Numerical renormalization group approach to a quartet quantum-dot array connected to reservoirs: gate-voltage dependence of the conductance

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(Dated: September 17, 2018)

Abstract

The ground-state properties of quartet quantum-dot arrays are studied using the numerical renormalization group (NRG) method with a four-site Hubbard model connected to two non-interacting leads. Specifically, we calculate the conductance and local charge in the dots from the many-body phase shifts, which can be deduced from the fixed-point eigenvalues of NRG. As a function of the on-site energy \( \epsilon_d \) which corresponds to the gate voltage, the conductance shows alternatively wide peak and valley. Simultaneously, the total number of electrons \( N_{el} \) in the four dots shows a quantized staircase behavior due to a large Coulomb interaction \( U \). The conductance plateaus of the Unitary limit emerging for odd \( N_{el} \) are caused by the Kondo effect. The valleys of the conductance emerge for even \( N_{el} \), and their width becomes substantially large at half-filling. It can be regarded as a kind of the Mott-Hubbard insulating behavior manifesting in a small system. These structures of the plateaus and valleys become weak for large values of the hybridization strength \( \Gamma \) between the chain and leads. We also discuss the parallel conductance for the array connected to four leads.

PACS numbers: 72.10.-d, 72.10.Bg, 73.40.-c
I. INTRODUCTION

The Kondo effect in quantum dots is a subject of current interest, and early theoretical predictions \[1, 2\] have already been confirmed by the experiments. \[3, 4\] Recently, the interplay of various effects such as Aharonov-Bohm, Fano, Josephson, and Kondo effects have been studied extensively, \[5, 6, 7, 8, 9, 10, 11\] and interesting phenomena caused by inter-electron interactions have been expected to be seen at low temperatures.

For studying the low-temperature transport of interacting electron systems, careful calculations are required. So far, some numerical approaches to conductance through small interacting systems have been examined by several groups. For instance, a Fermi-liquid based method, \[12\] density matrix renormalization method, \[13, 14\] and functional renormalization method, \[14, 15\] seem to be complement each other to give reliable information valid at low temperatures. The Wilson numerical renormalization group (NRG) method, which successively eliminates higher-energy states to obtain accurately the low-lying energy states, \[16, 17, 18\] has also been applied successfully to single and double quantum dots. \[5, 19, 20\] Recently, we have provided an explicit prescription to deduce the many-body phase shifts from the fixed-point energy levels of NRG. It is applicable to a wide class of the quantum-dot systems connected to noninteracting leads. With this method, we examined precisely the conductance of a Hubbard chain of finite size \(N_C\) connected to noninteracting leads, \[21, 22\] the low-temperature Fermi-liquid regime of which had been studied before with a perturbation theory. \[23, 24\] It was confirmed that at half-filling the conductance through the four dots, \(N_C = 4\), decreases exponentially with increasing \(U\) reflecting a Mott-Hubbard type insulating behavior. \[21\] In contrast to the chains in the even size, for odd \(N_C\) the Kondo resonance emerges at the Fermi level, and it contributes to the Unitary-limit conductance \(g = 2e^2/h\).

In quantum dots, the on-site potential \(\epsilon_d\) is a tunable parameter, and it corresponds to the gate voltage. We have reported the \(\epsilon_d\) dependence of the conductance of the triple quantum dots. \[22\] The purpose of the work is to study how the conductance through the four quantum-dot chain behaves as a function of the gate voltage. Owing to the Fermi-liquid properties at low temperatures, the conductance \(g\) and local charge \(N_{el}\) in the quantum dots are determined by the two phase shifts \(\delta_{\text{even}}\) and \(\delta_{\text{odd}}\), which are defined with respect to the even and odd \((s \text{ and } p)\) partial waves, respectively. \[22\] We calculate these two phase
shifts from the fixed-point eigenvalues of NRG. Furthermore, from these phase shifts, we can also deduce a parallel conductance through the quantum dots connected transversely to four noninteracting leads.

The results of the dc conductance show the typical Kondo plateaus of the Unitary limit $g \simeq 2e^2/h$ when the total number of electrons $N_{\text{el}}$ in the four dots is odd. On the other hand, the conductance shows wide minima for even $N_{\text{el}} \simeq 2, 4, 6$. The local charge $N_{\text{el}}$ shows a quantized staircase behavior as a function of $\epsilon_d$. Among the conductance minima, the one at half-filling $N_{\text{el}} \simeq 4$ is the widest, and it can be regarded as a kind of the Mott-Hubbard insulating behavior. The feature of the conductance near half-filling is quite different whether the number of quantum dots is even or odd, namely the Kondo plateau appears for odd $N_C$.

