Enhanced conductance through side-coupled double quantum dots

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Conductance, on-site, and intersite charge fluctuations and spin correlations in the system of two side-coupled quantum dots are calculated using Wilson’s numerical renormalization group (NRG) technique. We also show the spectral density calculated using the density-matrix NRG, which for some parameter ranges remedies inconsistencies of the conventional approach. By changing the gate voltage and the interdot tunneling rate, the system can be tuned to a nonconducting spin-singlet state, the usual Kondo regime with an odd number of electrons occupying the dots, the two-stage Kondo regime with two electrons, or a valence-fluctuating state associated with a Fano resonance. Analytical expressions for the width of the Kondo regime and the Kondo temperature are given. We also study the effect of unequal gate voltages and the stability of the two-stage Kondo effect with respect to such perturbations.

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I. INTRODUCTION

The advances in microfabrication have enabled studies of transport through single as well as coupled quantum dots, where at very low temperatures Kondo physics and magnetic interactions play an important role. A double-dot system represents the simplest possible generalization of a single-dot system which has been extensively studied in the past. Recent experiments demonstrate that an extraordinary control over the physical properties of double dots can be achieved, which enables direct experimental investigations of the competition between the Kondo effect and the exchange interaction between localized moments on the dots. One manifestation of this competition is a two-stage Kondo effect that has recently been predicted in multilevel quantum dot systems with explicit exchange interaction coupled to one or two conduction channels. Experimentally, it manifests itself as a sharp drop in the conductance versus gate voltage $G(V_g)$ (Ref. 7) or as nonmonotonic dependence of the differential conductance versus drain-source voltage $dI/dV_{ds}(V_{ds})$ (Ref. 8).

Fano resonances, which occur due to interference when a discrete level is weakly coupled to a continuous band, were recently observed in experiments on rings with embedded quantum dots and quantum wires with side-coupled dots. The interplay between Fano and Kondo resonances was investigated using equation-of-motion and slave-boson techniques.

In this work we study a double quantum dot (DQD) in a side-coupled configuration (Fig. 1), connected to a single conduction-electron channel. Systems of this type were studied previously using a noncrossing approximation, embedding technique, and slave-boson mean-field theory. Numerical renormalization group (NRG) calculations were also performed recently, where only narrow regimes of enhanced conductance were found at low temperatures. We will show that when the interdot overlap is large, wide regimes of enhanced conductance as a function of gate-voltage exist at low temperatures due to the Kondo effect, separated by regimes where localized spins on DQD’s are antiferromagnetically (AFM) coupled. Kondo temperatures $T_K$ follow a prediction based on Schrieffer-Wolff transformation and poor-man’s scaling. In the limit when the dot $a$ is only weakly coupled, the system enters the “two-stage” Kondo regime where we again find a wide regime of enhanced conductivity under the condition that the high and low Kondo temperatures ($T_K$ and $T'_K$ respectively) be well separated and the temperature of the system $T$ be in the interval $T'_K \ll T \ll T_K$.

II. MODEL AND METHOD

The Hamiltonian that we study reads

$$H = \delta_d(n_d - 1) + \delta_a(n_a - 1) - t \sum_{\sigma} (d_{\sigma}^a d_{\sigma} + a_{\sigma}^d a_{\sigma})$$

$$+ \frac{U_d}{2} (n_d - 1)^2 + \frac{U_a}{2} (n_a - 1)^2$$

$$+ \sum_{k\sigma} \epsilon_k c_{k\sigma}^d c_{k\sigma}^\dagger + \sum_{k\sigma} V_d(k)(c_{k\sigma}^d a_{\sigma} + d_{\sigma}^a c_{k\sigma}) \tag{1}$$

where $n_d = \sum_d d_{\sigma}^d d_{\sigma}$ and $n_a = \sum_a a_{\sigma}^a a_{\sigma}$. The operators $d_{\sigma}^a$ and $a_{\sigma}$ are creation operators for an electron with spin $\sigma$ on site $d$ or $a$. On-site energies of the dots are defined by $\epsilon = \delta - U/2$. For simplicity, we choose the on-site energies and Coulomb interactions to be equal on both dots, $\delta_d = \delta_a = \delta$ and $U_a = U_d = U$. Coupling between the dots is described by the interdot tunnel coupling $t_d$. Dot $d$ couples to both leads with equal hopping $t'$. As it couples only to symmetric combinations of

![Figure 1](color online) Side-coupled configuration of quantum dots.
the states from the left and right leads, we have used a unitary transformation\textsuperscript{19} to describe the system as a variety of the single-channel, two-impurity Anderson model. The operator \( c_{\nu,\sigma}^\dagger \) creates a conduction band electron with momentum \( k \), spin \( \sigma \), and energy \( E_{\nu} = -D \cos k \), where \( D = 2t \) is the half-bandwidth. The momentum-dependent hybridization function is \( V_d(k) = -(2/\sqrt{1+N^2})t' \sin k \), where \( N \) in the normalization factor is the number of conduction band states.

