The equation of motion method (EOM) is one of the approximations to calculate transport coefficients of interacting electron systems. The method is known to be useful to examine high-temperature properties. However, sometimes a naive application of the EOM fails to capture an important physics at low-energy scale, and it happens in recent preprints [cond-mat/0309458 and cond-mat/0308413] which study a series of quantum dots. These preprints concluded that a unitarity-limit transport due to the Kondo resonance, which has been deduced from a Fermi-liquid behavior at $T=0$, does not occur. We show that the EOM self-energy obtained with a finite cluster has accidentally a singular $1/\omega$ dependence around the Fermi energy, and it misleads one to the result incompatible with a Fermi-liquid ground state.

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I. BACKGROUND

A Hubbard chain of finite size $N$ connected to two noninteracting leads, which is illustrated in Fig. 1, has been studied as a model for a series of quantum dots [[1, 2, 3, 4, 5]]. Here $N$ corresponds to the number of quantum dots and should be small, while the number of the sites in the noninteracting leads at left and right are infinite, i.e., $N_L \to \infty$ and $N_R \to \infty$. It has been shown for the chain of an odd $N$ that the transmission probability reaches a unitarity-limit value at $T=0$ if the system has the electron-hole symmetry (half-filling) together with the inversion symmetry $(v_L = v_R)$ [[4]]. This conclusion has been deduced from a Fermi-liquid behavior of the self-energy summarized simply in Eq. (2).

Recently, the dc conductance at zero temperature has been calculated with an extended version of the equation of motion method (EOM) [[6]], which is essentially the Hubbard I approximation [[7]], at zero temperature [[1, 2]]. The results of these preprints contradict with the unitarity-limit transport mentioned above. The purpose of this report is to show that the discrepancy is caused just by a naive use of the EOM self-energy of obtained with a finite cluster, which accidentally has a singularity at low-energies and is not compatible with the Fermi-liquid ground state.

In Sec. II we describe briefly the results deduced from a Fermi-liquid property Eq. (6) to make our points clear. Then, in Sec. III the properties of the approximate self-energy in the EOM are discussed.

II. CONDUCTANCE AT ZERO TEMPERATURE

A. Formulation

The dc conductance at $T=0$ is determined by the value of a Green’s function $G_{N1}^+(\omega)$ at the Fermi energy $\omega = 0$ (1):

$$g_N = \frac{2e^2}{h} 4 \Gamma_R^*(0) \Gamma_L^*(0) \left| G_{N1}^+(0) \right|^2, \quad (1)$$

Here $G_{ij}^+(\omega)$ is the retarded Green’s in the real space ($1 \leq i,j \leq N$), see Fig. 1 and $\Gamma_\alpha(\omega) = -v_\alpha^2 \text{Im} g_\alpha^+(\omega)$ for $\alpha = L, R$ with $g_\alpha^+(g_R^*)$ being an interface Green’s function for the semi-infinite lead at left (right). The Dyson equation can be written in a $N \times N$ matrix form:

$$\{G(\omega)\}^{-1} = \{G^0(\omega)\}^{-1} - \Sigma(\omega). \quad (2)$$

Here $G^0 = \{G^0_{ij}\}$ is the noninteracting Green’s function for $U=0$ defined with respect to the total system connected via tunneling $v_L$ and $v_R$. The inverse matrix of the unperturbed Green’s function can be expressed as

$$\{G^0(\omega)\}^{-1} = \omega 1 - H_C^0 - V_{\text{mix}}(\omega), \quad (3)$$

$$H_C^0 = \begin{bmatrix} 0 & -t & 0 \\ -t & 0 & \ddots \\ \vdots & \ddots & \ddots & -t \\ 0 & -t & 0 \end{bmatrix}, \quad (4)$$

$$V_{\text{mix}}(\omega) = \begin{bmatrix} v_L^2 g_L^+(\omega) & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix} + \begin{bmatrix} v_R^2 g_R^+(\omega) & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & v_R^2 g_R^+(\omega) \end{bmatrix}. \quad (5)$$

Here $1$ is the $N \times N$ unit matrix. The self-energy due to the Coulomb interaction $\Sigma$ is also defined with respect
to the total system of continuous energy spectrum. Note that the Green’s function $G^r_{N}(0)$ appearing in Eq. 11 can be obtained by taking the inverse of the matrix in Eq. 2.

