active field of research in recent decades, for example, the fractional quantum Hall effect in a two-dimensional space under a magnetic field[1–4] and quantum dots in disordered semiconductors.[5–8] The coexistance of a strong correlation between electrons and disorder presents important problems of ''complex'' quantum systems, which are realized in solid-state materials.[9,10]

Let us review a way of understanding the fractional quantum Hall effect, which consists of three steps.[11] The first step considers wave functions of a single electron running through a disordered medium in a magnetic field.[12] The second step considers the electronic states of correlated electrons in a uniform space without disorder.[13,14] In the third step, these two systems are unified into a single system in which correlated electrons are in a disordered medium.

In the first step, we see that a single electron in a disordered medium can diffuse without spin-orbit interactions when the number of dimensions is larger than two.[15,16] Therefore, all wave functions of noninteracting electrons in two dimensions are localized by randomness when spin-orbit interactions are absent.[17,18] However, when a magnetic field is introduced in two-dimensional space, only the state in the center of each Landau level becomes extended and the state carries a nondissipative current in a bulk sample. When the Fermi energy is located between the energies of the extended states, Hall plateaus are seen in σ_{xy}. This is the integer quantum Hall effect.[19]

Let us turn to the second step, in which electrons are correlated in two dimensions, particularly under a strong magnetic field. It is useful to introduce composite fermions in two dimensions under a magnetic field.[20] Using the composite fermions, correlated electrons in two dimensions under a magnetic field can be expressed as almost independent fermions with a flux of ''virtual magnetic fields.'' An external magnetic field causes Landau-level splitting, resulting in a reduction of the degree of freedom for quanta, so quantum systems in two dimensions under a strong magnetic field are similar to quantum systems in one dimension. Note that we have integrable quantum models in one dimension.[21–23] An example is a many-body model with the δ-type interaction in one dimension,[24] and another example is the Hubbard model in a one-dimensional lattice.[25–27]

In the third step, we return to the fractional quantum Hall effect, in which we have extra plateaus in σ_{xy} when electron-electron interaction strongly affects electronic structures in two dimensions under a magnetic field. Because the interaction between composite fermions in two dimensions under a magnetic field is weak, the composite fermions can be independent. Therefore, the fractional quantum Hall effect in two dimensions with disorder can be understood as the integer quantum Hall effect of composite fermions in two dimensions with disorder. Thus, the key to this way of understanding the fractional quantum Hall effect is the decomposition of correlated electron systems into almost independent particles.

There is another kind of decomposition of correlated electron systems in a Hubbard chain under an overall confining potential.[28,29] In general, the overall confining potential destroys the integrability of an infinite Hubbard chain. However, under a certain strength of confining potential, Mott insulating electrons and electron tunneling through the Mott insulating electrons can be useful in understanding the electronic states of the Hubbard chain under an overall confining potential. In another words, the Hilbert space of the multielectron system is approximately decomposed into Mott insulating states with antiferromagnetic spin correlation and a single electron that tunnels through the Mott insulating electrons. When an even number of electrons are confined in a symmetric chain, there is electron tunneling through the Hubbard gap. If asymmetry is introduced into the chain, the tunneling amplitude is strongly suppressed.[30] When an odd number of electrons is confined in a symmetric chain, there is no electron tunneling through the Hubbard gap, though we know that asymmetry in an odd-number chain enhances the tunneling amplitude. These effects due to the number of electrons have been clarified by the calculations of eight-,

nine-, and ten-electron chains in Ref. 31. Note that the absolute value of the tunneling amplitude decreases as the number of the electrons confined in the chain increases. This is because the length of the tunneling barrier, i.e., Mott insulating electrons, increases as the number of electrons increases.

In the present paper, we analyze the effect of disorder on Hubbard-gap tunneling. The effect of disorder is important not only in analyzing the result of experiments because of the inevitable disorder in experimental situations, e.g., disordered quantum-dot chains,[32] but for analyzing multielectron effects on Hubbard-gap tunneling.

II. MODEL OF OUR QUANTUM-DOT CHAINS

Let us consider a chain of 13 sites of a single orbital in each quantum dot, which is described by a Hubbard-type model:

$$\hat{H}=-t\sum_{j=-L}^{L-1}\sum_{\sigma=\uparrow,\downarrow}\hat{c}_{j\sigma}^{\dagger}\hat{c}_{j+1\sigma}+\sum_{j=-L}^{L}(\Omega j^2+v_j)\hat{n}_j + \sum_{j=-L}^{L}(U+u_j)\hat{n}_{j\uparrow}\hat{n}_{j\downarrow}+\text{H.c.}, \tag{1}$$

where $\hat{n}_{j\sigma}=\hat{c}_{j\sigma}^{\dagger}\hat{c}_{j\sigma}$ and $\hat{n}_j=\hat{n}_{j\uparrow}+\hat{n}_{j\downarrow}$. $\hat{c}_{j\sigma}^{\dagger}$ creates an electron at the jth site with spin σ. t is the transfer between adjacent sites. $U+u_j$ is the strength of on-site electron-electron interaction and Ωj^2+v_j is the on-site potential energy of a single electron at the jth site. When $\Omega>0$, electrons in the Hubbard chain are confined by an overall parabolic potential. When we introduce randomness in our Hubbard chain, u_j and/or v_j are treated as random numbers.[33] In this paper we analyze the system of eight electrons in a chain having $L=6$ and $t=1$. The eigen energy of the eight-electron ground state E_0 and its eigenvector $|\Psi_0\rangle$ were calculated using the Lanczos method.[34] The ground state of our eight-electron chain has total spin $S=0$ because there is no possibility of ferromagnetism in single-band Hubbard systems. (This has been numerically checked when six electrons are considered in a chain with parabolic confinement.[28]) $S=0$ indicates that the z component of the total spin S_z is also zero.

