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Two-electron transport in a quantum waveguide having a single Anderson impurity

Jung-Tsung Shen^{1,3} and Shanhui Fan²

- ¹ Department of Electrical and Systems Engineering, Washington University in St. Louis, St. Louis, MO 63130, USA
- ² Ginzton Lab and Department of Electrical Engineering, Stanford University, Stanford, CA 94305, USA

E-mail: jushen@ese.wustl.edu

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Abstract. We consider the scattering problem of two-electron transport in one-dimensional channel coupled with an Anderson-type impurity. The treatment includes the backscattering of the electrons. We show that the transport properties are fundamentally different for spin singlet and triplet states, thus the impurity acts as a novel filter that operates based on the total spin angular momentum of the electron pairs, but not individual spins. The filter provides a deterministic generation of electron entanglement in spin, as well as energy and momentum space.

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³ Author to whom any correspondence should be addressed.

1. Introduction

There has been a significant interest in creating controllable entanglement between two electrons for the purpose of creating electron-based solid-state systems for quantum information processing [1]–[7]. Among many proposals to generate entanglement between electrons, that of mobile electron scattering in a one-dimensional channel is of particular interest. In such scattering processes, the strong correlations between flying electrons could be induced either via direct Coulomb interactions in quantum dots [4], or by a localized magnetic impurity [3]. Such a scattering process is important because it leads to a deterministic generation of entanglement, without the need for additional processes such as post-selection [6]. As a result, there has been substantial theoretical interest in understanding in detail the intrinsic behaviors of two-electron scattering by a quantum impurity, *in the absence of the Fermi sea* [3, 4, 7]. However, in all previous work, the treatment is perturbative, and yet it is well known that these few-electron systems have interesting properties beyond perturbation theory.

In this paper, we provide an exact solution of two-electron transport in one-dimensional channel coupled with an Anderson-type empty orbital. Our analysis shows that the transport properties are fundamentally different for spin-singlet and triplet states. For the singlet state, the strong on-site Coulomb repulsion can generate spatial electron-electron pairing via the scattering process. In addition, the energy spectra of the transmitted and reflected scattering states of the two entangled electrons exhibit a continuous distribution with side bands, a phenomenon analogous to photonic resonance fluorescence [8]. Furthermore, the transmitted two-electron state can manifest either bunching or anti-bunching behavior, in contrast to the case considered in [2] wherein the singlet states only show bunching behavior. This indicates that the spatial correlation between entangled electrons is a tunable dynamical process. On the other hand, in the triplet case, the transport properties of the two electrons are the same as those of two independent electrons, with no spatial electron-electron pairing. Finally, we show that based upon the different behaviors of the singlets and the triplets, the system acts as a novel filter that operates based on the total spin angular momentum of the electron pairs, but not individual spins, and that the filter provides a deterministic generation of electron entanglement in spin, as well as energy and momentum space.

In the following, we first introduce the system of interest and the Hamiltonian; we then discuss the scattering matrix (S-matrix) of the system and the decomposition of the two-electron Hilbert space. Using these techniques, the transport properties of the spin-singlet and triplet states are computed; the contrast between the transport properties of the spin-singlet and triplet states can be exploited to differentiate these two spin states. Finally, we briefly describe possible experimental implementations of the two-electron transport. Some relevant mathematical details are presented in the appendix.

2. The system and the Hamiltonian

To begin with, we set up the system as shown in figure 1. The electrons freely propagate in the one-dimensional channel, which couples to an Anderson-type empty orbital [9]. In real space,

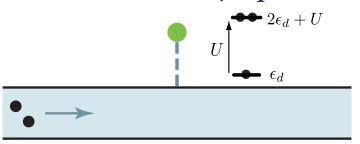


Figure 1. Schematics of the system. Two electrons (black dots) propagate in a one-dimensional channel (light blue) coupled to a quantum impurity (green dot). The coupling is indicated by the dashed line. Also shown is the energy diagram of the quantum impurity: when only one electron occupies the impurity, the energy is ϵ_d ; when two electrons with opposite spins occupy the impurity, the total energy is $2\epsilon_d + U$.

the Anderson Hamiltonian takes the following form [10, 11]:

$$H = \sum_{\sigma=\uparrow,\downarrow} \int dx \left\{ -i\hbar \, v_{g} c_{R\sigma}^{\dagger}(x) \frac{\partial}{\partial x} c_{R\sigma}(x) + i\hbar \, v_{g} c_{L\sigma}^{\dagger}(x) \frac{\partial}{\partial x} c_{L\sigma}(x) + \bar{V} \delta(x) \left(c_{R\sigma}^{\dagger}(x) d_{\sigma} + c_{R\sigma}(x) d_{\sigma}^{\dagger} + c_{L\sigma}^{\dagger}(x) d_{\sigma} + c_{L\sigma}(x) d_{\sigma}^{\dagger} \right) \right\}$$

$$+ \sum_{\sigma=\uparrow,\downarrow} \epsilon_{d} n_{d,\sigma} + U n_{d\uparrow} n_{d\downarrow}.$$

