Quasiparticle description for transport through a small interacting system

Akira Oguri
Department of Material Science, Faculty of Science, Osaka City University, Sumiyoshi-ku, Osaka 558-8585, Japan
(Received 1 February 2000; revised manuscript received 5 July 2000; published 22 February 2001)

We study the effects of electron correlation on transport through a small interacting system connected to reservoirs using an effective Hamiltonian which describes the free quasiparticles of a Fermi liquid. The effective Hamiltonian is defined microscopically with the value of the self-energy at $\omega=0$. Specifically, we apply the method to a Hubbard chain of finite size N $(=1,2,3,\ldots)$, and calculate the self-energy within the second order in U in the electron-hole-symmetric case. When couplings between the chain and the reservoirs on the left and right are small, the conductance for even N decreases with increasing N, showing a tendency toward a Mott-Hubbard insulator. This is caused by the off-diagonal element of the self-energy, and this behavior is qualitatively different from that in the special case examined in previous work. We also study the effects of the asymmetry in the two couplings. While a perfect transmission due to the Kondo resonance occurs for any odd N in the symmetric coupling, the conductance for odd N decreases with increasing N in the case of asymmetric coupling.

DOI: 10.1103/PhysRevB.63.115305 PACS number(s): 72.10.Bg, 73.40.−c

I. INTRODUCTION

Effects of interelectron interaction on transport through small interacting systems are a subject of current interest. For instance, the Kondo effect, expected to be observed in a quantum dot,[1–3] has been studied intensively from both theoretical[4,5] and experimental sides.[6–8] Also, the Tomonaga-Luttinger behavior expected in one-dimensional systems[9,10] has been investigated in a quantum wire.[11]

For studying the quantum transport of small systems theoretically, a formulation which is able to treat both interaction and interference effects in a unified way is necessary. Meir and Wingreen[12] presented one such framework using the nonequilibrium Keldysh formalism.[13,14] In particular, Eq. (6) of Ref. 12 is a general formula for the total current, and is available for various systems. While the quantum transport theory for nonequilibrium states is important to understand the physics in small systems, there are some ambiguities in determining the stationary state. Thus, it seems to be meaningful to describe a formulation based on the linear-response theory. In the Kubo formalism, the conductance for noninteracting electrons at $T=0$ can be expressed in terms of the Green's function at Fermi energy.[15–17] This is also true for interacting electrons if the ground state is a Fermi liquid.[18,19] The purpose of this paper is to apply a quasiparticle description of a Fermi liquid to the conductance of small interacting systems. At $T=0$, an effective Hamiltonian for free quasiparticles can be defined microscopically based on perturbation theory, which reproduces the value of the Green's function at $\omega=0$. This kind of effective Hamiltonian has been introduced, for instance, for a single Anderson impurity and for systems with a translational invariance.[20] One of the characteristics of a small interacting system is that the self-energy has off-diagonal elements. This is because generally the system consists of a number of resonant states and has no translational invariance.

Specifically, we apply this method to a Hubbard chain of finite size N $(=1,2,3,\ldots)$ connected to noninteracting leads. This system can be regarded as a model for a Mott-Hubbard insulator of nanometer scale. Also, for small N, the system can regarded as a model for a series of quantum dots, which has been examined by advanced numerical methods such as the numerical renormalization-group[21] and quantum Monte Carlo methods.[19,22,23] It may also be considered as a model for a quantum wire, which has been studied with the bosonization approach, taking into account the umklapp scattering. [24–28] We calculate all the elements of a $N\times N$ matrix self-energy within second order in U in the electron-hole-symmetric case. As in the perturbation theory for an Anderson Model by Yamada and Yosida,[29] we include the coupling between the Hubbard chain and two leads in the perturbed Hamiltonian. In a previous paper,[30] we reported the results obtained in a special case $v_L=v_R=t$, where v_L (v_R) is the tunneling matrix element between the chain and the left (right) lead, and t is the hopping matrix element of the chain. In this case, one can obtain the self-energy analytically owing to the property that the noninteracting system has a translational invariance. However, this particular feature is realized only in this case, and some behaviors seen in the results seem to depend on it: the reduction of the conductance for even N is proportional to U^4 for small U, and in the limit of large even N the conductance tends to be finite.

In the present work, we examine the dependence of the conductance on the coupling v_L and v_R, calculating the self-energy numerically. In contrast to the special case mentioned above, the results obtained in weak-coupling cases v_L, $v_R<t$ show quite different behaviors: the reduction of the conductance for even N is proportional to U^2 for small U, and the conductance tends to zero for large even N. Physically, the difference between the weak coupling cases v_L, $v_R<t$ and the special case $v_L=v_R=t$ is caused by whether or not N revels in the chain form distinguishable resonant states. The effect of the interaction is enhanced for weak-coupling cases. We also show generally, beyond second-order perturbation, that a perfect transmission occurs for odd N when the system has both inversion symmetry $v_L=v_R$ $(\equiv v)$ and electron-hole symmetry. This is due to Kondo resonance, and is independent of the values of v and U. We also examine the

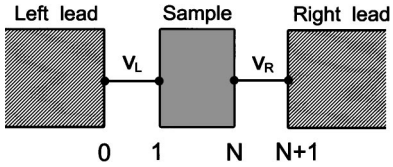

FIG. 1. Schematic picture of the system.

effects of the asymmetry in the coupling $v_L \neq v_R$, which disturbs the perfect transmission. We note that preliminary results were reported in a proceedings.[31]

In Sec. II, we introduce the effective Hamiltonian, and give an interpretation of the dc conductance and total charge displacement in terms of the free quasiparticles. In Sec. III, we show some properties of the quasiparticles in the electron-hole symmetric case without specifying details of the model. In Sec. IV, we apply the method to a Hubbard chain of finite size, and present the results obtained with the second-order perturbation theory. A summary is given in Sec. V.

II. EFFECTIVE HAMILTONIAN AND GROUND-STATE PROPERTIES

In this section, we introduce an effective Hamiltonian for free quasiparticles based on perturbation theory in the interelectron interaction. In this context, the dc conductance and total charge displacement at $T=0$ are described by scattering coefficients of the free quasiparticles. In what follows, we will discuss the formulation, assuming single-mode leads for simplicity. The formulation can be generalized to the multimode leads.

We start with a system which consists of three regions; a finite central region (C) and two noninteracting leads on the left (L) and right (R). The central region consists of N resonant levels, and the interaction is switched on only for electrons in this region. We assume that the two leads consist of infinite degrees of freedom, respectively, and are connected to the central region by the mixing matrix elements v_L and v_R, as illustrated in Fig. 1. The complete Hamiltonian is given by

$$\mathcal{H}=\mathcal{H}_L+\mathcal{H}_R+\mathcal{H}_C^0+\mathcal{H}_C^{int}+\mathcal{H}_{mix}, \tag{1}$$

$$\mathcal{H}_L=\sum_{ij\in L}\sum_{\sigma}(-t_{ij}^L-\mu\delta_{ij})c_{i\sigma}^\dagger c_{j\sigma}, \tag{2}$$

$$\mathcal{H}_R=\sum_{ij\in R}\sum_{\sigma}(-t_{ij}^R-\mu\delta_{ij})c_{i\sigma}^\dagger c_{j\sigma}, \tag{3}$$

$$\mathcal{H}_C^0=\sum_{ij\in C}\sum_{\sigma}(-t_{ij}^C-\mu\delta_{ij})c_{i\sigma}^\dagger c_{j\sigma}, \tag{4}$$

$$\mathcal{H}_C^{int}=\frac{1}{2}\sum_{\{j\}\in C}\sum_{\sigma\sigma'}U_{j_4j_3;j_2j_1}c_{j_4\sigma}^\dagger c_{j_3\sigma'}^\dagger c_{j_2\sigma'}c_{j_1\sigma}, \tag{5}$$

$$\mathcal{H}_{mix}=-\sum_{\sigma}v_L(c_{1\sigma}^\dagger c_{0\sigma}+c_{0\sigma}^\dagger c_{1\sigma}) -\sum_{\sigma}v_R(c_{N+1\sigma}^\dagger c_{N\sigma}+c_{N\sigma}^\dagger c_{N+1\sigma}). \tag{6}$$

Here $c_{j\sigma}^\dagger$ ($c_{j\sigma}$) creates (destroys) an electron with spin σ at site j, and μ is the chemical potential. t_{ij}^L, t_{ij}^R, and t_{ij}^C are the intraregion hopping matrix elements in regions L, R, and C, respectively. The coupling between the central region and the two leads are described by the mixing matrix element $\mathcal{H}_{mix}$. We assign the labels 1,2, . . . ,N to sites in the central region. Specifically, we assign the labels 1 and N to sites at the interface on the left and right, respectively. Correspondingly, the labels 0 and $N+1$ are assigned to the sites at the leadside of the interface on the left and right, respectively (see Fig. 1). The interelectron interaction $U_{j_4j_3;j_2j_1}$ is switched on in the central region, and has time-reversal symmetry: $U_{43;21}$ is real and $U_{43;21}=U_{34;12}=U_{12;34}=U_{42;31}=U_{13;24}$. We take all the hopping matrix elements to be real, and will use units $\hbar=1$ unless otherwise noted.

