

Interference and interaction effects in multilevel quantum dots

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(Received 13 June 2001; published 10 September 2001)

Using renormalization group techniques, we study spectral and transport properties of a spinless interacting quantum dot consisting of two levels coupled to metallic reservoirs. For strong Coulomb repulsion U and an applied Aharonov-Bohm phase ϕ , we find a large direct tunnel splitting $|\Delta| \sim (\Gamma/\pi) |\cos(\phi/2)| \ln(U/\omega_c)$ between the levels of the order of the level broadening Γ . As a consequence we discover a many-body resonance in the spectral density that can be measured via the absorption power. Furthermore, for $\phi = \pi$, we show that the system can be tuned into an effective Anderson model with spin-dependent tunneling.

DOI: 10.1103/PhysRevB.64.125309

PACS number(s): 73.63.Kv, 71.27.+a, 72.15.Qm, 73.23.Hk

Introduction. Electronic transport through ultrasmall quantum dots (QD's), where the charging energy is the largest energy scale, has been studied extensively over the past few years.¹ Due to the quantization of charge the transport is dominated by Coulomb blockade (CB). More recently experiments revealed that the transport can be even more intriguing by measuring the Kondo effect,^{2,3} as suggested in Ref. 4.

The Kondo effect occurs for a dot with one low-lying spin-degenerate level. In this Brief Report, we will study a dot consisting of two levels without spin or, equivalently, two dots in an Aharonov-Bohm (AB) geometry with one level per dot in the presence of an interdot Coulomb repulsion U . Such a system is of fundamental interest since the two possible paths through the dot (via level 1 or 2) can interfere with each other. The interference can be controlled by an AB flux and has attracted much interest due to the possibility of realizing AB interferometers⁵ or using the coherent properties in connection with quantum computing⁶ (for recent experimental realizations see Ref. 7). Furthermore, in many recent experiments performed in the strong tunneling regime, the level broadening is large and transport is inevitably controlled by multilevel physics.

The model. We consider a quantum dot consisting of two levels, labeled by $j = 1, 2$. Via tunnel barriers the dot is connected to two electronic reservoirs $r = L, R$. The orbital index j is not conserved during tunneling and hence does not exist in the leads. The Hamiltonian is written as $H = H_{\text{dot}} + H_{\text{res}} + H_T$, with $H_{\text{dot}} = \sum_j \epsilon_j c_j^\dagger c_j + U n_1 n_2$, $H_{\text{res}} = \sum_{kr} \epsilon_{kr} a_{kr}^\dagger a_{kr}$, and $H_T = \sum_{rkj} (t_{jk}^r a_{kr}^\dagger c_j + \text{H.c.})$. The tunnel matrix elements are assumed to be real except for an AB phase, i.e., we attach a phase factor $e^{i\phi}$ to t_{21}^L . The energy scale of the level broadening is defined by $\Gamma_j^r = 2\pi |t_{jk}^r|^2 \rho_0$, where ρ_0 is the density of states in the leads, which we assume to be independent of energy for the energy range of interest.

We neglect spin (assuming a large Zeeman splitting) since the aim is at analyzing explicitly the physical effects arising from the tunneling-induced interference between the two levels. Since both levels overlap with the reservoir states, there is an effective overlap matrix element $-\Delta/2$, which, surpris-

ingly, is shown to be zero for a noninteracting quantum dot, but for strong on-site Coulomb repulsion $U \gg |\epsilon|, \Gamma$, scales like

$$\Delta \sim \frac{\sqrt{\Gamma_1^R \Gamma_2^R} + \sqrt{\Gamma_1^L \Gamma_2^L} e^{i\phi}}{\pi} \ln(U/\omega_c). \quad (1)$$

Here, ϕ is the AB phase, and ω_c denotes a low-energy cutoff set by the maximum of the mean level position $\epsilon = (\epsilon_1 + \epsilon_2)/2$, the mean level broadening $\Gamma = (\Gamma_1 + \Gamma_2)/2$ (with $\Gamma_j = \Gamma_j^R + \Gamma_j^L$), the temperature T , or the bias voltage eV . The level splitting is given by