We use the Meir-Wingreen formula for conductance in the case of proportionate coupling\textsuperscript{20} which is known to apply under very general conditions (for example, the system need not be in a Fermi-liquid ground state) with spectral functions obtained using the NRG technique.\textsuperscript{21–24} At zero temperature, the conductance is

\[
G = G_0 \pi \Gamma \rho_d(0),
\]

where \( G_0 = 2e^2/h \), \( \rho_d(\omega) \) is the local density of states of electrons on site \( d \), and \( \Gamma(\omega) = (\tau' / \tau)^2 \).

The NRG technique consists of logarithmic discretization of the conduction band, mapping onto a one-dimensional chain with exponentially decreasing hopping constants, and iterative diagonalization of the resulting Hamiltonian.\textsuperscript{21} Only the low-energy part of the spectrum is kept after each iteration step; in our calculations we kept 1200 states, not counting spin degeneracies, using the discretization parameter \( \Lambda = 1.5 \).

III. STRONG INTER-DOT COUPLING

A. Conductance and correlation functions

In Fig. 2(a) we present conductance through a double quantum dot at different values of interdot couplings versus \( \delta \). Due to the formation of Kondo correlations, conductance is enhanced, reaching the unitary limit in a wide range of \( \delta \).

To better understand multitod problems in the case of strong interdot coupling, it is helpful to exactly diagonalize the part of the Hamiltonian that describes the dots and rewrite the entire Hamiltonian [Eq. (1)] in a form similar to the ionic model:\textsuperscript{25}

\[
H_0 = \sum_{k,\sigma} e_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_a E(a)|a\rangle\langle a|,
\]

\[
H_1 = \sum_{k,\sigma,\alpha,\beta} t_{k\sigma\beta-\alpha} |\alpha\rangle\langle \beta| c_{k,\sigma} + \sum_{k,\sigma} t_{k\sigma\alpha-\beta} |\beta\rangle\langle \alpha| c_{k,\sigma}^\dagger,
\]

where multi-indices \( \alpha \) and \( \beta \) stand for quantum numbers \( (Q, S, S_z, r) \). Here \( Q \) is the charge number \( Q = (n_a - 1) + (n_d - 1) \) and \( S \) and \( S_z \) are the spin and its component, while \( r \) numbers different states with the same \( Q, S, S_z \) quantum numbers. In the absence of a magnetic field, \( S_z \) is irrelevant and will be omitted from now on. Each \( (Q, S, r) \) multiplet is then \((2S+1)\)-fold degenerate. Finally, the effective hopping coefficients

\[
t_{k\sigma\beta-\alpha} = V_d(k)|\alpha\rangle\langle d'_{\beta}| \beta\rangle
\]

correspond to electrons hopping from the conduction band to the dots.

FIG. 2. (Color online) Conductance and correlation functions of DQD vs \( \delta \). Besides different values of \( t_d \), indicated in the figure, other parameters of the model are \( \Gamma / D = 0.03 \) and \( U / D = 1 \). Temperature is \( T / D = 10^{-6} \), which for all parameters used corresponds to a zero-temperature limit. In particular, in the Kondo plateaus, \( T \ll T_k \) for all \( \delta \).

The eigenvalue diagram in Fig. 3 represents the gate-voltage dependence of the multiplet energies \( E(Q, S, r) \). From this diagram we can read off the ground state and the excited states for each parameter \( \delta \).

Regimes of enhanced conductance appear in the intervals approximately given by \( \delta_1 \leq |\delta| < \delta_2 \), where \( \delta_1 = t_d(2\sqrt{1 + (U / 4t_d)^2} - 1) \) and \( \delta_2 = (U / 2 + t_d) \). These estimates are obtained from the lowest energies of states with zero, one, and two electrons on the isolated double quantum dot:

\[
E(-2, 0, 0) = U - 2\delta,
\]

\[
E(-1, 1, 0) = U / 2 - \delta - t_d,
\]

FIG. 3. (Color online) Eigenvalue diagram for the isolated DQD system. The diagram is symmetric, since for \( \delta \rightarrow -\delta \), \( E(Q, S, r) \rightarrow E(-Q, S, r) \). Points A and B correspond to valence-fluctuation regions when the charge on the dot changes, while point C corresponds to the center of the Kondo regime, when the Kondo temperature is the lowest. Parameters are \( U / D = 1 \) and \( t_d / D = 0.3 \).
The width of conductance peaks (measured at $G/G_0=1/2$) are therefore approximately given by

$$\Delta = \frac{U}{2} + 2t_d[1 - \frac{1}{4} + (U/4t_d)^2].$$

(7)

Note that in the limit of large $t_d$, $\Delta = U/2$, and in the limit of large $U$, $\Delta \approx 2t_d$. As it will become apparent later in this paper, this naive estimate fails when $t_d \rightarrow 0$. Comparison of conductance-peak widths with the analytical result as given in the text is shown in Fig. 4(a).

