Exact many-electron scattering states in a parallel-coupled double quantum-dot system

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Abstract. We study a parallel-coupled double quantum-dot (PDQD) system with both intradot and interdot Coulomb interactions by constructing many-electron scattering eigenstates explicitly. We obtain exact solutions of the two-electron scattering eigenstates whose incident states are plane-wave states. We find that, as a result of the Coulomb interactions, many-body bound states appear in the scattering eigenstates. The binding strength of the many-body bound states is shown to depend on the difference of gate energies of the two quantum dots, which is interpreted as an effect of geometrical interference.

1. Introduction
Interference is one of the fundamental properties of quantum systems. Mesoscopic systems have provided a useful ground to study quantum interference phenomena since the pioneering experiments [1–3]. One of the advantages of using mesoscopic samples is the variety of tunable parameters such as the Aharonov-Bohm magnetic flux, the source-drain voltage drop and gate voltages. By using the tunable samples with a multipath connecting two external leads, effects of the geometrical interference have been investigated by the measurement of their electrical conductance. In an experiment [1], it is shown for the Aharonov-Bohm ring with a quantum dot embedded within one of the ring’s arm that electron transport through the quantum dot contains a coherent component.

Recently, the effect of the geometrical interference has been discussed for quantum-dot systems that include the Coulomb interactions yielding the Kondo effect. The Kondo effect has been observed experimentally as a conductance peak near zero bias voltage at low temperatures [4–6] while, theoretically, it is understood by the Anderson model with a single quantum dot [7–12]. In order to study the interplay of the geometrical interference and the Coulomb interactions, the analysis has been extended to parallel-coupled double quantum-dot (PDQD) systems consisting of two quantum dots connected parallel to two external leads [13–19].

In this paper, we study a PDQD system to investigate the effect of the geometrical interference quantum mechanically. We assume both intradot and interdot Coulomb interactions around the quantum dots. We find that the difference of gate energies controlling the energy levels of the two quantum dots plays an important role from the viewpoint of the geometrical interference. We
explicitly construct two-electron scattering eigenstates whose incident states are free-electronic plane waves. We also consider the incident states associated with both triplet and singlet incident states, from which we obtain those associated with non-entangled incident states. The Coulomb interactions produce two-body bound states in the two-electron scattering eigenstates, which is similar to our previous works [20–22]. Furthermore, the binding strength of the two-body bound states depends on the difference of the two gate energies, which is considered as an effect of the geometrical interference.

The exact many-electron scattering eigenstates that we obtain are essential in extending the Landauer formula for electric current to interacting cases. Through an extension of the Landauer formula, we calculated electric current flowing through an open quantum dot described by the interacting resonant-level model [20, 22]. We obtained a universal form of the electric current using a renormalization-group technique and clarified that the negative differential conductance is due to the many-body bound states. Our result is consistent with that of the Green’s function approaches [23, 24] in the first order in the interaction parameter, which shows the validity of our extension of the Landauer formula.

The paper is organized as follows: in Section 2, we introduce the Hamiltonian of a PDQD system with both intradot and interdot Coulomb interactions. In Section 3, we present exact two-electron eigenstates after a brief explanation of one-electron cases. We consider the triplet and singlet two-electron eigenstates. Section 4 is devoted to concluding remarks.

2. Parallel-coupled double quantum-dot system
We study an open quantum-dot system consisting of two quantum dots ($\alpha = 1, 2$) that are connected parallel to two external leads ($\ell = 1, 2$) of noninteracting electrons. The Hamiltonian is expressed as follows:

$$H = \sum_{\ell=1,2} \int dx \left[ c^{\dagger}_{\ell\sigma}(x) \frac{1}{i} \frac{d}{dx} c_{\ell\sigma}(x) + \ell \sum_{\sigma=\uparrow,\downarrow} \epsilon_{\ell\sigma}(0) d_{\ell\sigma} + d_{\ell\sigma}^{\dagger} c_{\ell\sigma}(0) \right] + \sum_{\alpha=1,2} \epsilon_{d\alpha} n_{\alpha\sigma}$$

$$+ \sum_{\alpha=1,2} U_\alpha n_{\alpha\uparrow} n_{\alpha\downarrow} + U' \sum_{\sigma=\uparrow,\downarrow} n_{1\sigma} n_{2\sigma}. \tag{1}$$

