Nonequilibrium charge transport in an interacting open system: two-particle resonance and current asymmetry

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We use Lippman-Schwinger scattering theory to study nonequilibrium electron transport through an interacting open quantum dot. The two-particle current is evaluated exactly while we use perturbation theory to calculate the current when the leads are Fermi liquids at different chemical potentials. We find an interesting two-particle resonance induced by the interaction and obtain criteria to observe it when a small bias is applied across the dot. Finally, for a system without spatial inversion symmetry we find that the two-particle current is quite different depending on whether the electrons are incident from the left lead or the right lead.

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We study nonequilibrium steady state charge transport in an open quantum system in the presence of a repulsive Coulomb interaction in a localized region. One of the simplest realizations of our model is a quantum dot (QD) connected to two noninteracting leads at different chemical potentials. In the last two decades, there have been several theoretical and experimental studies of electron transport through a QD where electrons interact with each other only in the dot region. The presence of a chemical potential difference across the QD leads to nonequilibrium dynamics which opens up the possibility of exploring the interplay of nonequilibrium physics and interactions in this model. In this spirit, we will study two interesting phenomena in our model system, namely, two-particle resonance and current asymmetry.

The phenomenon of resonances is often realized in open quantum systems. Resonances are signatures of quasi-stationary states with a long life-time which eventually decay into the continuum coupled to them. There are many examples of resonances in different branches of physics, especially atomic and nuclear physics. Systems with or without interactions between the constituents like electrons, photons or phonons can exhibit resonances; for example, the symmetric Breit-Wigner or the asymmetric Fano resonances can occur in noninteracting systems, while the Kondo resonance occurs in correlated electronic systems. In a recent work, strongly correlated two-photon transport in a one-dimensional system was studied. In this paper, we study a two-electron resonance which occurs due to the interactions between electrons; this was recently observed in Ref. [9]. This resonance is clearly visible in the two-electron current. We demonstrate that it survives in the thermodynamic limit when one takes the leads to be Fermi seas of electrons. Our two-electron resonance can occur at small bias and when the one-particle current is small; it differs from the pair-tunneling resonance studied in Ref. [23] which requires a sufficiently large bias between the leads and coexists with one-particle transport.

A rectification of the current can be achieved in a system without spatial inversion symmetry. There are many theoretical and experimental studies of the diode effect in electron transport using the nonlinear regime of transport in asymmetric nanostructures. Coulomb blockade in triple QD or Pauli exclusion in coupled double QD. Current rectification has also been realized in thermal and optical systems. In our model, we find an asymmetry in the two-particle current when either the on-site energies in the dot or the couplings of the dot with the leads break left-right symmetry.

Recently we developed a technique employing the Lippman-Schwinger scattering theory to study nonequilibrium transport in an open system with electron-electron interactions in a localized region. In this paper we extend that method to investigate quantum transport in more realistic models. Compared to our previous study, here we incorporate on-site energy in the dot as well as arbitrary tunnelings between the dot and the leads. In experiments, the on-site energy in the dot is realized through a plunger gate attached to the dot while quantum point contacts between the dot and the leads control the tunneling strength. We show how the two-electron scattering states and the corresponding current can be evaluated for an arbitrary strength of the Coulomb interaction. We then use a two-particle scattering approximation to find the current in the presence of Fermi seas in the leads.

We study a model of a quantum dot coupled to leads on its left and right sides; we first consider spinless electrons for simplicity. The model is described by a tight-binding Hamiltonian; the dot consists of two sites (0, 1) with an interaction $U$ if both sites are occupied by electrons. The
Hamiltonian is

\[ H = H_{LR} + H_D + V, \]

\[ H_{LR} = - \sum_{x=-\infty}^{\infty} (c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x), \]

\[ H_D = \varepsilon_0 n_0 + \varepsilon_1 n_1 - (c_1^\dagger c_1 + c_{1}^\dagger c_0) \]
\[ - \gamma_0 (c_{-1}^\dagger c_0 + c_0^\dagger c_{-1}) - \gamma_1 (c_1^\dagger c_2 + c_2^\dagger c_1), \]

\[ V = U n_0 n_1, \]

where \( \hat{n}_x = c_x^\dagger c_x \) is the number operator at site \( x \), and \( \sum^\prime \) means summation over all integers omitting \( x = -1, 0, 1 \).