Next, we focus on various correlation functions. In Fig. 2(b) we show $S$, calculated from expectation value $(S_{tot})^2 = S(S+1)$, where $S_{tot} = S_a + S_d$ is the total spin operator. $S$ reaches value 1/2 in the regime where $G/G_0=1$. Enhanced conductance is thus followed by the local moment formation, indicative of the Kondo effect. This is further supported by the average double-dot occupancy $\langle n \rangle$, where $n=n_a+n_d$, which in the regime of enhanced conductivities approaches odd-integer values—i.e., $\langle n \rangle = 1$ and 3 [see Fig. 2(c)]. Transitions between regimes of nearly integer occupancies are rather sharp; they are visible as regions of enhanced charge fluctuations measured by $\Delta n^2 = \langle n^2 \rangle - \langle n \rangle^2$, as shown in Fig. 2(d). Finally, we show in Fig. 2(e) the spin-spin correlation function $(S_a, S_d)$. Its value is negative between two separated Kondo regimes where the conductance approaches zero—i.e., for $-\delta_i < \delta < \delta_i$; otherwise, it is zero. This regime further coincides with $\langle n \rangle \sim 2$. Each dot thus becomes nearly singly occupied, and spins on the two dots form a local singlet due to effective exchange coupling $J_{eff} = 4t_d^2/U$. Surprisingly, the absolute value of $(S_a, S_d)$ increases and it nearly reaches its limiting value—i.e., $(S_a, S_d) = -3/4$—as the inter-dot hopping $t_d$ and, with it, $J_{eff}$ decrease. This seeming contradiction is resolved by recognizing that $J_{eff}$ represents the exchange interaction based on the effective Heisenberg coupling between localized spins on DQQ’s only in the limit when $t_d \rightarrow 0$. Smaller absolute values of $(S_a, S_d)$ are thus due to a small amount of double occupancy at larger values of $t_d/U$.

In Fig. 4(b) we present Kondo temperatures $T_K$ vs $\delta$ extracted from the widths of Kondo peaks. Numerical results in the regime where $\langle n \rangle \sim 1$ and 3 fit the analytical expression obtained using the Schrieffer-Wolff transformation that leads to an effective single $S=1/2$ Kondo model. We obtain

$$T_K = \frac{0.182U}{\rho_0 J \exp[-1/\rho_0 J]},$$

(8)

with

$$\rho_0 J = \frac{2\Gamma \alpha}{\pi} \left[ \left( E \left( -1, \frac{1}{2}, 0 \right) - E(-2,0,0) \right)^2 \right. + \left. \left( E \left( -1, \frac{1}{2}, 0 \right) - E(0,0,0) \right)^2 \right],$$

(9)

where

$$\alpha = \left( \left| -1, \frac{1}{2}, 0 \right| d_1^\dagger \left| -2,0,0,0 \right\rangle \right|^2 = 1/2,$$

$$\beta = \left( \left| 0,0,0,0 \right| d_1^\dagger \left| -1, \frac{1}{2}, \frac{1}{2}, 0 \right\rangle \right|^2 = \frac{(4t_d^2 + U + \sqrt{16t_d^4 + U^2})^2}{8[16t_d^4 + U(U + \sqrt{16t_d^4 + U^2})^2]}.$$  

(10)

The factor of 0.182$U$ in Eq. (8) is the effective bandwidth. The same effective bandwidth was used to obtain $T_K$ of the Anderson model in the regime $U<D$.23,26

B. Spectral densities

We observed that the spectral density calculation using the conventional NRG approach27 fails for our model. The spectral densities manifest spurious discontinuities, and the normalization sum rule is violated for some choices of model parameters (Fig. 5). This happens because at the early stages of the NRG iteration the lowest-energy state does not yet correspond to the true ground state. We found that we obtain correct results using the density-matrix (DM) NRG.
FIG. 6. (Color online) Zero-temperature spectral density $\rho_d(\omega)$ sweeps for $t_d/D=0.3$. (a) Spectral density calculated using the conventional NRG approach. (b) Spectral density calculated using the density-matrix NRG approach. Note that the vertical line, representing the Kondo peak, has been artificially broadened. Its true width is given by $T_K$.

Features in the spectral density sweeps can be easily interpreted using eigenvalue diagram in Fig. 3. At low temperatures and for constant $\delta$, the spectral density $A(\omega)$ will be high whenever the energy difference $\Delta E=E_{1}-E_{0}$ between the ground state (0) and an excited state (1) is equal to $+\omega$ (particle excitations, $Q_{1}=Q_{0}+1, S_{1}=S_{0}\mp\frac{1}{2}$) or to $-\omega$ (hole excitations, $Q_{1}=Q_{0}-1, S_{1}=S_{0}\pm\frac{1}{2}$). At $\delta=0$ two broad peaks are seen located symmetrically at $\omega \sim \pm \delta_i$ (see Figs. 6 and 7, at $\delta/D=0$). At this point the model is particle-hole symmetric and therefore $E(Q,S,r)=E(-Q,-S,r)$ for all $Q,S,r$. Consequently, the spectrum is also symmetric, $\rho_d(\omega)=\rho_d(-\omega)$. With increasing $\delta$, the particle excitation energy $E(1,\frac{1}{2},0)-E(0,0,0)$ increases and the corresponding peak quickly washes out. The hole excitation energy $E(-1,\frac{1}{2},0)-E(0,0,0)$ decreases and the peak gains weight.