This paper is organized as follows. In Sec. II, we describe the outline of the formulation to deduce the conductance from the fixed-point energy levels of the NRG. In Sec. III, we show the NRG results. In Sec. IV, discussions are given.

II. MODEL AND FORMULATION

In this section, we describe briefly the relation between the phase shifts and fixed-point Hamiltonian of NRG.[22] As far as the zero-temperature value is concerned, the conductance can be calculated more accurately with this formulation than to calculate it directly from the current-current correlation function.

We start with a Hubbard chain of a finite size $N_C$, as illustrated in Fig. [I]. It is connected to two non-interacting leads on the left($L$) and right($R$) via the tunneling matrix elements $v_L$ and $v_R$, respectively. The Hamiltonian is given by

$$\mathcal{H} = \mathcal{H}_C^0 + \mathcal{H}_C^U + \mathcal{H}_{\text{mix}} + \mathcal{H}_{\text{lead}}$$  (1)
FIG. 1: Schematic picture of a series connection.

with

\[ H_C^0 = -t \sum_{i=1}^{N_C-1} \sum_{\sigma} \left( d_{i\sigma}^\dagger d_{i+1\sigma} + d_{i+1\sigma}^\dagger d_{i\sigma} \right) + \epsilon_d \sum_{i=1}^{N_C} \sum_{\sigma} d_{i\sigma}^\dagger d_{i\sigma} , \]  

(2)

\[ H_C^U = U \sum_{i=1}^{N_C} d_{i\uparrow}^\dagger d_{i\downarrow}^\dagger d_{i\downarrow} d_{i\uparrow} , \]  

(3)

\[ H_{\text{mix}} = v_L \sum_{\sigma} \left( d_{1\sigma}^\dagger \psi_{L\sigma} + \psi_{L\sigma}^\dagger d_{1\sigma} \right) + v_R \sum_{\sigma} \left( \psi_{R\sigma}^\dagger d_{N_C\sigma} + d_{N_C\sigma}^\dagger \psi_{R\sigma} \right) , \]  

(4)

\[ H_{\text{lead}} = \sum_{\nu=L,R} \sum_{k\sigma} \epsilon_{k\nu} c_{k\nu\sigma}^\dagger c_{k\nu\sigma} , \]  

(5)

where \( d_{i\sigma} \) annihilates an electron with spin \( \sigma \) at site \( i \) in the Hubbard chain, which is characterized by the nearest-neighbor hopping matrix element \( t \), onsite energy \( \epsilon_d \), and Coulomb interaction \( U \). In the lead on the left or right (\( \nu = L, R \)), the operator \( c_{k\nu\sigma}^\dagger \) creates a conduction electron with energy \( \epsilon_{k\nu} \), the wavefunction for which is denoted by \( \phi_{k\nu}(r) \). The linear combinations of the conduction electrons \( \psi_{L\sigma} \) and \( \psi_{R\sigma} \) mixed with the electrons in the interacting sites at \( i = 1 \) and \( N_C \), respectively, where \( \psi_{\nu\sigma} = \sum_k c_{k\nu\sigma} \phi_{k\nu}(r_{\nu}) \) and \( r_{\nu} \) is the position at the interface in the lead \( \nu \). We assume that the hybridization strength \( \Gamma_{\nu} \equiv \pi v_{\nu}^2 \sum_k |\phi_{k\nu}(r_{\nu})|^2 \delta(\omega - \epsilon_{k\nu}) \) is a constant independent of the frequency \( \omega \), and take the origin of the energy to be \( \mu = 0 \).
A. Ground-state properties and phase shifts