$$\delta\tilde{\epsilon} = \sqrt{\delta\epsilon^2 + |\Delta|^2}, \quad (2)$$

where $\delta\epsilon = \epsilon_2 - \epsilon_1$ denotes the level spacing. Consequently, the tunnel splitting gives rise to an interference- and interaction-induced level repulsion, i.e., an effect not being considered in models with levels labeled by a conserved quantum number (e.g., spin⁴) or in the absence of interactions.⁸ The energy scale of Δ is given by Γ and will influence the spectral properties as well as the conductance for low enough temperatures $T \lesssim \Gamma$. We emphasize that this energy scale is well separated from the Kondo temperature $T_K \sim \sqrt{\Gamma U} \exp(\pi\epsilon/\Gamma)$ ($\epsilon \ll -\Gamma$), which is exponentially small and determines the crossover to the occurrence of the Kondo effect for spin-degenerate levels.⁴ Most importantly, we will show in this Brief Report that for low-lying levels $\epsilon \approx -\Gamma$ (where the ground state is the singly occupied state), the effective level splitting shows up in a many-body resonance in the spectral density at the energy $\delta\tilde{\epsilon}$, which, e.g., can be measured by an absorption experiment but influences also the temperature and flux dependence of the linear conductance. For $\phi = \pi$ and $\Gamma_j^R = \Gamma_j^L$, the tunnel splitting is zero, and the system is shown to be equivalent to an Anderson model with Zeeman splitting $\delta\epsilon$. Thus, Kondo physics can be realized in a quantum dot without spin even if the quantum number labeling the levels is *not* conserved.

We note that multilevel dots in the presence of spin have been studied previously.⁹⁻¹¹ However, Ref. 9 studies the case of a conserved quantum number labeling the levels, and

Refs. 10 and 11 consider the cases $\delta\epsilon \gg \Gamma$ or $\phi = \pi$, where the effect of the tunnel splitting Δ can be neglected. The same applies to the AB geometry of Ref. 12 where the interdot Coulomb repulsion is absent.

Renormalization group study. An effective dot Hamiltonian can easily be derived from perturbation theory or, equivalently, by integrating out the reservoir states by the renormalization group. The dot is characterized by four states $|0\rangle$, $|1\rangle$, $|2\rangle$, and $|12\rangle$, with energies $E_0=0$, $E_1 = \epsilon_1$, $E_2 = \epsilon_2$, and $E_{12} = \epsilon_1 + \epsilon_2 + U$. Intuitively, the hybridization with the reservoirs will lower the energies of all these states. For the singly occupied states, however, this is less pronounced because it costs a finite energy U to occupy the dot with a second electron. Therefore, the level positions $\epsilon_j = E_j - E_0$ will be renormalized upwards. Furthermore, a coupling between the levels is generated since tunneling events can shift the electrons between the two levels. For an electron starting in level 1 there are two possibilities: either the electron first tunnels out and hops into level 2 or an electron first hops into level 2 and then the electron tunnels out of level 1. In the latter case, the intermediate state is the doubly occupied state and, due to Fermi statistics, the matrix element gets an additional minus sign. Therefore, for reservoir electrons with an energy $|\epsilon_k| \gg U$, these two terms will cancel each other and, consequently, there is no direct coupling between the levels in the noninteracting case. In contrast, for an interacting system, the doubly occupied state is suppressed, and there is a finite coupling Δ between the two levels. We note that this mechanism does not work for levels characterized by spin since the two tunneling processes described above would also change the spin in the reservoirs and, therefore, do not lead to a direct renormalization of the dot Hamiltonian.

Using the real-time renormalization group (RG) of Ref. 13 for the forward propagator we find that energy scales $\omega_c > U$ do not renormalize the states, i.e., we start the RG at $\omega_c = \min(D, U)$ where D is the bandwidth. In the basis of the three remaining states $|0\rangle$, $|1\rangle$, and $|2\rangle$, we obtain the flow equation ($t_c = 1/\omega_c$)

$$\frac{dH_{\text{dot}}}{dt_c} = -\frac{1}{2\pi(t_c - i0^+)} \begin{pmatrix} \Gamma/2 & 0 & 0 \\ 0 & \Gamma_1 & \Phi \\ 0 & \Phi^* & \Gamma_2 \end{pmatrix}, \quad (3)$$

where $\Phi = \sqrt{\Gamma_1^R \Gamma_2^R} + \sqrt{\Gamma_1^L \Gamma_2^L} e^{i\phi}$. Neglecting level broadening, the solution of this equation gives an upward level shift $E_{1/2} - E_0 = \epsilon_{1/2} + \lambda \Gamma_{2/1}$, with $\lambda = (1/2\pi) \ln(U/\omega_c)$, and a coupling $-\Delta/2 = -\Phi\lambda$ leading to Eq. (1). As a consequence we get two effective levels at $\tilde{\epsilon}_{1/2} = \epsilon + \lambda \Gamma \mp \delta\tilde{\epsilon}/2$, where the effective level splitting $\delta\tilde{\epsilon}$ is given by Eq. (2). While $\tilde{\epsilon}_1$ is quite close to the original level position, $\tilde{\epsilon}_2$ is strongly renormalized upwards. For $\Gamma_j^r \approx \Gamma/2$, $\delta\epsilon \ll \Gamma$, and $\phi \ll 1$ the lower (upper) level is coupled strongly (weakly) to the reservoirs. For the following discussion we will usually assume equal couplings $\Gamma_j^r = \Gamma/2$, i.e., $|t_j^r| = t_j = t$ and discuss the effect of asymmetries at the appropriate places.