Note that we have set the hopping \( \gamma_{x,x+1} = 1 \) for all \( x \) except \( x = -1 \) and 1 where it takes the values \( \gamma_0 \) and \( \gamma_1 \).

The energy of a single particle with wave number \( k \) is given by \( E_k = -2 \cos k \), where \( -\pi < k < \pi \). The wave function \( \phi_k(x) \) for a particle incident on the dot from the left or from the right can be found in terms of the dot parameters \( \varepsilon_1 \) and \( \gamma_1 \). The explicit expressions for these wave functions and the reflection and transmission amplitudes are as follows. For a particle incident from the left (with \( 0 < k < \pi \)), we have

\[ \phi_k(l) = e^{ikl} + rk e^{-ikl} \] for \( l \leq 1, \]
\[ \phi_k(l) = (1 + rk)/\gamma_0 \] for \( l = 0, \)
\[ \phi_k(l) = tk/e^{ikl}/\gamma_1 \] for \( l = 1, \]
\[ \phi_k(l) = tk e^{ikl} \] for \( l \geq 2, \]

\[ t_k = \frac{-2\gamma_0 \gamma_1 e^{-ik} \sin k}{(e_1 - E_k - \gamma_1^2 e^{ik})(e_0 - E_k - \gamma_0^2 e^{-ik}) - 1}, \]

\[ r_k = \frac{1}{(e_1 - E_k - \gamma_1^2 e^{ik})(e_0 - E_k - \gamma_0^2 e^{-ik}) - 1}. \]

For a particle incident from the right (with \( -\pi < k < 0 \)), we have

\[ \phi_k(r) = tk e^{ikl} \] for \( l \leq 1, \]
\[ \phi_k(r) = tk/\gamma_0 \] for \( l = 0, \)
\[ \phi_k(r) = tk e^{ikl}/\gamma_1 \] for \( l = 1, \]
\[ \phi_k(r) = tk e^{ikl} \] for \( l \geq 2, \]

\[ t_k = \frac{2\gamma_0 \gamma_1 e^{-ik} \sin k}{(e_1 - E_k - \gamma_1^2 e^{ik})(e_0 - E_k - \gamma_0^2 e^{-ik}) - 1}, \]

\[ r_k = \frac{e^{2ik}(1 - (e_1 - E_k - \gamma_1^2 e^{ik})(e_0 - E_k - \gamma_0^2 e^{-ik}))}{(e_1 - E_k - \gamma_1^2 e^{ik})(e_0 - E_k - \gamma_0^2 e^{-ik}) - 1}. \]

We note that the transmission probability \( |t_k|^2 \) is the same for wave numbers \( k \) and \(-k\); we will see below that the two-particle current will generally not have this symmetry as a result of the interaction. For a weakly coupled dot with \( \gamma_1 \rightarrow 0 \), there is a one-particle resonance in the transmission if the energy of the incoming particle is given by one of two special values,

\[ E_{1,\pm} = \frac{1}{2} \left[ e_0 + e_1 \pm \sqrt{(e_0 - e_1)^2 + 4} \right], \]

provided that the energy lies within the range \([-2, 2] \). If the energy lies outside the range \([-2, 2] \), it corresponds to a bound state rather than a transmission resonance. Eq. (4) corresponds to the one-particle eigenvalues of the two-site Hamiltonian \( \varepsilon_0 n_0 + \varepsilon_1 n_1 - (c_1^\dagger c_1 + c_{1}^\dagger c_0) \).

The two-particle scattering states can be found exactly in this model [10]. If \( H_0 = H_{LR} + H_D \) denotes the noninteracting Hamiltonian, and \( E_k \) and \( \phi_k(x) \) are the one-particle energies and wave functions, the noninteracting two-particle energies and wave functions are given by \( E_k = E_k + E_{2k} \) and \( \phi_k(x) = \phi_k(x_1)\phi_k(x_2) - \phi_k(x_2)\phi_k(x_1) \), where \( k = (k_1, k_2) \) and \( x = (x_1, x_2) \). A scattering eigenstate of the total Hamiltonian \( H = H_0 + V \) is then given by the Lippman-Schwinger equation \( |\psi\rangle = |\phi\rangle + G_0^+ (E)|\psi\rangle \), where \( G_0^+ (E) = 1/(E - H_0 + i\epsilon) \). In the position basis \( |x\rangle \), we obtain \( \psi_k(x) = \phi_k(x) + UK_{E_k}(x)\psi_k(0) \), where \( 0 \equiv (0, 1), K_{E_k}(x) = \langle x|G_0^+ (E_k)|0\rangle \) has the explicit form