Let us review the electronic states of our Hubbard chain without randomness. When $\Omega=0$, the electron gas has an almost constant density over the chain. Because the density of electrons is smaller than that of half-filled electrons, our electronic system is a metal of correlated electrons, i.e., a Luttinger liquid.[35–37] As the confining potential becomes stronger, i.e., Ω becomes larger, the density of the center region becomes higher. When the density of the center region reaches that of half-filled electrons, a Mott-Hubbard gap appears with an antiferromagnetic spin correlation.[38] Hubbard-gap tunneling between the left of the center and the right is seen in the chain through the Hubbard gap induced by the overall confining potential.[28] The tunneling effect is analyzed using the equal-time Green's function of the ground state $|\Psi_0\rangle$:

$$G_{i,j}^{\sigma}=\langle\Psi_0|\hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma}|\Psi_0\rangle, \tag{2}$$

because whether electrons with spin σ are localized or delocalized can be determined by the behavior of $G_{i,j}^{\sigma}$ $(i\neq j)$.

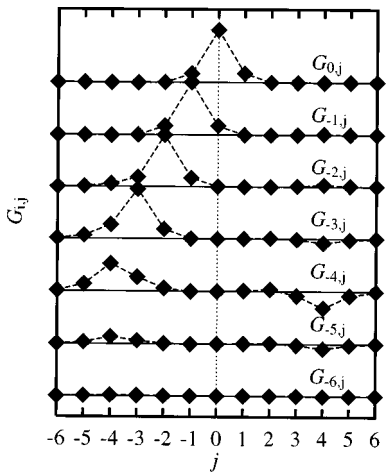

FIG. 1. The equal-time Green's function $G_{i,j}$ without randomness when $\Omega=0.4$ and $U=16$ are taken. The absolute value of $G_{-4,4}$ is large, though $|G_{-4,j}|$ $(-2\leqslant j\leqslant 2)$ is very small. This is a sign of Hubbard-gap tunneling.

Note that $G_{i,j}^{\uparrow}$ is equal to $G_{i,j}^{\downarrow}$ when an even number of electrons is confined in our Hubbard chain, so they are denoted by $G_{i,j}$. This is the result of the rotational invariance of the ground state having the total spin 0. Note that $2G_{j,j}=G_{j,j}^{\uparrow}+G_{j,j}^{\downarrow}$ is the density of electrons at the jth site in the ground state.

Figure 1 shows the equal-time Green's function $G_{i,j}$ when $U=16$, $u_j=0$, $\Omega=0.4$, and $v_j=0$. Note that we concentrate on an eight-electron system in a thirteen-site chain under an overall confining potential. In the chain, seven electrons constitute a Mott insulator in the center of the chain and the rest of electrons can tunnel through the Hubbard gap of the Mott insulator. In the center of the chain, where a quasi-Mott-Hubbard gap appears, $G_{i,j}$ decays rapidly as $|i-j|$ increases. The exponential decay of the Green's function indicates that the fermionic excitation is massive due to the quasi-Mott-Hubbard gap. The value $G_{-4,j}$ is large while $|j+4|\leqslant 1$, on the other hand, decays rapidly when $j>-2$ again. Further, $G_{-4,j}$ has a considerable value at $j=4$. This behavior of the equal-time Green's function indicates electron tunneling from the $j=-4$ site to the $j=4$ site through a Hubbard gap in the center of the chain. Thus, the amplitude of Hubbard-gap tunneling for an eight-electron system in a thirteen-site chain is

$$p=\left|\frac{G_{-4,4}}{G_{-4,-4}}\right|. \tag{3}$$

Figure 2 shows the equal-time Green's function $G_{-4,j}$ when $U=2,3,4,...,16$ is taken, and the rest of the parameters are the same as in Fig. 1. Though Hubbard-gap tunneling is well indicated by $G_{-4,j}$ when $U\geqslant 8$, wavy behavior of the equal-time Green's function when $U<8$ indicates that the electronic state of the chain is metallic. In the following section, randomness will be introduced in sites that have $j=-3$, $-2,...,3$ because we intend to analyze the effects of disorder on Hubbard-gap tunneling from the $j=-4$ site to the $j=4$. Note that if we introduced randomness in $|j|=4$ sites, the effect of off-resonance between the $j=4$ site and the $j=-4$ site would strongly reduce the tunneling amplitude.

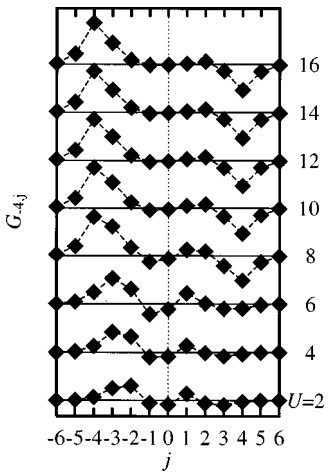

FIG. 2. The equal-time Green's function $G_{-4,j}$ without randomness $\Omega=0.4$ and $U=2,3,4,...,16$ are taken. When $U\geqslant 8$, Hubbard-gap tunneling is present.