In the following, we assume that the system has an inversion symmetry, $v_L = v_R (\equiv v)$ and $\Gamma_L = \Gamma_R (\equiv \Gamma)$. Then, it is convenient to introduce the orbitals which have even and odd parities

$$a_{j,\sigma} = \frac{d_{j,\sigma} + d_{N_C-j+1,\sigma}}{\sqrt{2}};$$

$$b_{j,\sigma} = \frac{d_{j,\sigma} - d_{N_C-j+1,\sigma}}{\sqrt{2}},$$

where $j = 1, 2, \ldots, N_C/2$ for even $N_C$. For odd $N_C$, there exists one extra unpaired orbital $a_{(N_C+1)/2,\sigma} \equiv d_{(N_C+1)/2,\sigma}$ in addition to the pairs labeled as $j = 1, 2, \ldots, (N_C - 1)/2$. Due to the inversion symmetry, at zero temperature $T = 0$ and Fermi energy $\omega = 0$, the retarded Green’s functions for $a_{1,\sigma}$ and $b_{1,\sigma}$ can be written in the forms,[22]

$$\langle \langle a_{1,\sigma}; a_{1,\sigma}^\dagger \rangle \rangle_{\omega=0} = \frac{1}{\Gamma} \frac{1}{\kappa_{\text{even}} + i} \equiv \frac{1}{\Gamma} \frac{1}{\sqrt{\kappa_{\text{even}}^2 + 1}} e^{i\delta_{\text{even}}},$$

$$\langle \langle b_{1,\sigma}; b_{1,\sigma}^\dagger \rangle \rangle_{\omega=0} = \frac{1}{\Gamma} \frac{1}{\kappa_{\text{odd}} + i} \equiv \frac{1}{\Gamma} \frac{1}{\sqrt{\kappa_{\text{odd}}^2 + 1}} e^{i\delta_{\text{odd}}}.$$  

Namely, each of these two retarded Green’s functions is determined by a single parameter, $\kappa_{\text{even}}$ or $\kappa_{\text{odd}}$, which contains all effects of the scatterings and interactions. The phase shifts $\delta_{\text{even}}$ and $\delta_{\text{odd}}$, correspond to the angle of these two Green’s functions in the complex plane.

The two phase shifts determine the ground-state properties of the series connection illustrated in Fig.[23] Specifically, using the Kubo formalism and Friedel sum rule, the dc conductance $g_{\text{series}}$ and total number of electrons in the Hubbard chain $N_{\text{el}} \equiv \sum_{i=1}^{N_C} \sum_{\sigma} \langle d_{i\sigma}^\dagger d_{i\sigma} \rangle$ can be expressed in the forms,[22]

$$g_{\text{series}} = \frac{2e^2}{h} \sin^2 \left( \frac{1}{2} \left( \delta_{\text{even}} - \delta_{\text{odd}} \right) \right),$$

$$N_{\text{el}} = \frac{2}{\pi} \left( \delta_{\text{even}} + \delta_{\text{odd}} \right).$$

These formulas are justified if the imaginary of the $N_C \times N_C$ matrix version of the retarded self-energy due to the interaction $\mathcal{H}_U^I$ vanishes, $\text{Im} \Sigma^+(0) = 0$, at $T = 0$ and $\omega = 0$.[22] [24]

Furthermore, from these two phase shifts defined with respect to the series connection, one can deduce the parallel conductance $g_{\text{parallel}}$ for the current flowing in the horizontal
FIG. 2: Schematic picture of a parallel connection.

direction in the geometry illustrated in Fig. 2.

\[ g_{\text{parallel}} = \frac{2e^2}{h} \left( \sin^2 \delta_{\text{even}} + \sin^2 \delta_{\text{odd}} \right) \].

(12)

This expression is equivalent to the multi-channel version of the Landauer formula,\cite{26} and it can also be derived from the Kubo formula.\cite{22, 27} Since two conducting channels can contribute to the total current, the maximum possible value of \( g_{\text{parallel}} \) is \( 4e^2/h \). Note that the tunneling matrix elements between the leads and interacting part are taken to be \( v/\sqrt{2} \) as shown in Fig. 2. Because of the inversion symmetry between left lead 1 (2) and right lead 1 (2), an odd combination of the states from these two leads is separated, and the interacting site for \( i = 1 \) (\( i = N_C \)) is coupled to an even combination by the matrix element \( v \). Therefore, the ground state properties for the parallel geometry are determined by the phase shifts \( \delta_{\text{even}} \) and \( \delta_{\text{odd}} \) that are defined with respect to the series connection in eqs. (8) and (9). Specifically, \( N_{el} \) for parallel connection is equal to that for the series connection, and is given by eq. (11).
B. Fixed-point Hamiltonian and phase shifts

