# Inducing Spin Correlations and Entanglement in a Double Quantum Dot through Nonequilibrium Transport

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For a double quantum dot system in a parallel geometry, we demonstrate that by combining the effects of a flux and driving an electrical current through the structure, the spin correlations between electrons localized in the dots can be controlled at will. In particular, a current can induce spin correlations even if the spins are uncorrelated in the initial equilibrium state. Therefore, we are able to engineer an entangled state in this double-dot structure. We take many-body correlations fully into account by simulating the real-time dynamics using the time-dependent density matrix renormalization group method. Using a canonical transformation, we provide an intuitive explanation for our results, related to Ruderman-Kittel-Kasuya-Yoshida physics driven by the bias.

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*Introduction.*—Considerable progress in nanotechnology in the last decades has made possible the fabrication of new artificial structures [1,2] such as quantum dots, quantum rings, or molecular conductors. The physics of quantum dots in a parallel geometry is intriguing, since it allows one to study interference effects between electrons traveling through different paths, most notably realized in the Aharanov-Bohm effect. Such structures have been studied in several experiments [3,4]. Besides the interest in practical applications in nanoelectronics or in fundamental many-body physics such as the Kondo effect [4–6], double quantum dots (DQDs) also play a vital role in the context of quantum information processing [7–9]. Generating, controlling, and detecting entangled states in condensed matter systems is one of the challenges for future quantum computation applications [10]. Various proposals for entangling spatially separated electrons have been put forward, such as, for instance, by splitting Cooper pairs [11,12] or by manipulating spins in quantum dots [13]. In a DQD, an entangled state can be realized by putting the electrons into a singlet state [7,8,14]. Means of detecting entangled states of electrons were discussed in, e.g., Refs. [11,15].

In this Letter, we demonstrate that an entangled state between electrons localized in a DQD embedded in an Aharonov-Bohm interferometer can be induced and controlled by sending an electrical current through the structure. In the presence of a flux, the initial state can even be fully uncorrelated yet the nonequilibrium dynamics results in nonzero spin correlations in the steady state. The sign and the strength of such steady-state spin correlations depend on voltage, interactions, and the flux. The generation of entanglement through nonequilibrium dynamics in quantum dots, with different setups, has been discussed in Ref. [16]. An additional motivation for our work stems from the current interest, both from theory [17,18] and from experiment (see, e.g., [19]), in the nonequilibrium dynamics of nanostructures with strong electronic correlations. We emphasize that we treat both interactions and nonequilibrium dynamics in a well-controlled manner using the time-dependent density matrix renormalization group (DMRG) method [20]. As we will see, the effect of inducing spin correlations is the largest at voltages $\sim\Theta(W/4)$ ($W$ is the bandwidth of the reservoirs) where Kondo correlations cease to matter [2,5].

*The model.*—We model the quantum dots as Anderson impurities resulting in the Hamiltonian [depicted in the inset of Fig. 1(a)],

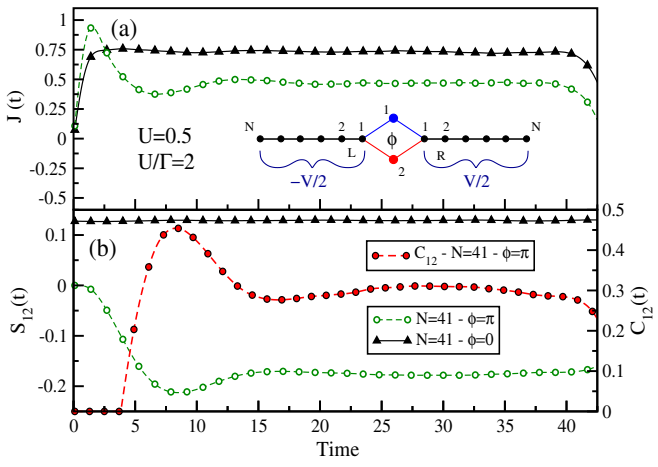


FIG. 1 (color online). (a) Current $J(t)$ for $\phi = 0$ and $\pi$. (b) Spin correlation $S_{12}(t)$ and concurrence $C_{12}(t)$. All for $N = 41$, $U = 0.5$, $V = 0.5$. Inset in (a): Sketch of the DQD structure.