Let us consider the degree of randomness in on-site electron-electron interaction and in single-particle energy. A simple estimation suggests that the ground-state energy of a single electron in a quantum dot is

$$\tilde{V}=\frac{\hbar^2}{2m_eR^2}, \tag{4}$$

and the energy of electron-electron interaction is

$$\tilde{U}=\frac{e^2}{4\pi\epsilon_0\epsilon_rR}, \tag{5}$$

where R is the diameter of each quantum dot. If we assume that the fluctuation in electron-electron interaction, i.e., $d\tilde{U}$ and the fluctuation in single-particle energy, i.e., $d\tilde{V}$ originate from the fluctuation in the diameter of quantum dots dR, we find that

$$d\tilde{V}=\frac{4\pi\epsilon_0\epsilon_r\hbar^2}{m_ee^2}\frac{d\tilde{U}}{R}. \tag{6}$$

The values $m_e=0.067m_0$, $\epsilon_r=10.9$, for GaAs result in

$$d\tilde{V}=8.6\times10^{-9}\frac{d\hat{U}}{R}, \tag{7}$$

where the units of the *Système International* are used. When R is much larger than 10 nm, $d\hat{V}$, i.e., randomness in single-particle energy, can be ignored. This is the case where electrons are confined by a depletion region of a semiconductor.[39–44] These quantum dots are considered in Sec. III A, where u_j $(j=-3,-2,...,3)$ is randomly distributed and $v=_j=0$. In our calculation, random variables are taken to be in a range of r, so

$$-\frac{r}{2}<u_j<\frac{r}{2} \tag{8}$$

will be taken for $j=-3,-2,...,3$.

When R is much smaller than 10 nm, $d\tilde{U}$ can be ignored. Section III B analyzes this case, where v_j $(j=-3,-2,...,3)$ is randomly distributed and $u_j=0$. Again, random variables are taken to be in a range of r, so

$$-\frac{r}{2}<v_j<\frac{r}{2} \tag{9}$$

will be taken for $j=-3,-2,...,3$. In a quantum dot with $R\sim10$ nm, $d\tilde{V}$ is comparable with $d\hat{U}$. Fabricating semiconductor quantum dots on the order of this size can be achieved using state-of-the-art technology. Using epitaxial growth techniques of compound semiconductors, a quantum dot confined by a herostructure on the order of 10 nm has been fabricated.[45–47] Whiskers of GaAs (Ref. 48) and of silicon[49] have been used to fabricate a quantum wire of this size. As suggested by the above expressions, the sign of $d\hat{V}$ is the same as that of $d\tilde{U}$, resulting in a correlation between the degree of randomness in single-particle energy and the degree of randomness in electron-electron interaction. If the size of quantum dots becomes smaller, the single-particle energy as well as the energy due to electron-electron interaction becomes larger. Note that the correlation between the degrees of the two kinds of randomness is not present if impurities in semiconductors cause randomness in single-particle energy. Section III C analyzes systems that have randomness both in on-site single-particle energy and in on-site electron-electron interaction. A system where v_j and u_j $(j=-3,-2,...,3)$ are randomly distributed and their degrees of randomness have no correlation, is compared to a system where $v_j=u_j$ are randomly distributed, but the degrees of randomness are correlated. In this section, the effect of the correlation between randomness in on-site single-particle energy and randomness in on-site electron-electron interaction is discussed.

The tunneling amplitude p will be statistically averaged in a whole random ensemble. We have numerical result p when we take u_j and v_j as an ensemble, so p is a function of u_j and v_j. The nth set of the random variables is denoted by $u_j^{(n)}$ and $v_j^{(n)}$, so we write the tunneling amplitude as

$$p(n)=p(u_j^{(n)},v_j^{(n)}). \tag{10}$$

The number of random samples is taken to be $N_s=200$, so we write the statistical average for p,

$$\langle p\rangle=\frac{1}{N_s}\sum_{n=1}^{N_s}p(n), \tag{11}$$

where $p(n)$ is the tunneling amplitude of the nth set of random variables. We also define the variance of the tunneling amplitude p as

$$\langle\delta p\rangle=\sqrt{\langle p^2\rangle-\langle p\rangle^2}, \tag{12}$$

where

$$\langle p^2\rangle=\frac{1}{N_s}\sum_{n=1}^{N_s}[p(n)]^2. \tag{13}$$

III. RESULTS

A. Randomness in on-site electron-electron interaction

The Mott-Hubbard gap is useful to describe a Mott insulator in which the upper Hubbard band is empty and the lower Hubbard band is fully occupied by electrons. The width of the gap, i.e., the energy at the bottom of the upper Hubbard band minus the energy at the top of the lower Hubbard band, is $\Delta = U_{\rm eff} - T_{\rm eff}$, where $U_{\rm eff}$ is the on-site energy due to electron-electron interaction and $T_{\rm eff}$ is the bandwidth of a single electron.[38] In Hubbard-gap tunneling, the height of the tunneling barrier is approximately proportional to Δ minus the Fermi energy. When Ω induces a Hubbard gap in the center of the chain, the left-hand and right-hand sides should have the discrete excitation spectra of a single electron. There is a single electron located to the left of the Mott-insulating electrons in the center of the chain in the eight-electron state $|L\rangle$ and there is a single electron located to the right of the Mott-insulating electrons in the eight-electron state $|R\rangle$. The ground state of our chain without randomness can be written as the bonding state of these multielectron states: $(|L\rangle + |R\rangle)/\sqrt{2}$, where there is resonant tunneling between the right-hand side and the left-hand side. The energy of $|L\rangle$ and $|R\rangle$, which depends on the strength of overall confining potential Ω, can be thought of as the Fermi energy of both ends of our chain. Because the barrier height for Hubbard-gap tunneling is the energy difference between the energy at the bottom of the upper Hubbard band and the Fermi energy of the left and right sides, the barrier height can be modulated by Ω.

When we introduce randomness in on-site electron-electron interaction in a region near the center of the chain, the effect of the randomness on Hubbard-gap tunneling is similar to that of a fluctuation in the barrier height on single-electron tunneling, as suggested by the above discussion of Hubbard-gap tunneling. Note that the effect of randomness in a tunneling barrier is small in single-electron tunneling. A lower barrier encourages tunneling and a higher barrier discourages tunneling. Therefore, the degree of randomness in a tunneling barrier has a little effect on the amplitude of single-electron tunneling. An analysis in single-electron tunneling is given in the appendix, which shows that fluctuations in the barrier height enhance the tunneling amplitude.