In the symmetric case we define $\sqrt{2}f_i = c_1 - (-1)^i c_2$. For $\phi = 0$, only the f_1 operator couples to the reservoirs, whereas

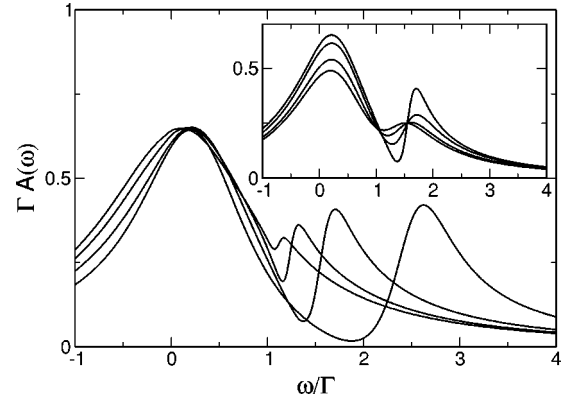


FIG. 1. Spectral density of the f_1 level for $\epsilon_1 = T = 0$, $U = 10\Gamma$, $\delta\epsilon = 0.25\Gamma$, 0.5Γ , 1Γ , 2Γ (from left to right). Inset: $\delta\epsilon = \Gamma$, $T = 0, 0.5\Gamma$, 1Γ , 1.5Γ (from top to bottom).

the level spacing $\delta\epsilon$ controls the coupling between the f_1 and f_2 level. The current operator in the right reservoir is given by $I_R = ie\sqrt{2}t\Sigma_k(a_{kR}^\dagger f_1 - \text{H.c.})$. We also note that for $\delta\epsilon = 0$ and $\phi = \pi$ the conductance is exactly zero since the $f_1(f_2)$ level couples only to the left (right) reservoir. This is an effect of destructive interference which interestingly persists also in the presence of interactions.

Spectral density and absorption power. In Fig. 1 we show the spectral density of the f_1 level for $\epsilon > 0$, where the ground state is given by the empty state. The results are obtained by using the full real-time renormalization group method of Ref. 13, which is known to yield excellent results in the regime where charge fluctuations dominate. The two peaks in the spectral density correspond to the renormalized level positions and change qualitatively as function of temperature T and $\delta\epsilon$ according to Eqs. (1) and (2). The distance between the resonances saturates for $\delta\epsilon < \Gamma$ at the energy scale Δ according to Eq. (2). In contrast, when ϵ is below the Fermi level, the lower level is occupied and particle excitations lead to a broad shoulder in the spectral density at the effective spacing $\delta\tilde{\epsilon}$; see inset of Fig. 2 (an additional weak feature occurs at negative frequencies but this is masked by

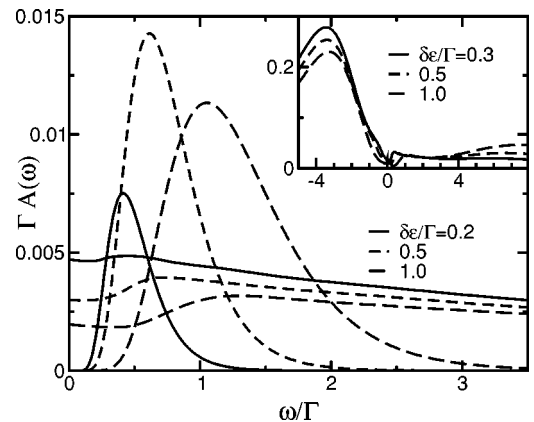


FIG. 2. Absorption power (scaled, single peaks) vs spectral density of the f_1 level (“shoulder” at the same position) for $\epsilon_1 = -10\Gamma$, $U = 50\Gamma$, and $T = 0$. In the inset, the spectral density is shown for $\epsilon_1 = -3.5\Gamma$ and $U = 10\Gamma$.