In the limit $N=1$, the model reduces to a single Anderson impurity in which the perturbation expansion is valid for all values of U.[32] Our basic idea is to apply the perturbation theory in $\mathcal{H}_C^{int}$ following Yamada and Yosida,[29] regarding the central region as one large impurity. Therefore, we take the unperturbed part of the Hamiltonian $\mathcal{H}^{(0)}$ to be connected by including the mixing term $\mathcal{H}_{mix}$ in it:

$$\mathcal{H}^{(0)}=\mathcal{H}_L+\mathcal{H}_R+\mathcal{H}_C^0+\mathcal{H}_{mix}. \tag{7}$$

Our working hypothesis is that the ground state is changed continuously against the adiabatic switching on of the interaction $\mathcal{H}_C^{int}$. The perturbation expansion can be done using the single-particle Green's function

$$G_{jj'}(i\varepsilon_l)=-\int_0^\beta d\tau\langle T_\tau c_{j\sigma}(\tau)c_{j'\sigma}^\dagger(0)\rangle e^{i\varepsilon_l\tau}, \tag{8}$$

where $\beta=1/T$, $\varepsilon_l=(2l+1)\pi/\beta$, $c_{j\sigma}(\tau)=e^{\tau\mathcal{H}}c_{j\sigma}e^{-\tau\mathcal{H}}$, and $\langle\cdots\rangle$ denotes the thermal average $\mathrm{Tr}[e^{-\beta\mathcal{H}}\cdots]/\mathrm{Tr}\,e^{-\beta\mathcal{H}}$. The spin index has been omitted from the left-hand side of Eq. (8), assuming the expectation value to be independent of whether spin is up or down. Since the interaction is switched on only for electrons in the central region, the Dyson equation is written as

$$G_{ij}(z)=G_{ij}^{(0)}(z)+\sum_{ll'\in C}G_{il}^{(0)}(z)\Sigma_{ll'}(z)G_{l'j}(z). \tag{9}$$

Here $G_{ij}^{(0)}(z)$ is the unperturbed Green's function corresponding to $\mathcal{H}^{(0)}$. The summations with respect to l and l' run over the sites in the central region, and $\Sigma_{ll'}(z)$ is the self-energy correction due to $\mathcal{H}_C^{int}$. Note that $G_{ij}(z)=G_{ji}(z)$ and $\Sigma_{ij}(z)=\Sigma_{ji}(z)$ because of the time-reversal symmetry of $\mathcal{H}$. In what follows, we will treat z as a complex variable, i.e., $G_{ij}(z)$ is the analytic continuation of $G_{ij}(i\varepsilon_l)$. When the perturbation expansion is valid, the single-particle

excitation at the Fermi energy $z=i0^+$ does not decay at $T=0$, owing to a property of the Fermi liquid:[33]

$$\mathrm{Im}\,\Sigma_{ij}^{+}(0)=0. \tag{10}$$

Here the superscript $(+)$ is the label for a retarded function: we will use a notation $\Sigma_{ij}^{\pm}(\omega)\equiv\Sigma_{ij}(\omega\pm i0^+)$.[33] Due to this property, the Dyson equation [Eq. (9)] for $\omega=0$ can be mapped onto a scattering problem of the free quasiparticles described by the effective Hamiltonian

$$\tilde{\mathcal{H}}_{qp}=\mathcal{H}_L+\mathcal{H}_R+\tilde{\mathcal{H}}_C+\mathcal{H}_{mix}, \tag{11}$$

$$\tilde{\mathcal{H}}_C=\sum_{ij\in C}\sum_{\sigma}(-\tilde{t}_{ij}^{C}-\mu\delta_{ij})c_{i\sigma}^{\dagger}c_{j\sigma}, \tag{12}$$

$$-\tilde{t}_{ij}^{C}=-t_{ij}^{C}+\mathrm{Re}\,\Sigma_{ij}^{+}(0). \tag{13}$$

The value of the Green's function corresponding to $\tilde{\mathcal{H}}_{qp}$ and the one corresponding $\mathcal{H}$ are the same at $T=0$ and $\omega=0$.

We now consider the conductance with the Kubo formalism. If the ground state is a Fermi liquid, the contributions of the vertex corrections for the dc conductance vanish at $T=0$.[18,19] Therefore, the dc conductance at $T=0$ is also written in terms of the Green's function at $\omega=0$ for interacting electrons:[34]

$$g_N=\frac{2e^2}{h}4\Gamma_R(0)G_{N1}^{+}(0)\Gamma_L(0)G_{1N}^{-}(0). \tag{14}$$

Here $\Gamma_L(\omega)=-\mathrm{Im}[v_L^2\mathrm{g}_L^{+}(\omega)]$ and $\Gamma_R(\omega)=-\mathrm{Im}[v_R^2\mathrm{g}_R^{+}(\omega)]$. g_L^{+} (g_R^{+}) is the Green's function at the interface $i=0$ $(i=N+1)$ of the isolated lead, and it is determined by $\mathcal{H}_L$ ($\mathcal{H}_R$). Note that Eq. (14) is also expressed in terms of the transmission probability of the free quasiparticles, $|\tilde{t}(0)|^2=4\Gamma_R(0)G_{N1}^{+}(0)\Gamma_L(0)G_{1N}^{-}(0)$.[14,35,36] Correspondingly, the reflection probability is given by $|\tilde{r}(0)|^2=|1-2i\Gamma_L(0)G_{11}^{+}(0)|^2=|1-2i\Gamma_R(0)G_{NN}^{+}(0)|^2$, and the unitarity $|\tilde{t}(0)|^2+|\tilde{r}(0)|^2=1$ is preserved owing to the property Eq. (10) [also see Eq. (22)]. Another quantity which can be related to the scattering coefficients is the displacement of the total charge:[33,37]

$$\Delta N_{tot}=\sum_{i\in C}\sum_{\sigma}\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle+\sum_{i\in L}\sum_{\sigma}[\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle-\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle_L]$$
$$+\sum_{i\in R}\sum_{\sigma}[\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle-\langle c_{i\sigma}^{\dagger}c_{i\sigma}\rangle_R]. \tag{15}$$

Here $\langle\cdots\rangle_L$ and $\langle\cdots\rangle_R$ denote the ground-state average of isolated leads described by $\mathcal{H}_L$ and $\mathcal{H}_R$, respectively. At $T=0$, ΔN_{tot} can be expressed in terms of the S matrix for the quasiparticles, following the derivation of the Friedel sum rule by Langer and Ambegaokar,[33] as

$$\Delta N_{tot}=\frac{1}{\pi i}\log[\det \boldsymbol{S}], \tag{16}$$

$$\boldsymbol{S}=\begin{bmatrix}1&0\\0&1\end{bmatrix}-2i\begin{bmatrix}\Gamma_L(0)&0\\0&\Gamma_R(0)\end{bmatrix}\begin{bmatrix}G_{11}^{+}(0)&G_{1N}^{+}(0)\\G_{N1}^{+}(0)&G_{NN}^{+}(0)\end{bmatrix}. \tag{17}$$

Therefore, the conductance and charge displacement are determined by the inter-boundary and intra-boundary elements of the Green's function such as $G_{N1}^{+}(0)$ and $G_{11}^{+}(0)$.

Next we discuss the structure of the Dyson equation [Eq. (9)] further in order to make the mathematical features of the perturbation theory in the presence of the reservoirs clear. For the Green's functions in the central region, Eq. (9) is written in a $N\times N$ matrix form:

$$\{\boldsymbol{\mathcal{G}}(z)\}^{-1}=\{\boldsymbol{\mathcal{G}}^{(0)}(z)\}^{-1}-\boldsymbol{\Sigma}(z). \tag{18}$$

Here $\boldsymbol{\mathcal{G}}(z)=\{G_{ij}(z)\}$, with $ij\in C$, and the inverse matrix of the unperturbed part can be expressed as $\{\boldsymbol{\mathcal{G}}^{(0)}(z)\}^{-1}=z\mathbf{1}-\boldsymbol{\mathcal{H}}_C^0-\boldsymbol{\mathcal{V}}_{mix}(z)$, with

$$\boldsymbol{\mathcal{H}}_C^0=\begin{bmatrix}-t_{11}^{C}-\mu&-t_{12}^{C}&\cdots&&\\-t_{21}^{C}&-t_{22}^{C}-\mu&&&\\\vdots&&\ddots&&\\&&&&-t_{NN}^{C}-\mu\end{bmatrix}, \tag{19}$$

$$\boldsymbol{\mathcal{V}}_{mix}(z)=\begin{bmatrix}v_L^2\mathrm{g}_L(z)&0&\cdots&0&0\\0&0&\cdots&0&0\\\vdots&\vdots&\ddots&\vdots&\vdots\\0&0&\cdots&0&0\\0&0&\cdots&0&v_R^2\mathrm{g}_R(z)\end{bmatrix}, \tag{20}$$

$$\boldsymbol{\Sigma}(z)=\begin{bmatrix}\Sigma_{11}(z)&\Sigma_{12}(z)&\cdots&&\\\Sigma_{21}(z)&\Sigma_{22}(z)&&&\\\vdots&&\ddots&&\\&&&&\Sigma_{NN}(z)\end{bmatrix}. \tag{21}$$