Here $c^{\dagger}_{\ell\sigma}(x)$ and $c_{\ell\sigma}(x)$ are the creation and annihilation operators of an electron with spin $\sigma$ on the lead $\ell$, while $d_{\ell\sigma}$ and $d_{\ell\sigma}^{\dagger}$ are those on the quantum dot $\alpha$. We also define the number operator $n_{\alpha\sigma} = d_{\ell\sigma}^{\dagger} d_{\ell\sigma}$ for electrons on the quantum dot $\alpha$. We assume that all the transfer integrals between the leads and the dots are equal to each other and denote them by $\ell = t/\sqrt{2}$. We denote the energy level on the quantum dot $\alpha$ by $\epsilon_{d\alpha}$ and call it the gate energy. We consider both intradot and interdot Coulomb interactions that are expressed by the parameters $U_\alpha(>0)$ and $U'(>0)$, respectively. It should be noted that the dispersion relation in each lead is linearized, which is valid in the vicinity of the Fermi energy under the assumption that the parameters $|t|, |\epsilon_{d\alpha}|, U_\alpha$ and $U'$ are small compared with the Fermi energy.

We explicitly construct scattering eigenstates whose incident states are free-electronic plane-wave states. Such scattering eigenstates are essential in extending the Landauer formula to interacting cases [20, 22]. From the viewpoint of geometrical interference, it is important to find out how the scattering eigenstates depend on the difference $\Delta \epsilon_{d} = \epsilon_{d1} - \epsilon_{d2}$ of the two gate energies. Hence we mainly consider the case $\epsilon_{d1} \neq \epsilon_{d2}$. We emphasize that the Bethe-ansatz eigenstates were previously obtained for the PDQD system only under the following two types of parameter conditions: i) $U_1 + 2\epsilon_{d1} = U_2 + 2\epsilon_{d2}$ and $U' = 0$ corresponding to well-separated two quantum dots; ii) $U_1 = U_2 = U'$ and $\epsilon_{d1} = \epsilon_{d2}$ corresponding to a quantum dot with degenerate two energy levels [18, 19]. In order to tune the gate-energy difference $\Delta \epsilon_{d}$ independently of the Coulomb interactions, however, we need the scattering eigenstates irrespective of such parameter
conditions. Indeed our scattering eigenstates are completely different from the Bethe-ansatz eigenstates [18, 19].

For the two-lead system, it is convenient to adopt the picture of even and odd leads through the transformation $c_{0\sigma}(x) = (c_{1\sigma}(x) + c_{2\sigma}(x))/\sqrt{2}$ and $c_{o\sigma}(x) = (c_{1\sigma}(x) - c_{2\sigma}(x))/\sqrt{2}$. Then the Hamiltonian becomes the sum of the even part $H_e$ and the odd part $H_o$ given by

$$H_e = \sum_\sigma \int dx \frac{d}{dx} c_{0\sigma}^\dagger(x) \frac{1}{i} \frac{d}{dx} c_{0\sigma}(x) + t \sum_{\alpha,\sigma} (c_{0\sigma}^\dagger(0) d_{\alpha\sigma} + d_{\alpha\sigma}^\dagger c_{0\sigma}(0)) + \sum_{\alpha,\sigma} \epsilon_{\alpha\sigma} n_{\alpha\sigma}$$

$$+ \sum_{\alpha} U_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} + U' \sum_{\sigma,\tau} n_{1\sigma} n_{2\tau},$$

$$H_o = \sum_\sigma \int dx \frac{d}{dx} c_{o\sigma}^\dagger(x) \frac{1}{i} \frac{d}{dx} c_{o\sigma}(x).$$

(2)

The odd part $H_o$ is the Hamiltonian of free electrons and is decoupled from the even part $H_e$. Let us define the number operators $N_{o\sigma} = \int dx c_{o\sigma}^\dagger(x) c_{o\sigma}(x)$ and $N_{e\sigma} = \int dx c_{e\sigma}^\dagger(x) c_{e\sigma}(x)$ for electrons on the leads. Then the set $(N_{e\uparrow} + n_{1\uparrow} + n_{2\uparrow}, N_{e\downarrow} + n_{1\downarrow} + n_{2\downarrow}, N_{o\uparrow}, N_{o\downarrow})$ of the number operators is a set of good quantum numbers and labels $N$-electron eigenstates. In order to obtain the scattering eigenstate whose incident state is a free-electronic plane-wave state in the picture of the leads 1 and 2, we need to take a linear combination of the eigenstates of all sectors [20–22, 25]. In what follows, we focus on the even part for explanatory purposes.

