Exact Scattering Eigenstates, Many-Body Bound States, and Nonequilibrium Current in an Open Quantum Dot System

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We obtain an exact many-body scattering eigenstate in an open quantum dot system. The scattering state is not in the form of the Bethe eigenstate in the sense that the wave number set of the incoming plane wave is not conserved during the scattering and many-body bound states appear. By using the scattering state, we study the average nonequilibrium current through the quantum dot under a finite bias voltage. The current-voltage characteristics that we obtained by taking the two-body bound state into account is qualitatively similar to several known results.

Mesoscopic transport of interacting electrons has attracted much interest recently [1–4]. A remarkable feature of the mesoscopic system is the coherence length greater than the sample size. A well-known approach to the electric current across the sample under a finite bias voltage is the Landauer formula, although the original one is restricted to the noninteracting case. The nonequilibrium Green's function is also employed to study the transport property [5–10]. To discuss the effect of interactions in this framework, however, we would have to resort to a perturbation technique, which is generally a hard task.

In this Letter, we present an exact many-body scattering eigenstate in an open quantum dot system and apply the eigenstate to analysis of the nonequilibrium current. The system is an open interacting resonant-level model (IRLM), which consists of two leads of noninteracting spinless electrons that interact with an electron on a quantum dot in between the two leads. Each lead is connected to a large reservoir. First, we explicitly construct two- and three-electron scattering states, which are plane waves before scattering and, at the quantum dot, are partially scattered to a many-body bound state due to the Coulomb interaction. Second, by using the scattering states, we calculate the quantum-mechanical expectation value of the current through the quantum dot in the second order of the inverse system length. Third, we study the statistical average of the nonequilibrium current for a finite bias voltage, assuming that electrons are completely thermalized in each reservoir before returning to the lead.

Our study of the nonequilibrium current is a genuine extension of the Landauer formula. Our scattering states of the *open* system are suitable for describing incident electrons thermalized to a free-electron state in each reservoir. Some used the Bethe ansatz [11–13] to study the transport properties of quantum dot systems [14], where the Landauer formula was formally applied to the quasiparticles in a *closed* system in equilibrium. However, the periodic boundary conditions imposed on the Bethe state are clearly different from the conditions adopted for the Landauer formula, the conditions that the incident electrons are asymptotically free. Recently, there have been a few attempts to study the transport properties with a scattering state in the framework of the Lippmann-Schwinger (LS) equation [15,16]. Our scattering state is a solution of the LS equation associated with the open IRLM.

A remarkable point of our solution is the appearance of *a many-body bound state* in the scattering eigenstate. Another many-body bound state given by the Bethe ansatz method is known to be the ground state of the Anderson model in equilibrium [17]. Our bound state, on the other hand, is generated as a result of the scattering of an incident free-electronic plane-wave state (Fig. 1). The interaction around the dot is a necessary condition of the appearance of the bound state. The nonequilibrium current is affected by the interaction through the bound state.

The open IRLM out of equilibrium has been studied with various approaches [18–22]. We express the quantum-mechanical expectation value of the current as a series of the inverse system length to consider the average current, while the perturbative result [20] gives the average current as a series of the interaction parameter. The qualitative behavior of the current-voltage characteristics that we obtain is similar to the results in Refs. [19–21]. We remark that, in our results, the effect of the interaction appears in the quantum-mechanical expectation value, which differs from the result in Ref. [18].

The Hamiltonian of the open IRLM is given by

$$H = \sum_{\alpha}\left(\int_{-L/2}^{L/2} dx\, c_{\alpha}^{\dagger}(x)\frac{1}{i}\frac{d}{dx}c_{\alpha}(x) + \bar{t}[c_{\alpha}^{\dagger}(0)d + d^{\dagger}c_{\alpha}(0)]\right)$$
$$+ \epsilon_d d^{\dagger}d + \sum_{\alpha} U c_{\alpha}^{\dagger}(0)c_{\alpha}(0)d^{\dagger}d, \qquad (1)$$