At $\delta=\delta_1$, $E(0,0,0)=E(-1,\frac{1}{2},0)$ (point A in Fig. 3) and the system enters the Kondo regime: a sharp many-body resonance appears which remains pinned at the Fermi level throughout the Kondo region (see Figs. 6 and 7, at $\delta/D=0.62$). The Kondo effect occurs whenever the ground state is a doublet, $S=1/2$, and there are excited states with $S'=0,1, Q'=Q\pm1$. We recognize such regions by characteristic triangular level crossings in the eigenvalue diagram, one of which is marked as triangle $ABC$ in Fig. 3. The high-energy peaks at $\omega=E(0,0,0)-E(-1,\frac{1}{2},0)>0$ and $\omega=E(-1,\frac{1}{2},0)-E(-2,0,0)<0$ in the spectral density are also characteristic: they correspond to particle and hole excitations that are at the heart of the Kondo effect.

In the case of the DQD we also see additional structure for $\delta_1<\delta<\delta_2$: a broad peak at $\omega=E(0,1,0)-E(-1,\frac{1}{2},0)$ which corresponds to virtual triplet excitations from the ground state. These excitations could also be taken into account in the calculation of the effective exchange interaction, Eq. (9); however, due to their high energy, they only lead to an exponentially small renormalization of the Kondo temperature, which may be neglected.

In the inset of Fig. 7 we show scaling of Kondo peaks versus $\omega/T_K$. In the case of perfect scaling, all curves should exactly overlap. However, Kondo temperatures of different peaks differ by almost four orders of magnitudes, as seen in Fig. 4(b). Moreover, Kondo peaks become asymmetric near the edges of the Kondo region—i.e., for $\delta=\delta_1$ and $\delta=\delta_2$. Note also that for each point in Fig. 4(b) there is a respective spectral density presented in the inset of Fig. 7.

C. Effect of the on-site-energy splitting

In real double-quantum-dot systems, it is difficult to produce dots and electrodes with identical properties. In particular, it is not easy to achieve equal on-site energies $\delta_i=\delta_a=\delta$ for a wide range of parameters $\delta$. Therefore it is necessary to study the robustness of the physical regimes with respect to the splitting of the on-site energies.

We now generalize slightly our model to allow for unequal on-site energies by introducing a new parameter $\kappa$, so that on-site energies are $\delta_i=\delta+\kappa$ and $\delta_a=\delta-\kappa$. The DQD part of the Hamiltonian is now

$$H_0 = (\delta + \kappa)(n_d - 1) + (\delta - \kappa)(n_a - 1) - t_d \sum_\sigma (d_\sigma^\dagger a_\sigma + a_\sigma^\dagger d_\sigma)$$

$$+ \frac{U}{2} (n_d - 1)^2 + \frac{U}{2} (n_a - 1)^2.$$ 

(11)

Only $\kappa>0$ has to be considered, because $H_0(\delta,-\kappa)$ $-H_0(\delta,\kappa)$ when particle-hole transformation $d_\mu^\dagger \rightarrow d_\mu^\dagger a_\mu^\dagger$ $-a_\mu^\dagger$ is performed.
FIG. 8. (Color online) Conductance as a function of gate-voltage \( \delta_d \) for different gate-voltage asymmetries \( \kappa \). The label SIAM corresponds to results for conductance of the corresponding single-impurity Anderson model. The temperature is \( T/D = 10^{-9} \).

By diagonalization \( H_0 \) exactly, we find that the effect of \( \kappa \) is to shift states while the general eigenvalue structure is maintained and is similar to that shown in Fig. 3. We therefore still expect to see two Kondo peaks as \( \delta \) is swept for a constant \( \kappa \).

In the limit of large \( \kappa \) and for \( \delta \) such that \( \delta_d \rightarrow 0 \) and \( \delta_i \rightarrow \pm \infty \), the side-coupled dot becomes irrelevant and we recover the familiar single-impurity Anderson model with conduction plateau in the region \( -U/2 \leq \delta_d < U/2 \) with \( T_K \) given by Eq. (8) with

\[
\rho_0 J = \frac{2 \Gamma}{\pi} \left( \frac{1}{|\delta_d - U/2|} + \frac{1}{|\delta_d + U/2|} \right).
\]

This scenario is corroborated by NRG calculations (Fig. 8). The approach to the limit can be determined using expressions (8) and (9), with \( \kappa \)-dependent \( a(\kappa) \), \( b(\kappa) \), and \( E_1(\kappa), E_2(\kappa) \). The result is shown in Fig. 9(a). The \( \kappa \) dependence is nonmonotonic, which can be traced to the nonmonotonic behavior of the coefficient \( b(\kappa) \). At \( \kappa/D = 1 \) the asymptotic value \( T_K/D = 1.04 \times 10^{-7} \) is nearly reached.

In the limit of large \( \kappa \), but for \( \delta \) such that \( \delta_d \rightarrow 0 \) and \( \delta_i \rightarrow \pm \infty \), the embedded dot will be either fully occupied or empty with very little charge fluctuations, while the side-coupled dot will maintain \( S = 1/2 \) spin moment. This moment will be screened, but due to the suppression of the virtual electron hopping through the dot \( d \), the corresponding Kondo temperature rapidly drops with increasing \( \kappa \) [Fig. 9(b)]. Keeping the temperature constant and increasing \( \kappa \), the Kondo plateau in the region \( -U/2 \leq \delta_d < U/2 \) will therefore quickly evolve into two peaks separated by a Coulomb blockade valley and for very large \( \kappa \) it will not conduct at all. This prediction can also be verified using NRG (Fig. 10).