\[ K_{E_k}(x) = \frac{1}{2} \pi \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} dq dq_2 \phi_q(0)\phi_q^\dagger(0) \]
\[ \times \frac{\phi_{q_1}(x_1)\phi_{q_1}(0)}{E_{k} - E_{q} + i\epsilon} - \frac{\phi_{q_1}(x_1)\phi_{q_2}(0)}{E_{k} - E_{q} + i\epsilon}. \]

Finally, \( J_S = 2 \text{Im} \langle S_k|c_{x_2}^\dagger c_{x_2}|S_k\rangle \) and

\[ \langle S_k|c_{x_2}^\dagger c_{x_2}|S_k\rangle = \frac{|\phi_k(0)|^2}{1/[U - K_{E_k}(0)]^2} \int_{-\pi}^{\pi} dq I_0(q) I_1^* (q), \]

where \( I_s(q) = \int_{-\pi}^{\pi} dq \phi_q(0) \phi_q(x + s)/2\pi \) for \( s = 0, 1 \).

For a small interaction strength \( U \), we see that \( J_C \) and \( J_S \) are generally of order \( U \) and \( U^2 \) respectively. On the
other hand, they have non-zero and finite limits when $U \to \infty$. We can use Eqs. (7-8) to compute $(j_2)$ at any convenient value of $x$. (The extra factor of $N$ that $j_1$ has with respect to $j_2$ and $j_S$ will disappear when we consider the thermodynamic limit below).

We have used Eqs. (7-8) to numerically compute the correction to the current $\delta j(k_1,k_2) \equiv j_c + j_s$ caused by the interaction. [In the numerical calculations, the integrals were approximated by summations with a small grid size $dq$ and several small values of $\epsilon$ satisfying $dq \ll \epsilon \ll 1$. The results were then linearly extrapolated to the limit $\epsilon \to 0$.] We discover two interesting phenomena: (i) First, we find that $\delta j(k_1,k_2)$ as a function of $U$ has peaks at certain values of the energies of the two incident states. We will call this an interaction induced two-particle resonance; this was recently noticed in Ref. [9]. To understand this, let us first set the dot-lead couplings $\gamma_i = 0$. In that case a state in which sites 0 and 1 are occupied by one particle each is an eigenstate of $H_0$ with energy $e_0 + e_1$, and of $H$ with energy $e_0 + e_1 + U$. Then $K_{E_k}(0) = \langle 0 | 1/(E_k - H_0 + i\epsilon) | 0 \rangle$ will be purely real and equal to $1/(E_k - e_0 - e_1)$ if $E_k \neq e_0 + e_1$. We now turn on small values of the $\gamma_i$, and consider two particles coming from the leads with a total energy $E_k = E_{k_1} + E_{k_2}$, where $E_{k_1}$ are not at the one-particle resonance energies $E_{1\pm}$, so that $j_1$ is close to 0. We expect that if $E_k \neq e_0 + e_1$, the real and imaginary parts of $K_{E_k}(0)$ will remain close to $1/(E_k - e_0 - e_1)$ and 0 respectively. It is now clear from the pre-factors in the expressions in Eqs. (7-8) that $\delta j(k_1,k_2)$ will show a peak, as a function of $U$, at $1/U - K_{E_k}(0) = 0$, i.e., at $E_k = E_{2r}$, where the two-particle resonance energy is given by