B. Fermi-liquid behavior

At $T = 0$, $\omega = 0$ not only the Fermi-liquid but also some other “liquid” states of interacting electron systems show a behavior,

$$\text{Im} \Sigma(0) = 0, \quad \text{and} \quad \text{Re} \Sigma(0) \text{ is finite.}$$  

This property of the self-energy, the electron-hole symmetry, and the inversion symmetry are the three keys to lock the conductance for odd $N$ at the unitarity-limit value. No other assumptions have been made in the proof \[8\]. The perturbation expansion in $U$ preserves the properties of Eq. (6) also for $N \geq 2$ owing to the presence of the noninteracting leads. The contributions of the hybridization $\Gamma_L$ and $\Gamma_R$ in the unperturbed part $G^0$ make it possible to take into account the virtual processes in which electrons visit inside the noninteracting leads of continuous spectrum during the multi-scattering by $U$.

For even $N$, the conductance decreases with increasing $N$ showing a tendency towards the development of a Mott-Hubbard insulator gap $\Delta_{\text{gap}}$. Although we are interested in the system of small $N$, a question arises: what can we see in the limit of $N \to \infty$? Note that the results mentioned above hold just at $T = 0$. To describe the thermodynamic limit properly, we must consider the physics at finite but sufficiently low temperatures. For odd $N$, the Kondo resonance of width $T_K$ is situated in the Hubbard gap. As $N$ increases, $T_K$ decreases and finally $T_K \to 0$ at $N \to \infty$ because the developing gap disturbs the electrons to form the Kondo singlet. Thus, the value of the conductance $g_N$ for odd $N$ ($= 2M + 1$) must depend on the order to take the two limit $N \to \infty$ and $T \to 0$:

- if we take $T \to 0$ first and then $N \to \infty$, we see the physics at $T < T_K$, i.e., the Kondo behavior,

$$\lim_{M \to \infty} \left[ \lim_{T \to 0} g_{2M+1} \right] = 2e^2/h ,$$

- if we take $N \to \infty$ first and then $T \to 0$, we see the physics at $T > T_K$, i.e., Mott-Hubbard behavior,

$$\lim_{T \to 0} \left[ \lim_{M \to \infty} g_{2M+1} \right] = 0 .$$

Note that, for even $N$ ($= 2M$), the result does not depend on the order to take these two limits,

$$\lim_{M \to \infty} g_{2M} = 0 .$$

At the temperatures $T_K < T < \Delta_{\text{gap}}$, we see the insulating behavior for large $N$ independent of whether $N$ is even or odd. To observe the Kondo behavior at an accessible temperature $T$, the resonance width $T_K$ should be sufficiently large, so that the number of the quantum dots $N$ should be small.

III. APPLICABILITY OF EOM AT LOW TEMPERATURES

A. Method

In the EOM calculation of Refs. \[1\] and \[2\] the self-energy has been calculated using a finite cluster of the size $N_{cl}$ decoupled from the total system. Typically, the cluster introduced for the calculation consists of $N$ interacting sites, several noninteracting sites in the left lead $N'_L$, and that in the right lead $N'R$:

$$N_{cl} = N + N'_L + N'R .$$  

Using the ground state of the decoupled cluster obtained with an exact diagonalization, a $N_{cl} \times N_{cl}$ cluster Green’s function $g_{\text{cl}}$ has been calculated \[1\], \[2\]. The EOM self-energy $\Sigma_{\text{cl}}$ can be obtained from the Dyson equation for the decoupled cluster,

$$\Sigma_{\text{cl}}(\omega) = \left\{ \tilde{g}_{\text{cl}}^0(\omega) \right\}^{-1} - \left\{ g_{\text{cl}}(\omega) \right\}^{-1} .$$  

Here $\tilde{g}_{\text{cl}}^0$ is the $U = 0$ Green’s function for the decoupled cluster, which describes a discrete energy spectrum. Then, an approximate Green’s function which takes into account the rest of the system can be calculated by substituting $\Sigma_{\text{cl}}(\omega)$ for the self-energy $\Sigma(\omega)$ defined with respect to the total system.