IV. WEAK INTERDOT COUPLING

A. Conductance and correlation functions

We now turn to the limit when \( t_d/D \rightarrow 0 \). Unless otherwise specified, we choose the effective temperature \( T \) to be finite—i.e., \( T / D \rightarrow 10^{-9} D \), since calculations at much lower temperatures would be experimentally irrelevant. In this case one naively expects to obtain essentially identical conductance as in the single-dot case. As \( \delta \) decreases below \( \delta \sim U/2 \), \( G/G_0 \) indeed follows result obtained for the single-dot case as shown in Fig. 11(a). In the case of DQD’s, however, a sharp Fano resonance appears at \( \delta = U/2 \). This resonance coincides with the sudden jump in \( S, \langle n \rangle \), as well as with the spike in \( \Delta n^2 \), as shown in Figs. 11(b)–11(d), respectively. Fano resonance is a consequence of a sudden charging of the nearly decoupled dot \( a \), as its level \( \epsilon \) crosses the chemical potential of the leads—i.e., at \( \epsilon = 0 \). Meanwhile, the electron density on the dot \( d \) remains a smooth function of \( \delta \), as seen from \( \langle n_d \rangle \) in Fig. 11(c). With increasing \( t_d \), the width of the resonance increases, as shown for \( t_d/D = 0.01 \) in Fig. 11(f). For \( t_d = 0.1 \), the resonance merges with the Kondo plateau and disappears [see Fig. 2(a)].

The resonance at \( \delta \sim U/2 \) can be explained using a simple semianalytical model. For \( t_d = 0 \), we write the exact Green’s function of the impurity \( d \) at \( a = 0 \) as \( \chi_0^d = 1/(\Gamma - \Gamma \cot \phi) \), where \( \phi \) is the scattering phase shift for single impurity
Fig. 11. (Color online) Conductance and correlation functions at \( t_d/D = 0.001 \) (a)–(e), \( t_d/D = 0.01 \) (f) and (g), and a blow-up of (f) in the inset of (g). Dashed lines in (a) represent \( G/G_0 \) and (b) \( S \) of a single quantum dot with otherwise identical parameters. Dashed line in (c) represents \( (n_d) \) of DQD, and finally dashed line in the inset of (g) represents the semianalytical model described in the text. In (h) a schematic plot of different temperatures and interactions is presented as explained in the text. NRG values of the gap in \( \rho_{J}(\omega) \) at \( \omega = 0 \) and \( T \ll T_K \) are presented with open circles and squares for \( t_d/D = 0.001 \) and 0.01, respectively. Values of \( J_{\text{eff}} \) and analytical results of \( T_K^0 \) are presented as dashed and dot-dashed lines for \( t_d/D = 0.001 \) and 0.01, respectively. For analytical estimates of \( T_K^0 \) different values of \( \alpha = 2.2 \) and 1.3, respectively, were used. Other parameters of the model are \( \Gamma/D = 0.03, U/D = 1 \).

model that we calculate using NRG. The side-coupled dot is taken into account from the Dyson’s equation

\[
G_d = G_0 d(1 - t_d^2 G_0 G_d^2).
\]

For the Fano resonance at \( \epsilon = \delta - U/2 \), we keep only the low-energy pole in the Green's function,

\[
G_0(\omega) = \frac{z}{\omega - \epsilon + i \eta},
\]

where \( z = 1/2 \) for \( \epsilon < 0 \) and \( z = 1 \) for \( \epsilon > 0 \). The conductance is

\[
G = G_0 \frac{2\Gamma^2 e^2}{\epsilon^2} \sin^2 \phi - \frac{4\Gamma^2 e^2}{\epsilon^2} \cos(2\phi) - 2\Gamma^2 e^2 \Gamma \sin(2\phi).
\]

Just below \( \delta < U/2 \), \( T \) falls in the interval, given by \( T_K^0 \ll T \ll T_K \), where

\[
T_K^0 \sim T_K \exp(-\alpha T_K^0/\Gamma_{\text{eff}})
\]

denotes the lower Kondo temperature, corresponding to the gap in the spectral density \( \rho_{J}(\omega) \) at \( \omega = 0 \) and \( \alpha \) is of the order of 1 (Ref. 17). Note that NRG values of the gap in \( \rho_{J}(\omega) \) (open circles and squares), calculated at \( T \ll T_K^0 \), follow analytical results for \( T_K^0(\delta) \) when \( J_{\text{eff}} < T_K \) [see Fig. 11(h)], while in the opposite regime—i.e., for \( J_{\text{eff}} > T_K \) —they approach \( J_{\text{eff}} \).