The two phase shifts $\delta_{\text{even}}$ and $\delta_{\text{odd}}$ can be deduced from the fixed-point eigenvalues NRG. In the NRG approach, a sequence of the Hamiltonian $H_N$ is introduced, by carrying out the logarithmic discretization for the conduction band with the half-width $D$,\cite{16,17,18} as

$$H_N = \Lambda^{(N-1)/2} \left( H_C^0 + H_C^U + H_{\text{mix}} + H_{\text{lead}}^{(N)} \right),$$  \hspace{1cm} (13)

$$H_{\text{mix}} = \bar{v} \sum_{\sigma} \left( f_{0,L\sigma}^\dagger d_{1,\sigma} + d_{1,\sigma}^\dagger f_{0,L\sigma} \right)$$

$$+ \bar{v} \sum_{\sigma} \left( f_{0,R\sigma}^\dagger d_{N_C,\sigma} + d_{N_C,\sigma}^\dagger f_{0,R\sigma} \right),$$  \hspace{1cm} (14)

$$H_{\text{lead}}^{(N)} = D \frac{1 + 1/\Lambda}{2} \sum_{\nu=L,R} \sum_{\sigma} \sum_{n=0}^{N-1} \xi_n \Lambda^{-n/2}$$

$$\times \left( f_{n+1,\nu\sigma}^\dagger f_{n,\nu\sigma} + f_{n,\nu\sigma}^\dagger f_{n+1,\nu\sigma} \right),$$  \hspace{1cm} (15)

where $\bar{v} = \sqrt{2D\Gamma \Lambda/\pi}$, $A_\Lambda = \frac{1+1/\Lambda}{2\log \Lambda}$, and

$$\xi_n = \frac{1 - 1/\Lambda^{n+1}}{\sqrt{1 - 1/\Lambda^{2n+1}} \sqrt{1 - 1/\Lambda^{2n+3}}}. \hspace{1cm} (16)$$

As in the case of the single Anderson (or Kondo) impurity,\cite{16,17,18} the low-lying eigenvalues of $H_N$ for the finite Hubbard chain converge, for large $N$, to the fixed-point values which have one-to-one correspondence to the free quasi-particles of a local Fermi liquid.\cite{21,22}

The fixed-point Hamiltonian describing the free quasi-particles can be written in the form

$$H_{\text{qp}}^{(N)} = \Lambda^{(N-1)/2} \left( H_C^{\text{eff}} + H_{\text{mix}} + H_{\text{lead}}^{(N)} \right),$$  \hspace{1cm} (17)

where $H_C^{\text{eff}} \equiv H_C^0 + \sum_{i,j=1}^{N_C} \text{Re} \ \Sigma_{ij}^+(0) d_{i\sigma}^\dagger d_{j\sigma}$. The many-body corrections enter through the real part of self-energy at $T = 0$, $\omega = 0$. With NRG, one can calculate accurately the quasi-particle energies $\varepsilon^{\gamma_*}$ with parity $\gamma$ (= “even” or “odd”) from the fixed-point eigenvalues of $H_N$. Then, the parameters $\kappa_{\text{even}}$ and $\kappa_{\text{odd}}$ defined in eqs. \cite{8} and \cite{9} can be deduced from the quasi-particle energy $\varepsilon^{\gamma_*}$,\cite{22}

$$\kappa_\gamma = \left( \bar{v}^2/\Gamma D \right) \lim_{N \to \infty} D \Lambda^{(N-1)/2} g_N(\varepsilon^{\gamma_*}).$$  \hspace{1cm} (18)

Here, $g_N(\omega) = \sum_{m=0}^N |\varphi_m(0)|^2/(\omega - \varepsilon_m)$ is the Green’s function for one of the isolated leads described in $H_{\text{lead}}^{(N)}$. The eigenvalue and eigenfunction of for one isolated lead are denoted by $\varepsilon_m$ and $\varphi_m(n)$, respectively, for $0 \leq n \leq N$.\footnote{7}
In this section, we apply the formulation described in the above to the four-site Hubbard chain, $N_C = 4$, attached to the reservoirs. In each step of the iteration, the Hilbert space for $H_{N+1}$ is constructed from that for $H_N$ and extra 16 states with respect to the two orbitals $f_{N+1,R\sigma}^\dagger$ and $f_{N+1,L\sigma}^\dagger$. We have kept the lowest 1716 eigenstates for constructing the Hilbert space for the next step. With this procedure the discretized Hamiltonian $H_N$, which consists of $2(N+1)+N_C$ sites, can be diagonalized exactly up to $N = 0$ for $N_C = 4$. We have checked that the conductance of the the noninteracting case $U = 0$ are reproduced sufficiently well with this procedure also for a rather large value of the discretization parameter $\Lambda = 6.0$, as shown in Fig. 3. We have also confirmed that the numerical results for the fixed-point eigenvalues of $H_N$ can be mapped onto the energy spectrum of the free quasi-particles in all parameter sets we have examined. It justifies the assumption of the local Fermi liquid we have made in the previous section.