The applicability of this method is determined by the separation of the eigenvalues of the cluster $\Delta \epsilon$. This is because $\Sigma_{\text{cl}}$ has been calculated for the discrete energy spectrum, and the correlation effects on the low-lying states below this energy separation have not been taken into account. Therefore, the application of EOM can be justified at high-energies (or high-temperatures) above the energy separation $\Delta \epsilon$. The information about the many-body effects on the low-lying states is still missing even though one gets a continuous spectrum after taking into account the connection to the rest of the system. Therefore, if a fine structure is seen in the obtained continuous spectrum, that structure is expected to be real only when the energy scale is consistent with the resolution $\Delta \epsilon$. In principle, the energy resolution can be improved systematically by increasing the size of the cluster successively, and the numerical renormalization group (NRG) can be regarded as one of such approaches \[3\], \[4\]. Since the cluster is introduced just for the approximation and have no physical meanings, the results of the observable quantities must not have a strong dependence on the value of $N'_L$ and $N'R$. 

B. The 1/ω singularity of the EOM self-energy

In Refs. [1] and [2], the calculations have been carried out for the cluster with an odd number of sites $N_{cl}$. At half-filling, the ground state of the cluster is doublet with the total spin $S_{tot} = 1/2$. According to the appendix of Ref. [2], the cluster Green’s function $\hat{g}_{cl}$ is defined using the equal-weight sum of $S_{tot}^z = 1/2$ and $-1/2$ in Ref. [2], while the work in Ref. [1] considers only the cluster state with $S_{tot}^z = 1/2$. Furthermore, in Fig. 9 of Ref. [2], these two procedures are shown to lead quite different results. This means that huge ambiguities exist in the EOM results at low energies. In these two procedures, however, the equal-weight sum seems to be better because it restores the rotational symmetry, so that we will use this convention in the following discussion of the behavior of the EOM self-energy. As typically seen in Fig. 9 of Ref. [2], the results in Ref. [1] have also been affected by the singularity, although the position of the pole might shift due to the absence of the rotation symmetry of the spin in the convention used in Ref. [1].

The presence of the 1/ω singularity of the EOM self-energy for the cluster of an odd size can be deduced along the discussion similar to that in the section V of Ref. [2]. Using the SU(2) symmetry of the axial charge holding in the electron-hole symmetric case (see Appendix A), the cluster Green’s function can be expressed as,

$$\hat{g}_{cl;ij}(ω) = \frac{S_g + 1}{2S_g + 1} \sum_{i'} C_i(1/2, S_g + 1/2; r'|0, S_g; r_g) \times C_j(1/2, S_g + 1/2; r'|0, S_g; r_g) \times \left\{ \frac{1}{ω - \omega_{S_g}^+(r')} + \frac{(-1)^{i+j}}{ω + \omega_{S_g}^+(r')} \right\}$$

$$+ \frac{S_g}{2S_g + 1} \sum_{i'} C_i(1/2, S_g - 1/2; r'|0, S_g; r_g) \times C_j(1/2, S_g - 1/2; r'|0, S_g; r_g) \times \left\{ \frac{1}{ω - \omega_{S_g}^-(r')} + \frac{(-1)^{i+j}}{ω + \omega_{S_g}^-(r')} \right\},$$

$$ω_{S_g}^±(r') = E_{1/2, S_g±1/2}(r') - E_{0, S_g}(r_g).$$

Here $S_g$, $J_g$, and $r_g$ are the quantum numbers of the ground state, the energy of which is denoted by $E_{J_g, S_g}(r_g)$. Note that $J_g$ must be zero for $U > 0$. Furthermore, for $U > 0$, the excitation energy must be finite $ω_{S_g}^±(r') > 0$ in the case of $N \geq 2$ as long as the cluster size $N_{cl}$ is finite. Thus, for $N \geq 2$, the full Green’s $\hat{g}_{cl}(ω)$ does not have a pole at $ω = 0$ independent of whether $N_{cl}$ is even or odd. In contrast, the noninteracting Green’s function $\hat{g}_{cl}^0(ω) = 0$ for odd $N_{cl}$, while it does not for even $N_{cl}$. Therefore the EOM self-energy $\hat{Σ}_{cl}(ω)$, which can be calculated using Eq. (8), must have a pole at $ω = 0$ for odd $N_{cl}$ because the structure of the energy spectrum of $\hat{g}_{cl}(ω)$ and that of $\hat{g}_{cl}^0(ω)$ are completely different. On the other hand, for even $N_{cl}$ the the energy spectrum of $\hat{g}_{cl}(ω)$ and $\hat{g}_{cl}^0(ω)$ belong to the same category having no zero mode, so that $\hat{Σ}_{cl}(ω)$ does not have a singularity at $ω = 0$ and shows a behavior consistent with that of the Fermi liquid Eq. (4). Therefore, the presence of the zero-energy pole can be summarized as Table I (see also Appendix B for $N = 1$). Note that in the case of “Yes”, it does not necessary mean that all the matrix elements have the pole.