Here $\mathbf{1}$ is the $N\times N$ unit matrix. $\boldsymbol{\mathcal{V}}_{mix}$ corresponds to the contribution of the mixing with the reservoirs. In particular, the two nonzero elements $v_L^2\mathrm{g}_L$ and $v_R^2\mathrm{g}_R$ have finite imaginary parts corresponding to Γ_L and Γ_R defined just below Eq. (14). These imaginary parts change the discrete levels of $\boldsymbol{\mathcal{H}}_C^0$ to continuous peaks with finite level widths, and thus the unperturbed part of the Green's function $\boldsymbol{\mathcal{G}}^{(0)}(z)$ describes a system of N resonant scatterers. Therefore, owing to the contribution of the mixing, the mathematical structure of the perturbation theory in the presence of the reservoirs becomes similar to that of an Anderson model with a number of orbits rather than the usual Hubbard model without reservoirs. In this matrix form, the quasiparticle description is summarized as follows. Due to the property $\mathrm{Im}\,\boldsymbol{\Sigma}^{+}(0)=0$ at $T=0$, the Green's function at $\omega=0$ is written as $\{\boldsymbol{\mathcal{G}}^{+}(0)\}^{-1}=\boldsymbol{\mathcal{K}}-\boldsymbol{\mathcal{V}}_{mix}^{+}(0)$, where $\boldsymbol{\mathcal{K}}$ is the renormalized hopping matrix corresponding to $-\tilde{\mathcal{H}}_C$ defined by Eq. (12):

$$\boldsymbol{\mathcal{K}}=-[\boldsymbol{\mathcal{H}}_C^0+\mathrm{Re}\,\boldsymbol{\Sigma}^{+}(0)]. \tag{22}$$

Then a relation corresponding to the optical theorem can be obtained as $\mathcal{G}^+(0)-\mathcal{G}^-(0)=\mathcal{G}^+(0)[\mathcal{V}^+_{mix}(0)-\mathcal{V}^-_{mix}(0)]\mathcal{G}^-(0)$, which certifies the unitarity of the scattering coefficients. Here the superscript $+$ $(-)$ means a retarded (advanced) function.

The quasiparticle approach cannot be applied to a non-Fermi-liquid ground state where the perturbation theory with respect to the interelectron interaction breaks down. However, in a finite interacting system connected to reservoirs, as illustrated in Fig. 1, a crossover from a high-temperature phase to a low-temperature Fermi liquid phase is expected in many cases. This is because, due to the connection with the reservoirs, not only the energy scale corresponding to the level spacing of the isolated interacting system of size N but also the level width introduced through Γ_L and Γ_R, i.e., the imaginary part of the mixing term Eq. (20), plays the role of a cutoff. In this sense, as mentioned above, the system can be regarded as a generalized Anderson impurity with N resonant states.

When the interacting region is described by an one-dimensional chain, a Tomonaga-Luttinger (TL) behavior[38] seems to be seen for large N. However, as discussed by Kane and Fisher for a finite TL model of size L connected to Fermi-liquid reservoirs,[9] the crossover from a high-temperature TL phase to a low temperature Fermi liquid phase occurs at a characteristic energy $T_0 \simeq v_F/L$, where v_F is the Fermi velocity. Since this simple discussion does not take into account various effects such as the back and umklapp scatterings, the characteristic energy will be different depending on the details of the situations. Specifically, in the electron-hole-symmetric case of the Hubbard chain examined in the following sections, the characteristic energy depends on whether N is even or odd, and it should be the Mott-Hubbard gap E_G or the Kondo temperature T_K. Again, due to the contribution of the mixing, the low-energy excitations below the characteristic energy scale are described by Fermi liquid as far as N is finite. For even N, a Mott-Hubbard gap opens in the thermodynamic limit of the usual Hubbard model without reservoirs, and a corresponding tendency should be seen in the present system of finite N. However, there still remains a finite density of states at the Fermi energy caused by a mixing with the reservoirs, although the spectral weight in the region corresponding to the gap will decrease with increasing N. For odd N, there is an additional spectral weight at the Fermi energy in the Mott-Hubbard gap, i.e., Kondo resonance of width T_K. Thus an insulator-like low conductivity should be seen at the temperature range $T_K<T<E_G$, and a metallic behavior of the Fermi liquid will be seen at low temperatures $T<T_K$. Note that T_K can be defined only for open system connected to reservoirs, while E_G is a constant defined in the thermodynamic limit of the isolated system. Furthermore, T_K should decrease with increasing N, and in most of cases T_K should vanish in the limit of $N\to\infty$. Therefore, if the limit $N\to\infty$ is taken, keeping T finite, the even-odd behavior disappears, and at $T<E_G$ the insulating behavior meeting with an intuitive picture is expected to be seen. This limit corresponds to the thermodynamic limit of the macroscopic system. However, there is another nontrivial limit which describes the low-temperature physics of mesoscopic systems, i.e., the limit $T\to 0$, keeping N finite. The ground state of the small system belongs to this limit, and in the case of a small Hubbard chain the even-odd behavior can be seen at low temperatures since T_K is finite for small N. This kind of mesoscopic limit is expected to be realized in quantum dots or quantum wires of nanometer size, and our aim here is to develop a Fermi-liquid theory for the mesoscopic systems.

Another possible non-Fermi-liquid state is the ground state of the multichannel Kondo system.[39] Shimizu, Sakai and Suzuki showed, with a numerical renormalization-group approach, that a non-Fermi-liquid ground state is also realized in an extended version of the Anderson model.[40] Thus, if the parameters of the Hamiltonian equation (1) satisfy certain conditions, a similar situation seems to be realized.

III. QUASIPARTICLES IN THE ELECTRON-HOLE-SYMMETRIC CASE

The effective Hamiltonian has some notable properties in the electron-hole-symmetric case, where the average number of electrons in each site is unity. In this section, we provide a simplified expression of the conductance in the electron-hole symmetric case. Equations (31) and (33) will be used for the finite Hubbard chain in Sec. IV. In particular, from Eq. (31), we can deduce quite generally that perfect transmission occurs for odd N when the system has an additional inversion symmetry.

In the electron-hole-symmetric case, the off-diagonal element of the renormalized parameter $\tilde{t}^C_{ij}$ is zero when i and j belong to the same sublattice, i.e., $-\tilde{t}^C_{ij}-\mu\delta_{ij}=0$ for $|i-j|=0,2,4,\ldots$, and $\mathrm{Re}\,\mathcal{V}^+_{mix}(0)=0$. Thus the matrix $\mathcal{K}$ defined by Eq. (22) has a checkered structure, and the Green's function at $T=0$, $\omega=0$ is written in the form

$$\{\mathcal{G}^+(0)\}^{-1}=\begin{bmatrix} 0 & \tilde{t}^C_{12} & 0 & \tilde{t}^C_{14} & \cdots \\ \tilde{t}^C_{21} & 0 & \tilde{t}^C_{23} & 0 & \cdots \\ 0 & \tilde{t}^C_{32} & 0 & \tilde{t}^C_{34} & \cdots \\ \tilde{t}^C_{41} & 0 & \tilde{t}^C_{43} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} + \begin{bmatrix} i\Gamma_L(0) & & & \\ & \mathbf{0} & & \\ & & & i\Gamma_R(0) \end{bmatrix}, \tag{23}$$

and $G^+_{ij}(0)$ is obtained by taking the inverse of Eq. (23). Specifically, using the explicit form of $G^+_{1N}(0)$, the dc conductance g_N can be obtained from Eq. (14). For $N=1$ and 2, the dc conductance is written in the forms

$$g_1=\frac{2e^2}{h}\frac{\Gamma_L\Gamma_R}{[(\Gamma_L+\Gamma_R)/2]^2}, \tag{24}$$

$$g_2=\frac{2e^2}{h}\frac{\Gamma_L\Gamma_R\{\tilde{t}^C_{12}\}^2}{[(\Gamma_L\Gamma_R+\{\tilde{t}^C_{12}\}^2)/2]^2}. \tag{25}$$

Here $\Gamma_L \equiv \Gamma_L(0)$ and $\Gamma_R \equiv \Gamma_R(0)$, and we will use this simplified notation in what follows. For $N \geqslant 3$, $G^+_{1N}(0)$ is written in the forms

$$G^+_{1N}(0) = (-1)^{N+1} \frac{\det \mathcal{K}_{N1}}{\det\{\mathcal{G}^+(0)\}^{-1}}, \tag{26}$$

$$\det\{\mathcal{G}^+(0)\}^{-1} = \begin{cases} i\Gamma_L \det \mathcal{K}_{11} + i\Gamma_R \det \mathcal{K}_{NN} & \text{for odd } N \\ -\Gamma_L \Gamma_R \det \mathcal{K}^{NN}_{11} + \det \mathcal{K} & \text{for even } N. \end{cases} \tag{27}$$