 

$$H = H_l + H_{\mathrm{hy1}} + H_{\mathrm{hy2}} + H_{\mathrm{int}}, \tag{1}$$

$$H_l = \sum_{\alpha=L,R} \sum_{i=1;\sigma}^{N-1} [-t_0(c^\dagger_{\alpha i\sigma} c_{\alpha i+1\sigma} + \mathrm{H.c.})] + \sum_{\alpha=L,R} \sum_{i=1;\sigma}^{N} \mu_\alpha n_{\alpha i\sigma}, \tag{2}$$

$$H_{\mathrm{hy1}} = -t_1'[d^\dagger_{1\sigma} c_{L1\sigma} + c^\dagger_{R1\sigma} d_{1\sigma} + \mathrm{H.c.}], \tag{3}$$

$$H_{\mathrm{hy2}} = -t_2'[d^\dagger_{2\sigma} c_{L1\sigma} + e^{i\phi} c^\dagger_{R1\sigma} d_{2\sigma} + \mathrm{H.c.}], \tag{4}$$

$$H_{\mathrm{int}} = \sum_{j=1,2;\sigma} [U n_{j\sigma} n_{j\bar{\sigma}} + V_g n_{j\sigma}]. \tag{5}$$

The system size is $2N + 2$ where $N$ is the number of sites in the left or right lead. The two dots are at the center of the system labeled by $j = 1, 2$. The Hamiltonian consists of four parts: First, the noninteracting leads $H_l$ with a constant hopping matrix element $t_0 = 1$ used as the unit of energy ($\hbar = 1$, $e = 1$). Second, the terms $H_{\mathrm{hy1}}$ and $H_{\mathrm{hy2}}$ give rise to the hybridization between the localized levels of the dots and the leads. We consider fully symmetric tunnel couplings, i.e., $|t_1'| = |t_2'| = t'$ (see the Supplemental Material [21] for a discussion of asymmetric couplings). We define the tunneling strength by $\Gamma = 2\pi t'^2 \rho_{\mathrm{leads}}(E_F) = 2t'^2$, where $\rho_{\mathrm{leads}}(E_F)$ is the local density of states (LDOS) of the leads at the Fermi energy $E_F$. In the hopping matrix element between the second dot and the right lead we incorporate an arbitrary phase $\phi$. Finally, there is the interacting region $H_{\mathrm{int}}$ with the two quantum dots, which are both subject to the same Coulomb repulsion $U$ and a gate potential $V_g = -U/2$ such that both dots are kept at half-filling. The operator $c^\dagger_{\alpha l\sigma}$ ($c_{\alpha l\sigma}$) creates (annihilates) an electron at site $l$ in the $\alpha = L, R$ lead with spin $\sigma$ while $d^\dagger_{j\sigma}$ ($d_{j\sigma}$) acts on dot $j$; $n_{\alpha l\sigma} = c^\dagger_{\alpha l\sigma} c_{\alpha l\sigma}$ as usual. In Eq. (2), $\mu_L$ and $\mu_R$ mimic the chemical potentials of the leads.

The ground state and the linear conductance of DQDs Eq. (1) were extensively studied in Ref. [22]. A closely related DQD model with a finite flux $\phi$ and with spin-polarized electrons was discussed in Ref. [23].

The phase included in Eq. (4) may have a different meaning depending on the specific physical realization. The most obvious one is to associate $\phi$ with a magnetic flux that pierces the ring structure containing the two dots and the first site from each lead as shown in Fig. 1(b). As usual, one can use a gauge transformation such that the flux appears in only one of the four hopping matrix elements. Another situation described by Eq. (4) is a single quantum dot with two levels where by symmetry the levels can couple with a phase difference to the leads.

We use DMRG [20] to obtain the steady state in the presence of a finite bias voltage by time-evolving the wave function $|\Psi(t)\rangle$ and then measuring its properties such as the current and spin correlations as a function of time $t$. This method has been successfully used to study nonequilibrium transport through nanostructures with electronic correlations [17,24,25]. We evaluate the spin correlations from [26]

$$S_{12}(t) = \langle \Psi(t)|\vec{S}_1 \cdot \vec{S}_2|\Psi(t)\rangle. \tag{6}$$

The current between two sites in the leads is defined as

$$J_{l,m}(t) = it_0 \sum_\sigma \langle \Psi(t)|c^\dagger_{l\sigma} c_{m\sigma} - c^\dagger_{m\sigma} c_{l\sigma}|\Psi(t)\rangle. \tag{7}$$

In the figures, we display the current $J = (J_{L2,L1} + J_{R1,R2})/2$ averaged over the first link in the left and right lead.