$$(1)$$

The first two terms describe the kinetic energy of the right-moving (R) and left-moving (L) electrons in the one-dimensional continuum, respectively, where v_g is the group velocity. $c_{R,\sigma}^{\dagger}(x)$ $(c_{R,\sigma}(x))$ is the creation (annihilation) operator of the right-moving electron with spin σ and similarly for $c_{L,\sigma}^{\dagger}(x)$ $(c_{L,\sigma}(x))$. The third term describes the processes of electron hopping on and off the impurity at x=0 ('hybridization'), where \bar{V} is the coupling strength, and the operator d_{σ}^{\dagger} (d_{σ}) creates (annihilates) an electron of spin σ on the impurity. $n_{d,\sigma} \equiv d_{\sigma}^{\dagger} d_{\sigma}$ is the electron number operator on the impurity. ϵ_d is the energy of the empty orbital of the impurity, degenerate for both spins of the electron. The last term with U>0 is the energy cost to put two electrons with opposite spin on the same impurity orbital. Double occupation of electrons is energetically unfavorable, and becomes prohibited in the limit $U \to +\infty$. The Hamiltonian of (1) describes the situation where the electrons can propagate in both directions, and is referred to as 'two-mode' model.

By employing the transformation $c_{\rm e\sigma}^{\dagger}(x) \equiv (c_{\rm R\sigma}^{\dagger}(x) + c_{\rm L\sigma}^{\dagger}(-x))/\sqrt{2}$, and $c_{\rm o\sigma}^{\dagger}(x) \equiv (c_{\rm R\sigma}^{\dagger}(x) - c_{\rm L\sigma}^{\dagger}(-x))/\sqrt{2}$, the original two-mode Hamiltonian is transformed into two decoupled 'one-mode' Hamiltonians describing an even and an odd subspaces, i.e. $H = H_{\rm e} + H_{\rm o}$:

$$H_{e} = \sum_{\sigma} \int dx (-i)\hbar \ v_{g} c_{e\sigma}^{\dagger}(x) \frac{\partial}{\partial x} c_{e\sigma}(x) + \int dx V \delta(x) \left(c_{e\sigma}^{\dagger}(x) \sigma_{-} + c_{e\sigma}(x) \sigma_{+} \right)$$

$$+ \sum_{\sigma} \epsilon_{d} n_{d,\sigma} + U n_{d\uparrow} n_{d\downarrow},$$

$$H_{o} = \sum_{\sigma} \int dx (-i)\hbar \ v_{g} c_{o\sigma}^{\dagger}(x) \frac{\partial}{\partial x} c_{o\sigma}(x),$$

$$(2)$$

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with $[H_e, H_o] = 0$. H_o is an interaction-free Hamiltonian, while H_e describes a nontrivial interacting model with coupling strength $V \equiv \sqrt{2}\bar{V}$. H_e has also been used to describe the S-wave scattering of electrons off a single magnetic impurity in three dimensions. Also, with the substitution $V \to \sqrt{|t_L|^2 + |t_R|^2}$, H_e describes the one-dimensional transport problem of electrons tunneling into a small quantum dot, with t_L and t_R being the tunneling amplitude from the left lead and right lead, respectively [12]. For notational simplicity, v_g and \hbar are set to 1 hereafter.

3. The S-matrix and the decomposition relation

The transport properties is fully encoded in the S-matrix, **S**. For a prepared *free* incoming state (in-state) $|\Psi_{\rm in}\rangle$, the free state describing the outcome (out-state) is given by $|\Psi_{\rm out}\rangle = \mathbf{S}|\Psi_{\rm in}\rangle$ [13, 14]. Since both $c_{\rm R\sigma}^{\dagger}(x)$ and $c_{\rm L\sigma}^{\dagger}(x)$ are linear combinations of $c_{\rm e\sigma}^{\dagger}(x)$ and $c_{\rm o\sigma}^{\dagger}(x)$, any *free* two-electron state $|\Psi_2\rangle$ can be written as

$$|\Psi_2\rangle = |\Psi\rangle_{ee} + |\Psi\rangle_{eo} + |\Psi\rangle_{oe} + |\Psi\rangle_{oo}, \tag{3}$$

where the subscript 'ee', for example, labels the subspace spanned by $c_{e\sigma}^{\dagger}(x_1)c_{e\sigma'}^{\dagger}(x_2)|\emptyset\rangle$. (The spin labels are suppressed for simplicity.) Moreover, since the Hamiltonians, (1) and (2), do not mix the e and o subspaces, the following *decomposition relation* holds [14]

$$\mathbf{S}|\Psi_{2}\rangle = \mathbf{S}_{ee}|\Psi\rangle_{ee} + \mathbf{S}_{eo}|\Psi\rangle_{eo} + \mathbf{S}_{oe}|\Psi\rangle_{oe} + \mathbf{S}_{oo}|\Psi\rangle_{oo},\tag{4}$$

where S_{ee} is the two-electron S-matrix in the 'ee' subspace governed by H_e ; $S_{eo} = S_{oe} = S_e S_o$, with S_e being the one-electron S-matrix in the e subspace, and $S_o = 1$, the identity operator, being the one-electron S-matrix in the o subspace governed by H_o ; $S_{oo} = 1$.