Here $\mathcal{K}_{ij}$ is a $(N-1)\times(N-1)$ matrix obtained from $\mathcal{K}$ by deleting the ith row and the jth column. Similarly, $\mathcal{K}^{NN}_{11}$ is a $(N-2)\times(N-2)$ matrix obtained from $\mathcal{K}$ by deleting the first and Nth rows, and the first and Nth columns. Due to the checkered structure of Eq. (23), the determinants satisfy a relation

$$(\det \mathcal{K}_{N1})^2 = \begin{cases} \det \mathcal{K}_{11} \det \mathcal{K}_{NN} & \text{for odd } N \\ -\det \mathcal{K} \det \mathcal{K}^{NN}_{11} & \text{for even } N. \end{cases} \tag{28}$$

Although the details are given in Appendix A, the origin of the even-odd dependence can be understood just seeing typical examples:

$$\mathcal{K} = \begin{bmatrix} 0 & \tilde{t}^C_{12} & 0 & \tilde{t}^C_{41} & 0 \\ \tilde{t}^C_{12} & 0 & \tilde{t}^C_{23} & 0 & \tilde{t}^C_{52} \\ 0 & \tilde{t}^C_{23} & 0 & \tilde{t}^C_{34} & 0 \\ \tilde{t}^C_{41} & 0 & \tilde{t}^C_{34} & 0 & \tilde{t}^C_{45} \\ 0 & \tilde{t}^C_{52} & 0 & \tilde{t}^C_{45} & 0 \end{bmatrix} \quad \text{for } N=5, \tag{29}$$

$$\mathcal{K} = \begin{bmatrix} 0 & \tilde{t}^C_{12} & 0 & \tilde{t}^C_{41} & 0 & \tilde{t}^C_{61} \\ \tilde{t}_{12^C} & 0 & \tilde{t}^C_{23} & 0 & \tilde{t}^C_{52} & 0 \\ 0 & \tilde{t}^C_{23} & 0 & \tilde{t}^C_{34} & 0 & \tilde{t}^C_{63} \\ \tilde{t}^C_{41} & 0 & \tilde{t}^C_{34} & 0 & \tilde{t}^C_{45} & 0 \\ 0 & \tilde{t}^C_{52} & 0 & \tilde{t}^C_{45} & 0 & \tilde{t}^C_{56} \\ \tilde{t}^C_{61} & 0 & \tilde{t}^C_{63} & 0 & \tilde{t}^C_{56} & 0 \end{bmatrix} \quad \text{for } N=6. \tag{30}$$

The antidiagonal elements, $\mathcal{K}_{j,N+1-j}$ for $j=1,2,\ldots,N$, are zero for odd N, while they are not for even N. Furthermore, $\det \mathcal{K}$ is zero for odd N, while it is finite and can be divided into two determinants for even N. Using Eqs. (26)–(28) with Eq. (14), the dc conductance for odd $N\,(=2M+1)$ is written in the form

$$g_{2M+1} = \frac{2e^2}{h} \frac{\tilde{\Gamma}_L \tilde{\Gamma}_R}{[(\tilde{\Gamma}_L + \tilde{\Gamma}_R)/2]^2}, \tag{31}$$

where $\tilde{\Gamma}_L = \lambda \Gamma_L$, $\tilde{\Gamma}_R = \Gamma_R/\lambda$, and

$$\lambda = \sqrt{\frac{\det \mathcal{K}_{11}}{\det \mathcal{K}_{NN}}}. \tag{32}$$

We note that the parameter λ can be simplified as in Eq. (A10) by using the checkered structure further. If the system has an inversion symmetry $\Gamma_L = \Gamma_R$ in addition to the electron-hole symmetry, the parameter is fixed as $\lambda = 1$. This is because the matrix $\mathcal{K}$ becomes symmetric with respect to the antidiagonal line. Therefore, due to the combination of the symmetries, the perfect transmission occurs at $g_{2M+1} = 2e^2/h$, independent of M and the details of the interaction, as far as the perturbation expansion is valid. Physically, this is caused by the Kondo resonance appearing at the Fermi energy $\omega = 0$. On the other hand, for even $N\,(=2M)$, the dc conductance is written in the form

$$g_{2M} = \frac{2e^2}{h} \frac{\Gamma_L \Gamma_R \tilde{v}_C^2}{[(\Gamma_L \Gamma_R + \tilde{v}_C^2)/2]^2}, \tag{33}$$

$$\tilde{v}_C^2 = -\frac{\det \mathcal{K}}{\det \mathcal{K}^{NN}_{11}}. \tag{34}$$

We note that the parameter $\tilde{v}_C$ can also be simplified as Eq. (A6). The two expressions for the dc conductance [Eqs. (31) and (33)], are the main results of this section.

We next examine the Friedel sum rule. Using the property Eq. (27) and the expression of the total charge displacement [Eqs. (16) and (17)], we obtain $\det \boldsymbol{S} = 1$ for even N, and $\det \boldsymbol{S} = -1$ for odd N. This is consistent with the fact that the average number of electrons in each site is unity. In order to realize the electron-hole symmetry, the bare matrix element t^C_{ij} should also have a checkered structure, as assumed for the renormalized parameter $\tilde{t}^C_{ij}$, i.e., the system must be classified into two sublattices. Note that, since only symmetry is assumed so far, the bare hopping matrix element is not necessarily restricted to the nearest-neighbor element. Furthermore, the system may possibly be disordered through the randomness in the off-diagonal element of t^C_{ij}.

IV. TRANSPORT THROUGH A FINITE HUBBARD CHAIN

In this section, we will use the effective Hamiltonian to investigate the conductance of a finite Hubbard chain connected to two semi-infinite leads. The system is considered as a model for a series of quantum dots or atomic wires of nanometer size. We calculate the renormalized hopping matrix element $\tilde{t}^C_{ij}$ up to second order in U, and obtain the dc conductance using expressions given in Sec. III. We note that the second-order perturbation theory was used by several groups for studying transport properties of a single impurity[5,41–43] and systems consisting of a number of resonant levels.[44,45] For $N \geqslant 2$, the off-diagonal part of the self-energy plays an important role in the conductance at $T=0$, as seen below. To our knowledge, however, effects of the off-diagonal part have not been examined sufficiently so far.

The schematic picture of the model is illustrated in Fig. 2: the system consists of N interacting sites at the center $1 \leqslant i \leqslant N$, and two noninteracting leads at $-\infty < i \leqslant 0$ and $N+1 \leqslant i < +\infty$. The explicit form of the Hamiltonian is given by

$$H = H_0 + H_I, \tag{35}$$

$$H_0=-\sum_{i=-\infty}^{+\infty}\sum_{\sigma} t_i(c_{i+1\sigma}^{\dagger}c_{i\sigma}+c_{i\sigma}^{\dagger}c_{i+1\sigma}) -\mu\sum_{i=-\infty}^{+\infty}\sum_{\sigma} c_{i\sigma}^{\dagger}c_{i\sigma}+\sum_{i=1}^{N}\sum_{\sigma}\left(\epsilon_0+\frac{U}{2}\right)n_{i\sigma}, \quad (36)$$

$$H_I=U\sum_{i=1}^{N}\left[n_{i\uparrow}n_{i\downarrow}-\frac{1}{2}(n_{i\uparrow}+n_{i\downarrow})\right], \quad (37)$$

where U is the repulsive interaction in the chain, ϵ_0 is the on-site energy, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. We take the hopping matrix element to be $t_i=t$ for every link except for the coupling between the chain and leads, i.e., $t_0=v_L$ and $t_N=v_R$. Thus the level width caused by the coupling with the leads is given by $\Gamma_{\alpha}(0)=\pi v_{\alpha}^2 D(0)$ for $\alpha=L,R$ with $D(0)=\sqrt{4t^2-\mu^2}/(2\pi t^2)$. In what follows, we concentrate on the electron-hole-symmetric case taking the parameters to be $\mu=0$ and $\epsilon_0=-U/2$.