Our simulations start from the system in equilibrium with a finite $\Gamma \neq 0$ and a charge per spin of $\langle n_{j\sigma}\rangle = 0.5$ on both dots. At time $t = 0$, we turn on a bias voltage $V = \mu_L - \mu_R$ that drives the system out of equilibrium. We work at large values of $\Gamma = 0.25$ such that the transient dynamics to reach the steady state is short [25]. The two quantum dots are treated as a supersite permitting the use of a Trotter-Suzuki breakup of $\exp(-iHt)$ [27]. The time step is $\delta t \sim 0.1$ and we enforce a fixed discarded weight [27] of $10^{-5}$ or less, keeping a maximum of 2000 DMRG states. All runs are performed at an overall half-filling of dots and leads.

*Results.*—In Fig. 1, we elucidate the time dependence of the current and spin correlations, comparing the behavior of $\phi = 0$ to $\phi = \pi$. Similar to a single quantum dot [25], the current undergoes transient dynamics, and then takes a quasistationary value (i.e., a plateau in time), which we shall refer to as the steady-state regime. Note that on finite systems, there is a system-size dependent revival time, resulting in a decay of the steady state current and a sign change (realized for $t \gtrsim 38$). For a discussion of transient time scales as well as an analysis of time dependent data for currents, see Ref. [25].

For the spin correlations shown in Fig. 1(b), we first observe that in the initial state, $S_{12} > 0$ for $\phi = 0$ whereas the correlation vanishes for $\phi = \pi$. The application of the bias voltage does virtually not affect the value of $S_{12}$ for $\phi = 0$, which remains positive. The more interesting behavior is realized for $\phi = \pi$. As a function of time, $S_{12}$ decreases and approaches a roughly constant value. The transient time is comparable to the one for the current and is of order $1/\Gamma$. Moreover, the transients are suppressed by increasing the bias, similar to a single quantum dot [25]. This finite and large spin correlation between the spins localized in the dots that emerges in the steady state and that is induced by driving a current through the structure is the main aspect of our work. It implies that nonequilibrium dynamics can be used to prepare a DQD in a correlated and thus entangled state.

To link the spin correlations to entanglement we use the concurrence $C_{12}$ [28,29]. For instance, the concurrence approaches $C_{12} = 1$ if the spin correlation is $-3/4$ and if there are no charge fluctuations on the dots [21]. In Fig. 1(b) we include the concurrence versus time calculated for $\phi = \pi$. We observe that for $t = 0$ the concurrence is zero

showing that the dots are not entangled. Applying the bias, and after reaching the steady state for the spin correlations, the concurrence takes a value $C_{12} \sim 0.3$ corresponding to a finite entanglement between the dots.

The qualitative behavior of the spin correlations can be understood by using a canonical transformation of the states of the leads, which is given by (see, e.g., Refs. [23,30])

$$c_{\gamma l\sigma} = (c_{Rl\sigma} \pm c_{Ll\sigma})/\sqrt{2}, \tag{8}$$

where $\gamma = s$, $a$ are the symmetric and antisymmetric combinations, respectively. The result of this transformation is sketched in Fig. 2, where the leads shown there now represent the new states obtained from Eq. (8). In the absence of a bias voltage, there is no direct coupling between these new states, as depicted in Figs. 2(a.1) and (b.1). Most importantly, the dots are coupled to only the symmetric states for $\phi = 0$, whereas for $\phi = \pi$, dot $j = 1$ is coupled to the symmetric states and dot $j = 2$ to the antisymmetric ones. For $\phi = 0$, the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction gives rise to a ferromagnetic correlation between the dots since each path that connects them involves an odd number of sites and since the leads are at half-filling [22]. For $\phi = \pi$, the dots are part of two decoupled subsystems and therefore, $S_{12}$ vanishes.

Upon applying a bias, one effectively obtains a ladder geometry where the voltage acts as a transverse coupling between the symmetric and antisymmetric states of Eq. (8) as shown in Figs. 2(a.2) and (b.2). For $\phi = 0$, the coupling $V$ only marginally affects the correlations. By contrast, for $\phi = \pi$ and $V \neq 0$, the dots are now connected through paths with an even number of sites in the effective leads and therefore, in the *ground state* of such a geometry, one expects a finite negative spin correlation. Our numerical results shown in Fig. 1(b) unveil that the same behavior occurs in *nonequilibrium* as well. While here we focus on fully symmetric tunnel couplings, the main results can be recovered in the case of asymmetric couplings [21], and