3. Many-electron scattering eigenstates

3.1. One-electron cases

Before discussing the two-electron cases, it is instructive to consider one-electron eigenstates. The general form of the one-electron states with spin $\sigma$ is given by

$$|1, \sigma\rangle = \left(\int dx g(x)c_{0\sigma}^\dagger(x) + \sum_\alpha e_{\alpha} d_{\alpha\sigma}^\dagger\right)|0\rangle.$$  

(3)

Here $|0\rangle$ is the vacuum state while $g(x)$ and $e_{\alpha}$ are wave functions to be determined. The eigenvalue problem $H|1, \sigma\rangle = E|1, \sigma\rangle$ is equivalent to the following Schrödinger equations:

$$\left(\frac{1}{i} \frac{d}{dx} - E\right)g(x) + i\delta(x) \sum_\alpha e_{\alpha} = 0, \quad ig(0) + (\epsilon_{\alpha\sigma} - E)e_{\alpha} = 0.$$  

(4)

The eigenfunction $g(x)$ is a plane wave in both the regions $x < 0$ and $0 < x$. By integrating the first equation from $x = 0$ to $0+$, we find that $g(x)$ is discontinuous at $x = 0$. Hence we assume from physical intuition that the value of $g(x)$ at $x = 0$ is determined by $g(0) = (g(0+) + g(0-))/2$ [20–22, 26]. By solving the Schrödinger equations under the assumption, the eigenfunctions with energy eigenvalue $E = k$ are given by

$$g_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} (\theta(-x) + e^{i\delta_k} \theta(x)), \quad e^{i\delta_k} = \frac{1 - \sum_\alpha \frac{i t^2}{4(k-\epsilon_{\alpha\sigma})}}{1 + \sum_\alpha \frac{i t^2}{4(k-\epsilon_{\alpha\sigma})}},$$

$$e_{\alpha, k} = \frac{1}{2\sqrt{\pi}} \frac{t}{k-\epsilon_{\alpha\sigma}} \left[1 + \sum_\beta \frac{i t^2}{3(k-\epsilon_{\alpha\beta})}\right], \quad (\alpha = 1, 2).$$

(5)

Here we remark that, in the case $\epsilon_{d1} \neq \epsilon_{d2}$, the transmission probability of an electron from the lead 1 to the lead 2 has two peaks at $k = \epsilon_{d1}, \epsilon_{d2}$ but is not a superposition of Lorentzians; this is considered to be an effect of the geometrical interference.
3.2. Two-electron cases (triplet state)

We next consider the triplet eigenstates of two electrons. The general form of the two-electron triplet states is given by

\[ |2, T\rangle = \left( \int dx_1 dx_2 g(x_1, x_2) c_{e_1}^\dagger(x_1) c_{e_2}^\dagger(x_2) + \sum_\alpha \int dx e_\alpha(x)(c_{e_1}^\dagger(x)d_{\alpha_1}^\dagger + c_{e_2}^\dagger(x)d_{\alpha_2}^\dagger) + \sum_{\alpha \neq \beta} f_{\alpha\beta}d_{\alpha_1}^\dagger d_{\beta_1}^\dagger \right) |0\rangle, \tag{6} \]

where \( g(x_1, x_2) \) is antisymmetric with respect to the exchange of variables \( x_1 \) and \( x_2 \) and \( f_{\alpha\beta} \) is also antisymmetric with respect to the exchange of indices \( \alpha \) and \( \beta \). The corresponding Schrödinger equations are given as follows:

\[ \left( \frac{1}{i} \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) - E \right) g(x_1, x_2) - i \sum_\alpha \left( \delta(x_1) e_\alpha(x_2) - e_\alpha(x_1) \delta(x_2) \right) = 0, \]

\[ \left( \frac{1}{i} \frac{d}{dx} + e_\alpha - E \right) e_\alpha(x) + \bar{t} g(x, 0) - \bar{t} \delta(x) \sum_{\beta \neq \alpha} f_{\alpha\beta} = 0, \quad (\alpha = 1, 2), \tag{7} \]

where \( \bar{t} = (\epsilon_{d1} + \epsilon_{d2})/2 \). We find that the eigenfunction \( g(x_1, x_2) \) is discontinuous at \( x_1 = 0 \) and \( x_2 = 0 \) and \( e_\alpha(x) \) is discontinuous at \( x = 0 \). In a way similar to the one-electron case, we assume that the values of the eigenfunctions at the discontinuous points are determined by \( g(x, 0) = -g(0, x) = (g(0, 0) + g(x, 0))/2 \) and \( e_\alpha(0) = (e_\alpha(0) + e_\alpha(0))/2 \). The strength of the intradot Coulomb interactions \( U_\alpha \) does not appear in the Schrödinger equations (7) since the doubly occupied state on a quantum dot is the singlet state, which we consider in the next subsection. It should be remarked that, in the case \( \epsilon_{d1} = \epsilon_{d2} \) of equal gate energies, the Schrödinger equations for the pair \{\( e_1(x) - e_2(x) \), \( f_{12} \)\} are decoupled from those for the pair \{\( g(x_1, x_2) \), \( e_1(x) + e_2(x) \)\}. Hence the case is equivalent to that with a single quantum dot.

Our purpose is to construct eigenstates satisfying a scattering boundary condition that the incident state is a free-electronic plane wave,

\[ g(x_1, x_2) = \frac{1}{2\sqrt{2\pi}} \sum_Q \text{sgn}(Q) e^{i(k_1 x_{Q_1} + k_2 x_{Q_2})} \quad \text{for} \; x_1, x_2 < 0. \tag{8} \]

Here the sum on \( Q \) runs over permutations of \((1, 2)\), that is, \((Q_1, Q_2) = (1, 2), (2, 1)\), and \( \text{sgn}(1, 2) = -\text{sgn}(2, 1) = 1 \). Such scattering states are appropriate for the situation that electrons are equilibrated to the Fermi degenerate state in a reservoir at the end of each lead before being emitted towards the quantum dots. This is the essential difference from the Bethe-ansatz eigenstates \([18, 19]\).

We can solve the Schrödinger equations (7) explicitly in a way similar to our previous papers \([20–22]\). As a result, the eigenfunctions with energy eigenvalue \( E = k_1 + k_2 \) are given as follows:

\[ \sqrt{2} g_{k_1 k_2}(x_1, x_2) = \sum_Q \text{sgn}(Q) \left( g_{k_1}(x_{Q_1}) g_{k_2}(x_{Q_2}) - i \Delta \epsilon_d \sum_{s = \pm} Z_{k_1 k_2}(x_{Q_1} Q_2) e^{iE_{Q_2}x_2} \theta(x_{Q_1}) \right), \]

\[ \sqrt{2} e_{1, k_1 k_2}(x) = g_{k_1}(x) e_{1, k_2} - g_{k_2}(x) e_{1, k_1} + \sqrt{2} \sum_{s = \pm} \left( \lambda_s - \frac{t^2}{4} \right) Z_{k_1 k_2}^s(-x) e^{iE_{Q_1}}, \]

\[ \sqrt{2} e_{2, k_1 k_2}(x) = g_{k_1}(x) e_{2, k_2} - g_{k_2}(x) e_{2, k_1} + \sqrt{2} \sum_{s = \pm} \left( \lambda_s + \frac{t^2}{4} \right) Z_{k_1 k_2}^s(-x) e^{iE_{Q_1}}, \]