Within second order, the self-energy correction is described by Fig. 3, and the value at $T=0$ and $\omega=0$ is obtained from the expression

$$\Sigma_{ij}^{(2)}(i0^+)=-U^2\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\epsilon d\epsilon'}{(2\pi)^2}G_{ij}^{(0)}(i\epsilon)G_{ij}^{(0)}(i\epsilon') \times G_{ji}^{(0)}(i\epsilon+i\epsilon') \quad (38)$$

for $1\leqslant i,j\leqslant N$. Here $G_{ij}^{(0)}(i\epsilon)$ is the unperturbed Green's function corresponding to H_0, and thus $\Sigma_{ij}^{(2)}(i0^+)$ depends on v_L and v_R through $G_{ij}^{(0)}$. Note that the value of the retarded function at $\omega=0$ can be obtained from the Matsubara function, i.e., $\Sigma_{ij}^{(2)}(i0^+)=\Sigma_{ij}^{(2)}(i\epsilon)|_{\epsilon\to 0^+}$. The imaginary part of the self-energy vanishes owing to the Fermi-liquid property, i.e., $\mathrm{Im}\,\Sigma_{ij}^{(2)}(i0^+)=0$. Furthermore, $\Sigma_{ij}^{(2)}(i0^+)=0$ for even $|i-j|$, since $G_{ij}^{(0)}(-i\epsilon)=(-1)^{|i-j|+1}G_{ij}^{(0)}(i\epsilon)$ in the electron-hole-symmetric case. We have performed the integration (38) numerically to estimate the renormalized matrix element $\tilde{t}_{ij}^{C}$ defined by Eq. (13) within second order, and obtained the dc conductance g_N using Eqs. (31) and (33). As an example, we show the result of the self-energy for $N=6$:

$$\boldsymbol{\Sigma}^{(2)}(i0^+)=-t\left(\frac{U}{2\pi t}\right)^2\tilde{\boldsymbol{\Sigma}}^{(2)}, \quad (39)$$

$$\tilde{\boldsymbol{\Sigma}}^{(2)}=\begin{bmatrix} 0 & 0.8596 & 0 & -0.1642 & 0 & 0.0783 \\ 0.8596 & 0 & 0.3969 & 0 & -0.0352 & 0 \\ 0 & 0.3969 & 0 & 0.7543 & 0 & -0.1642 \\ -0.1642 & 0 & 0.7543 & 0 & 0.3969 & 0 \\ 0 & -0.0352 & 0 & 0.3969 & 0 & 0.8596 \\ 0.0783 & 0 & -0.1642 & 0 & 0.8596 & 0 \end{bmatrix}. \quad (40)$$

Here the coupling is taken to be $v_L/t=v_R/t=0.8$. The matrix element for a given distance $|i-j|$ shows an oscillatory behavior, i.e., $\Sigma_{l,l+2m+1}^{(2)}(i0^+)$ is an oscillatory function of l. In contrast, in the special case $v_L=v_R=t$, $\Sigma_{l,l+2m+1}^{(2)}(i0^+)$ is independent of l and the integration Eq. (38) can be done analytically.[30] Note that $\Sigma_{ij}^{(2)}(i0^+)$ is also an oscillatory function of $|i-j|$, and the absolute value tends to decrease with increasing $|i-j|$.

A. Symmetric connection $v_L=v_R$

We now examine the case where the system has an inversion symmetry, $v_L=v_R\equiv v$, in addition to an electron-hole symmetry. In this case, as shown generally in the Sec. III, perfect transmission occurs for odd N independent of U. Physically, this is due to the contribution of the Kondo resonance appearing at the Fermi energy. Thus, we have made a numerical calculation only for even N. The result of g_N is plotted as a function of the size N in Fig. 4, where the parameters are taken to be $v/t=0.8$ and $U/(2\pi t)=0.4$. The result shows a typical even-odd oscillatory behavior, and the conductance for even N decreases with increasing N. This reduction is caused by the oscillatory l dependence of the self-energy $\Sigma_{l,l+2m+1}^{(2)}$. In Fig. 5, the envelope of g_N for even $N\,(=2M)$ is plotted vs M for several values of the repulsion $U/(2\pi t)=0.0,0.2,0.4,0.6$, and 0.8, taking the mixing matrix element to be $v/t=0.8$. The conductance g_{2M} decreases with increasing M and increasing U. In the noninteracting case, g_{2M} is independent of M, since the parameter defined by Eq.

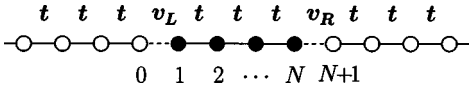

FIG. 2. Schematic picture of the model: (●) interacting region; (○) ideal leads.

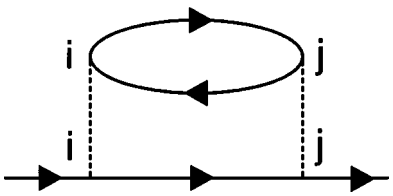

FIG. 3. Second-order self-energy $\Sigma_{ij}^{(2)}(i\omega)$.

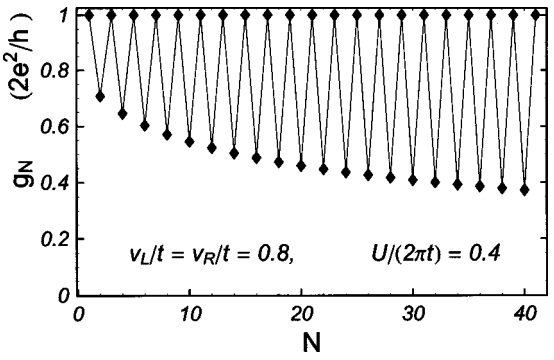

FIG. 4. Conductance g_N as a function of the size N in the inversion-symmetric case. Here $v/t=0.8$ and $U/(2\pi t)=0.4$.

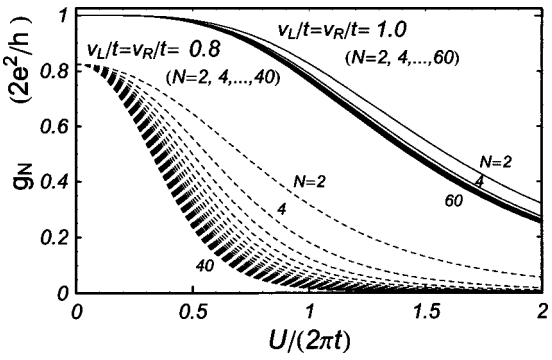

FIG. 6. Conductance vs U, for even N $(=2,4,6,\ldots)$. Here $v/t=0.8$ for dashed lines, and $v/t=1.0$ for solid lines. Totally, 20 dashed lines and 30 solid lines are plotted.

(34) is simply $\tilde{v}_C=t$. The reduction of the conductance seems to show a tendency toward a Mott-Hubbard insulator. However, the result shows a rather moderate decay, i.e., it does not show an exponential dependence. Since the range of U in which the second-order perturbation theory is able to provide quantitatively reliable results depends on the size M, contributions of higher-order terms should be examined in order to clarify the correct asymptotic behavior for large M.

In Fig. 6, the conductance is plotted as a function of U for a number of even N $(=2,4,6,\ldots)$ taking the parameters to be $v/t=0.8$ (dashed lines) and $v/t=1.0$ (solid lines). As can be seen in the behavior of the dashed lines, the reduction of g_{2M} is proportional to U^2 for small U when $|v/t|<1.0$. The curvature increases with size M. In order to see this quantitatively, we expand the conductance in powers of U as $g_{2M}=(2e^2/h)[C_0-C_2\{U/(2\pi t)\}^2+\cdots]$, and plot the ratio C_2/C_0 as a function of M in Fig. 7 for several values of v/t $(=0.1,0.2,\ldots,0.9)$. C_2 increases with size M, and seems to diverge in the limit of large M, showing a power-law behavior. Note that the transmission probability in the noninteracting case C_0 depends on the mixing matrix element v but is independent of the size M, as mentioned above. Furthermore, since the self-energy is calculated up to order U^2, the result of C_2 is exact. The ratio C_2/C_0 increases with decreasing v. This means that the effect of the interaction is enhanced when the coupling between the sample and leads is weak. In the special case $v=t$, the reduction of g_{2M} is proportional to U^4 for small U, i.e., $g_{2M}=(2e^2/h)[1-C_4\{U/(2\pi t)\}^4+\cdots]$. This is because the unperturbed system described by H_0 has a translational invariance accidentally in this case, and the reflection probability is zero at $U=0$. The solid lines for $N\gtrsim 10$ in Fig. 6 almost overlap each other. In Fig. 8, C_4 is plotted vs M. This result is also exact, and the coefficient C_4 converges to a finite value for large M: $C_4\simeq 0.5293$ for $N=250$. In Appendix B, the convergence of C_4 in the limit of $M\to\infty$ is confirmed with another approach. Therefore, when $v=t$, g_{2M} is finite even in the limit of large M at least for small U.[30] For large values of U, both the dashed and solid lines in Fig. 6 tend to zero, showing a $1/U^4$ dependence. However this behavior depends on the approximation: as can be confirmed from Eqs. (33) and (34), $\tilde{v}_C\propto U^n$ and $g_{2M}\propto 1/U^{2n}$ for large U when the self-energy is estimated within an nth order perturbation in U.