$$E_{2r} = e_0 + e_1 + U. \quad (9)$$

Fig. 1 illustrates the effects of two-particle resonance. The main plot shows a peak in $\delta j(k_1,k_2)$ at $U \approx 1.45$ compared to $U = 1.48$ expected from Eq. (9). The deviation is presumably due to the small but finite values of $\gamma_0$ and $\gamma_1$. The right inset shows what happens when one of the incident energies is at a one-particle resonance; then the two-particle resonance, occurring at $U = 2.6$ for $(k_1,k_2) = (1.772,2.1)$ and $U = 0.6$ for $(k_1,k_2) = (0.64,2.1)$, produces a rapid variation in the current with $U$ due to the denominator $1/U - K_{E_k}(0)$ in Eq. (7) going through zero. The left inset of Fig. 1 shows what happens when both the incident energies correspond to one-particle resonances; the interaction causes backscattering and suppresses the one-particle resonance by a large amount because the pre-factor of $\phi_k(0)$ in Eqs. (7-8) is large for one-particle resonances.

(ii) Secondly, we find that $\delta j(k_1,k_2) \neq -\delta j(-k_1,-k_2)$ if the system is not invariant under the parity transformation $x \leftrightarrow 1-x$, i.e., if either $e_0 \neq e_1$ or $\gamma_0 \neq \gamma_1$.

The reason for current asymmetry is the re-distribution of the electrons' momentum after scattering from the dot along with the absence of spatial inversion symmetry in the model. It can be understood quantitatively if $\gamma_0$ and $\gamma_1$ are both small but differ greatly in magnitude, and if $k_1, k_2$ have the same sign. We see from Eqs. (7-8) that the strength of the interaction depends on the probability $|\phi_k(0)|^2$ of finding the two particles at sites 0 and 1. If both the particles come from the left (right) lead, their joint amplitude of reaching sites 0 and 1 is proportional to $\gamma_0^2 (\gamma_1^2)$ if $k_1, k_2 > 0$ ($<0$); hence $\delta j$ will be quite different in the two cases if $\gamma_0$ and $\gamma_1$ have very different values. For instance, if $e_0 = -0.8$, $e_1 = -0.3$, $\gamma_0 = 0.1$, $\gamma_1 = 0.3$, $U = 1$, $k_1 = 1$, and $k_2 = 2$, we find numerically that $\delta j(k_1,k_2) = 0.031$ and $\delta j(-k_1,-k_2) = -1.014$. We note that the ratio $|\delta j(-k_1,-k_2)/\delta j(k_1,k_2)| \approx 33$ which is of the same order of magnitude as $\gamma_1^4/\gamma_0^4 \approx 81$.

We now examine whether the two-particle resonance remains visible when we consider a many-electron system. Let us compute the current when the left (right) leads are at zero temperature and chemical potentials $\mu_L (\mu_R)$. This requires us to find $N$-particle scattering states and then take the limit $N \to \infty$. It is difficult to find such states exactly in our model. We therefore make the approximation of considering only two-particle scattering [10]; this is justified if either the density is so low that three-electron scattering can be ignored [29], or if $U \ll 2\pi \sin k_F/k_F$. The latter condition arises as follows. In the simple case with $e_0 = e_1 = 0$ and $\gamma_0 = \gamma_1 = 1$, the interaction $V$ in Eq. (11) can be written in a Hartree-Fock approximation as $U(|\langle n_0|n_1 + n_1|n_0\rangle)$, where the mean density is related to the Fermi momentum as $\langle n_1 \rangle = k_F/\pi$. At the Fermi momentum $k_F$, the reflection probability for this one-
particle problem is much less than 1 if $U \langle n_i \rangle$ is much less than the Fermi velocity $2\sin k_F$. We thus require that $U \ll 2\pi \sin k_F/k_F$. Within the two-particle approximation, we write $|\psi_{i\kappa\nu}\rangle = |\phi_{i\kappa\nu}\rangle + |S_{i\kappa\nu}\rangle$, where the amplitude of scattering from a wave vector $k_N = \{k_1, k_2, \ldots, k_N\}$ to a wave vector $q_N = \{q_1, q_2, \ldots, q_N\}$ is given by

$$
\langle q_N | S_{i\kappa\nu} \rangle = \sum_{q_1, q_2} (-1)^{P + P'} \langle q_2 | S_{i\kappa\nu} \rangle \langle q_{N-2} | \Phi_{N-2} \rangle,
$$