A. Series connection

We now show the $\epsilon_d$ dependence of the conductance of the quantum dots in the series connection. As already mentioned, the onsite potential $\epsilon_d$ is a tunable parameter that is
FIG. 4: (a) The conductance $g_{\text{series}}$, (b) local charge $N_{\text{el}}$, phase shifts $2\delta_{\text{even}}/\pi$ and $2\delta_{\text{odd}}/\pi$ as functions of $\epsilon_d/U$ for $U/(2\pi t) = 1.0$, $\Gamma/t = 0.12$, $t/D = 0.1$, and $\Lambda = 6.0$. The dashed vertical lines in (b) correspond to the values of $\epsilon_d$, at which $N_{\text{el}}$ jumps in the limit of $\Gamma \to 0$.

controlled by the gate voltage in real quantum dots systems. In Fig. 4 (a) the conductance $g_{\text{series}}$, (b) total charge $N_{\text{el}}$ in the four-site Hubbard chain, the phase shifts $\delta_{\text{even}}$ and $\delta_{\text{odd}}$ are plotted as functions of $\epsilon_d/U$, where the parameters are chosen to be $U/(2\pi t) = 1.0$, $\Gamma/t = 0.12$, $t/D = 0.1$ and $\Lambda = 6.0$. The vertical dashed lines in (b) correspond to the values of $\epsilon_d$ at which $N_{\text{el}}$ jumps discontinuously in the limit of $\Gamma \to 0$. The Kondo plateaus of the Unitary limit $g_{\text{series}} \simeq 2e^2/h$ are seen in the regions corresponding to the odd occupations $N_{\text{el}} \simeq 1, 3, 5, 7$, where the value of the phase shifts is almost locked such that $\delta_{\text{even}} - \delta_{\text{odd}} \simeq \pi/2$. On the other hand, for even occupancies $N_{\text{el}} \simeq 2, 4, 6$, the conductance is suppressed substantially, and the phase shifts are locked at $\delta_{\text{even}} - \delta_{\text{odd}} \simeq 0$ or $\pi$. The conductance valley at half-filling becomes wider and deeper than the other valleys. Although the size of chain is not so large, i.e., $N_C = 4$, the feature of the valley at half-filling can be
FIG. 5: (a) The conductance $g_{\text{series}}$, (b) local charge $N_{\text{el}}$, phase shifts $2\delta_{\text{even}}/\pi$ and $2\delta_{\text{odd}}/\pi$ as functions of $\epsilon_d/U$. Here, $U/(2\pi t) = 0.2$, $\Gamma/t = 0.12$, $t/D = 0.1$, and $\Lambda = 6.0$. The dashed vertical lines in (b) correspond to the values of $\epsilon_d$ at which $N_{\text{el}}$ jumps in the limit of $\Gamma \to 0$.

understood as a kind of the Mott-Hubbard insulating behavior. We will discuss later the behavior of the conductance near half-filling more quantitatively. In Fig. 4 the hybridization energy scale $\Gamma$ is chosen to be much smaller than the hopping matrix element $t$. Therefore, the local charge $N_{\text{el}}$ shows a clear staircase step behavior. In the limit of $\Gamma \to 0$, the local charge jumps discontinuously at the values of $\epsilon_d$ corresponding to the dashed lines. Note that unless the Coulomb interaction, the phase shifts do not show the $\pi/2$ steps corresponding to the plateaus for odd $N_{\text{el}} = 1, 3, 5, \text{and } 7$. When the onsite potential $\epsilon_d/U$ decreases from 0.4 to 0, the phase shift for the even partial wave $\delta_{\text{even}}$ increases from 0 to $\pi$ via two successive $\pi/2$ steps, while that for the odd partial wave $\delta_{\text{odd}}$ remains almost unchanged at 0. Then, in the region of $-0.5 < \epsilon_d/U < 0.0$, $\delta_{\text{odd}}$ shows one $\pi/2$ step, while the even part remains to be $\delta_{\text{even}} \simeq \pi$. Similar features are seen also for $\epsilon_d/U < -0.5$. In fact, the two regions
FIG. 6: The conductance near half-filling for several values of the Coulomb interaction $U/(2\pi t) = 0.2, 0.5, 1.0$ and 1.5. Here, $\Gamma/t = 0.12$, $t/D = 0.1$, and $\Lambda = 6.0$.