In Fig. 3, the tunneling amplitude $\langle p\rangle$ and its variance $\langle \delta p\rangle$ are plotted as a function of $\log_{10}(r)$, where r is the degree of randomness, as defined in Sec. II. In these figures, Ω is taken to be 0.4 and U is taken to be 4,6,8,...,16. When $U=4$, $\langle p\rangle$ is small and almost constant over the whole range of randomness. When $U=6$, $\langle p\rangle$ is slightly larger than when $U=4$, and remains almost constant over the whole range of randomness. At the same time, fluctuation of the tunneling amplitude $\langle \delta p\rangle$ is very small even when a high degree of randomness is introduced. Note that the values $\langle p\rangle$ and $\langle \delta p\rangle$ when $U=4$ and 6 are very different from others when U has a larger value, as suggested in Sec. II. When our Hubbard chain has these parameters, the electronic structure of our chain is similar to that of a Luttinger liquid, i.e., a metal of correlated electrons. Note that over the whole range of randomness $\langle p\rangle$ is almost independent of $\log_{10}(r)$ and $\langle \delta p\rangle$ is almost zero. Only when $\log_{10}(r)$ exceeds -1, $\langle \delta p\rangle$ has non-

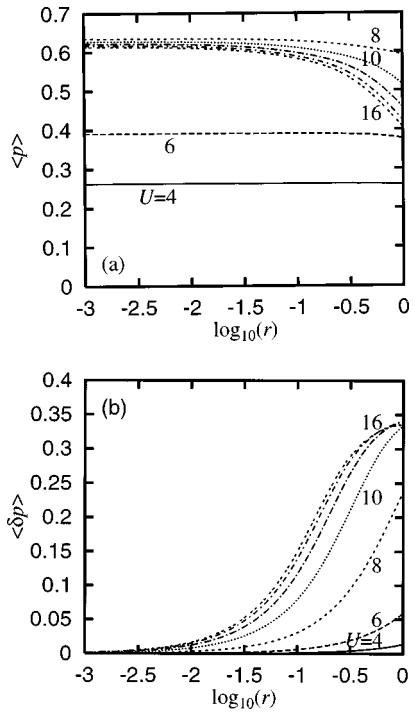

FIG. 3. (a) The average tunneling amplitude $\langle p\rangle = \langle |G_{-4,4}/G_{-4,-4}|\rangle$ and (b) its variance as a function of the degree of randomness when the on-site electron-electron interaction is randomly distributed. Ω is fixed at 0.4 and U is taken to be 4,6,8,...,16.

zero value. These behaviors suggest that the Luttinger liquid is not sensitive to randomness in on-site electron-electron interaction.

As we investigate Hubbard-gap tunneling, we are interested in the results when $U \geqslant 8$, as suggested in Fig. 2 of Sec. II. The tunneling amplitude $\langle p\rangle$ when $U=8$ is largest in Fig. 3(a) and decreases slightly as r increases. As the mean strength of electron-electron interaction, i.e., U increases, the value $\langle p\rangle$ decreases over the whole range of randomness. We see that the tunneling amplitude $\langle p\rangle$ decreases as r increases when $U \geqslant 8$. As U becomes larger, the decrease $\langle p\rangle$ becomes more pronounced. This is because the barrier of Hubbard-gap tunneling becomes higher as the electron-electron interaction becomes stronger. Though $\langle p\rangle$ decreases slightly as r increases, $\langle \delta p\rangle$ increases sharply as r increases, as seen in Fig. 3(b). This means that randomness in on-site electron-electron interaction hardly affects the mean rate of Hubbard-gap tunneling, though the fluctuation of the tunneling rate is enlarged. This tendency is similar to that in a single-electron tunneling through a potential barrier. Note that $\langle \delta p\rangle$ increases rapidly when $\log_{10}(r)$ exceeds -1, particularly in the curve when $U=16$.

In Fig. 4, the tunneling amplitude $\langle p\rangle$ and its variance $\langle \delta p\rangle$ are plotted as a function of $\log_{10}(r)$, where Ω is taken to be 0.1,0.2,...,0.7 and U is fixed at 16. Comparing the tunneling amplitude $\langle p\rangle$ when $U=4$ and $\Omega=0.4$ in Fig. 3(a), we conclude that the electronic state of the chain having $0.1 \leqslant \Omega \leqslant 0.2$ is that of a Luttinger liquid. The confining potential of the chain is so weak that a quasi-Hubbard-gap could not be induced in the center of the chain. Note that $\langle \delta p\rangle$ when $\Omega=0.1$ is so small that one cannot see it in Fig. 4(b), and $\langle \delta p\rangle$ remains very small even when $\Omega=0.2$. We are

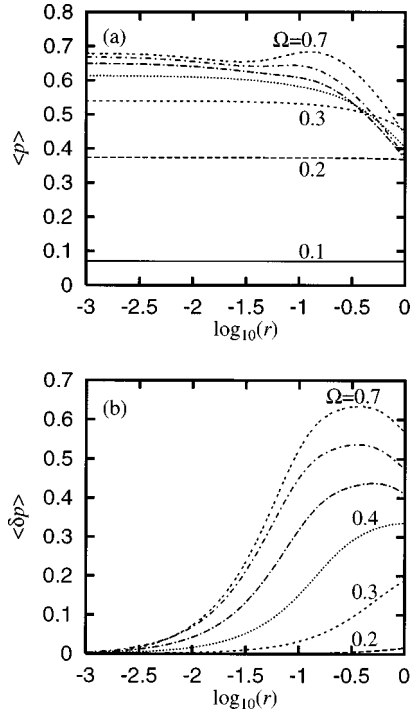

FIG. 4. (a) The average tunneling amplitude $\langle p\rangle = \langle |G_{-4,4}/G_{-4,-4}| \rangle$ and (b) its variance as a function of the degree of randomness when the on-site electron-electron interaction is randomly distributed. Ω is taken to be 0.1,0.2,...,0.7 and U is fixed at 16.

