Hubbard Gap Tunneling in Quantum Dot Chains: An Investigation Using Absorption Spectra

Ryuichi Ugajin
Sony Corporation Research Center, 174, Fujitsuka-cho, Hodogaya-ku, Yokohama 240, Japan
(Received 2 July 1997)

In a Hubbard chain under an overall confining potential, electrons localized by electron-electron interaction in the center of the chain coexist with electron tunneling through a quasi-Hubbard gap in the center, as suggested by the equal-time Green's function. This mixture of particlelike electrons and wavelike electrons is analyzed using absorption spectra. The effect is expected in a chain of tunneling-coupled nanostructures, e.g., coupled quantum dots. [S0031-9007(97)04924-7]

PACS numbers: 73.20.Dx, 78.66.–w

Quanta sometimes behave like particles and sometimes behave like waves. Quanta seeming to be particles, i.e., appearing to be an eigenstate of point $|x\rangle$, and quanta seeming to be waves, i.e., appearing to be an eigenstate of momentum $|p\rangle$, are different aspects of the same thing, as when a cylinder viewed from above seems to be circular, but when viewed from the side seems to be rectangular. The coexistence of these two different aspects of quanta provides interesting problems for condensed-matter physics, where the interplay between extended waves and localized particles is important in determining the behavior of electrons. One example is the Kondo effect of magnetic impurities in a diluted metal [1,2]; another example is a heavy-electron metal in which a localized f electron is coupled to conducting electrons [3,4], where localized states are embedded in a three-dimensional solid-state material. Still another example is metal-insulator transitions, in which an insulator of localized electrons is transferred to a metal of extended electrons through a transition point. When electrons are localized by randomness, the metal-insulator transition, i.e., Anderson transition, is well known to be a second-order phase transition [5,6]. When electrons are localized by electron-electron interaction on a lattice, the metal-insulator transition, i.e., Mott transition, may be a first-order phase transition [7,8]. Though the kinetic term in a Hamiltonian highlights the wave nature of electrons, the electron-electron interaction term, written in position eigenstates, emphasizes the particle nature over the wave nature.

As the number of dimensions is reduced, mean-field analysis can no longer be applied to determine the behavior of electrons in a solid-state material, particularly the coexistence of the wave nature and the particle nature, though we know the mean-field approximation works in these problems in three dimensions. This is because fluctuation from the mean-field solution becomes more important as the number of dimensions decreases. A great effort has been made to understand correlated electrons in low-dimensional lattices [9,10] and in low-dimensional structures, i.e., quantum Hall systems in two dimensions [11,12], quantum wires [13,14], and quantum dots [15–17]. The size of the confining structure can be smaller than 15 nm if compound semiconductor heterostructures, e.g., GaAs/AlGaAs, are used [18]. In tunneling-coupled quantum dots, we can expect various phenomena caused by the interplay between electron tunneling through the potential barrier of a heterostructure and electron-electron interaction [19]. In an array of tunneling-coupled quantum dots, we can expect electrons to have various phases when the array is half filled, and these systems can be mapped to Hubbard-type models for low-energy excitation [20–22]. If an array of very small quantum dots of GaAs is embedded in bulk AlAs, a field effect caused by a depletion region causes parabolic confinement over the array. This system can be realized using whiskers of compound semiconductors [23] and can be described by a Hubbard chain under an overall confining potential [24].

In the present Letter, another kind of coexistence, a mixture of localized electrons and extended electrons, which is the result of electron tunneling through a Mott insulator of localized electrons in a Hubbard chain under an overall confining potential, is discussed. We calculate the absorption spectra of several electrons in the chain, the result of which suggests some features of the two opposite aspects of correlated electrons.

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

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

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 jth site with spin σ. t is the transfer between adjacent sites and U is the on-site Coulomb interaction. When $\Omega > 0$, electrons in the Hubbard chain are confined by an overall parabolic potential. E introduces asymmetry in the chain, as in the Stark effect [25]. In this Letter we analyze the system of six electrons in the chain having $L = 5$, $t = 1$, and $U = 16$. The eigen energy E_n and its eigenstate $|n\rangle$ were calculated using numerical diagonalization of a Hamiltonian constructed by six-electron states, as $\hat{c}_{i\uparrow}^{\dagger} \hat{c}_{j\uparrow}^{\dagger} \hat{c}_{k\uparrow}^{\dagger} \hat{c}_{l\downarrow}^{\dagger} \hat{c}_{m\downarrow}^{\dagger} \hat{c}_{n\downarrow}^{\dagger} |0\rangle$. Note that we do not need