Thus, for a given two-electron in-state $|\Psi_2\rangle$, to compute the out-state $S|\Psi_2\rangle$, one first decomposes the in-state $|\Psi_2\rangle$ into ee, oo, eo and oe subspaces, followed by computing the scattering states in each subspace, and finally transforms the results back to the original RR, LL, RL and LR spaces, using (4). Note that the Hamiltonian in (1) conserves the total spins of the two electrons, thus the singlet and the triplet states do not mix with each other by scattering. Below we treat these cases separately.

4. The transport properties of the spin-singlet state

Any two-electron spin singlet eigenstate of the Hamiltonian H_e is of the form [10]

$$|\Phi\rangle \equiv \left\{ \int dx_1 dx_2 \, g(x_1, x_2) c_{e\uparrow}^{\dagger}(x_1) c_{e\downarrow}^{\dagger}(x_2) + \int dx \, e(x) \left[c_{e\uparrow}^{\dagger}(x) d_{\downarrow}^{\dagger} - c_{e\downarrow}^{\dagger}(x) d_{\uparrow}^{\dagger} \right] + f d_{\uparrow}^{\dagger} d_{\downarrow}^{\dagger} \right\} |\emptyset\rangle,$$
(5)

where $g(x_1, x_2)$ is the two-electron wave function of the singlet state $c_{e\uparrow}^{\dagger}(x_1)c_{e\downarrow}^{\dagger}(x_2)|\emptyset\rangle$, e(x) is the amplitude of the singlet state $[c_{e\uparrow}^{\dagger}(x)d_{\downarrow}^{\dagger}-c_{e\downarrow}^{\dagger}(x)d_{\uparrow}^{\dagger}]|\emptyset\rangle$, wherein one electron is at the impurity; f is the amplitude of the doubly occupied state of the impurity, $d_{\uparrow}^{\dagger}d_{\downarrow}^{\dagger}|\emptyset\rangle$. $g(x_1, x_2)$ is a symmetric function of x_1 and x_2 (see the appendix). $g(x_1, x_2)$, f and e(x) can be analytically solved (see [10, 14]).

In order to construct the S-matrix, one interprets $g(x_1, x_2)$ in the third quadrant $(x_1, x_2 < 0)$ as the in-state, and in the first quadrant $(x_1, x_2 > 0)$ as the out-state. This interpretation can be rigorously proved using Lippmann–Schwinger formalism [14]. We note that

$$g(x_1, x_2) \equiv \begin{cases} ee \langle x_1, x_2 | W_{k,p} \rangle_{ee}, & \text{for } x_1, x_2 < 0; \\ t_k t_{p ee} \langle x_1, x_2 | W_{k,p} \rangle_{ee}, & \text{for } x_1, x_2 > 0; \end{cases}$$
(6)

where $t_k \equiv (k - \epsilon_d - i\Gamma/2)/(k - \epsilon_d + i\Gamma/2)$ with $\Gamma \equiv V^2$ is the one-mode single electron transmission amplitude, and similar for t_p .

$$|W_{k,p}\rangle_{\text{ee}} \equiv \frac{(k-p)(E-2\epsilon_d-U)|S_{k,p}\rangle_{\text{ee}} - iU\Gamma|A_{k,p}\rangle_{\text{ee}}}{\sqrt{(k-p)^2(E-2\epsilon_d-U)^2 + U^2\Gamma^2}},$$
(7)

with

$$\langle x_{1}, x_{2} | S_{k,p} \rangle_{ee} \equiv S_{k,p}(x_{1}, x_{2}) = \frac{e^{ikx_{1}}e^{ipx_{2}} + e^{ikx_{2}}e^{ipx_{1}}}{2\pi\sqrt{2}},$$

$$\langle x_{1}, x_{2} | A_{k,p} \rangle_{ee} \equiv A_{k,p}(x_{1}, x_{2}) = \frac{\operatorname{sgn}(x) \left(e^{ikx_{1}}e^{ipx_{2}} - e^{ikx_{2}}e^{ipx_{1}} \right)}{2\pi\sqrt{2}},$$
(8)

and normalized as $_{\text{ee}}\langle W_{k',p'}|W_{k,p}\rangle_{\text{ee}} = \delta(k-k')\delta(p-p')$. As a result, we have $\mathbf{S}_{\text{ee}}|W_{k,p}\rangle_{\text{ee}} = t_k t_p |W_{k,p}\rangle_{\text{ee}}$.

To describe the entire scattering properties, we would need to ensure that we provide the mapping for all states in the free two-electron Hilbert space. Thus, a completeness check on $\{|W_{k,p}\rangle_{\rm ee}\}$ is crucial. Remarkably, we found that the completeness depends upon the sign of $E-2\epsilon_d-U$. When $E-2\epsilon_d-U\geqslant 0$, the set $\{|W_{k,p}\rangle_{\rm ee}:k\leqslant p\}$ alone forms an orthonormal complete set of basis that spans the free two-electron Hilbert space. However, when $E-2\epsilon_d-U\leqslant 0$, an additional *two-electron bound state* $|B_E\rangle_{\rm ee}$, defined as

$$\langle x_1, x_2 | B_E \rangle_{\text{ee}} \equiv B_E(x_1, x_2) = \frac{\sqrt{\Gamma'}}{\sqrt{4\pi}} e^{iEx_c - \Gamma'|x|/2}, \tag{9}$$

is needed, such that $\{|W_{k \leq p}\rangle_{\text{ee}}, |B_E\rangle_{\text{ee}}\}$ together forms a complete and orthonormal basis set. Here, $_{\text{ee}}\langle B_{E'}|B_E\rangle_{\text{ee}} = \delta(E-E')$, and $_{\text{ee}}\langle W_{k,p}|B_E\rangle_{\text{ee}} = 0$. $\Gamma' \equiv (U\Gamma)/(U+2\epsilon_d-E) > 0$ defines the effective size of the bound state $|B_E\rangle_{\text{ee}}$. Such bound state has been noted in other context before [15]. We show here that including it is crucial for describing the transport properties.