where $c_{\alpha}^{\dagger}(x)$ and $c_{\alpha}(x)$ are creation- and annihilation-operators of the electrons in the lead $\alpha(=1, 2)$, $d^{\dagger}$ and d are those in the quantum dot, $\bar{t} = t/\sqrt{2}$ is the transfer integral between each lead and the dot, ϵ_d is the gate energy of the dot, and $U(>0)$ expresses the Coulomb repulsion. The dispersion relation in the leads is linearized in the vicinity of the Fermi energy to be $E = k$, under the
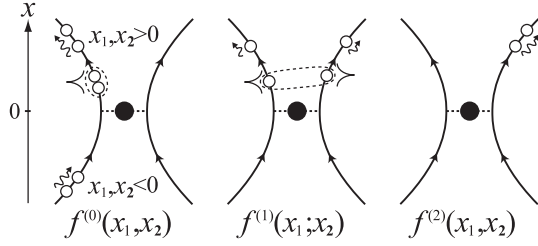
FIG. 1. A two-electron scattering state which contains incoming plane waves only in the left lead.

assumption that t, ϵ_d, and U are small compared with the Fermi energy [11–13]. We treat the system as an open system in the limit $L \to \infty$. The lead α is connected infinitely far way to a large reservoir characterized by the Fermi distribution with the chemical potential μ_α. Our goal is to calculate the statistical average of the current

$$I = i\bar{t}\sum_\alpha (-)^{\alpha+1}[c_\alpha^\dagger(0)d - d^\dagger c_\alpha(0)] \qquad (2)$$

for the system under a finite bias voltage, $\mu_1 > \mu_2$.

We consider the general form of eigenstates. After the transformation $c_{1/2}(x) = [c_e(x) \pm c_o(x)]/\sqrt{2}$, the Hamiltonian (1) is decomposed into the even and odd parts. Because $[H, N_e + N_d] = [H, N_o] = 0$ for the number operators $N_{e/o} = \int dx c_{e/o}^\dagger(x)c_{e/o}(x)$ and $N_d = d^\dagger d$, the set $\{N_e + N_d, N_o\}$ gives a good quantum number. The N-electron state $|N, n\rangle$ in the sector with $N_o = n$ is expressed in the form

$$|N, n\rangle = \left(\int dx^{N-n}dy^n g^{(n)}(x; y)c_e^\dagger(x_1)\cdots c_e^\dagger(x_{N-n})\right.$$
$$\times c_o^\dagger(y_1)\cdots c_o^\dagger(y_n)$$
$$+ \int dx^{N-n-1}dy^n e^{(n)}(x; y)c_e^\dagger(x_1)\cdots c_e^\dagger(x_{N-n-1})$$
$$\left.\times d^\dagger c_o^\dagger(y_1)\cdots c_o^\dagger(y_n)\right)|0\rangle, \qquad (3)$$

where we put $e^{(N)}(x; y) = 0$. The functions $g^{(n)}(x; y)$ and $e^{(n)}(x; y)$ are antisymmetric with respect to $\{x_i\}$ as well as $\{y_i\}$. The one-electron eigenstate $|1, n; k\rangle$, $(n = 0, 1)$ with the energy eigenvalue $E = k$ is obtained by inserting the eigenfunctions $g^{(0)}(x) = g_k(x)$, $e^{(0)} = e_k$ or $g^{(1)}(y) = h_k(y)$ into the general form (3), where

$$g_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}\left(\theta(-x) + \frac{e_k}{e_k^*}\theta(x)\right),$$
$$h_k(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}, \qquad e_k = \frac{1}{\sqrt{2\pi}}\frac{t}{k - \epsilon_d + i\bar{t}^2}, \qquad (4)$$

with the step function $\theta(x)$. The linear combination $|k\rangle = (|1, 0; k\rangle + |1, 1; k\rangle)/\sqrt{2}$ gives a scattering state containing an incoming electron only in the lead 1. If we imposed periodic boundary conditions to the leads, the wave number k allowed for the eigenfunction $g^{(1)}(x)$ would be different from that for $g^{(0)}(x)$. Thus, even in the noninteracting

case, the scattering state $|k\rangle$ is inconsistent with the periodic boundary conditions.