As shown in Fig. 11(a) for \( 0.3D \leq \delta < U/2 \), \( G/G_0 \) calculated at \( T = 10^{-4}D \) follows results obtained in the single-quantum-dot case and approaches the value 1. The spin quantum number \( S \) in Fig. 11(b) reaches the value \( S \sim 0.8 \), consistent with the result obtained for a system of two decoupled spin-1/2 particles, where \( \langle \hat{S}_z \rangle = 3/2 \). This result is also in agreement with \( n \sim 2 \) and the small value of the spin-spin correlation function \( \langle \hat{S}_x \cdot \hat{S}_y \rangle \), presented in Figs. 11(c) and 11(e), respectively.
manifests as two successive decreases of the susceptibility, at $T \sim T_K$ from around 0.5 to 0.25 and at $T \sim T'_K$ from around 0.25 to 0.17. We now investigate how this behavior changes when $\kappa \neq 0$ by comparing temperature-dependent susceptibilities calculated for a range of parameters $\kappa$.

We find that the two-stage Kondo effect is robust against $\kappa \neq 0$ perturbation. In fact, it survives until $\kappa = U/2$ (see Fig. 12). For $\kappa < U/2$ the main effect of $\kappa$ is to reduce the lower Kondo temperature $T'_K$. For $\kappa > U/2$, dot $a$ becomes irrelevant at low temperatures and dot $d$ is in the usual Kondo regime.

The transition from $\kappa < U/2$ to $\kappa > U/2$ is continuous despite a rather abrupt change in $\chi_{imp}$ caused by a rapid change in occupation of dot $a$ that occurs with increasing $\kappa$ on an energy scale proportional to $t_d^2$. For $\kappa = U/2$, $\epsilon_a = \delta_0 - U/2 = 0$ and the side-coupled dot is in the valence-fluctuation regime. For two uncoupled dots, one in the local-moment regime and the other in the valence-fluctuation regime, the magnetic moment $k_B T\chi/(g\mu_B)^2$ is expected to be $1/4 + 1/6 = 5/12$. At high temperatures, $\chi$ is indeed in the vicinity of this value.

V. CONCLUSIONS

In this paper we have explored different regimes of the side-coupled DQD. When quantum dots are strongly coupled, wide regions of enhanced, nearly unitary conductance exist due to the underlying Kondo physics. Analytical estimates for their positions and widths, as well as for the corresponding Kondo temperatures, are given and numerically verified. When two electrons occupy a DQD, the conductance is zero due to the formation of a spin-singlet state which is effectively decoupled from the leads. In this regime most physical properties of the coupled DQD’s can be predicted using the eigenvalue diagram of the isolated DQD system. This happens because energy separations of different DQD states are much larger than the Kondo temperature. Introducing the on-site-energy splitting between DQD’s induces new, even though not unexpected, effects within the Kondo regime. With increasing level splitting, the Kondo plateau is expanded when the level of the embedded dot is kept near the local particle-hole limit. In the other case, when, in contrast, the level of the side-coupled dot is kept near the particle-hole limit, Kondo plateau splits at finite $T$ due to abrupt decrease of $T_K$ with increasing level splitting.

When quantum dots are weakly coupled Fano resonance appears in the valence-fluctuation regime. Its width is enhanced as a consequence of interactions which should facilitate experimental observation. Unitary conductance exists when two electrons occupy a DQD due to a two-stage Kondo effect as long as the temperature of the system is well below $T_K$ and above $T'_K$. The experimental signature of the two-stage Kondo effect in the weakly coupled regime should materialize through the interdot-coupling sensitive width of the enhanced conductance versus gate voltage. Experimental observation of the two-stage Kondo effect would require no external magnetic field as used in Ref. 7. The interdot-coupling strength can be experimentally varied using gate electrodes.1–4

![FIG. 12. (Color online) Dynamic magnetic susceptibility $k_B T \chi(T)/(g\mu_B)^2$ for different $\kappa$. Parameters are $U/D = 1$, $\Gamma/D = 0.03$, $t_d/D = 8 \times 10^{-5}$, and $\delta/D = 0$. These calculations were performed using a different NRG discretization scheme (Ref. 29) with $\Lambda = 4$ and keeping 600 states.](image)
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APPENDIX: DENSITY-MATRIX NRG IN A \((Q,S)\) SUBSPACE BASIS

The density-matrix numerical renormalization group was originally implemented for a NRG iteration that uses subspaces with well-defined charge \(Q\) and spin projection \(S\). and it was used to determine the effect of magnetic field on spin-projected spectral densities. In the absence of a magnetic field, when rotational invariance in the spin space is recovered, it is advantageous to use subspaces with well-defined charge \(Q\) and spin \(S\), which leads to greatly enhanced numerical efficiency.

Here we show how the DM-NRG can be implemented in a \((Q,S)\) subspace basis in the case of a single conduction channel.