The mixing matrix element v determines the bare level width of the resonant states, which in the present case is given by $\Gamma=v^2/t$. Since we are now considering an electron-hole-symmetric case, the Fermi level for even N is located between the two resonant states corresponding to the highest occupied and lowest unoccupied levels. In Fig. 9, g_{2M} is plotted vs U for several values of v/t $(=0.4,0.5,0.6,\ldots,1.0)$, where solid (dashed) lines are the results for $N=40$ $(N=4)$. The value of the conductance it-

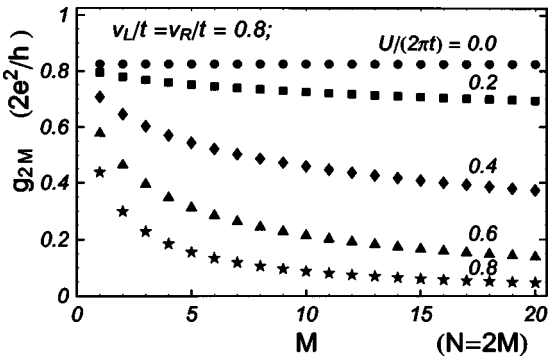

FIG. 5. Conductance for even N $(=2M)$ as a function of the size M. Here $v/t=0.8$, and the repulsion $U/(2\pi t)$ is taken to be (●) 0.0, (■) 0.2, (◆) 0.4, (▲) 0.6, and (★) 0.8.

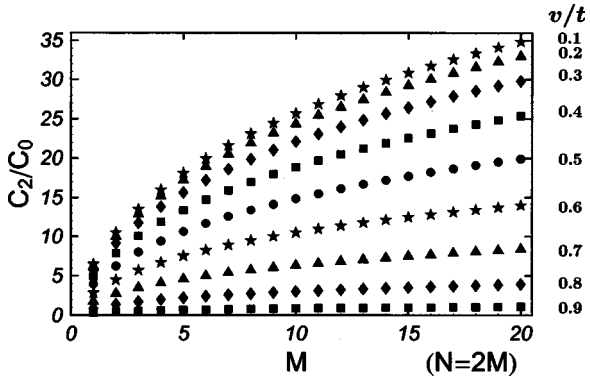

FIG. 7. The ratio C_2/C_0 is plotted for several v/t $(=0.1,0.2,\ldots,0.9)$ as a function of the size M. Here $g_{2M}=(2e^2/h)[C_0-C_2\{U/(2\pi t)\}^2+\cdots]$.

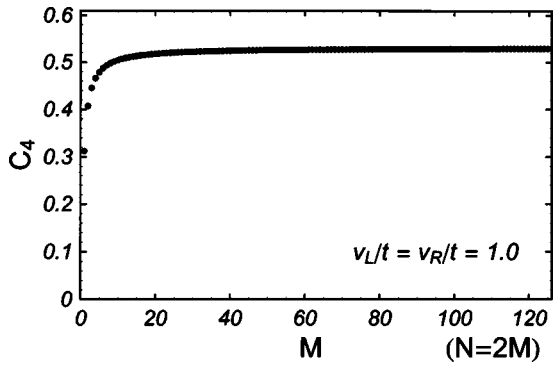

FIG. 8. The coefficient C_4 in the case of $v/t=1.0$ is plotted as a function of the size M. Here $g_{2M}=(2e^2/h)[1-C_4\{U/(2\pi t)\}^2+\cdots]$.

self decreases with v, but the qualitative feature of the U dependence is similar in the cases of $|v/t|<1.0$. In Fig. 10, we show the conductance as a function of M for several v/t $(=0.4,0.5,\ldots,1.0)$ taking the repulsion to be $U/(2\pi t)=0.3$. In this figure, the conductance is normalized by the noninteracting value $g_{2M}^{(0)}\equiv(2e^2/h)C_0$ which depends on v. The normalized conductance decreases with v. This also means that the effect of the interaction is enhanced when the level width of the resonant states is small.

B. Asymmetric connection $v_L\neq v_R$

We next examine the case where the inversion symmetry is broken, $v_L\neq v_R$, but the electron-hole symmetry is still preserved in the equilibrium state by the condition $\mu=0$ and $\epsilon_0=-U/2$. As one typical example, we take the mixing parameters to be $v_L/t=0.8$ and $v_R/t=0.6$ in this subsection. In Figs. 11(a) and 11(b), the conductance is plotted as a function of the size N, taking $U/(2\pi t)$ to be (a) 0.2 and (b) 0.4, respectively. The result shows an even-odd oscillatory behavior like that in the case of $v_L=v_R$ discussed above. However, in the case of $v_L\neq v_R$, perfect transmission does not occur, as can be deduced from Eq. (31), so that we have also made a numerical calculation for odd N. Although the Kondo resonance is still present at the Fermi level owing to the electron-hole symmetry, the conductance is reduced. Nevertheless, the Kondo state contributes to higher transmission

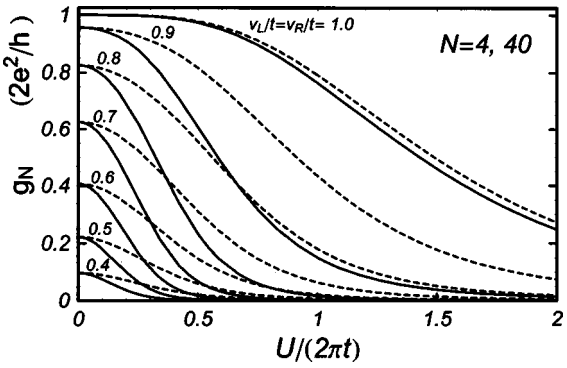

FIG. 9. Conductance vs U, for $N=4$ (dashed lines) and $N=40$ (solid lines). Here v/t is taken to be 0.4,0.5, . . . ,0.9, and 1.0.

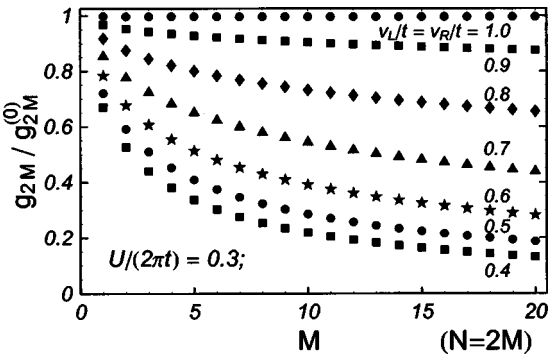

FIG. 10. Conductance for even N $(=2M)$ as a function of the size M. Here $U/(2\pi t)=0.3$, and the conductance is normalized by the value for $U=0$, i.e., $g_{2M}^{(0)}\equiv(2e^2/h)C_0$. The mixing matrix element v/t is taken to be (■) 0.4, (●) 0.5 (⋆) 0.6, (▲) 0.7, (◆) 0.8, (■) 0.9, and (●) 1.0.

for odd N. In Fig. 12, g_N is plotted as a function of U for a number of N $(=1,2,3,\ldots,40)$. For even N, the qualitative features of the results are similar to those in the inversion-symmetric case (see Fig. 6). On the other hand, for odd N, the features of the curves are somewhat different. However, the results for large values of U have some limitations, because the parameter λ defined by Eq. (32) tends to show an incorrect limit for large U when the self-energy is estimated within a finite order in U, i.e., λ tends to the ratio of the highest-order term of the numerator and that of the denominator of Eq. (A10). In the noninteracting case the conductances for even and odd N, g_{2M} and g_{2M+1}, are independent of the size M, respectively, since $\tilde{v}_C=t$ and $\lambda=1$. For small

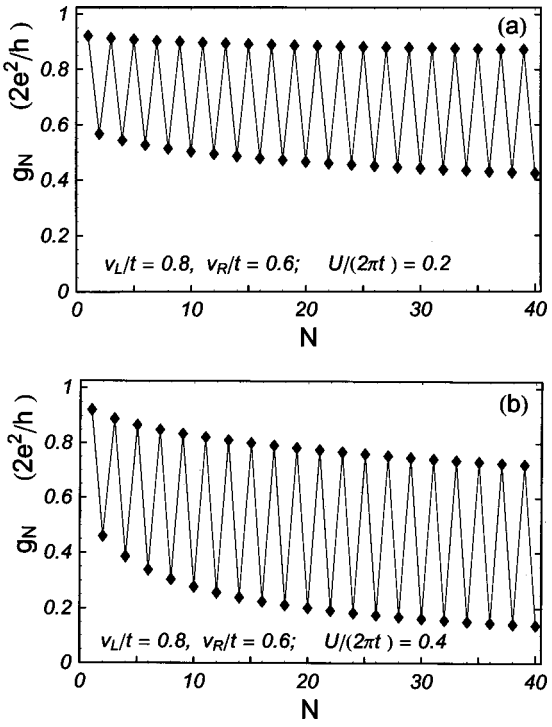

FIG. 11. Conductance g_N as a function of the size N in the inversion asymmetric case. Here $v_L/t=0.8$, $v_R/t=0.6$, and $U/(2\pi t)$ is taken to be (a) 0.2 and (b) 0.4.