$\epsilon_d/U < -0.5$ and $\epsilon_d/U > -0.5$ are relating each other via an electron-hole transformation. In the case of the linear chain of the quantum dots, the resonance states of the even parity for the even partial wave and that of the odd one cross the Fermi level alternatively. Thus, the $\pi/2$ steps took place for even and odd phase shifts alternatively.

We next examine the ground-state properties for small $U$. The results of the conductance and local charge for $U/(2\pi t) = 0.2$ are shown in Fig. 5 where $\Gamma/t = 0.12$ and $t/D = 0.1$. The peaks of the conductance becomes very narrow compared to those for larger $U$ shown in Fig. 4. Nevertheless, the shape of the peaks seen deviates from a simple Lorentzian shape as a result of the many-body effects due to the small but finite $U$. The conductance valley at half-filling $N_{el} \simeq 4$ is slightly wider than the other ones at $N_{el} \simeq 2$ and 6. However, the difference is not so large. In Fig. 5 (b), the steps for the local charge are seen clearly for even occupancies $N_{el} \simeq 2$, 4, and 6. However, for odd occupancies, only a weak structure can be recognized just for $N_{el} \simeq 1$ and 7. Therefore, when a resonance state passes through the Fermi level, two electrons occupy the state almost simultaneously. Correspondingly, the phase shifts $\delta_{\text{even}}$ and $\delta_{\text{odd}}$ do not show clear $\pi/2$ steps, although the weak structure can be seen for $N_{el} \simeq 1$ and 7.

In order to see how the conductance valley at half-filling evolves with the repulsive interaction, the conductance is plotted for several values of $U/(2\pi t) = 0.2, 0.5, 1.0$ and 1.5 in Fig. 6 where the other parameters are chosen to be $\Gamma/t = 0.12$, $t/D = 0.1$, and $\Lambda = 6.0$. As $U$ increases, the valley becomes wider, and the edge at the both side becomes sharper.
Furthermore, the minimum value of the conductance at the electron-hole symmetric case $\epsilon_d = -U/2$ decreases exponentially with increasing $U$, which has been confirmed precisely in a previous work. These results imply that for even $N_C$ the conductance valley at half-filling approaches to the insulating gap, even though the size of the chain examined here is just $N_C = 4$. However, because $N_C$ is finite, the low-lying energy states of the whole system including the noninteracting leads are described by the Fermi-liquid fixed point. Therefore, the ground state is not an exact insulating state, but a highly renormalized metallic state with heavy quasi-particles. For large even $N_C$, however, the conductance is expected to show an exponential dependence $g \propto e^{-N_C/\xi}$, where $\xi \sim \hbar v_F/\Delta_{\text{gap}}$ is a correlation length determined by the Hubbard gap $\Delta_{\text{gap}}$ and Fermi velocity $v_F$.

So far, the hybridization energy scale $\Gamma$ is taken to be much smaller than the hopping matrix element $t$ between the dots, $\Gamma = 0.12t$. In order to study the ground-state properties for larger $\Gamma$, we have carried out the calculations taking the hybridization to be $\Gamma/t = 0.5$. The results are show in Fig. 7 where $U/(2\pi t) = 1.0$, $t/D = 0.02$ and $\Lambda = 6.0$. The local charge $N_{\text{el}}$, which shows a staircase behavior for small $\Gamma$, becomes a gentle slope in Fig. 7(b). This is because the large hybridization makes the resonance peaks broad, and it reduces effectively the correlation effects. Therefore, the peaks of conductance become round. Furthermore, the conductance valleys especially the ones corresponding to $N_{\text{el}} \simeq 2$ and 6 become shallow. The valley at half-filling is still deeper than the other two valleys because of the correlations that lead the Mott-Hubbard behavior in the thermodynamic limit.