The density matrix at the last iteration step (estimated using the truncated basis) is

\[
\rho = \frac{1}{Z_{QSS_0}} \exp(-\beta E_{QSS_0}) |QSS_0\rangle \langle QSS_0|,
\]

where \(\omega\) enumerates different states in each \((Q,S)\) subspace and the grand-canonical statistical sum \(Z\) is

\[
Z = \text{Tr}[\exp(-\beta H)] = \sum_{QSS_0} \exp(-\beta E_{QSS_0}). \tag{A2}
\]

Unitary transformation of states from the \(N\)th to the \((N+1)\)th stage is

\[
|QSS_{N+1}\rangle = \sum_{r\alpha} U_{QSS}(r\alpha) |QSS,r\alpha\rangle_{N+1}, \tag{A3}
\]

where \(U_{QSS}\) are the corresponding unitary transformation matrices obtained during the diagonalization step of the NRG and the \(|QSS,r\alpha\rangle_{N+1}\) states are defined as

\[
|QSS,r\alpha\rangle_{N+1} = |Q + 1, S_\alpha, r\rangle_{N},
\]

\[
|QSS,r\alpha\rangle_{N+1} = u f_{(N+1)}^{\alpha} \left| Q, S - \frac{1}{2}, S_z - \frac{1}{2}, r \right\rangle_{N},
\]

\[
+ v f_{(N+1)}^{\alpha} \left| Q, S - \frac{1}{2}, S_z + \frac{1}{2}, r \right\rangle_{N},
\]

\[
|QSS,r\alpha\rangle_{N+1} = w f_{(N+1)}^{\alpha} \left| Q, S + \frac{1}{2}, S_z - \frac{1}{2}, r \right\rangle_{N},
\]

\[
+ y f_{(N+1)}^{\alpha} \left| Q, S + \frac{1}{2}, S_z + \frac{1}{2}, r \right\rangle_{N},
\]

\[
|QSS,r\alpha\rangle_{N+1} = f_{(N+1)}^{\alpha} f_{(N+1)}^{\alpha} \left| Q - 1, S_\alpha, r\right\rangle_{N}, \tag{A4}
\]

where \(f_{(N+1)}^{\alpha}\) is the creation operator for electrons on the \((N+1)\)th site of the “hopping Hamiltonian” and \(u, v, w, y\) are the Clebsch-Gordan coefficients.

The density matrix in the basis of \(|QSS,c\alpha\rangle_{N+1}\) states is

\[
\rho = \sum_{QSS,c\alpha} \exp(-\beta E_{QSS}) \sum_{r\alpha', r'\alpha} U_{QSS}(c\alpha) U_{QSS}(c\alpha') \left| QSS,c\alpha\right\rangle \langle QSS,c\alpha'\right|.
\]

\[
\times \langle QSS,r\alpha \left| QSS,r'\alpha' \right\rangle. \tag{A5}
\]

We now perform a partial trace over the states on the additional \((N+1)\)th site to obtain projector operators defined on the chain of length \(N\). Diagonal projectors (those with \(\alpha = \alpha'\)) are

\[
\text{Tr}_{N+1}(|QSS,c\alpha\rangle \langle QSS,c\alpha'|) = |Q + 1, S_\alpha, r\rangle_{N} \langle Q + 1, S_\alpha, r'|_{N},
\]

\[
\text{Tr}_{N+1}(|QSS,c\alpha\rangle \langle QSS,c\alpha'|) = |Q - 1, S_\alpha, r\rangle_{N} \langle Q - 1, S_\alpha, r'|_{N},
\]

\[
\text{Tr}_{N+1}(|QSS,c\alpha\rangle \langle QSS,c\alpha'|) = |Q + 1, S_\alpha, r\rangle_{N} \langle Q + 1, S_\alpha, r'|_{N},
\]

\[
+ \langle QSS,c\alpha \left| QSS,c\alpha' \right\rangle. \tag{A6}
\]

The out-of-diagonal \(\alpha=2, \alpha'=3\) terms give zero when summed over

\[
\sum_{S,z=S} \text{Tr}_{N+1}|QSS,c\alpha\rangle \langle QSS,c\alpha'| = 0,
\]

\[
\sum_{S,z=S} \text{Tr}_{N+1}|QSS,c\alpha\rangle \langle QSS,c\alpha'| = 0. \tag{A7}
\]
where we took into account that \( v_{SS}=0 \) and \( u_{SS}=0 \) in order to expand the range of the summation index \( S \). Similarly we show that \( \alpha=3 \) and \( \alpha' = 2 \) terms are dropped.

The \( \alpha=\alpha'=2 \) terms can be simplified after summing over \( S \):

\[
\sum_{S} Tr_{N+1}(QSSr_{2})(QSSr'_{2})
\]

\[
= \sum_{S} \left( u_{SS}^2 + v_{SS}^2 \right)
\times \left( Q_S - \frac{1}{2} S_c - \frac{1}{2} r \right)
\times \left( Q_S - \frac{1}{2} S_c - \frac{1}{2} r' \right)
\]

\[
= \frac{2S+1}{2S} \sum_{S=(-S/2)}^{(S+1)/2} \left( Q_S - \frac{1}{2} S_c \right)
\times \left( Q_S - \frac{1}{2} S_c - \frac{1}{2} r \right)
\times \left( Q_S - \frac{1}{2} S_c - \frac{1}{2} r' \right).
\]

(A8)

The spin multiplicity of \( QS \) is \( 2S+1 \), while the spin multiplicity of \( Qr \) is \( 2S+1 \). The factor \( (2S+1)/2S \) is therefore merely a normalization factor. In the last line we emphasized that in the \( N \)-site space the \( S_c \) runs over all possible values for \( S= \frac{1}{2} \).