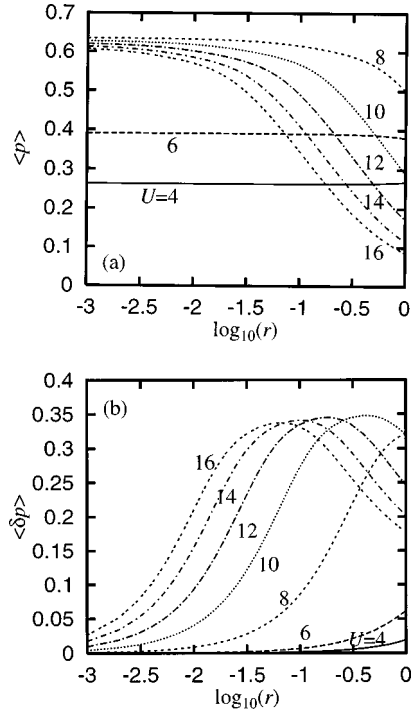

FIG. 5. (a) The average tunneling amplitude $\langle p\rangle = \langle |G_{-4,4}/G_{-4,-4}| \rangle$ and (b) its variance as a function of the degree of randomness when the single-particle energy is randomly distributed. Ω is fixed at 0.4 and U is taken to be 4,6,8,...,16.

reminded that this behavior of $\langle \delta p\rangle$ is similar to that of the chain having $U=4$ and $\Omega=0.4$, as shown in Fig. 3(b). As the strength of the confining potential, i.e., Ω becomes strong, $\langle p\rangle$ and $\langle \delta p\rangle$ become just as in a chain having Hubbard-gap tunneling. Though the tunneling amplitude $\langle p\rangle$ when $\Omega > 0.5$ is slightly larger than $\langle p\rangle$ when $\Omega=0.4$, the variance at $\log_{10}(r)\sim -1$ becomes larger as Ω increases from 0.4. As Ω becomes larger, the Fermi energy of both sides of the center increases, resulting in the large tunneling amplitude. This interpretation is supported by the fact that the tunneling amplitude $\langle p\rangle$ when $\Omega=0.7$ is enhanced at $\log_{10}(r)\sim -1$, as seen in Fig. 4(a). As discussed in the appendix, the tunneling amplitude of a single electron through a potential barrier is enlarged by randomness within a potential barrier. The term appearing in the appendix that makes the tunneling stronger is proportional to the inverse of the barrier height minus the energy of a particle. Therefore, this effect has a large contribution to the tunneling amplitude when the Fermi energy of both sides in our Hubbard chain is large, i.e., Ω is large.

B. Randomness in on-site single-particle energy

In a Hubbard chain without randomness, we know that the amplitude of Hubbard-gap tunneling strongly depends on whether the number of electrons in the chain is even or odd.[28] Note that, when the number of electrons is odd, the ground states degenerate; one of the ground states has the total spin $\uparrow$ and the other has the total spin $\downarrow$. To construct a ground state like the spin-density-wave state,[50] we must place an electron with spin $\sigma=\uparrow$ at the center of the chain, i.e., $j=0$. Next we place a pair of electrons with spin $\sigma=\downarrow$ at $|j|=1$, place a pair of electrons with $\sigma=\uparrow$ at $|j|=2$, and so on. This state is written as

$$|\Phi^{\mathrm{SDW}}_{N,\sigma}\rangle \sim \hat{c}^{\dagger}_{-N,\sigma}\hat{c}^{\dagger}_{-N+1,-\sigma}\cdots\hat{c}^{\dagger}_{N-1,-\sigma}\hat{c}^{\dagger}_{N,\sigma}|0\rangle, \qquad (14)$$

where $2N+1$ is the number of electrons. Note that an electron with spin σ cannot tunnel through the region from $j=-N$ to $j=N$ because electrons with spin σ exist in this region. On the other hand, if an even number of electrons is confined in the chain, the above discussion does not apply because the ground state has total spin 0 and becomes rotationally invariant. In this electronic system, Hubbard-gap tunneling can be seen. It should be noted that when asymmetry is introduced in the chain, Hubbard-gap tunneling can be seen when an odd number of electrons are confined in the Hubbard chain.[30] Moreover, the effect of the double occupancy in sites near the center is important in determining the electronic structure of a chain having Hubbard-gap tunneling. This is because no electrons can tunnel through a doubly occupied site, as stated in Pauli's principle.[31] Thus, the birth of doubly occupied sites due to an increase of the confining potential, stops Hubbard-gap tunneling in the Hubbard chain. We conclude that Fermi statistics are important in understanding Hubbard-gap tunneling because the tunneling barrier consists of electrons as well as tunneling particles.

In Fig. 5, the tunneling amplitude $\langle p\rangle$ and its variance $\langle \delta p\rangle$ are plotted as a function of $\log_{10}(r)$, where Ω is fixed as 0.4 and U is taken to be 4,6,8,...,16. The tunneling amplitudes when $U=4$ and 6 are similar to those with $U=4$ and 6 in Fig. 3(a). As suggested in the previous section, an electronic system like the Luttinger liquid is stable in the face of randomness. On the other hand, when $U \geqslant 8$, the tunneling

amplitude is very different from that in Fig. 3(a). The tunneling amplitude $\langle p\rangle$ decreases rapidly when $\log_{10}(r)$ exceeds -1.5, the amplitude of Hubbard-gap tunneling is strongly reduced by randomness in single-particle energy. Let us turn to deviation in the tunneling amplitude, i.e., $\langle \delta p\rangle$. Recall that $\langle \delta p\rangle$ increases as $\log_{10}(r)$ when Hubbard-gap tunneling is present, as seen in Figs. 3(b) and 4(b). In Fig. 5(b), however, we see peaks in $\langle \delta p\rangle$ when $U>8$. Note that $\langle \delta p\rangle$ starts to increase at smaller r as the strength of on-site electron-electron interaction, i.e., U becomes larger. On the other hand, the strong reduction of the tunneling amplitude $\langle p\rangle$ causes the reduction of $\langle \delta p\rangle$ because the latter is a variance of the former. Therefore, we have peaks in $\langle \delta p\rangle$.