 0031-9007/98/80(3)/572(4)$15.00

to consider six-electron states except states having $S_z = 0$, where S_z is the total spin of six electrons in the z direction. This is because the ground state of our Hubbard chain should have $S_z = 0$ and because the dipole approximation, which is justified by the small size of our tunneling-coupled quantum dots, will not allow optical transitions with a spin flip. The absorption spectra are obtained by calculating the matrix element of the dipole operator

$$\hat{D} = \sum_{j=-L}^{L} j\hat{n}_j \,. \tag{2}$$

Dipole transition from the ground state $|\Psi_0\rangle$ to the nth excited state $|\Psi_n\rangle$, which has absorption energy $E_n - E_0$, is possible when $\Gamma = |\langle\Psi_n|\hat{D}|\Psi_0\rangle|^2 \neq 0$. A single optical transition from the ground state of six electrons has a large Γ, and Γ of the other optical transitions is small enough to ignore. Numerical calculations were performed using a Cray J916.

When $\Omega = 0$, 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 [26]. 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, the Mott-Hubbard gap appears, with an antiferromagnetic spin correlation. Hubbard gap tunneling is seen in the chain through the Hubbard gap induced by the overall confining potential [24]. This electronic system can be analyzed using the equal-time Green's function of the ground state $|\Psi_0\rangle$:

$$G_{i,j} = \langle\Psi_0|\hat{c}^{\dagger}_{i\uparrow}\hat{c}_{j\uparrow}|\Psi_0\rangle = \langle\Psi_0|\hat{c}^{\dagger}_{i\downarrow}\hat{c}_{j\downarrow}|\Psi_0\rangle \,, \tag{3}$$

because whether electrons are localized or delocalized can be determined by the behavior of $G_{i,j}$ $(i \neq j)$. In Fig. 1, $G_{-3,j}$ is plotted as a function of j with various E, where Ω is taken to be 1. Note that $G_{-3,-3}$ is the expectation value of the density of electrons at the $j = -3$ site. First we analyze $G_{-3,j}$ when $E = 0$. In this region of the confining potential, $G_{-3,3}$ has a considerable value, as shown in Fig. 1, although $G_{-3,j}$ is very small when $-2 < j < 2$. The figure shows that an electron at the $j = -3$ site can tunnel to the $j = 3$ site through the barrier of Mott-insulating electrons in the center. The value $G_{-3,j}/G_{-3,3}$ may be useful in determining the amplitude of the Hubbard gap tunneling. In a Mott insulator of a Hubbard chain of finite sites, the equal-time Green's function decays exponentially as the distance between sites increases—the fermionic excitation is massive because of the Hubbard gap. Thus, if the Hubbard chain of finite sites is surrounded by metallic electrons, we can expect tunneling through the Mott insulator.

When E introduces asymmetry into the chain, we see a reduction in the tunneling amplitude, as shown in Fig. 1. $G_{-3,j}/G_{-3,3}$ decreases rapidly as E increases. When $\Omega = 1$ induces a Hubbard gap in the center of the chain, the left and right sides from the center region should have discrete excitation spectra of a single electron. The least-energy state of the left-hand side, denoted by $|L\rangle$, can be resonantly coupled to the least-energy state of the right-hand side, denoted by $|R\rangle$, so resonant tunneling through the Hubbard gap can occur. If E is taken to be a nonzero value, "off resonance" between these two sides causes a reduction in the tunneling amplitude. Note that this description cannot be applied in all details to our system because our system has six electrons whose wave functions are totally asymmetric and $|L\rangle$ and $|R\rangle$ are really six-electron states [25]. Thus, the total Hilbert space of our six-electron system is decomposed, approximately, into two sectors—in one, electrons are localized by electron-electron interaction and, in the other, electrons are extended through the Hubbard gap.

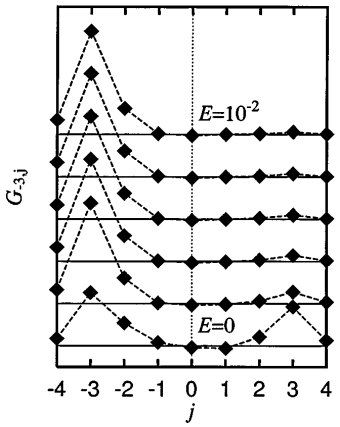

FIG. 1. Equal-time Green's function of the six-electron ground state $G_{-3,j}$ as a function of j. The strength of the external electric field E is taken to be 0, 0.2×10^{-2}, $0.4 \times 10^{-2}, \ldots, 1 \times 10^{-2}$, and successive traces are displayed upward by 0.2. $\Omega = 1$ is taken so as to allow the chain to have Hubbard gap tunneling.