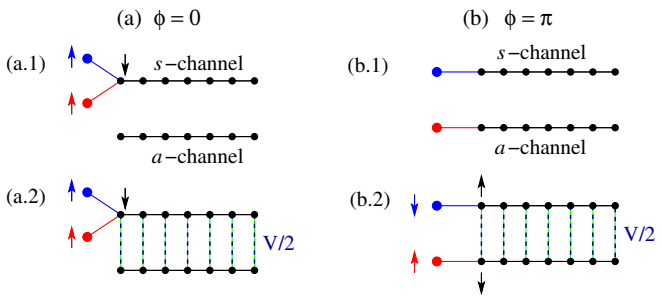


FIG. 2 (color online). Illustration of the canonical transformation Eq. (8). (a) $\phi = 0$. (b) $\phi = \pi$. (a.1), (b.1): $V = 0$; (a.2), (b.2): $V \neq 0$. The application of the bias leads to a ladder structure where the bias acts like a transverse hopping matrix element between the symmetric ($s$ channel) and antisymmetric states ($a$ channel) defined in Eq. (8).

therefore, fine-tuning of parameters is not necessary to observe a change of $S_{12}$ induced by a bias $V$.

After qualitatively explaining the emergence of finite spin correlations in the current-carrying stationary state, we next study the dependence of the steady-state properties on the bias potential. We denote the steady-state values by $\langle S_{12}\rangle$ and $\langle J\rangle$, obtained from averaging over time-dependent data in the steady-state regime (compare Ref. [25]). Figure 3(a) shows $\langle J\rangle/V$ versus $V$ for phases $\phi = 0$ and $\pi$. For $\phi = 0$, $\langle J\rangle/V$ approaches a constant value at low bias [22]. For $\phi = \pi$, the linear conductance vanishes due to the Aharanov-Bohm effect [23]. A finite voltage causes a finite current to flow in both cases, but $\langle J\rangle/V$ for $\phi = 0$ is always larger than in the $\phi = \pi$ case.

In Fig. 3(b), we display the steady-state spin correlations $\langle S_{12}\rangle$ versus $V$. First, let us emphasize that data for the steady-state values obtained from systems of different lengths are included, showing that all our main results are quantitatively robust against finite-size effects. For $\phi = 0$, a constant value of $\langle S_{12}\rangle > 0$ is found. A slight decrease appears for $V \gtrsim 1$, which we trace back to the variation of the LDOS of the leads seen by the dots. Since in our simulations we work with tight-binding bands with a finite bandwidth and band curvature, this LDOS decreases with $V$. For the case of $\phi = \pi$, the value of the steady-state correlations can be tuned by the bias voltage and in fact, $\langle S_{12}\rangle$ increases with $U$. Therefore, to obtain a strong correlation a large voltage is needed putting the system out of the Kondo regime. As the figure clearly shows, we can get to $\langle S_{12}\rangle \approx -0.25$ for $U/\Gamma = 2$. We therefore realize a mixed state with singlet correlations dominating over triplet correlations. If there were no charge fluctuations then this value of $S_{12}$ would correspond to a Werner state [31,32] with 50% of the weight in the singlet. In our

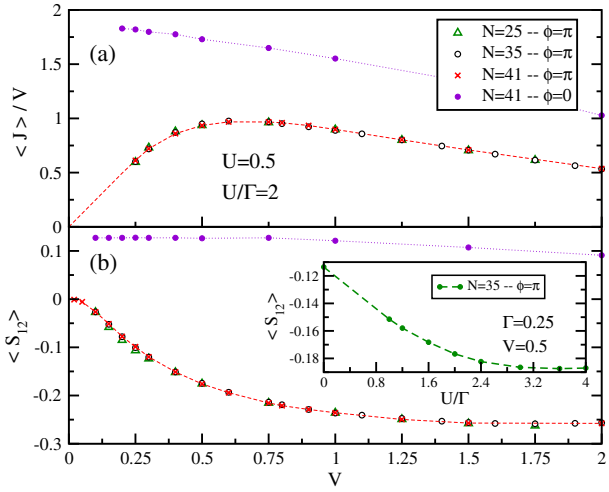


FIG. 3 (color online). (a) $\langle J\rangle/V$ vs $V$ for $\phi = 0$ and $\phi = \pi$ in units of twice the conductance quantum $G_0$. (b) Steady-state spin correlations $\langle S_{12}\rangle$ vs bias $V$. The figure shows data for different system sizes $N = 25, 35, 41$ for $\phi = \pi$. In (a) and (b), $U/\Gamma = 2$. Inset in (b): Steady-state spin correlations vs $U/\Gamma$ for $V = 0.5$.

case, however, the current needed to obtain the entangled state typically induces charge fluctuations at large $V$. Therefore, $\langle S_{12}\rangle \leq -1/4$ implies an even larger relative contribution of the singlet over the triplet than in a situation without any charge fluctuations. The fact that a finite voltage unavoidably induces charge fluctuations is the reason why the steady-state spin correlations do not reach their largest possible value $-3/4$.