For $N = 2$, the eigenvalue problem $H|2, n\rangle = E|2, n\rangle$ is cast into a set of the Schrödinger equations:

$$\left(\frac{1}{i}(\partial_1 + \partial_2) - E\right)g^{(0)}(x_1, x_2)$$
$$- \frac{t}{2}[\delta(x_1)e^{(0)}(x_2) - e^{(0)}(x_1)\delta(x_2)] = 0,$$
$$\left(\frac{1}{i}\frac{d}{dx} + U\delta(x) + \epsilon_d - E\right)e^{(0)}(x) + 2tg^{(0)}(x, 0) = 0,$$
$$\left(\frac{1}{i}(\partial_1 + \partial_2) - E\right)g^{(1)}(x_1; x_2) + t\delta(x_1)e^{(1)}(x_2) = 0, \qquad (5)$$
$$\left(\frac{1}{i}\frac{d}{dx} + U\delta(x) + \epsilon_d - E\right)e^{(1)}(x) + tg^{(1)}(0; x) = 0,$$
$$\left(\frac{1}{i}(\partial_1 + \partial_2) - E\right)g^{(2)}(x_1, x_2) = 0.$$

We construct the eigenfunctions $g^{(0)}(x_1, x_2)$, $g^{(1)}(x_1; x_2)$, and $g^{(2)}(x_1, x_2)$ by imposing the conditions that, in the region $x_1, x_2 < 0$, they are free-electronic plane waves. The eigenfunction $g^{(0)}(x_1, x_2)$ is discontinuous at $x_1 = 0$ and $x_2 = 0$, $g^{(1)}(x_1; x_2)$ at $x_1 = 0$, and $e^{(0,1)}(x)$ at $x = 0$. The value of the functions at the discontinuous point cannot be determined by Eqs. (5). We then set $g^{(0)}(x, 0) = [g^{(0)}(x, 0+) + g^{(0)}(x, 0-)]/2$ and so on. The function $g^{(2)}(x_1, x_2)$ should be a free-electron eigenfunction. The eigenfunctions with the energy eigenvalue $E = k_1 + k_2$, $(k_1, k_2 \in \mathbb{R})$ are then given as follows:

$$2g^{(0)}(x_1, x_2) = \sum_Q \text{sgn}(Q)[g_{k_1}(x_{Q_1})g_{k_2}(x_{Q_2})$$
$$+ uZ_{12}(x_{Q_1 Q_2})e^{iEx_{Q_2}}\theta(x_{Q_1})],$$
$$e^{(0)}(x) = g_{k_1}(x)e_{k_2} - g_{k_2}(x)e_{k_1} + \frac{u}{it}Z_{12}(-x)e^{iEx},$$
$$g^{(1)}(x_1; x_2) = g_{k_1}(x_1)h_{k_2}(x_2) - uX_1(x_{12})e^{iEx_2}\theta(x_1),$$
$$e^{(1)}(x) = e_{k_1}h_{k_2}(x) + \frac{u}{it}X_1(-x)e^{iEx},$$
$$2h^{(2)}(x_1, x_2) = \sum_Q \text{sgn}(Q)h_{k_1}(x_{Q_1})h_{k_2}(x_{Q_2}), \qquad (6)$$

where $Q = (Q_1, Q_2)$ is a permutation of $(1, 2)$, $x_{ij} = x_i - x_j$, $u = 2U/(2 + iU)$, and

$$Z_{ij}(x) = (k_i - k_j)e_{k_i}e_{k_j}e^{i(\epsilon_d - i\bar{t}^2)x}\theta(-x),$$
$$X_i(x) = \frac{t}{\sqrt{2\pi}}e_{k_i}e^{i(\epsilon_d - i\bar{t}^2)x}\theta(-x). \qquad (7)$$

The set $\{k_1, k_2\}$ in each of the eigenfunctions $g^{(0)}(x_1, x_2)$ and $g^{(1)}(x_1; x_2)$ is not conserved during the scattering; the plane wave with $\{k_1, k_2\}$ is partially scattered to that with $\{\epsilon_d - i\bar{t}^2, E - \epsilon_d + i\bar{t}^2\}$ in $x_1, x_2 > 0$. In this sense, they are not the Bethe eigenfunctions [18,23]. We have found similar eigenfunctions in the Anderson model [24].