\[ \sqrt{2} f_{12, k_1 k_2} = e_{1, k_1} e_{2, k_2} - e_{1, k_2} e_{2, k_1} - \frac{2n}{i\hbar} Z_{k_1 k_2}^s. \tag{9} \]
Here \( g_k(x) \) and \( e_{\alpha,k} \) are the one-electron eigenfunctions presented in Eqs. (5) and we used the notation \( \lambda_{\pm} = (i\Delta\epsilon_d \pm \eta)/2 \), \( \eta = \sqrt{t^4/4 - \Delta\epsilon_d^2} \) and

\[
Z_{k_1k_2} = -\frac{it}{2\eta} (e_{1,k_1}e_{2,k_2} - e_{1,k_2}e_{2,k_1}) \frac{U'}{k_1+k_2-2\epsilon_d-U'+i\frac{U'}{2}},
\]

\[
Z_{k_1k_2}^\pm(x) = \pm Z_{k_1k_2} e^{i(\epsilon_d-i\frac{t^2}{4\eta})x} \theta(-x).
\]

We note that the eigenfunctions (9) are regular in the limit \( \eta \to 0 \) although \( Z_{k_1k_2} \) includes the factor \( 1/\eta \).

For \( \epsilon_{d_1} \neq \epsilon_{d_2} \), the terms with \( Z_{k_1k_2}^\pm(x) \) in the eigenfunctions are interpreted as two-body bound states since they exponentially decay as \( e^{-|x|/\xi_{\pm}} \), the binding strength being \( 1/\xi_{\pm} = t^2/4 \mp \text{Re}(\eta/2) \). Thus we have two types of the binding strength of the two-body bound states that depend on the gate-energy difference \( \Delta\epsilon_d \) of the two quantum dots. This is an effect of the geometrical interference. The behavior of the binding strength \( 1/\xi \) is drawn in Fig. 1. We find that, in the case \( \epsilon_{d_1} = \epsilon_{d_2} \), the terms including the factor \( Z_{k_1k_2} \) vanish and hence the two-electron eigenfunctions become free electronic.

![Figure 1. Binding strength \( 1/\xi_{\pm} \) of the two-body bound states.](image)

### 3.3. Two-electron cases (singlet state)

Third, we turn to the singlet eigenstates of two electrons. The general form of the two-electron singlet states is given by

\[
|2,S\rangle = \left( \int dx_1dx_2 g(x_1,x_2) c_{e_1}^\dagger(x_1)c_{e_2}^\dagger(x_2) + \sum_{\alpha} \int dx e_{\alpha}(x)(c_{e_1}^\dagger(x)d_{\alpha_1}^\dagger - c_{e_1}^\dagger(x)d_{\alpha_1}^\dagger) + \sum_{\alpha,\beta} f_{\alpha\beta}d_{\alpha_1}^\dagger d_{\beta_1}^\dagger \right) |0\rangle,
\]

where \( g(x_1,x_2) \) is now symmetric with respect to the exchange of variables \( x_1 \) and \( x_2 \) and \( f_{\alpha\beta} \) is also symmetric with respect to the exchange of indices \( \alpha \) and \( \beta \). The Schrödinger equations
the eigenfunctions are given as follows:

\[
\begin{align*}
\left( \frac{1}{i} \left( \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \right) - E \right) g(x_1, x_2) + i \sum_{\alpha} \left( \delta(x_1) e_\alpha(x_2) + e_\alpha(x_1) \delta(x_2) \right) &= 0, \\
\left( \frac{1}{i} \frac{d}{dx} + \epsilon_{d\alpha} - E \right) e_\alpha(x) + i g(x, 0) + i \delta(x) \sum_{\beta} f_{\beta\alpha} &= 0, \quad (\alpha = 1, 2), \\
(\epsilon_{d\alpha} + \epsilon_{d\beta} + U_{\alpha\beta} - E) f_{\alpha\beta} + i(e_{\alpha}(0) + e_{\beta}(0)) &= 0, \quad (\alpha, \beta = 1, 2),
\end{align*}
\]

where \( U_{\alpha\alpha} = U_\alpha \) and \( U_{12} = U_{21} = U' \).