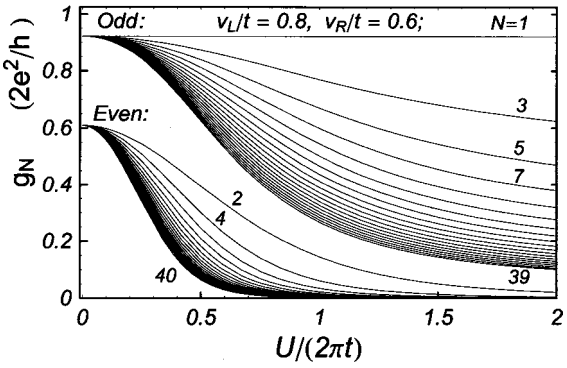

FIG. 12. Conductance vs U, for a number of N $(=1,2,3,\ldots,40)$. Here $v_L/t=0.8$ and $v_R/t=0.6$.

U, the reduction of the conductance is proportional to U^2 and the curvature increases with the size M, except for the single-impurity case $N=1$. In Fig. 13, the coefficient C_2 defined by $g_N=(2e^2/h)[C_0-C_2\{U/(2\pi t)\}^2+\cdots]$ is plotted as a function of N. In the figure, the envelops for even N is upward from that for odd N. The coefficient C_2 increases with size N, showing an oscillatory behavior, and it probably diverges in the limit of large N.

V. SUMMARY

We have applied a quasiparticle description of a Fermi liquid to transport through a small interacting system connected to reservoirs. With this approach, we have studied the properties of quasiparticles in an electron-hole-symmetric case. In this case, effects of electron correlation come in the theory through the off-diagonal part of the self-energy, and the conductance can be written in a simplified form [Eq. (31) or (33)] depending on whether the number of the interacting sites N is even or odd. It is shown, using Eq. (31), that perfect transmission occurs quite generally for odd N if the system has an inversion symmetry in addition to an electron-hole symmetry. We apply the method to a small Hubbard chain of finite size N, with second-order perturbation theory in U, and examine the conductance as a function of N and U, and the coupling between the chain and the leads, i.e., v_L and v_R. Effects of electron correlation are enhanced in the weak-coupling case $v_L, v_R < t$. In this case, the conductance for even N tends to zero for large N. This behavior is qualitatively different from that in the special case $v_L=v_R=t$. This seems to be caused by the difference in the structure of the resonant states. Quantitatively, the range of U in which the second-order perturbation theory is able to provide reliable results tends to be narrow with increasing N, and thus higher-order terms should be included in order to refine the results obtained for large U, and to clarify the asymptotic behavior for large N.

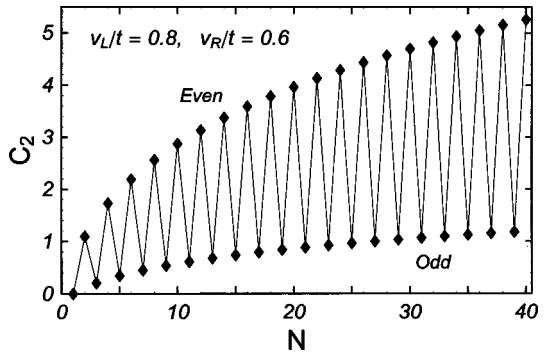

FIG. 13. The coefficient C_2 as a function of the size N. Here $v_L/t=0.8$, $v_R/t=0.6$, and $g_N=(2e^2/h)[C_0-C_2\{U/(2\pi t)\}^2+\cdots]$.

Throughout this work, we have assumed that the interaction is switched on only in the sample region at the center. When the interaction is also switched on in the two leads, a description in terms of the quasiparticles is still possible if the ground state is changed continuously against this interaction. However, some modifications are necessary. The interaction in the leads will cause a renormalization of the incoming and outgoing fields corresponding to initial and final states of the scattering matrix, i.e., a renormalization of the external lines. Furthermore, the quasiparticle description can be extended to finite temperatures by taking into account the residual interaction among the quasiparticles or the contributions of vertex corrections. In particular, an overall picture of the even-odd property described in the last part of Sec. II will be confirmed microscopically based on finite-temperature theory.

ACKNOWLEDGMENTS

We would like to thank H. Fukuyama, H. Ishii, W. Izumida, N. Nagaosa, S. Nonoyama, and O. Sakai for valuable discussions. This work was partially supported by the Grant-in-Aid for Scientific Research from the Ministry of Education, Science and Culture, Japan.

APPENDIX A: $\mathcal{K}$ MATRIX IN THE ELECTRON-HOLE-SYMMETRIC CASE

Here we summarize properties of the renormalized hopping matrix $\mathcal{K}$, and provide the derivation of Eq. (28). In the electron-hole-symmetric case, $\mathcal{K}$ has a checkered structure as shown in Eqs. (29) and (30). Thus $\det\mathcal{K}=0$ for odd N. For even $N\,(=2M)$, the determinant can be divided into two parts:

$$\begin{vmatrix} 0 & \tilde{t}^C_{12} & 0 & \tilde{t}^C_{14} & \cdots \\ \tilde{t}^C_{21} & 0 & \tilde{t}^C_{23} & 0 & \cdots \\ 0 & \tilde{t}^C_{32} & 0 & \tilde{t}^C_{34} & \cdots \\ \tilde{t}^C_{41} & 0 & \tilde{t}^C_{43} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{vmatrix} = (-1)^M \det \boldsymbol{Q} \det \boldsymbol{Q}'. \tag{A1}$$

Here $\boldsymbol{Q}$ and $\boldsymbol{Q}'$ are $M\times M$ matrices defined by

$$\boldsymbol{Q}=\begin{bmatrix} \tilde{t}^C_{12} & \tilde{t}^C_{14} & \cdots \\ \tilde{t}^C_{32} & \tilde{t}^C_{34} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}, \quad \boldsymbol{Q}'=\begin{bmatrix} \tilde{t}^C_{21} & \tilde{t}^C_{23} & \cdots \\ \tilde{t}^C_{41} & \tilde{t}^C_{43} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}. \tag{A2}$$

Since the renormalized parameter is real and $\tilde{t}^C_{ij}=\tilde{t}^C_{ji}$ owing to the time-reversal symmetry, $\det \boldsymbol{Q}=\det \boldsymbol{Q}'$. Consequently, for even N $(=2M)$, the determinant of the matrices $\boldsymbol{\mathcal{K}}$, $\boldsymbol{\mathcal{K}}^{NN}_{11}$, and $\boldsymbol{\mathcal{K}}_{N1}$ can be factorized as

$$\det \boldsymbol{\mathcal{K}}=(-1)^M\{\det \boldsymbol{Q}\}^2, \tag{A3}$$

$$\det \boldsymbol{\mathcal{K}}^{NN}_{11}=(-1)^{M-1}\{\det \boldsymbol{Q}^{NN}_{11}\}^2, \tag{A4}$$

$$\det \boldsymbol{\mathcal{K}}_{N1}=\det \boldsymbol{Q}\det \boldsymbol{Q}^{NN}_{11}. \tag{A5}$$

Here $\boldsymbol{Q}^{NN}_{11}$ is a $(M-1)\times(M-1)$ matrix extracted from $\boldsymbol{\mathcal{K}}^{NN}_{11}$ in a similar way as was done for extracting $\boldsymbol{Q}$ from $\boldsymbol{\mathcal{K}}$. Using Eqs. (A3)–(A5), we obtain Eq. (28) for even N, i.e., $(\det \boldsymbol{\mathcal{K}}_{N1})^2=-\det \boldsymbol{\mathcal{K}}\det \boldsymbol{\mathcal{K}}^{NN}_{11}$. Furthermore, $\tilde{v}_C$, defined by Eq. (34), is simplified as

$$\tilde{v}_C=\left|\frac{\det \boldsymbol{Q}}{\det \boldsymbol{Q}^{NN}_{11}}\right|. \tag{A6}$$

For odd N $(=2M+1)$, the $2M\times 2M$ matrices $\boldsymbol{\mathcal{K}}_{11}$ and $\boldsymbol{\mathcal{K}}_{NN}$ have properties similar to those described above. Consequently, the determinants can be factorized as

$$\det \boldsymbol{\mathcal{K}}_{11}=(-1)^M\{\det \boldsymbol{Q}_{11}\}^2, \tag{A7}$$

$$\det \boldsymbol{\mathcal{K}}_{NN}=(-1)^M\{\det \boldsymbol{Q}_{NN}\}^2, \tag{A8}$$

$$\det \boldsymbol{\mathcal{K}}_{N1}=\det \boldsymbol{Q}_{11}\det \boldsymbol{Q}_{NN}. \tag{A9}$$

Here $\boldsymbol{Q}_{11}$ and $\boldsymbol{Q}_{NN}$ are $M\times M$ matrices extracted from $\boldsymbol{\mathcal{K}}_{11}$ and $\boldsymbol{\mathcal{K}}_{NN}$, respectively, as done above. Using Eq. (A7)–(A9), we obtain Eq. (28) for odd N, i.e., $(\det \boldsymbol{\mathcal{K}}_{N1})^2=\det \boldsymbol{\mathcal{K}}_{11}\det \boldsymbol{\mathcal{K}}_{NN}$. Also, λ defined by Eq. (32) is simplified as

$$\lambda=\left|\frac{\det \boldsymbol{Q}_{11}}{\det \boldsymbol{Q}_{NN}}\right|. \tag{A10}$$