The S-matrix for the singlet state in the ee subspace, S_{ee} , thus can be diagonalized as

$$\mathbf{S}_{ee} \equiv \begin{cases} \sum_{k \leq p} t_k t_p |W_{k,p}\rangle \langle W_{k,p}|, & E - 2\epsilon_d - U \geqslant 0; \\ \sum_{k \leq p} t_k t_p |W_{k,p}\rangle \langle W_{k,p}| + \sum_E t_E |B_E\rangle \langle B_E|, & E - 2\epsilon_d - U < 0; \end{cases}$$
(10)

where

$$t_E \equiv \frac{(E - 2\epsilon_d - U)(E - 2\epsilon_d - 2i\Gamma) - \Gamma^2}{(E - 2\epsilon_d - U)(E - 2\epsilon_d + 2i\Gamma) - \Gamma^2},\tag{11}$$

is the transmission amplitude for the two-electron bound state as a whole. The two-electron bound state, $|B_E\rangle$, has a spatial extent of $1/\Gamma'$. It behaves as an effective single composite particle with an energy E=k+p, and remains integral when passing through the impurity, acquiring a phase shift t_E . By tuning Γ' via ϵ_d or U, the quantum impurity therefore provides a

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local means of manipulating composite particles of electrons. The other three remaining terms in (4) can be easily computed [14], and altogether, (4) provides a complete description of the transport properties.

Using the S-matrix, (10), we now compute the transport properties for the singlet state. Consider a singlet in-state

$$|\Psi_{\rm in}\rangle^{\rm s} \equiv |S_{k_1,p_1}\rangle_{\rm R\uparrow R\downarrow} = \int \mathrm{d}x_1 \mathrm{d}x_2 \, S_{k,p}(x_1,x_2) c_{\rm R\uparrow}^{\dagger}(x_1) c_{\rm R\downarrow}^{\dagger}(x_2) |\emptyset\rangle \tag{12}$$

incident from the left. The out-state, $\mathbf{S}|\Psi_{\rm in}\rangle^{\rm s}$, gives the amplitudes for all possible outcomes: both electrons transmitted $(t_2^{\rm s}(x_1,x_2) \equiv \langle \emptyset | c_{\rm R\downarrow}(x_2) c_{\rm R\uparrow}(x_1) | \Psi_{\rm out}\rangle^{\rm s})$, both reflected, and one electron transmitted and one reflected. All of these amplitudes have exact analytic forms. Below, we focus on $t_2^{\rm s}(x_1,x_2)$, which contains the spatial correlation properties of the two transmitted electrons.

Using (4) and (10), one has [14]

$$t_2^{s}(x_1, x_2) = \bar{t}_k \bar{t}_p S_{k,p}(x_1, x_2) + \frac{1}{4} \sum_{\Delta' \le 0} B S_{E,\Delta'}(x_1, x_2), \tag{13}$$

where $\bar{t}_{k,p} \equiv (t_{k,p} + 1)/2$ are the two-mode single-electron transmission amplitudes, and $\Delta \equiv (k-p)/2$ is the energy difference between the two electrons. *B* represents the resonance fluorescence similar to that in quantum optics [8, 16]. When $E - 2\epsilon_d - U < 0$, *B* is given by

$$B = \frac{U}{U - \delta E - i\Gamma} \left(\frac{16i\Gamma^2}{\pi} \frac{\delta E + i\Gamma}{\left[4\Delta^2 - (\delta E + i\Gamma)^2 \right] \left[4\Delta'^2 - (\delta E + i\Gamma)^2 \right]} \right)$$

$$- \left\{ \frac{32iU^4\Gamma^6(U - \delta E)^2}{\pi(U - \delta E - i\Gamma)} \frac{1}{\left[4\Delta^2(U - \delta E)^2 + U^2\Gamma^2 \right] \left[4\Delta'^2(U - \delta E)^2 + U^2\Gamma^2 \right]} \right.$$

$$\times \frac{1}{\left[\delta E(\delta E - U) + i\Gamma(\delta E - 2U) \right] \left[\delta E(\delta E - U) + 2i\Gamma(\delta E - U) - \Gamma^2 \right]} \right\}, \quad (14)$$

where $\delta E \equiv E - 2\epsilon_d$. When $E - 2\epsilon_d - U \geqslant 0$, $\{|W_{k \leqslant p}\rangle_{ee}\}$ alone is a complete set of basis. In this regime,