The second term of each of the first four eigenfunctions (6) comes from the Coulomb interaction. The imaginary part of the wave numbers, $i\bar{t}^2$, indicates the appearance of *a two-body bound state* $e^{-\bar{t}^2|x_{12}|}$. The interaction is a necessary condition of the appearance of the bound state, and the strength of binding is determined by $\bar{t}$. A similar two-photon bound state has been found in a one-dimensional waveguide coupled to a two-level system [25], where the bound state has been obtained through an "S-matrix" and the eigenstate including the bound state has not been constructed.

We obtain two-electron eigenstates by inserting the eigenfunctions (6) into the form (3); we denote them by $|2, n; k_1, k_2\rangle$, ($n = 0, 1, 2$). We notice that, by exchanging k_1 and k_2 in $|2, 1; k_1, k_2\rangle$, we have another eigenstate $|2, 1; k_2, k_1\rangle$ with the same energy. The four eigenstates satisfy the orthonormal relations in the limit $L \to \infty$:

$$\langle 2, n; k_1, k_2 | 2, n; k_1', k_2' \rangle = \delta(k_1 - k_1')\delta(k_2 - k_2')$$
$$- \delta(k_1 - k_2')\delta(k_2 - k_1'), \quad (n = 0, 2)$$
$$\langle 2, 1; k_1, k_2 | 2, 1; k_1', k_2' \rangle = \delta(k_1 - k_1')\delta(k_2 - k_2'). \quad (8)$$

In principle, we can construct eigenstates for a few electrons. For example, the three-electron eigenfunctions in the sector with $N_o = 0$ are given by

$$3!g^{(0)}(x_1, x_2, x_3) = \sum_P \text{sgn}(P)g_{k_{P_1}}(x_1)g_{k_{P_2}}(x_2)g_{k_{P_3}}(x_3) + \frac{u}{2}\sum_{P,Q}\text{sgn}(PQ)g_{k_{P_1}}(x_{Q_1})Z_{P_2P_3}(x_{Q_2Q_3})e^{i(k_{P_2}+k_{P_3})x_{Q_3}}\theta(x_{Q_2})$$

$$- \frac{u^2}{2i}\sum_{P,Q}\text{sgn}(PQ)h_{k_{P_1}}(x_{Q_2})Z_{P_2P_3}(x_{Q_1Q_3})e^{i(k_{P_2}+k_{P_3})x_{Q_3}}\theta(x_{Q_3Q_2})\theta(x_{Q_2Q_1})\theta(x_{Q_1}),$$

$$2!e^{(0)}(x_1, x_2) = \sum_P \text{sgn}(P)g_{k_{P_1}}(x_1)g_{k_{P_2}}(x_2)e_{k_{P_3}} + \frac{u}{2it}\sum_{P,R}\text{sgn}(PR)g_{k_{P_1}}(x_{R_1})Z_{P_2P_3}(-x_{R_2})e^{i(k_{P_2}+k_{P_3})x_{R_2}}$$

$$+ \frac{u}{2}\sum_{P,R}\text{sgn}(PR)Z_{P_2P_3}(x_{R_1R_2})e^{i(k_{P_2}+k_{P_3})x_{R_2}}e_{k_{P_1}}\theta(x_{R_1}) \quad (9)$$

$$- \frac{u^2}{2t}\sum_{P,R}\text{sgn}(PR)h_{k_{P_1}}(x_{R_1})Z_{P_2P_3}(-x_{R_2})e^{i(k_{P_2}+k_{P_3})x_{R_2}}\theta(x_{R_2R_1})\theta(x_{R_1}).$$

Here, $P = (P_1, P_2, P_3)$ and $Q = (Q_1, Q_2, Q_3)$ are permutations of (1, 2, 3) and $R = (R_1, R_2)$ is that of (1, 2). The third term of the eigenfunction $g^{(0)}(x_1, x_2, x_3)$ indicates a new three-body bound state. The eigenstates in other sectors with $N_o = 1, 2, 3$ are constructed in similar ways.