Using the EOM self-energy with the Dyson equation which connects the cluster to the remaining system, an approximate Green’s function $\hat{G}^{N \times N}_{cl}$ can be calculated. Alternatively, the same $\hat{G}^{N \times N}_{cl}$ can also be calculated by substituting the $N \times N$ partitioned part of $\hat{Σ}_{cl}$, which corresponds to the interacting region, into the Dyson equation of $N \times N$ form Eq. (12), and then taking the inverse of the matrix. Therefore, if one uses the cluster of odd $N_{cl}$ for calculating the value of $\hat{G}^{N \times N}_{cl}(ω)$ at $ω = 0$, one obtains the result $\hat{G}^{1 \times 1}_{N_{cl}}(0) = \hat{g}_{N_{cl}}^0(0) = 0$ for odd $N_{cl}$ because of the zero-energy pole of $\hat{Σ}_{cl}(ω)$. In contrast, if one uses the cluster of even $N_{cl}$ in the same situation, the result must be different. This also suggests that the EOM is not suitable for studying the low-temperature properties.

C. Interpretation of the zero-energy pole of $\hat{Σ}_{cl}$

The oscillatory behavior caused by the cluster size $N_{cl}$ has been seen also in the NRG calculation [4, 10]. For even $N_{cl}$, the ground-state is singlet and the self-energy can be expanded with respect to $ω$ at the Fermi energy $ω = 0$, which agrees with the local Fermi-liquid theory of Nozières [11] and the perturbation theory of Yamada and Yoshida [8]. For odd $N_{cl}$, the ground state is doublet, and the self-energy has the zero-energy pole. Nevertheless, the energy spectrum of the low-lying states shows the correct Fermi-liquid behavior even for odd $N_{cl}$ [10]. Furthermore, the residue of the zero-energy pole decreases with increasing $N_{cl}$ and vanishes in the $N_{cl} \to \infty$ limit. Therefore, it is quite dangerous to examine the low-temperature properties only by the Green’s function obtained with a finite cluster of an odd number sites $N_{cl}$.

Similar oscillation takes place in an antiferromagnetic Heisenberg chain. The spin susceptibility of the chain of an odd number sites has a Curie term. Since the weight of the Curie term is proportional to $1/N_{cl}$ and vanishes at $N_{cl} \to \infty$, usually the cluster of an even number sites is used for studying the properties in the thermodynamic limit, although the cluster of an odd number sites can also

| TABLE I: Pole at $ω = 0$ for the interacting sites of $N \geq 2$ |
|-----------------|-----------------|-----------------|
| Even $N_{cl}$   | $\hat{g}_{cl}(ω)$ | $\hat{g}_{cl}^0(ω)$ | $\hat{Σ}_{cl}(ω)$ |
| Odd $N_{cl}$    | None            | None            | Yes             |
| Even $N_{cl}$   | None            | None            | None            |


be used if the contribution of the Curie term is subtracted properly.

IV. CONCLUSION

In conclusion, the EOM self-energy obtained for a finite cluster of an odd number of sites has the zero-energy pole, the residue of which must vanish in the limit of large cluster $N_{cl} \to \infty$. The absence of the unitarity-limit transport reported in Refs. [1] and [2] can be explained to be caused by a naive use of this singular self-energy.