Let us explain why the strong reduction takes place in the tunneling amplitude. When the single-particle energy of the jth site is slightly lower than the single-particle energy of the $(j-1)$th site and of the $(j+1)$th site, an electron is apt to sit at the jth site. Let us put other electrons in this region. Because of the large energy due to electron-electron interaction, electrons other than the electron located at the jth site are located at sites other than the jth site. However, there is a small probability of a double occupancy at the jth site. When the difference in single-particle energy between the jth site and the neighboring sites becomes larger, the probability of a double occupancy at the jth site increases. When our Hubbard chain has randomness in single-particle energy, several sites that have locally minimum energy possibly have up and down electrons and they may be doubly occupied sites. Therefore, the effect due to randomness in single-particle energy is similar to that due to asymmetry in the Hubbard chain without randomness. Double occupancy at any site drastically reduces Hubbard-gap tunneling; the reduction is governed by the prohibition rule derived from the Fermi statistics.

In Fig. 6, the tunneling amplitude $\langle p\rangle$ and its variance $\langle \delta p\rangle$ are plotted as a function of $\log_{10}(r)$, where Ω is taken to be 0.1, 0.2,...,0.7 and U is fixed at 16. Though $\langle \delta p\rangle$ with $\Omega=0.1$ in Fig. 6(a) is similar to that with $\Omega=0.2$ in Fig. 4(a), we see that $\langle \delta p\rangle$ with $\Omega=0.2$ in Fig. 6(a) is different from that with $\Omega=0.2$ in Fig. 4(a). $\langle \delta p\rangle$ with $\Omega=0.2$ in Fig. 4(a) is almost constant, but $\langle \delta p\rangle$ with $\Omega=0.2$ in Fig. 6(a) decreases when $\log_{10}(r)$ exceeds -1.5. This means that a Luttinger liquid with $\Omega=0.2$ is sensitive to the randomness in single-particle energy but not to the randomness in electron-electron interaction. When there is randomness in single-particle energy, all wave functions of a single electron are localized in one dimension, as in the Anderson localization postulate. We know the localization length may be dependent on the degree of impurity scattering. Therefore, the tunneling amplitude may be affected by the localization length of our Hubbard chain, which has randomness in single-particle energy. When $\Omega>0.2$, $\langle \delta p\rangle$ has a peak at $\log_{10}(r)\sim-1.2$, as in Fig. 5(b). It is notable that the tunneling amplitude $\langle p\rangle$ when $\Omega=0.7$ is enhanced in the region where $\log_{10}(r)\sim-1.5$, as seen in Fig. 6(a). In Fig. 4(a), $\langle p\rangle$ when $\Omega=0.7$ is enhanced where $\log_{10}(r)\sim-1$.

C. Randomness in both on-site parameters

In a chain of 10-nm quantum dots embedded in a bulk semiconductor, fluctuation in the size of these quantum dots causes randomness in both single-particle energy and on-site electron-electron interaction, as noted in Sec. II. Note that there exists a correlation between the degree of randomness in single-particle energy and the degree of randomness in on-site electron-electron interaction when the two kinds of randomness originate from fluctuations in the size of quantum dots. However, the degree of randomness in the single-particle energy of each quantum dot is possibly independent of the degree of randomness in the on-site electron-electron interaction of each quantum dot, when impurities distributed in a semiconductor cause randomness in the single-particle energy of quantum dots.

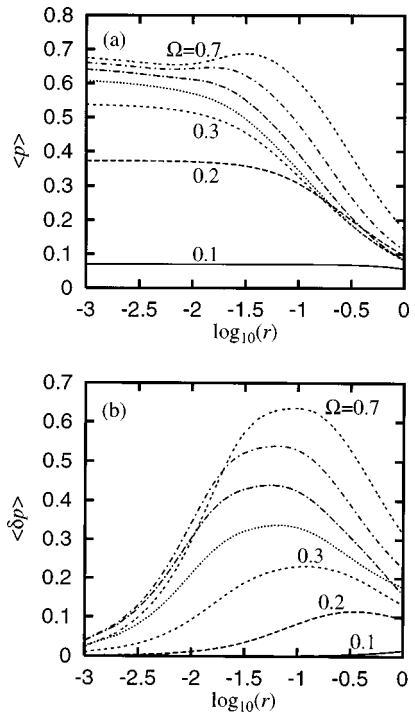

FIG. 6. (a) The average tunneling amplitude $\langle p\rangle = \langle |G_{-4,4}/G_{-4,-4}|\rangle$ and (b) its variance as a function of the degree of randomness when the single-particle energy is randomly distributed. Ω is taken to be 0.1,0.2,...,0.7 and U is fixed at 16.