**B. Parallel connection**

We have also calculated the parallel conductance $g_{\text{parallel}}$ using eq. (12) with the phase shifts obtained for the series connection. The results are shown in Fig. 8 as functions of $\epsilon_d/U$ for $U/(2\pi t) = 1.0$. In the figures, both the series and parallel conductances are plotted for comparison, and for the hybridization two different values are examined, (a) $\Gamma/t = 0.12$ and (b) $\Gamma/t = 0.5$. For small $\Gamma$, the parallel and series conductances are almost coincide with each other as seen in Fig. 8(a). The difference becomes larger, however, for large $\Gamma$, as seen in the lower panel (b). The valleys of the conductance are deeper for the parallel connection than that of the series connection. This seems to be caused by the fact the even and odd
FIG. 7: (a) The conductance $g_{\text{series}}$, (b) local charge $N_{\text{el}}$, phase shifts $2\delta_{\text{even}}/\pi$ and $2\delta_{\text{odd}}/\pi$ as functions of $\epsilon_d/U$. Here, $U/(2\pi t) = 1.0$, $\Gamma/t = 0.5$, $t/D = 0.02$, and $\Lambda = 6.0$. The dashed vertical lines in (b) correspond to the values of $\epsilon_d$ at which $N_{\text{el}}$ jumps in the limit of $\Gamma \to 0$.

Parts of the partial waves contribute to the parallel conduction separately through eq. (12). The parallel conductance for large $\Gamma$, shown in Fig. 8 (b), is slightly larger than $2e^2/h$ at the first and fourth peaks. As mentioned in the previous section, the upper bound of $g_{\text{parallel}}$ is $2e^2/h \times 2$, because two conducting channels can contribute to the current in the geometry shown in Fig. 2. However, in the present case, the parallel conductance does not reach the upper bound. Similar feature has also been confirmed to be seen for the triple dots in a previous work.[22] As mentioned, in the case of the linear chain of the quantum dots, the resonance state of the even parity and that of the odd parity passes through the Fermi level alternatively when $\epsilon_d$ increases (or decreases). Therefore, only a single resonance state can contribute to the tunneling current for given $\epsilon_d$, so that the peak value of the conductance for the linear chain is bounded at $g_{\text{parallel}} \simeq 2e^2/h$ despite having the two conducting channels. To reach the Unitary-limit value $4e^2/h$ for two conducting channels, the quantum dots are
FIG. 8: The series (solid line) and parallel (dotted line) conductances for $U/(2\pi t) = 1.0$ as functions of $\epsilon_d/U$. Here, (a) $\Gamma/t = 0.12$, $t/D = 0.1$, and (b) $\Gamma/t = 0.5$, $t/D = 0.02$.

required to have a degeneracy in the discrete energy levels. It is not the case of the linear chain considered in the present work.

IV. DISCUSSIONS

As discussed in Sec. III, a kind of the Mott-Hubbard insulating behavior is seen at half-filling in the conductance through the one-dimensional array consisting of the even number of quantum dots $N_C$. The situation is quite different for the array with odd $N_C$, because the Kondo resonance contributes to the current as shown in Fig. 9 where the series conductance and total charge $N_{el}$ in triple dots ($N_C = 3$) are plotted as functions of $\epsilon_d/U$. Near half-filling, the conductance shows a plateau of the height $g_{\text{series}} \simeq 2e^2/h$ in stead of a wide gap $\Delta_{\text{gap}}$ as seen in Fig. 6 for even $N_C$. The plateau becomes wider with
FIG. 9: NRG results for the conductance $g_{\text{series}}$ and local charge $N_{\text{el}}$ for triple dots $N_C = 3$ as functions of $\epsilon_d/U$. Here, $U/(2\pi t) = 1.0$, $\Gamma/t = 0.12$, $t/D = 0.1$, and $\Lambda = 6.0$. The dashed vertical lines correspond to the values of $\epsilon_d$ at which $N_{\text{el}}$ jumps in the limit of $\Gamma \to 0$.