$$B = \mathcal{P} \frac{4}{\Delta^{2} - \Delta^{\prime 2}} \frac{U\Gamma}{\pi} \left\{ \frac{\Delta^{2}(\delta E - U)(\delta E - i\Gamma - 2\Delta)(\delta E - i\Gamma + 2\Delta)}{\left[(\delta E + i\Gamma)^{2} - 4\Delta^{2}\right] \left[4(\delta E - U)^{2}\Delta^{2} + U^{2}\Gamma^{2}\right]} - \frac{\Delta^{\prime 2}(\delta E - U)(\delta E - i\Gamma - 2\Delta^{\prime})(\delta E - i\Gamma + 2\Delta^{\prime})}{\left[(\delta E + i\Gamma)^{2} - 4\Delta^{\prime 2}\right] \left[4(\delta E - U)^{2}\Delta^{\prime 2} + U^{2}\Gamma^{2}\right]} \right\} - \frac{U^{2}\Gamma^{3}}{\pi} \left\{ \frac{16\delta E \left(\delta E + i\Gamma\right)}{\left[(\delta E - U)^{2}\left(\delta E + i\Gamma\right)^{2} + U^{2}\Gamma^{2}\right] \left[4\Delta^{2} - (\delta E + i\Gamma)^{2}\right] \left[4\Delta^{\prime 2} - (\delta E + i\Gamma)^{2}\right]} - \frac{4U\left(\delta E - U\right)\left(\delta E - U - i\Gamma\right)\left[\delta E(\delta E - U) - i\Gamma(\delta E - 2U)\right]}{\left[\left[\delta E \left(\delta E - U\right)^{2} + 2i\Gamma\left(\delta E - U\right)^{2} - (\delta E - 2U)\Gamma^{2}\right] \left[4\Delta^{2}(\delta E - U)^{2} + U^{2}\Gamma^{2}\right] \left[4\Delta^{\prime 2}(\delta E - U)^{2} + U^{2}\Gamma^{2}\right]} \right\},$$
(15)

where \mathcal{P} denotes Cauchy principal value. The difference between (14) and (15) is the contribution from the bound state. The background fluorescence indicates that only the total

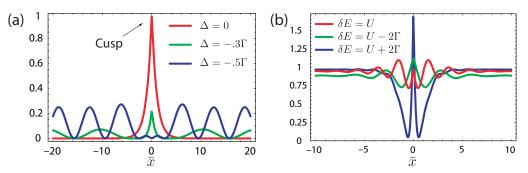


Figure 2. Singlet $|t_2^s(x_1, x_2)|^2$ (normalized by $(\sqrt{2}/2\pi)^2$). $U = 6\Gamma$ for both cases. $\bar{x} \equiv \Gamma(x_1 - x_2)$. (a) $\delta E = 0$. The wavefunction transitions from bunching $(|t_2^s(\bar{x} = 0)|^2 \simeq 1$, when $\Delta = 0$) to antibunching $(|t_2^s(\bar{x} = 0)|^2 = 0$ when $\Delta = -0.5\Gamma$). (b) $\Delta = 0$.

energy, but not the individual energy of each electron, is conserved. Thus, as one electron inelastically scattering off a transient composite object formed by the quantum impurity and the other electron, the individual energy of each electron is redistributed over a continuous range, described by B [14, 16]. The background fluorescence arises purely from on-site interaction. For the limiting case $U \rightarrow 0$, it completely disappears.

We now explain (13). The first term in (13) describes independent transport of electrons, while the second term describes correlated transport. In general, the effect of correlation occurs when $x_1 \simeq x_2$. Since the poles for Δ in B are all complex, the correlated term decays to zero when $|x_1 - x_2| \gg 0$. The poles in B also indicate single-electron and two-electron resonances. Specifically, when $|\delta E| \simeq 2|\Delta|$, one electron has energy close to ϵ_d and is on resonance with the impurity. On the other hand, when $\delta E \simeq U \neq 0$, the *electron pair* is on resonance with the impurity. The correlation typically attains its maximum degree when both conditions are simultaneously satisfied.

We look at the effects of spatial correlation due to the presence of these resonances, when only the single-electron resonance is present. Figure 2(a) plots $|t_2^s(x_1, x_2)|^2$ for the case $\delta E = 0$ and $U = 6\Gamma$. The transmitted singlet state transitions from bunching to antibunching when Δ varies from 0 to -0.5Γ . Thus, the bunching behavior of the singlet state is a dynamical process depending upon the tunable parameters of the system, and could be tuned via a gate voltage which changes U or ϵ_d . Note also that when $U \to \infty$, B is greatly simplified, and the scattering properties are in fact equivalent to the strongly correlated two-photon transport of one-dimensional Dicke model [14, 16].

For the case where *both* electrons satisfy the single-electron resonance condition, i.e. $E = 2\epsilon_d$ and $\Delta = 0$, (13) yields

$$t_2^{\rm s}(x_1, x_2) = \frac{\sqrt{2}}{2\pi} e^{iEx_c} \left[-\left(1 + \frac{U\Gamma}{(U - i\Gamma)(2iU + \Gamma)}\right) e^{-\Gamma|x|/2} \right],$$
 (16)

as shown in figure 2(a). $|t_2^s(x_1, x_2)|^2$ decays exponentially as $|x| \equiv |x_1 - x_2|$ becomes large, and thus the two transmitted electrons form a *bound state*. When |x| is small, $|t_2^s|^2 \propto 1 - \Gamma|x|$ shows a cusp at x = 0, so is $|r_2|^2$. These features should manifest in the measurement of the $g^{(2)}(\tau)$ function in each case.