APPENDIX B: REFLECTION COEFFICIENT IN A SPECIAL CASE

Here we show another approach to clarifying the asymptotic behavior of the coefficient C_4 introduced in Sec. IV in the case of $v_L=v_R=t$. In this case, the Dyson equation (9) is written, in terms of the scattering matrix $\mathcal{T}_{ll'}$, as

$$G_{jj'}=G^{(0)}_{jj'}+\sum_{l,l'=1}^{N} G^{(0)}_{jl}\mathcal{T}_{ll'}G^{(0)}_{l'j'}. \tag{B1}$$

The transmission and reflection coefficients are also written in terms of $\mathcal{T}_{ll'}$ as $\tilde{t}(0)=1-i\mathcal{T}_{k_Fk_F}(i0^+)/v_F$ and $\tilde{r}(0)=-i\mathcal{T}_{-k_Fk_F}(i0^+)/v_F$,[18,19] where $v_F=2t$, $k_F=\pi/2$, and

$$\mathcal{T}_{kk'}=\sum_{l,l'=1}^{N} e^{-ikl}\mathcal{T}_{ll'}e^{ik'l'}. \tag{B2}$$

Since the unperturbed system has a translational invariance in the present case, the lowest-order scattering matrix is given by $\mathcal{T}^{(2)}_{ll'}=\Sigma^{(2)}_{ll'}$. Thus, using a wave-number representation of $\Sigma^{(2)}_{ll'}$,[30] the lattice sum Eq. (B2) can be done explicitly, and the reflection coefficient is expressed as

$$\begin{aligned}\tilde{r}^{(2)}_N=&-\frac{i}{v_F}e^{ik_F(N+1)}U^2\int\frac{dk_3dk_2dk_1}{(2\pi)^3}\\&\times\frac{\cos k_FN-\cos[(k_1+k_2-k_3)N]}{\cos k_F-\cos(k_1+k_2-k_3)}\\&\times\mathrm{P}\frac{f_{k_3}(1-f_{k_2})(1-f_{k_1})+(1-f_{k_3})f_{k_2}f_{k_1}}{\xi_{k_3}-\xi_{k_2}-\xi_{k_1}}.\end{aligned} \tag{B3}$$

Here $\xi_k=-2t\cos k$, $f_k=[e^{\beta\xi_k}+1]^{-1}$, and P denotes the Cauchy principal value. It can be confirmed from Eq. (B3) that $\tilde{r}^{(2)}_N=0$ for odd N. For large even N, the contribution of the fast varying $\cos[(k_1+k_2-k_3)N]$ part becomes small, and the dominant contribution comes form the $\cos k_FN$ part. Thus, for large even N $(=2M)$, the reflection coefficient is written in the form $\lim_{M\to\infty}\tilde{r}^{(2)}_{2M}=\sqrt{C^\infty_4}\{U/(2\pi t)\}^2$ with

$$\sqrt{C^\infty_4}\equiv\frac{1}{4\pi}\mathrm{P}\int_{-\pi/2}^{\pi/2}\frac{dk_3dk_2dk_1}{[\cos k_1+\cos k_2+\cos k_3]\cos(k_1+k_2+k_3)}. \tag{B4}$$

The coefficient $\sqrt{C^\infty_4}$ is finite, and estimated numerically as $\sqrt{C^\infty_4}\simeq 0.729$. Thus, in the limit of large even N, the dc conductance in the case of $v_L=v_R=t$ is written in the form $\lim_{M\to\infty}g_{2M}=(2e^2/h)[1-C^\infty_4\{U/(2\pi t)\}^4+\cdots]$.

[1] T. K. Ng and P. A. Lee, Phys. Rev. Lett. **61**, 1768 (1988).
[2] L. I. Glazman and M. E. Raikh, Pis'ma Zh. Éksp. Teor. Fiz. **47**, 378 (1988) [JETP Lett. **47**, 452 (1988)].
[3] A. Kawabata, J. Phys. Soc. Jpn. **60**, 3222 (1991).
[4] Y. Meir, N. S. Wingreen, and P. A. Lee, Phys. Rev. Lett. **66**, 3048 (1991); **70**, 2601 (1993).
[5] S. Hersfield, J. H. Davies, and J. W. Wilkins, Phys. Rev. B **46**, 7046 (1992).
[6] D. C. Ralph and R. A. Buhrman, Phys. Rev. Lett. **72**, 3401 (1994).
[7] D. Goldharber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav, and M. A. Kastner, Nature (London) **391**, 156 (1998).
[8] S. M. Cronenwett, T. H. Oosterkamp, and L. P. Kouwenhoven, Science **281**, 540 (1998).
[9] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. **68**, 1220 (1992).
[10] A. Furusaki and N. Nagaosa, Phys. Rev. B **47**, 4631 (1993).
[11] S. Tarucha, T. Honda, and T. Saku, Solid State Commun. **94**, 413 (1995).
[12] Y. Meir and N. S. Wingreen, Phys. Rev. Lett. **68**, 2512 (1992).
[13] L. V. Keldysh, Zh. Éksp. Teor. Fiz. **47**, 1515 (1964) [Sov. Phys. JETP **20**, 1018 (1965)].

[14] C. Caroli, R. Combescot, P. Nozières, and D. Saint-James, J. Phys. C **4**, 916 (1971).
[15] E. N. Economou and C. M. Soukoulis, Phys. Rev. Lett. **46**, 618 (1981).
[16] D. S. Fisher and P. A. Lee, Phys. Rev. B **23**, 6851 (1981).
[17] P. A. Lee and D. S. Fisher, Phys. Rev. Lett. **47**, 882 (1981).
[18] A. Oguri, J. Phys. Soc. Jpn. **66**, 1427 (1997).
[19] A. Oguri, Phys. Rev. B **56**, 13 422 (1997); **58**, 1690(E) (1998).
[20] A. C. Hewson, Adv. Phys. **43**, 543 (1994); *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, 1993).
[21] W. Izumida, O. Sakai, and Y. Shimizu, J. Phys. Soc. Jpn. **66**, 717 (1997); **67**, 2444 (1998).
[22] O. Sakai, S. Suzuki, W. Izumida, and A. Oguri, J. Phys. Soc. Jpn. **68**, 1640 (1999).
[23] A. Oguri, H. Ishii, and T. Saso, Phys. Rev. B **51**, 4715 (1995).
[24] V. V. Ponomarenko and N. Nagaosa, Phys. Rev. Lett. **81**, 2304 (1998).
[25] A. A. Odintsov, Y. Tokura, and S. Tarucha, Phys. Rev. B **56**, R12 729 (1997).
[26] O. A. Starykh and D. L. Maslov, Phys. Rev. Lett. **80**, 1694 (1998).
[27] M. Mori, M. Ogata, and H. Fukuyama, J. Phys. Soc. Jpn. **66**, 3363 (1997).
[28] S. Fujimoto and N. Kawakami, J. Phys. Soc. Jpn. **65**, 3700 (1996).
[29] K. Yosida and K. Yamada, Suppl. Prog. Theor. Phys. **46**, 244 (1970); K. Yamada, Prog. Theor. Phys. **53**, 970 (1975).
[30] A. Oguri, Phys. Rev. B **59**, 12 240 (1999).
[31] A. Oguri, Physica B **284-288**, 1932 (2000).
[32] V. Zlatić and V. Horvatić, Phys. Rev. B **28**, 6940 (1983).
[33] J. S. Langer and V. Ambegaokar, Phys. Rev. **121**, 1090 (1961).
[34] We note that Eq. (14) has been derived for noninteracting systems by Caroli *et al.*[14] Also, Pernas *et al.* obtained a similar expression for interacting systems with the single-site approximation, neglecting the off-diagonal part of the self-energy (Ref. 44).
[35] R. Landauer, Philos. Mag. **21**, 863 (1970).
[36] M. Büttiker, Y. Imry, R. Landauer, and S. Pinhas, Phys. Rev. B **31**, 6207 (1985).
[37] D. C. Langreth, Phys. Rev. **150**, 516 (1966).
[38] See, for instance, J. Sólyom, Adv. Phys. **28**, 201 (1979).
[39] See, for instance, D. L. Cox and A. Zawadowski, Adv. Phys. **47**, 599 (1998).
[40] Y. Shimizu, O. Sakai, and S. Suzuki, J. Phys. Soc. Jpn. **67**, 2395 (1998).
[41] A. Yeyati, A. Martín-Rodero, and F. Flores, Phys. Rev. Lett. **71**, 2991 (1993).
[42] T. Mii and K. Makoshi, Jpn. J. Appl. Phys. **35**, 3706 (1996).
[43] O. Takagi and T. Saso, J. Phys. Soc. Jpn. **68**, 1997 (1999).
[44] P. L. Pernas, F. Flores, and E. V. Anda, J. Phys. Condens. Matter **4**, 5309 (1992).
[45] Y. Kawahito, H. Kasai, H. Nakanishi, and A. Okiji, J. Appl. Phys. **85**, 947 (1999).