By solving these, we obtain the two-electron eigenfunctions with energy \( E = k_1 + k_2 \):

\[
\begin{align*}
\sqrt{2} g_{k_1k_2}(x_1, x_2) &= \sum_Q \left( g_{k_1}(x_Q) g_{k_2}(x_{Q'}) - i \sum_{s=\pm} \left( 1 - \frac{4\lambda_s}{t^2} \right) C_{k_1k_2}^s(x_Q, Q') e^{iE_Qx-Q'} \theta(x_Q) \right), \\
\sqrt{2} e_{1k_1k_2}(x) &= g_{k_1}(x) e_{1k_2} + g_{k_2}(x) e_{1k_1} + \sqrt{2} \sum_{s=\pm} C_{k_1k_2}^s(-x) e^{iE_x}, \\
\sqrt{2} e_{2k_1k_2}(x) &= g_{k_1}(x) e_{2k_2} + g_{k_2}(x) e_{2k_1} - \sqrt{2} \sum_{s=\pm} \frac{4\lambda_s}{t^2} C_{k_1k_2}^s(-x) e^{iE_x}.
\end{align*}
\]

Here \( g_k(x) \) and \( e_{\alpha,k} \) are the one-electron eigenfunctions presented in Eqs. (5) and \((Q_1, Q_2) = (1, 2), (2, 1)\). We also used the notation

\[
C_{k_1k_2}^\pm(x) = C_{k_1k_2}^\pm e^{i(\epsilon_\alpha - i\frac{e^2}{4}x^2)} \theta(-x),
\]

where the coefficients \( C_{k_1k_2}^\pm \) on the right-hand side are determined by the coupled equations

\[
\begin{align*}
C_{k_1k_2}^+ + C_{k_1k_2}^- &= \frac{((1 - A_1)(1 + A_2) - (A_1 + A_2)B)E_1 - 2BE_2}{(1 + A_1)(1 + A_2) + (2 + A_1 + A_2)B} - F_1, \\
- \frac{4\lambda_+}{t^2} C_{k_1k_2}^+ - \frac{4\lambda_-}{t^2} C_{k_1k_2}^- &= \frac{((1 + A_1)(1 - A_2) - (A_1 + A_2)B)E_2 - 2BE_1}{(1 + A_1)(1 + A_2) + (2 + A_1 + A_2)B} - F_2
\end{align*}
\]

with the coefficients

\[
A_\alpha = \frac{i^2}{4} \left( \frac{1}{E - 2\epsilon_{d\alpha} - U_\alpha} \right), \quad B = \frac{i^2}{4} \left( \frac{1}{E - 2\epsilon_d - U'} \right), \\
E_\alpha = \frac{1}{2\sqrt{\pi}} (e_{\alpha,k_1} e_{\delta k_2} + e_{\alpha,k_2} e_{\delta k_1}), \quad F_\alpha = \frac{1}{2\sqrt{\pi}} (e_{\alpha,k_1} e_{\delta k_2} + e_{\alpha,k_2} e_{\delta k_1}).
\]

The eigenfunctions \( f_{\alpha\beta,k_1k_2} \) are readily obtained from the third equation of the Schrödinger equations (12). Similarly to the triplet case, two-body bound states that exponentially decay as \( e^{-|x|/\xi} \) appear in the terms with \( C_{k_1k_2}^\pm(x) \). The two types of the binding strength also behave as Fig. 1. For \( \epsilon_{d1} = \epsilon_{d2} \), the two-body bound states with the binding strength \( \xi^- \) survive, which is different from the triplet case.

4. Concluding remarks

We have studied a parallel-coupled double quantum-dot (PDQD) system with both intradot and interdot Coulomb interactions, constructing the exact solution of many-electron scattering eigenstates. We have obtained the two-electron scattering eigenstates whose incident states are triplet or singlet plane-wave states. The two-electron scattering eigenstates whose incident
states are non-entangled states are readily constructed by taking the linear combination $|2, \uparrow\downarrow_i\rangle = (|2, T_i\rangle + |2, S_i\rangle)/\sqrt{2}$. The Coulomb interactions produce two-body bound states in the two-electron scattering eigenstates. The binding strength of the two-body bound states depends on the gate-energy difference of the two quantum dots, which is interpreted as an effect of the geometrical interference. Our exact solutions play an essential role in the calculation of physical quantities such as the electric current for the system under a finite bias voltage, which will be reported elsewhere.

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