Now we construct a scattering eigenstate by taking a linear combination of the four two-electron eigenstates as

$$|k_1, k_2\rangle = A|2, 0; k_1, k_2\rangle + B_1|2, 1; k_1, k_2\rangle$$
$$+ B_2|2, 1; k_2, k_1\rangle + C|2, 2; k_1, k_2\rangle. \quad (10)$$

Going from the eigenfunctions in terms of the even and odd parts back to the ones in terms of the leads 1 and 2, we have $f^{(0/2)}(x_1, x_2) = \langle 0|c_{1/2}(x_2)c_{1/2}(x_1)|k_1, k_2\rangle$ and $f^{(1)}(x_1; x_2) = \langle 0|c_2(x_2)c_1(x_1)|k_1, k_2\rangle$. By choosing $A = B_1 = B_2 = C = 1/2$ in Eq. (10), we obtain the scattering state which contains an incoming two-electron plane wave only in the lead 1, i.e., $f^{(1)}(x_1; x_2) = f^{(2)}(x_1, x_2) = 0$ for $x_1, x_2 < 0$, which is depicted in Fig. 1. In the same way, by choosing $A = -B_1 = B_2 = -C = 1/2$, we obtain the scattering state which contains an incoming one-electron plane wave in each lead, i.e., $f^{(0,2)}(x_1, x_2) = 0$ for $x_1, x_2 < 0$. We denote the former or latter scattering state by $|k_1, k_2\rangle_{\pm}$. Each scattering state is shown to be a solution of the LS equation whose incident state is a free-electron plane-wave state, where the incident state means an eigenstate of the Hamiltonian (1) with $\bar{t} = 0$. On the other hand, the scattering state constructed from the Bethe eigenstates [18,23] is interpreted as the solution associated with an incident state

that depends on the parameter U. We remark that the scattering states are also constructed from a superposition of an infinite number of the degenerate Bethe eigenstates [23].

We use the two-electron scattering states to calculate the quantum-mechanical expectation value of the current I in Eq. (2). The expectation value with respect to the scattering state $|k_1, k_2\rangle_{\pm}$, ($k_1 < k_2$) is calculated as

$$\frac{\langle k_1, k_2|I|k_1, k_2\rangle_{\pm}}{\langle k_1, k_2|k_1, k_2\rangle_{\pm}} = \frac{1}{L}[I_0(k_1) \pm I_0(k_2)] + \frac{1}{L^2}I_{\pm}(k_1, k_2),$$

$$I_0(k) = -\frac{t}{2\sqrt{2\pi}}\text{Im}(e_k),$$

$$I_{\pm}(k, h) = \frac{k-h}{t\sqrt{2\pi}}[\text{Re}(e_h)\text{Im}(ue_k^2) \pm \text{Re}(e_k)\text{Im}(ue_h^2)],$$

$$(11)$$

where $L = \delta(0)$ is the length of the system. The first term of order L^{-1} gives the current of noninteracting electrons. The correction term of order L^{-2} containing $I_{\pm}(k_1, k_2)$ is due to the two-body bound state.

We find that, in the limit $L, N \to \infty$, the correction term in Eqs. (11) contributes to the current. We speculate from the result of $N = 2$ that, for general N, similar n-body bound states ($1 < n \leq N$) contribute to the term of order L^{-n} in the expectation value. We assume that the contribution from the two-body bound state is given by the function $I_{\pm}(k, h)$ in Eqs. (11). Let $|k\rangle$ be an N-electron scattering state with an incoming N_{α}-electron plane wave characterized by distinct wave numbers $\{k_i^{\alpha}\}$ in the lead α.