In Fig. 7, the tunneling amplitude $\langle p\rangle$ and its variance $\langle \delta p\rangle$ are plotted as a function of $\log_{10}(r)$, where there is a correlation between the degree of randomness in single-particle energy and the degree of randomness in on-site electron-electron interaction, so $v_j=u_j$ for $j=-3,-2,...,3$ is randomly distributed. In Fig. 8, the tunneling amplitude $\langle p\rangle$ and its variance $\langle \delta p\rangle$ are plotted as a function of $\log_{10}(r)$, where there is no correlation between the degree of randomness in single-particle energy and the degree of randomness in on-site electron-electron interaction, so v_j is randomly distributed for $j=-3,-2,...,3$ and u_j is also randomly distributed for $j=-3,-2,...,3$. Note that the value of v_j is independent of the value of u_j in each ensemble. In both figures, Ω is fixed at 0.4 and U is taken to be 4,6,8...,16.

We see that Fig. 7 is almost identical to Fig. 5 in Sec. III B where only single-particle energy is randomly distributed. On the other hand, Fig. 8 is different from Fig. 7, particularly when the large U ($\geqslant 8$) causes Hubbard-gap tunneling. The tunneling amplitude $\langle p\rangle$ when $U=8$ in Fig. 8(a) remains constant up to $\log_{10}(r)\sim-0.5$, then decreases. This

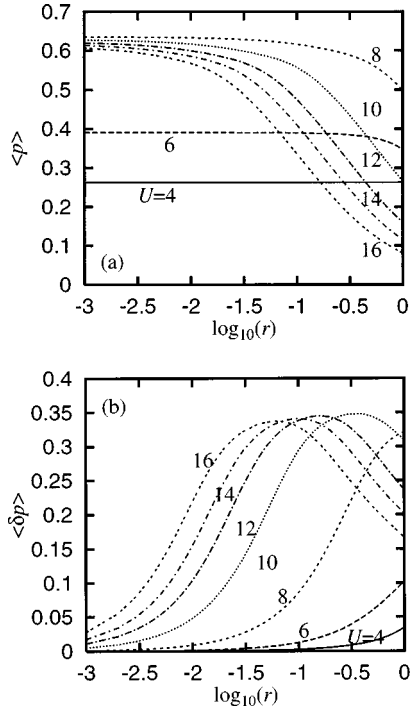

FIG. 7. (a) The averaged tunneling amplitude $\langle p\rangle = \langle |G_{-4,4}/G_{-4,-4}| \rangle$ and (b) its variance as a function of the degree of randomness when randomness in the size of quantum dots causes randomness both in on-site electron-electron interaction and in single-particle energy. Note that the degree of randomness in single-particle energy is correlated to the degree of randomness in on-site electron-electron interaction. Ω is fixed at 0.4 and U is taken to be 4,6,8,...,16.

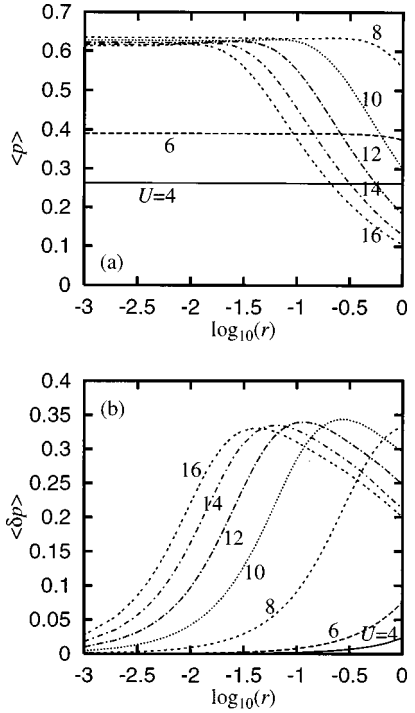

FIG. 8. (a) The averaged tunneling amplitude $\langle p\rangle = \langle |G_{-4,4}/G_{-4,-4}| \rangle$ and (b) its variance as a function of the degree of randomness both in single-particle energy and in on-site electron-electron interaction. Note that there is no correlation between randomness in single-particle energy and randomness in on-site electron-electron interaction. Ω is fixed at 0.4 and U is taken to be 4,6,8,...,16.

behavior of the tunneling amplitude is different from $\langle p\rangle$ when $U=8$ in Fig. 7(a), where the value gradually decreases as $\log_{10}(r)$ increases. When we turn our attention to the tunneling amplitude when $U>8$, we see the more rapid decrease of Hubbard-gap tunneling in Fig. 8(a) caused by the randomness. The tunneling amplitude when $U=10$ starts to decrease at $\log_{10}(r)\sim -1$; the tunneling amplitude when $U=12$ starts to decrease at $\log_{10}(r)\sim -1.5$; the tunneling amplitude when $U=14$ starts to decrease at $\log_{10}(r)\sim -1.8$; and so on. We have seen that as $\log_{10}(r)$ increases the tunneling amplitude decreases smoothly in Fig. 7(a) and that in Fig. 8(a), the tunneling amplitude falls off suddenly at value r, which depends on the strength of electron-electron interaction. The above result suggests that the degree of correlation between the two kinds of randomness has an effect on Hubbard-gap tunneling.

As discussed previously, the effect of double occupancy caused by randomness in single-particle energy is crucial in determining the behavior of Hubbard-gap tunneling in disordered quantum-dot chains. When randomness in single-particle energy and randomness in electron-electron interaction originate from fluctuations in the size of quantum dots, a smaller dot has larger single-particle energy and larger Coulomb energy, but a larger dot has smaller single-particle energy and smaller Coulomb energy. Therefore, these two kinds of randomness must have the same sign in order to produce the effect of double occupancy. Recall that double occupancy takes place at a site that has relatively small single-particle energy and relatively small Coulomb energy. When there is no correlation between the two kinds of randomness however, one may compensate the other. We suppose that when the degree of randomness is small the compensation works well so the tunneling amplitude is almost constant, but there is less compensation as the degree of randomness becomes larger. The strong effect of randomness in single-particle energy suggests that there is a rapid decrease in the tunneling amplitude as the degree of randomness increases.