The steady-state values further depend on $U/\Gamma$. To elucidate this, we plot $\langle S_{12}\rangle$ versus $U$ in the inset of Fig. 3(b) for a fixed value of $V = 0.5$, by increasing $U/\Gamma$ to 4, i.e., in a regime where charge fluctuations are still relevant even in equilibrium. As expected, the larger $U$, the more strongly charge fluctuations are suppressed, leading to larger steady-state spin correlations. Therefore, either a large $U/\Gamma$ at a fixed voltage or applying a large voltage order of $V \sim t$ induces the largest steady-state correlations. Fortunately, many experiments with DQDs realize $U/\Gamma \gtrsim 10$ [4,5], thus relaxing the requirement on voltage. An important role of $U$ is to define a local spin as in many other quantum information application of quantum dots [8].

So far we have investigated the dependence of correlations on $V$, $U$, and $\phi$ in nonequilibrium, comparing the cases of $\phi = 0$ to $\phi = \pi$. An additional degree of tunability can be added if the phase can take arbitrary values (see Fig. S1 in the Supplemental Material [21]). As expected from the discussion of Fig. 2, $\langle S_{12}\rangle$ is positive for small $\phi$ at $V = 0$ and then decreases to zero as $\phi = \pi$ is approached. This transition to the uncorrelated case of $\phi = \pi$ is continuous. At a finite voltage, it is possible to go from positive steady-state correlations to negative ones by changing $\phi$. For the parameters of Fig. 3(a), the steady-state correlations change sign at $\phi_c \approx 0.18\pi$ (see Fig. S1). This value depends both on $U$ and $V$. To summarize, the steady-state correlations can be tuned both in sign and magnitude by changing $V$, $\phi$, and $U$. We have further verified that the steady-state correlations are independent of the initial conditions [21].

Based on the qualitative picture developed so far, we conclude that the steady-state correlations are a result of mixing the symmetric and antisymmetric states of lead electrons in nonequilibrium. At finite $U$, this may be viewed as an RKKY effect in nonequilibrium. A discussion on how to estimate the effective indirect coupling $J_{\mathrm{eff}}(V)$ induced by the bias can be found in the Supplemental Material [21]. As is well known from the physics of the RKKY effect in equilibrium, the spin correlation induced by indirect exchange is destroyed for temperatures larger than $\Gamma$ [33]. For the nonequilibrium version of RKKY discussed here, we expect that temperatures should be smaller than the effective strength $J_{\mathrm{eff}}(V)$ shown in [21] for thermal fluctuations not to affect the induced correlations.

Finally, we study the behavior of $S_{12}$ under quenches of parameters of the Hamiltonian Eq. (1). We proceed as before, i.e., a finite bias voltage $V > 0$ is turned on at $t = 0$, and in addition we instantaneously change some of the tunnel couplings at a time $t_q \geq 0$.

We find that if we disconnect the quantum dots from the leads at time $t_q > 0$ by setting $t_1' = t_2' = 0$ after the steady state has been established, as expected, the spins remain in a correlated state after isolating them from the reservoirs (see Fig. S4(b) in Ref. [21]).

In a second example, after reaching the steady state, we isolate one of the dots while the current continues to flow through the other. This results in the loss of the spin correlations after a short transient time (see Fig. S4(c) in [21]). Therefore, control over the tunneling matrix elements allows one to put the system back into its original uncorrelated state. Both the generation of entanglement and the removal happen on short time scales, similar to the proposals discussed in Ref. [16].

*Summary.*—In this work, we demonstrated that spin correlations between spatially separated electrons localized in a parallel DQD embedded in the rings of an Aharonov-Bohm interferometer can be induced and modified by driving a current through the structure. The steady-state correlations depend on voltage, the flux, and Coulomb interactions. Control over the individual tunneling couplings would allow one to isolate the entangled spins from the environment or to remove the entanglement again. The mechanism behind this time-dependent formation of correlations can be thought of as an RKKY effect in nonequilibrium. Our results may be relevant for applications of DQD structures in quantum information processing.

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