Now we examine the electronic system using absorption spectra. Figure 2(a) shows the absorption energy when Ω is changed from 0 to 1. Figure 2(b) shows the dipole matrix element Γ of the allowed transition from the ground state. When $\Omega \sim 0$, i.e., in a Hubbard chain without confinement, absorption with a considerable energy exists in the absorption spectra. In the Hubbard chain, electrons are strongly correlated, but metallic. This electronic system has photon absorption just as a Fermi liquid (more exactly, a Luttinger liquid) has. Therefore, the absorption is due to the transition from the ground state of the electron liquid to the first excited state, in which an electron-hole pair is created. The energy difference between the ground state and the final state of absorption is enlarged because of the finite length of the chain. However, the matrix element of the dipole transition is rather small because the effective size of an electron at the Fermi level is reduced by electron correlation in the chain.

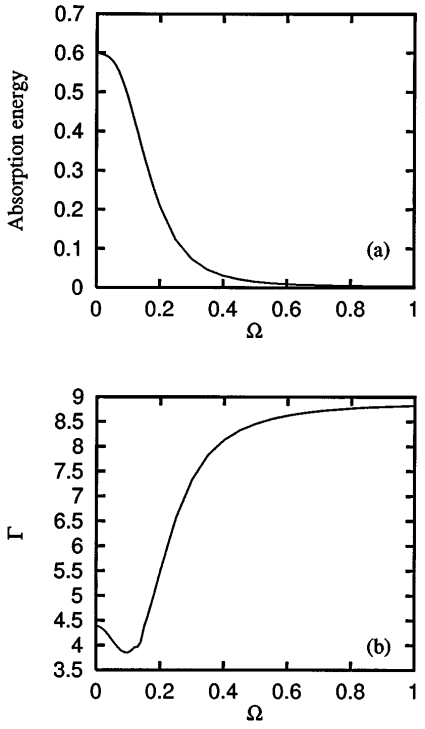

FIG. 2. (a) Absorption energy and (b) optical transition coefficient Γ as a function of the strength of the confining potential Ω when $E = 0$.

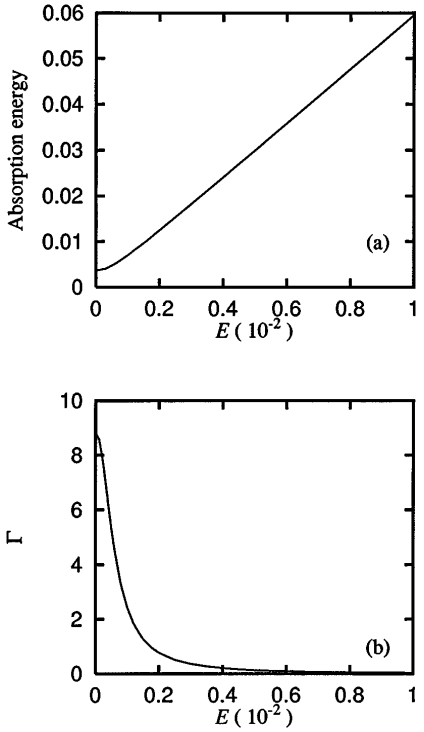

FIG. 3. (a) Absorption energy and (b) optical transition coefficient of Γ as a function of the strength of the external electric field E when $\Omega = 1.0$.

As Ω increases, the absorption energy becomes smaller, together with the matrix element of the dipole transition. However, when Ω exceeds 0.1, the dipole matrix element increases because of Hubbard gap tunneling. As suggested previously, the six-electron state $|L\rangle$, in which there is a single electron located to the left of the Mott-insulating electrons in the center of the chain, and the six-electron state $|R\rangle$, in which there is a single electron located to the right of the Mott-insulating electrons, are useful in describing Hubbard gap tunneling [27]. In a six-electron chain under an overall confining potential, a tunneling electron can absorb a photon through the dipole transition from the ground state of the "bonding state" $(|L\rangle + |R\rangle)/\sqrt{2}$ to the excited state of the "antibonding state" $(|L\rangle - |R\rangle)/\sqrt{2}$. This electron extends through the chain via the Hubbard gap embedded in the center of the chain. Thus, the dipole-matrix element of the transition is large.

Let us turn to absorption spectra of our Hubbard chain under an external electric field—we will see the Stark effect on the Hubbard gap tunneling when $\Omega = 1$. Figure 3(a) shows the absorption energy when external electric field E is changed from 0 to 0.01. Figure 3(b) shows the dipole-matrix element Γ of the allowed transition from the ground state. As is expected, the absorption is weakened by introducing E and the energy of the absorption becomes larger when E increases. If the ground state is written as $\alpha|L\rangle + \beta|R\rangle$ and the excited state as $\beta|L\rangle - \alpha|R\rangle$, where $\alpha^2 + \beta^2 = 1$, α is very different from