The speculated form of the expectation value is

$$\frac{\langle k|I|k\rangle}{\langle k|k\rangle} = \frac{1}{L}\sum_\alpha \sum_{i=1}^{N_\alpha}(-)^{\alpha+1}I_0(k_i^\alpha) + \frac{1}{L^2}\Bigg(\sum_\alpha \sum_{i<j}(-)^{\alpha+1}I_+(k_i^\alpha, k_j^\alpha)$$

$$+ \sum_{i,j}I_-(k_i^1, k_j^2)\Bigg) + O\Big(\frac{1}{L^3}\Big).$$

We have verified this for $N = 3$. We neglect the terms of order higher than L^{-2} in the expansion [16]. By taking the limit $L, N_\alpha \to \infty$, the sum $\sum_{i=1}^{N_\alpha}$ divided by L should be replaced by the integral on k with the zero-temperature Fermi distribution $f_\alpha(k) = \theta(\mu_\alpha - k)$. For $\mu_{1/2} = \pm V/2$, the average current is then given by

$$\langle I\rangle = \int_{-V/2}^{V/2}dk I_0(k) + \frac{1}{2}\int_{-V/2}^{V/2}dk\int_{-V/2}^{V/2}dh I_+(k, h)$$

$$+ \int_{-\Lambda}^{V/2}dk\int_{-\Lambda}^{-V/2}dh I_-(k, h), \qquad (12)$$

where $-\Lambda$ is the low-energy cutoff. We have

$$\langle I\rangle = \frac{t^2}{4\pi}j_- + \frac{t^2}{8\pi^2}\frac{4U}{4+U^2}\Big(J - \frac{U}{2}J'\Big),$$

$$J = 2(\bar\Lambda + j_+)j_2 + (j_- - j_1)\log\frac{(\epsilon_\Lambda^2 + 1)^2}{(\epsilon_+^2 + 1)(\epsilon_-^2 + 1)},$$

$$J' = 2(\bar\Lambda + j_+)j_1 + \Big(j_2 + \frac{1}{2}\log\frac{\epsilon_+^2 + 1}{\epsilon_-^2 + 1}\Big)\log\frac{(\epsilon_\Lambda^2 + 1)^2}{(\epsilon_+^2 + 1)(\epsilon_-^2 + 1)},$$

$$(13)$$

where $\epsilon_\pm = (\epsilon_d \pm V/2)/\bar{t}^2$, $\epsilon_\Lambda = (\epsilon_d + \Lambda)/\bar{t}^2$, $\bar\Lambda = 2[\Lambda/\bar{t}^2 - \arctan(\epsilon_\Lambda)]$, $j_\pm = \arctan(\epsilon_+) \pm \arctan(\epsilon_-)$, and $j_s = \epsilon_+^{2-s}/(\epsilon_+^2 + 1) - \epsilon_-^{2-s}/(\epsilon_-^2 + 1)$, $(s = 1, 2)$. The current includes higher-order terms in U and, at $\epsilon_d = 0$, agrees with the perturbative result [20] in the first order in U. The linear divergence in $\Lambda \to \infty$ is due to the linearized dispersion relation in Eq. (1). In Fig. 2, we plot the current-voltage characteristics at $\epsilon_d = 0$ by setting $\Lambda = V/2$. The regime of negative differential conductance appears for $U > 2$ [19,21].

In summary, we have studied the nonequilibrium current in an open quantum dot system by using exact scattering
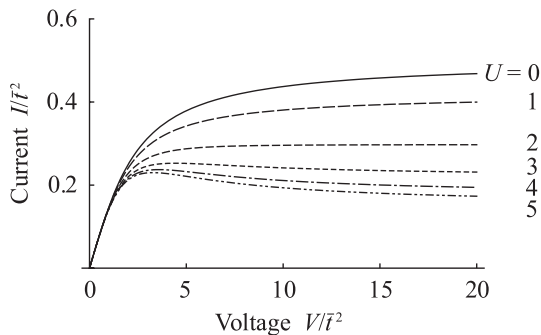
eigenstates. We have found that the interaction effect appears through the many-body bound states. By taking the two-body bound state into account, we have calculated the average current, which agrees with the perturbative result [20] at $\epsilon_d = 0$ and has a behavior similar to the other results [19,21]. In order to compare our result, including the case $\epsilon_d \neq 0$, with the result in Ref. [20] precisely, we need to consider contributions from other many-body bound states in Eq. (13). They would enable us to regularize the logarithmic divergences in Eq. (13) with the RG technique [19,26].

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FIG. 2. A current-voltage characteristics of the average nonequilibrium current for $\epsilon_d = 0$ and $U = 0, 1, 2, 3, 4, 5$.