increasing $U$. However, the Kondo temperature $T_K$ decreases with increasing $U$, and thus the conductance plateau can be observed only at low temperatures $T \lesssim T_K$. If the single-particle spectral function is calculated at half-filling as a function of the frequency $\omega$, the narrow Kondo peak will be seen at $0 < |\omega| \lesssim T_K$. Then, there will be a pseudo-gap region at $T_K \lesssim |\omega| < \Delta_{\text{gap}}$, where the spectral weight almost vanishes. The width of the Kondo plateau at half-filling will be almost the same as the excitation gap $2\Delta_{\text{gap}}$ seen in the spectral function. The Kondo temperature $T_K$ for half-filling decreases with increasing $N_C$, and finally the resonant state vanishes as $T_K \to 0$ in the limit of $N_C \to \infty$. Therefore, for large $N_C$, the conductance plateau emerges only at very low temperatures. If the thermodynamic limit $N_C \to \infty$ is taken first at finite temperature $T \neq 0$ and then the limit $T \to 0$ is taken next, the conductance will vanish because of the Mott-Hubbard
FIG. 10: (Color online) EOM (equation of motion) results for the series conductance for the quantum-dot array of the size (a) $N_C = 3$ and (b) $N_C = 4$ obtained from eq. (20), where $U/(2\pi t) = 1.0$ and $\Gamma/t = 0.12$. The results describe a typical feature of a Coulomb oscillation at high temperatures $T_K \ll T \ll U$. The dashed lines show the local charge $N_{el}$ in the isolated molecule for $\Gamma = 0$. 
behavior.

So far, we have concentrated on the transport properties at zero temperature. For comparison, we now consider the conductance at high temperatures. For qualitatively understanding of the physics at high-energy energy scale, the equation motion (EOM) method can be used. It is equivalent basically to the Hubbard I approximation, and in the present case we start with a *molecule limit*, where $\Gamma = 0$ and the quantum-dot array can be regarded like an artificial *molecule* described by the Hamiltonian $H_C^0 + H_U^C$ defined in eqs. (2) and (3). With this method, the full Green’s function $G^{(\text{EOM})}_{ij}(\omega)$ is obtained by substituting the self-energy defined with respect to the *molecule* $\Sigma_{ij}^{(\text{mol})}(\omega)$, which is calculated exactly, into the $N_C \times N_C$ matrix Dyson equation,

$$ \left\{ G^{(\text{EOM})}(\omega) \right\}^{-1} = \left\{ G^{(0)}(\omega) \right\}^{-1} - \Sigma^{(\text{mol})}(\omega). $$

(19)

Here, $G^{(0)}(\omega) = \{G^{(0)}_{ij}(\omega)\}$ is the noninteracting Green’s function defined with respect to the whole system including the two leads, and is determined by the Hamiltonian $H_C^0 + H_{\text{mix}} + H_{\text{lead}}$. Then, a typical value of the conductance at high-temperatures $T_K \ll T \ll U$ is estimated by using an approximate formula following Kawabata,

$$ g_{\text{series}} \sim \frac{e^2}{h} \times 4\Gamma^2 \left| G^{(\text{EOM})}_{N_{C1}}(0) \right|^2, $$

(20)

where a factor $1/2$ has been introduced phenomenologically taking into account the fact that at high-energies the resonance tunneling using the Hubbard band occurs not simultaneously for the up and down spin components. In Fig. 10, the conductance obtained from eq. (20) is plotted for (a) $N_C = 3$ and (b) $N_C = 4$, where the same parameter value is chosen for $U$ and $\Gamma$ as those in Figs. 9 and 4. At high temperatures, the conductance almost vanishes both for even and odd $N_{\text{el}}$. The peaks of the Coulomb oscillation appear at the values of $\epsilon_d$, where $N_{\text{el}}$ jumps discontinuously by an addition of one electron. If the temperature decreases, the bottom of the valleys at odd $N_{\text{el}}$ will rise, and it develops at $T \lesssim T_K$ to the Kondo plateaus of the Unitary limit which we have described in the previous section. Particularly, the wide gap for the triple dots near half-filling seen in Fig. 10 (a) evolves to the broad plateau in Fig. 9.

In summary, we have studied the ground-state properties of an array consisting of four quantum dots based on a Hubbard chain attached to two non-interacting leads. Using NRG approach, we have deduced the phase shifts, by which the conductance and local charge
away from half-filling can be determined, from the low-energy eigenvalues near the Fermi-liquid fixed-point. We have also discussed the parallel conductance of the quantum-dot array connected transversely to four leads. Our formulation to calculate the two phase shifts for even and odd partial waves is quite general, and will be applied to various quantum-dot systems in the Kondo regime.

Acknowledgments

The authors are grateful to A. C. Hewson for valuable discussions. Numerical computation was partly carried out using Computer Facility of Yukawa Institute.

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