$$
\langle q_2 | S_{i\kappa\nu} \rangle = \frac{\phi_{q_2}(0)|\phi_{q_2}(0)\rangle}{(1/U - K_{q_2}(0))(E_{q_2} - E_{q_2} + i\epsilon)}
$$

where $q_2$ ($k_2$) denotes a pair of momenta chosen from the set $q_N$ ($k_N$), $q_{N-2}$ ($k_{N-2}$) denotes the remaining $N - 2$ momenta, and $P$ ($P'$) is the appropriate number of permutations. Using Eq. 10, we can calculate the current expectation value for the state $|\psi_{i\kappa\nu}\rangle$. The non-interacting current is $j_{i\kappa\nu} = 2N^{N-1} \sin k_j |t_{k_j}|^2$. The correct normalization is obtained by dividing by a factor of $N^2$; in the thermodynamic limit $N, N' \rightarrow \infty$, this gives $j_{i\kappa\nu} = \int_{-k_R}^{k_L} \int_{-k_R}^{k_L} dk_1 dk_2 (2\pi)^2 |t_{k_1}|^2$. Here $-k_R (k_L)$ is the Fermi wave number of the right (left) lead lying in the range $[-\pi, 0]$ ($[0, \pi]$); it is related to the corresponding chemical potentials by $\mu_{R/L} = -2\cos k_{R/L}$. Inserting factors of $h$ and the charge $e$, the above expression for $j_{i\kappa\nu}$ gives the current for the non-interacting system to be $I = (e/h) \int_{-k_R}^{k_L} \int_{-k_R}^{k_L} dk_1 dk_2 (2\pi)^2 |t_{k_1}|^2$, where $E = -2\cos k$. We now compute the correction to this current, $\delta j_{i\kappa\nu}$, caused by the interaction. Using the normalization given above, we find that

$$
\delta j_{i\kappa\nu} = (1/2N^2) \sum_{r,s} \delta j_{r\kappa, s\nu};
$$

where $r$ and $s$ are used to indicate the two different momenta that contribute to the correction, and $\delta j_{r\kappa, s\nu}$ is the contribution from the interaction between the two-electron states $|\psi_{r\kappa}\rangle$ and $|\psi_{s\nu}\rangle$. The inset of Fig. 2 shows the current versus the bias for $U = 0.52$ which corresponds to the first peak in the main figure, and $U = 1.1$ which lies between the peaks; we see that the conductance is much larger in the first case. In all our calculations, we have ensured that the bias is not large enough for either of the chemical potentials to lie close to a one-particle resonance; otherwise the two-electron resonance might get masked by a one-particle resonance.

The analysis in this paper can be readily extended to the case of spin-1/2 electrons. We consider a simple model of a dot consisting of only one site (at $x = 0$) where there is an on-site energy $e_0$ and an interaction of the form $U n_{1\uparrow} n_{1\downarrow}$. This can lead to scattering between two electrons in the singlet channel but not in the triplet channel. The scattering and the resultant correction to the current can again be studied using the Lippmann-Schwinger formalism. We again find that a two-electron resonance can occur at an energy given by $2e_0 + U$ if the dot-lead couplings are small. In addition to this, the interaction can now also lead to spin entanglement [30]. Namely, if a spin-up and a spin-down electron are incident on the dot in a spin-uncorrelated state with a total energy which is equal to the two-particle resonance energy, the two electrons will emerge in a singlet state after scattering.

To summarize, we have studied a model of a quantum dot which is a small region in which electrons interact. The scattering of two particles due to the interaction is studied exactly. We find that a two-particle resonance occurs if the incident energies and the dot parameters satisfy a certain relation. Further, the interaction generally leads to an asymmetry in the current if the incident wave numbers are reversed; for a many-electron system with no inversion symmetry and strong Coulomb interactions, the current asymmetry can be shown by using a master equation approach [31]. We then use a two-electron perturbative approach to show that the two-particle resonance can survive for the many-electron system which arises when the leads are Fermi seas with certain chemi-
FIG. 2: (Color online) Plots of total current \( j = j_f + \delta j \) versus \( U \), for \( e_0 = e_1 = -0.6 \), \( \gamma_0 = \gamma_1 = 0.2 \), and bias = 0.02, 0.04, 0.08. Inset shows \( j \) versus bias for \( U = 0.52 \) and 1.1.

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