APPENDIX A: AXIAL CHARGE

In the electron-hole symmetric case, the Hamiltonian $\hat{H}$ commute with the total axial charge defined by $[12]$

$$\hat{J}^2 = \hat{J}^2_z + (\hat{J}_- + \hat{J}_+/2),$$  \hspace{1cm} (A1)

$$\hat{J}_z = \sum_i \frac{1}{2} \left(c_i^\dagger c_i^\dagger + c_i c_i - 1\right),$$  \hspace{1cm} (A2)

$$\hat{J}_+ = \sum_i (-1)^i c_i c_i^\dagger ,$$  \hspace{1cm} (A3)

$$\hat{J}_- = \sum_i (-1)^i c_i^\dagger c_i .$$  \hspace{1cm} (A4)

Note that the $z$ component corresponds to the charge of the U(1) symmetry as $\hat{Q} = 2\hat{J}_z$. The operators $\hat{J}_z$ and $\hat{J}_\pm$ satisfy the commutation relations of the angular momentum as the total spin operators $\hat{S}_z$ and $\hat{S}_\pm$ do. Thus, the eigenstates can be classified according to the quantum numbers corresponding to $\hat{J}^2$, $\hat{J}_z S^2$, and $\hat{S}_z$.

$$\hat{H} \langle J, J_z, S, S_z; r \rangle = E_{J, S}(r) \langle J, J_z, S, S_z; r \rangle .$$  \hspace{1cm} (A5)

Eq. (5) can be derived using the Wigner-Eckart theorem for the spin and for the axial charge,

$$\langle J, J_z, S, S_z; r | c_{i\sigma} | J', J'_z, S', S'_z; r' \rangle$$

$$= \langle S', S_z' | 1/2, \sigma | S, S_z \rangle \langle J', J'_z' | 1/2, 1/2 | J, J_z \rangle \times C_i(J, S; r | J', S'; r' \rangle ,$$  \hspace{1cm} (A6)

where the Clebsh-Gordan coefficient appears for the total spin $(S', S'_z; 1/2, \sigma | S, S_z)$ and for the total axial charge $(J', J'_z; 1/2, 1/2 | J, J_z)$.

Note that the invariant matrix element $C_i(\alpha' | \alpha)$ has the following properties against the exchange of the arguments $\alpha'$ and $\alpha$,

$$C_i(J, S - \frac{1}{2}; r') \langle J - \frac{1}{2}, S; r \rangle$$

$$= (-1)^i \sqrt{\frac{2S + 1}{2S}} \sqrt{\frac{2J + 1}{2J}} C_i(J - \frac{1}{2}, S; r | J, S - \frac{1}{2}; r'),$$  \hspace{1cm} (A7)

$$C_i(J, S + \frac{1}{2}; r') \langle J - \frac{1}{2}, S; r \rangle$$

$$= (-1)^{i+1} \sqrt{\frac{2S + 1}{2S + 2}} \sqrt{\frac{2J + 1}{2J + 1}} C_i(J - \frac{1}{2}, S; r | J, S + \frac{1}{2}; r').$$  \hspace{1cm} (A8)

APPENDIX B: EOM RESULTS FOR $N = 1$

A cluster consisting of a single Anderson impurity at the center $i = 0$, the left lead of $N'_L$ sites at $i < 0$, and the right lead of $N'_R$ sites at $i > 0$ can be separated into two independent parts by a Unitary transformation $a_{i\sigma} = (c_{i\sigma} + c_{-i\sigma})/\sqrt{2}$ and $b_{i\sigma} = (c_{i\sigma} - c_{-i\sigma})/\sqrt{2}$ for $i = 1, 2, 3, \ldots$ when $N'_L = N'_R (= N'_0)$. Only the orbits of $a_{i\sigma}$ couple with the Anderson impurity to form a cluster of the size $N'_a (= N'_0 + 1)$, and the orbits of $b_{i\sigma}$ form a noninteracting band of the size $N'_b$. Thus, the EOM self-energy $\Sigma_{cl}(\omega)$ can be calculated using only the cluster of the interacting part, and the properties corresponding to Table II can be shown to hold by replacing $N_{cl}$ with $N'_a$: $\Sigma_{cl}(\omega)$ is zero at $\omega = 0$ and conductance reaches the unitarity limit for even $N'_a$, while $\Sigma_{cl}(\omega)$ has a pole at $\omega = 0$ and the conductance becomes zero for odd $N'_a$. Obviously, the conductance calculated from the self-energy having the zero-energy pole contradict with the correct unitarity-limit behavior known in the thermodynamic limit $N'_a \to \infty$. Note that in Ref. [1], the self-energy for even $N'_a$ is used for $N = 1$, while the self-energy having a pole around Fermi energy is used for $N = 3, 5, 7$ (see also Fig. 9 of Ref. [2]).

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