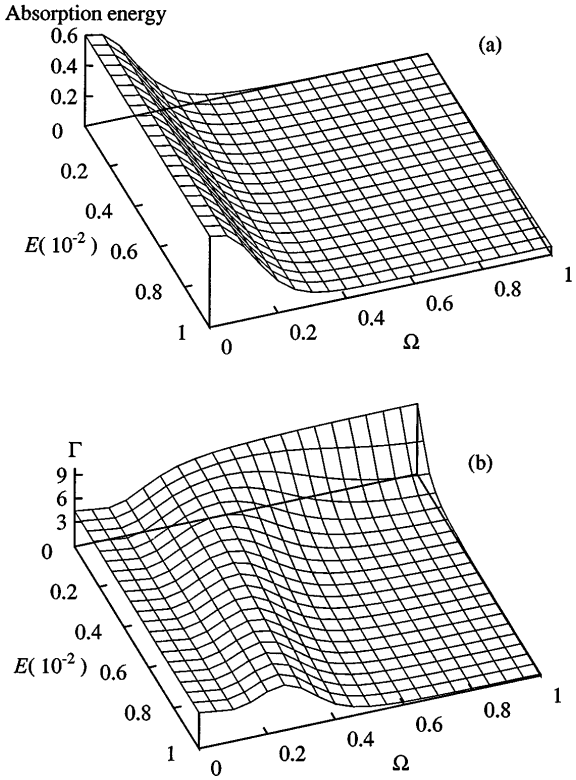

FIG. 4. (a) Absorption energy and (b) optical transition coefficient of Γ as a function of Ω and E.

β when our chain is under an external electric field. Because $\langle R|\hat{D}|L\rangle$ is very small, the matrix element of the dipole transition is weakened and the absorption energy is increased by the Stark effect, as in a single electron tunneling through a potential barrier.

For comparison, we plot the absorption energy and Γ of the Hubbard chain as a function of Ω and E in Fig. 4. When there is no confinement in the chain, we cannot see strong dependence of absorption on the strength of the external electric field E. This is because this system is identical to that of metallic electron gas under an external electric field and is very different from the system having Hubbard gap tunneling.

[1] J. Kondo, in *Solid State Physics, Volume 23*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1969).

[2] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

[3] Z. Fisk, D. W. Hess, C. J. Pethick, D. Pines, J. L. Smith, J. D. Thompson, and J. O. Willis, Science **239**, 33 (1988).

[4] P. G. McQueen, D. W. Hess, and J. W. Serene, Phys. Rev. Lett. **71**, 129 (1993).

[5] E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).

[6] P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).

[7] N. F. Mott, Philos. Mag. **6**, 287 (1961); *Metal-Insulator Transitions* (Taylor & Francis Ltd., London, 1974).

[8] X. Y. Zhang, M. J. Rosenberg, and G. Kotliar, Phys. Rev. Lett. **70**, 1666 (1993).

[9] P. W. Anderson, Science **235**, 1196 (1987).

[10] H. Fukuyama, H. Matsukawa, and Y. Hasegawa, J. Phys. Soc. Jpn. **58**, 364 (1989).

[11] R. B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983).

[12] B. I. Halperin, Phys. Rev. Lett. **52**, 1583 (1984).

[13] J. M. Luttinger, J. Math. Phys. (N.Y.) **4**, 1154 (1963).

[14] B. Sutherland, Phys. Rev. A **4**, 2019 (1971); Phys. Rev. A **5**, 1372 (1972).

[15] G. W. Bryant, Phys. Rev. Lett. **59**, 1140 (1987).

[16] T. Chakraborty, Comments Condens. Matter Phys. **16**, 35 (1992).

[17] R. Ugajin, Physica (Amsterdam) **237A**, 220 (1997).

[18] J. Oshinowo, M. Nishioka, S. Ishida, and Y. Arakawa, Appl. Phys. Lett. **65**, 1421 (1994).

[19] R. Ugajin, Appl. Phys. Lett. **68**, 2657 (1996); J. Appl. Phys. **81**, 2693 (1997).

[20] C. A. Stafford and S. Das Sarma, Phys. Rev. Lett. **72**, 3590 (1994).

[21] R. Ugajin, Phys. Rev. B **53**, 10 141 (1996).

[22] R. Ugajin, J. Phys. Soc. Jpn. **65**, 3952 (1996).

[23] T. Sato, K. Hiruma, M. Shirai, K. Tominaga, K. Haraguchi, T. Katsuyama, and T. Shimada, Appl. Phys. Lett. **66**, 159 (1995).

[24] R. Ugajin, Physica (Amsterdam) **229B**, 146 (1997).

[25] R. Ugajin, J. Phys. Soc. Jpn. **66**, 425 (1997).

[26] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[27] R. Ugajin, Physica (Amsterdam) **240B**, 128 (1997).