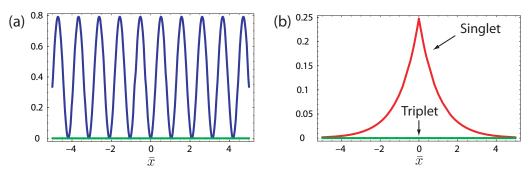


Figure 3. (a) Triplet $|t_2^t(x_1, x_2)|^2$ for $\delta E = 4\Gamma$ (blue curve) and 6Γ (green curve). $\Delta = -3\Gamma$. The triplet is always antibunched. (b) Singlet–triplet filtering. $\delta E = 6\Gamma = U = -2\Delta$. The singlet case $(|t_2^t|^2)$ is denoted by the red curve and the triplet case $(|t_2^t|^2)$ by the green curve. Both $|t_2^{t,s}|^2$ are normalized by $(\sqrt{2}/2\pi)^2$.

Figure 2(b) plots $|t_2^s(x_1, x_2)|^2$ for the case when only two-electron resonance manifests, with $\delta E \simeq U = 6\Gamma$ and $\Delta = 0$. In this case, away from x = 0, since neither electron is at the single-electron resonance, the wavefunction approaches that of two independent electrons for $\Delta = 0$, with a near-unity transmission coefficient. In the vicinity of x = 0, the electrons can exhibit a strong bunching effect, but no strong anti-bunching is observed.

5. The transport properties of the spin-triplet state

The triplet cases $(S = 1, S_z = 0, 1)$ can be solved straightforwardly in the same fashion. Here we will summarize the key findings: (1) $f \equiv 0$, which indicates that double occupation of electrons at the impurity are always prohibited; and (2) independent of E, the set $\{|T_{k,p}\rangle_{ee} : k \leq p\}$, with $|T_{k,p}\rangle_{ee}$ defined as

$$\langle x_1, x_2 | T_{k,p} \rangle_{\text{ee}} \equiv T_{k,p}(x_1, x_2) = \frac{e^{ikx_1} e^{ipx_2} - e^{ikx_2} e^{ipx_1}}{2\pi\sqrt{2}},$$
(17)

alone forms an orthonormal complete set in the free two-electron Hilbert space. The S-matrix in the ee subspace is

$$\mathbf{S}_{ee} = \sum_{k,p} t_k t_p |T_{k,p}\rangle \langle T_{k,p}|. \tag{18}$$

For a triplet in-state with $S_z = 0$,

$$|\Psi_{\rm in}\rangle^{\rm t} \equiv |T_{k_1,p_1}\rangle_{\rm R\uparrow R\downarrow} = \int \mathrm{d}x_1 \mathrm{d}x_2 \, T_{k,p}(x_1,x_2) c_{\rm R\uparrow}^{\dagger}(x_1) c_{\rm R\downarrow}^{\dagger}(x_2) |\emptyset\rangle, \tag{19}$$

the corresponding wavefunction describing both electrons being transmitted is

$$t_2^{\mathsf{t}}(x_1, x_2) = \bar{t}_k \bar{t}_p T_{k,p}(x_1, x_2) \propto \sin[\Delta(x_1 - x_2)]. \tag{20}$$

Thus, the transport properties of the two electrons in triplet are the same as those of two independent electrons. Figure 3(a) plots $|t_2^t(x_1, x_2)|^2$ for $\Delta = -3\Gamma$. When $\delta E = 6\Gamma = -2\Delta$, t_2^t vanishes, since one electron is on resonance with the impurity and the corresponding single-electron transmission amplitudes in (20) vanishes.

6. Spin singlet-triplet filter

The different transport properties of the singlet and the triplet states allow one to construct a novel *deterministic* filter that operates on the total spin angular momentum of the electron pair but not individual spins. In the triplet case, the transmission amplitude for the electron pair is zero when one electron is on resonance with the impurity with energy ϵ_d . In the singlet case, the electron pair can go through the impurity by forming a bound pair of singlet state. Thus, the filter deterministically generates a two-electron state that is entangled in spin, energy and momentum space (figure 3(b)). The transmission amplitude attains maximum value when the singlet approximately satisfies both the single-electron and two-electron resonance conditions simultaneously.

7. Possible experimental implementations

We now briefly discuss the possible experimental implementations. To prepare for the twoelectron input state, one can use a potential barrier to generate collimated two-electron state [17, 18]. For each transmitted electron, the energy distribution n(E) is given by the product of the Fermi distribution function $f(E, \mu; \beta)$ (β is the inverse temperature) and the probability of the electron transmitting through the barrier T(E):

$$n(E) = f(E, \mu; \beta)T(E), \tag{21}$$

which is strongly peaked at the Fermi level μ , with a specific shape and broadening linewidth depending upon the details of the barrier [17, 18]. These thermionically emitted electrons are input to a ballistic conductor coupled to an Anderson impurity with an empty orbital. The ballistic conductor can be a carbon nanotube [19], graphene nanostrip [20], semiconductor nanowire [21] or a one-dimensional constriction defined by a split-gate geometry in a two-dimensional electron gas [22, 23]. By convoluting the electron energy distributions with the constant energy in-states of equations (12) and (19), the two-electron wave packet could be expressed as a linear superposition of the constant energy in-states of equations (12) and (19), and the outcome of the two-electron scattering can be straightforwardly computed. Moreover, one could study the temperature dependence of the two-electron correlations.