By analogy we show that the \( \alpha=\alpha'=3 \) terms also simplify:

\[
\sum_{S} Tr_{N+1}(QSSr_{3})(QSSr'_{3})
\]

\[
= \frac{2S+1}{2S} \sum_{S=-(S+1)/2}^{(S+1)/2} \left( Q_S + \frac{1}{2} S_c \right)
\times \left( Q_S + \frac{1}{2} S_c - \frac{1}{2} r \right)
\times \left( Q_S + \frac{1}{2} S_c - \frac{1}{2} r' \right).
\]

(A9)

Again, the spin multiplicity of \( QS \) is \( 2S+2 \), and the factor \( (2S+1)/2S \) takes care of the correct normalization.

Nonzero partial traces of projector operators are therefore

\[
\sum_{S} Tr_{N+1}(QSSr_{\alpha})(QSSr'_{\alpha'})
\]

\[
= \delta_{\alpha\alpha'}\delta_{\alpha\alpha'} \sum_{S_{\alpha\alpha'}} \left| Q_{\alpha} S_{\alpha} S_{\alpha} r_{\alpha} \right| \left| Q_{\alpha'} S_{\alpha'} S_{\alpha'} r'_{\alpha'} \right|.
\]

(A10)

with \( c_1=c_4=1, \ c_2=(2S+1)/2S, \ c_3=(2S+1)/(2S+2) \), \( Q_1 = Q + 1, \ Q_2 = Q, \ Q_3 = Q - 1, \ S_1 = S_4 = S, \ S_2 = S - \frac{1}{2}, \ S_3 = S + \frac{1}{2} \), and the corresponding \( S_{\alpha\alpha'} \) ranges over all possible values for a given \( S_{\alpha} \). The reduced density matrix remains diagonal in its \((Q,S)\) subspace index.

In general we therefore have

\[
\rho_{\text{reduced}}^N = \sum_{QSS_{\alpha\alpha'}} \sum_{QSS_{\alpha'\alpha'}} \left| QSS_{\alpha}(QSS_{\alpha'}) \right| \left| QSS_{\alpha}(QSS_{\alpha'}) \right|.
\]

\[
= \sum_{QSS_{\alpha\alpha'}} \sum_{QSS_{\alpha'\alpha'}} U_{QSS_{\alpha}(\alpha')}(QSS_{\alpha'}(\alpha'))\delta_{QSS_{\alpha}(QSS_{\alpha'})}.
\]

\[
\times \sum_{S_{\alpha\alpha'}} \left| Q_{\alpha} S_{\alpha} S_{\alpha} r_{\alpha} \right| \left( Q_{\alpha'} S_{\alpha'} S_{\alpha'} r'_{\alpha'} \right).
\]

(A11)

This is to be compared with

\[
\rho_{\text{reduced}}^N = \sum_{QSS_{\alpha\alpha'}} \sum_{QSS_{\alpha'\alpha'}} \left| QSS_{\alpha}(QSS_{\alpha'}) \right| \left| QSS_{\alpha}(QSS_{\alpha'}) \right|.
\]

(A12)

We finally obtain the recursion relation for calculation of coefficients \( C_{N,S} \) in the reduced density matrix:

\[
C_{N,S}^{QSS_{\alpha\alpha'}} = \sum_{QSS_{\alpha'\alpha'}} C_{N,S}^{QSS_{\alpha}(\alpha')}(QSS_{\alpha'}(\alpha')) U_{QSS_{\alpha}(\alpha')} U_{QSS_{\alpha'}(\alpha')}.
\]

\[
+ \sum_{QSS_{\alpha\alpha'}} \sum_{QSS_{\alpha'\alpha'}} C_{N,S}^{QSS_{\alpha}(\alpha')}(QSS_{\alpha'}(\alpha')) U_{QSS_{\alpha}(\alpha')} U_{QSS_{\alpha'}(\alpha')}.
\]

\[
+ \frac{2S+2}{2S+1} \sum_{QSS_{\alpha\alpha'}} \sum_{QSS_{\alpha'\alpha'}} C_{N,S}^{QSS_{\alpha}(\alpha')}(QSS_{\alpha'}(\alpha')) U_{QSS_{\alpha}(\alpha')} U_{QSS_{\alpha'}(\alpha')}.
\]

\[
\times \left( Q_{\alpha}(r2) U_{QSS_{\alpha}(\alpha')} U_{QSS_{\alpha'}(\alpha')} \right).
\]

(A13)

This is the main result of the derivation. Using known \( U_{QSS} \) matrices, recursion in Eq. (A13) is applied after the first NRG run to calculate reduced density matrices for all chain lengths. In another NRG run, the spectral density functions are then calculated with respect to the reduced density matrices:

\[
A_{d\alpha}(\omega) = \sum_{ijm} \left( \langle j|d_{i}^\dagger|m \rangle \langle j|d_{j}^\dagger|m \rangle \right) \rho_{ij}^\text{reduced} + \langle j|d_{i}^\dagger|m \rangle \times \langle j|d_{j}^\dagger|m \rangle \rho_{ij}^\text{reduced} \delta(\omega - (E_j - E_m)).
\]

(A14)