IV. SUMMARY

We have investigated the effect of randomness on Hubbard-gap tunneling in a Hubbard chain under an overall confining potential. Two kinds of randomness—in on-site single-particle energy and in on-site electron-electron interaction—are considered not only separately but simultaneously. Because of the randomness in on-site single-particle energy, the variance of the tunneling amplitude has a peak when the degree of randomness changes. This peak is caused by the interplay between single-particle tunneling and Hubbard-gap tunneling in a Hubbard chain where the Fermi statistics of electrons have a strong influence. The effect of the degree of randomness on on-site electron-electron interaction is similar to the effect of barrier height on single-electron tunneling. These effects of randomness on Hubbard-gap tunneling are important in determining the electronic structures of tunneling-coupled nanostructures, e.g., coupled quantum dots.

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APPENDIX

When a single particle tunnels through a potential barrier, the WKB method gives a good approximation of the tunneling amplitude.[51] We consider a quantum particle that tunnels through a potential $V(x)$ in one dimension. When a single tunneling barrier is considered, $V(x)$ can be taken as

$$V(x)=\begin{cases} V_0 & \text{where } 0\leqslant x\leqslant d \\ 0 & \text{elsewhere,} \end{cases} \tag{A1}$$

where d is the width of the tunneling barrier. Let us define the value q, which is proportional to the tunneling amplitude through a potential barrier as

$$q(E)=\exp\left[-\frac{2}{\hbar}\int_0^d dx\sqrt{2m_e[V(x)-E]}\right], \tag{A2}$$

where E is the energy of a quantum particle and m_e is its mass. Randomness over a tunneling barrier can be introduced using a single-particle potential $V_{\rm dis}(x)$:

$$V_{\rm dis}(x)=\begin{cases} V_0+v_1 & \text{where } 0\leqslant x\leqslant d/N \\ V_0+v_2 & \text{where } d/N\leqslant x\leqslant 2d/N \\ \vdots & \\ V_0+v_N & \text{where } d(N-1)/N\leqslant x\leqslant d \\ 0 & \text{otherwise,} \end{cases} \tag{A3}$$

where v_j is randomly distributed from $-r/2$ to $r/2$ and N is an integer. Let us denote the tunneling amplitude q when a quantum particle runs through a potential barrier $V_{\rm dis}(x)$. The tunneling amplitude q can be written as

$$q(E)=q(E,v_1,v_2,\ldots,v_N)=\exp\left[-\alpha\sum_{j=1}^{N}\sqrt{V_0+v_j-E}\right], \tag{A4}$$

where

$$\alpha=\sqrt{2m_e}\,\frac{2d}{\hbar N}. \tag{A5}$$

Let us introduce the average of the tunneling amplitude in the random distribution as

$$\langle q\rangle=\frac{1}{r^N}\int_{-r/2}^{r/2}dv_1dv_2\cdots dv_N\exp\left(-\alpha\sum_{j=1}^{N}\sqrt{V_0+v_j-E}\right), \tag{A6}$$

when there is no spatial correlation in randomness. This expression is reduced into

$$\langle q\rangle=Q^N, \tag{A7}$$

where

$$Q=\frac{1}{r}\int_{-r/2}^{r/2}dv\ \exp(-\alpha\sqrt{V_0+v-E}). \tag{A8}$$

We have an expression for Q:

$$Q=\frac{1}{r}\int_{-r/2}^{r/2}dv\ \exp\left[-\alpha\sqrt{V_0-E}\sum_{m=0}^{\infty}\frac{c_m}{m!}\left(\frac{v}{V_0-E}\right)^m\right], \tag{A9}$$

where the sequence c_m is determined by $c_{m+1}=(\frac{1}{2}-m)c_m$ and $c_0=1$, so that

$$\sqrt{1+x}=\sum_{m=0}^{\infty}\frac{c_m x^m}{m!}. \tag{A10}$$

When the mean height of the barrier is large, i.e., $r\ll(V_0-E)$, we obtain the correction on the order of r^2 as

$$\begin{aligned} Q&\sim\frac{1}{r}\int_{-r/2}^{r/2}dv\ \exp\left[-\alpha\sqrt{V_0-E}\left(1+\frac{1}{2(V_0-E)}\,v\right)\right] \\ &=\frac{e^{\beta r/2}-e^{-\beta r/2}}{\beta r}\,e^{-\alpha\sqrt{V_0-E}} \\ &=e^{-\alpha\sqrt{V_0-E}}\left[1+\frac{(\beta r)^2}{24}+\frac{(\beta r)^4}{1920}+\cdots\right], \end{aligned} \tag{A11}$$

where

$$\beta=\frac{\alpha}{2\sqrt{V_0-E}}. \tag{A12}$$

We now have an expression for $\langle q\rangle$,

$$\begin{aligned} \langle q\rangle&=e^{-\alpha N\sqrt{V_0-E}}\left[1+\frac{(\beta r)^2}{24}\right]^N+\cdots \\ &=\exp\left(-\frac{2d}{\hbar}\sqrt{2m_e(V_0-E)}\right)\left(1+\frac{m_e d^2}{12\hbar^2(V_0-E)}\,\frac{r^2}{N}\right) \\ &\quad+\cdots, \end{aligned} \tag{A13}$$

when N is large and r is small. The first term in the above expression is common in an analysis of tunneling amplitude using the WKB method and the second term is a correction that reflects the degree of randomness in a tunneling barrier. The correction is positive, so a weak randomness, i.e., a small r, slightly enhances the tunneling amplitude. Note that the correction is proportional to $(V_0-E)^{-1}$. Therefore, the correction becomes smaller as the barrier becomes higher. It is remarkable that the effect of off resonance between the initial and final states strongly reduces the tunneling amplitude, resulting in the Anderson localization of electrons in a random potential.

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