We now discuss the general criterion to observe the strong correlation between electrons. Intuitively, for the two electrons to be able to establish correlations via interacting with the impurity, the second electron must arrive at the impurity before the first electron escape; that is, the difference between the arrival times of the two incoming electrons (Δt) must be smaller than the lifetime of the excited state of the impurity of single-electron occupancy:

$$\Delta t \lesssim \hbar / \Gamma = \frac{v_g \hbar^2}{V^2},\tag{22}$$

where Γ is the decay rate of the excited state of the impurity of single-electron occupancy, given above in the expression of single-electron transmission amplitude t_k (we have put back \hbar and $v_{\rm g}$), which can also be verified via a direct time-dependent calculation. For the quantum dots described in [24, 25], $\Gamma \sim 10 \,\mu\text{eV}$, and thus $\Delta t \lesssim 0.1 \,\text{ns}$. The constraint on the distance between the two incoming electrons is given by $\Delta x = v_{\rm g} \Delta t$.

As a final remark, here we show that the electron pairing can be generated by strong onsite Coulomb repulsion. Since the same one-mode model also describes the S-wave scattering in two and three dimensions, we speculate that such a pairing mechanism could be important in bulk materials involving Anderson impurities.

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Appendix. Spin-singlet and triplet state representations

In this appendix, we provide some details for the second quantization formalisms. We restrict the discussion to the one-mode case, and thus suppress the subscript e.

The creation operator $c_s^{\dagger}(x)$ creates a particle at x with spin s, while the annihilation operators $c_s(x)$ annihilates a particle at x with spin s. They satisfies the commutation relations: $\{c_{s_1}(x_1), c_{s_2}^{\dagger}(x_2)\} = \delta_{s_1, s_2}\delta(x_1 - x_2), \{c_{s_1}^{\dagger}(x_1), c_{s_2}^{\dagger}(x_2)\} = 0 \text{ and } \{c_{s_1}(x_1), c_{s_2}(x_2)\} = 0.$ The bases of the Hilbert space can be obtained via successive application of the creation

operators upon vacuum state:

1. One-particle basis:

$$|x,s\rangle \equiv c_s^{\dagger}(x)|\emptyset\rangle,$$
 (A.1)

2. Two-particle basis:

$$|x_1, s_1; x_2, s_2\rangle \equiv c_{s_1}^{\dagger}(x_1)c_{s_2}^{\dagger}(x_2)|\emptyset\rangle, \tag{A.2}$$

and similarly,

3. N-particle basis:

$$|x_1, s_1; \dots; x_N, s_N\rangle \equiv \prod_{n=1}^N c_{s_n}^{\dagger}(x_n)|\emptyset\rangle. \tag{A.3}$$

Using these bases, an N-particle state with spin s_1, \ldots, s_N is expressed as

$$|\phi\rangle \equiv \int \left(\prod_{i=1}^{N} dx_{i}\right) \phi(x_{1}, \dots, x_{N}) |x_{1}, s_{1}; \dots; x_{N}, s_{N}\rangle,$$
 (A.4)

where $\phi(x_1, \ldots, x_N)$ represents the N-particle wavefunction.

These basis states form a complete set of basis of the Hilbert space:

$$\mathbb{I} = |\emptyset\rangle\langle\emptyset| + \sum_{s} \int \mathrm{d}x |x, s\rangle\langle x, s| + \sum_{s_1, s_2} \int \mathrm{d}x_1 \mathrm{d}x_2 |x_1, s_1; x_2, s_2\rangle\langle x_1, s_1; x_2, s_2|
+ \dots + \sum_{\{s_i\}} \int \left(\prod_{i}^{N} \mathrm{d}x_i\right) |x_1, s_1; \dots; x_N, s_N\rangle\langle x_1, s_1; \dots; x_N, s_N| + \dots,$$
(A.5)

where \mathbb{I} is the identity operator.

It is often convenient to use bases that are also eigenstates of the total spin operator. For the two-particle case, this leads to the definitions of singlet and triplet states, which are the linear superposition of the two-particle basis states

1. Singlet basis state:

$$|T_{0,0}\rangle \equiv |S\rangle \equiv \frac{1}{\sqrt{2}} \left(c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) - c_{\downarrow}^{\dagger}(x_1) c_{\uparrow}^{\dagger}(x_2) \right) |\emptyset\rangle, \tag{A.6}$$

which is anti-symmetric with respect to the spin labels;

2. Triplet basis states:

$$|T_{1,1}\rangle \equiv c_{\uparrow}^{\dagger}(x_1)c_{\uparrow}^{\dagger}(x_2)|\emptyset\rangle,$$
 (A.7)

$$|T_{1,0}\rangle \equiv \frac{1}{\sqrt{2}} \left(c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) + c_{\downarrow}^{\dagger}(x_1) c_{\uparrow}^{\dagger}(x_2) \right) |\emptyset\rangle, \tag{A.8}$$

$$|T_{1,-1}\rangle \equiv c_{\downarrow}^{\dagger}(x_1)c_{\downarrow}^{\dagger}(x_2)|\emptyset\rangle,$$
 (A.9)

which are symmetric with respect to the spin labels.

The singlet and triplet states obey the ortho-normalization relations

$$\langle S'|S\rangle = \delta(x_1 - x_1')\delta(x_2 - x_2') + \delta(x_1 - x_2')\delta(x_2 - x_1'), \tag{A.10}$$

$$\langle T'_{1,m'}|T_{1,m}\rangle = \delta_{m',m} \left[\delta(x_1 - x'_1)\delta(x_2 - x'_2) - \delta(x_1 - x'_2)\delta(x_2 - x'_1)\right],\tag{A.11}$$

$$\langle S|T\rangle = 0, (A.12)$$

where the primed states have all the coordinate and spin labels primed.

A singlet state can be written in two different expressions

$$\int dx_1 dx_2 h(x_1, x_2) |S\rangle = \int dx_1 dx_2 h(x_1, x_2) \frac{1}{\sqrt{2}} \left(c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) - c_{\downarrow}^{\dagger}(x_1) c_{\uparrow}^{\dagger}(x_2) \right) |\emptyset\rangle$$

$$= \int dx_1 dx_2 h(x_1, x_2) \frac{1}{\sqrt{2}} \left(c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) + c_{\uparrow}^{\dagger}(x_2) c_{\downarrow}^{\dagger}(x_1) \right) |\emptyset\rangle$$

$$= \int dx_1 dx_2 \frac{1}{\sqrt{2}} \left(h(x_1, x_2) + h(x_2, x_1) \right) c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) |\emptyset\rangle$$

$$\equiv \int dx_1 dx_2 g_s(x_1, x_2) c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) |\emptyset\rangle. \tag{A.13}$$

Here $h(x_1, x_2)$ is an arbitrary function, while $g_s(x_1, x_2) = g_s(x_2, x_1)$ is a symmetric function with respect to x_1 and x_2 .

Similarly, the triplet state $|T_{1.0}\rangle$ can be expressed in two ways:

$$\int dx_1 dx_2 h(x_1, x_2) |T_{1,0}\rangle = \int dx_1 dx_2 h(x_1, x_2) \frac{1}{\sqrt{2}} \left(c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) + c_{\downarrow}^{\dagger}(x_1) c_{\uparrow}^{\dagger}(x_2) \right) |\emptyset\rangle$$

$$= \int dx_1 dx_2 h(x_1, x_2) \frac{1}{\sqrt{2}} \left(c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) - c_{\uparrow}^{\dagger}(x_2) c_{\downarrow}^{\dagger}(x_1) \right) |\emptyset\rangle$$

$$= \int dx_1 dx_2 \frac{1}{\sqrt{2}} \left(h(x_1, x_2) - h(x_2, x_1) \right) c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) |\emptyset\rangle$$

$$\equiv \int dx_1 dx_2 g_a(x_1, x_2) c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) |\emptyset\rangle, \tag{A.14}$$

where $g_a(x_1, x_2) = -g_a(x_2, x_1)$ is an anti-symmetric function with respect to x_1 and x_2 .

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As a side note, a state with total $S_z = 0$ can in general be written as

$$\int \mathrm{d}x_1 \mathrm{d}x_2 \, g(x_1, x_2) c_{\uparrow}^{\dagger}(x_1) c_{\downarrow}^{\dagger}(x_2) |\emptyset\rangle, \tag{A.15}$$

with $g(x_1, x_2)$ arbitrary. To see this, one only needs to show that the above state is a linear superposition of $|S\rangle$ and $|T_{1,0}\rangle$, since

$$\int dx_{1}dx_{2} g(x_{1}, x_{2})c_{\uparrow}^{\dagger}(x_{1})c_{\downarrow}^{\dagger}(x_{2})|\emptyset\rangle = \frac{1}{\sqrt{2}} \int dx_{1}dx_{2} \frac{1}{\sqrt{2}} \left(g(x_{1}, x_{2}) + g(x_{2}, x_{1})\right) c_{\uparrow}^{\dagger}(x_{1})c_{\downarrow}^{\dagger}(x_{2})|\emptyset\rangle + \frac{1}{\sqrt{2}} \int dx_{1}dx_{2} \frac{1}{\sqrt{2}} \left(g(x_{1}, x_{2}) - g(x_{2}, x_{1})\right) c_{\uparrow}^{\dagger}(x_{1})c_{\downarrow}^{\dagger}(x_{2})|\emptyset\rangle = \frac{1}{\sqrt{2}} \int dx_{1}dx_{2} g(x_{1}, x_{2})|S\rangle + \frac{1}{\sqrt{2}} \int dx_{1}dx_{2} g(x_{1}, x_{2})|T_{1,0}\rangle,$$
(A.16)

where we have used (A.13) and (A.14).

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