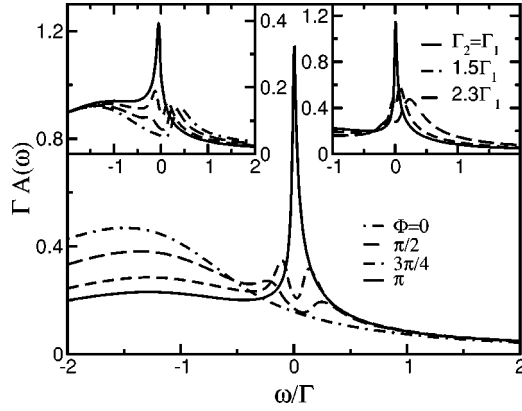


FIG. 3. Effect of a finite AB phase on the single-particle spectrum. The spectral density of the f_1 level is shown for $\epsilon_1 = -1.6\Gamma$, $\delta\epsilon = 0$, $U = 8.1\Gamma$, and $T = 0$. Left inset: Partial spectral density corresponding to the level c_1 . Same parameters as above, but with a finite level splitting $\delta\epsilon = 0.08\Gamma$. Right inset: f_1 spectral density for different broadening strengths $\Gamma_1 \neq \Gamma_2$ of levels c_1 and c_2 .

the broad resonance at $\tilde{\epsilon}_1$). These results have been obtained by using Wilson's nonperturbative numerical renormalization group (NRG)¹⁴ which, up to some overbroadening effects at higher frequencies, gives very precise results for the spectral density near the Fermi level and for the positions of all resonances. Since the location of the shoulder is not at the Fermi level, it is more suitable to test its position via the absorption power rather than the linear conductance. Therefore, we have shown in Fig. 2 the result for the spectral density of the transition operator $c_1^\dagger c_2 + c_2^\dagger c_1$. The peak position of the absorption power agrees very precisely with the position of the shoulder in the spectral density of the f_1 level. We emphasize that the shoulder is absent without the tunnel splitting, i.e., it is a generic effect which will also be present in the asymmetric case $\Gamma_1 \neq \Gamma_2$. In this case, however, the broadening of the shoulder (which is determined by Γ) will increase relative to its height (which is determined by Δ).

Figure 3 shows the spectral density of the f_1 level for different AB phases ϕ (also obtained by NRG). For $\delta\epsilon = 0$, the position of the shoulder varies proportional to $|\Delta| \sim (\Gamma/\pi)|\cos(\phi/2)|\ln(U/|\epsilon|)$, according to Eq. (1) (for $\phi = 0$, the amplitude of the shoulder is zero since the f_2 level is decoupled from the reservoirs). Furthermore, the resonances at finite frequency become more pronounced and, for $\phi = \pi$, merge into a Kondo resonance at the Fermi level with width given by the Kondo temperature T_K . This effect can easily be understood, since for $\phi = \pi$, the tunneling Hamiltonian reads $H_T = t \sum_{kj} (b_{kj}^\dagger c_j + \text{H.c.})$ with $\sqrt{2}b_{ki} = a_{kR} - (-1)^i a_{kL}$. Hence, for this special case, the pseudospin j is effectively a conserved quantum number and we obtain the Hamiltonian of the usual Anderson model, which, for a low-lying level ϵ is equivalent to the Kondo model.¹⁵

We note that this realization of Kondo physics without explicit spin degrees of freedom is quite different from other realizations, where metallic¹⁶ or two-level systems¹⁷ have been used. Furthermore, there are three experimentally tunable ways to destroy the Kondo resonance. First, a finite

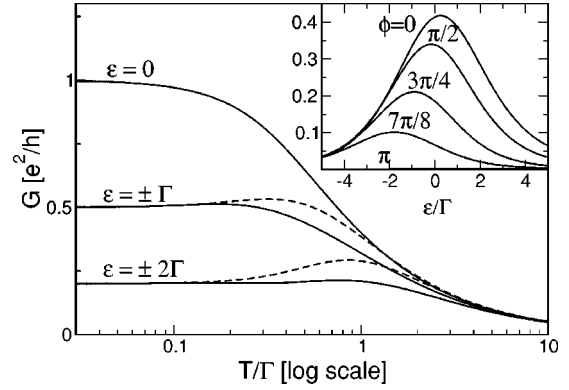


FIG. 4. The linear conductance for $\delta\epsilon = 0$, $D = 50\Gamma$, and $U = \infty$. Main panel: T dependence with $\phi = 0$ (dashed lines indicate the positive energies). Inset: ϕ dependence for $T = \Gamma$.

level spacing $\delta\epsilon \neq 0$ acts like an effective Zeeman splitting. This splits the Kondo resonance and decreases its height, see the left inset of Fig. 3. Second, an AB phase away from $\phi = \pi$ leads to an effective coupling Δ between the two levels. At $\Delta \sim T_K$ a phase transition will occur quite analog to the competition between Ruderman-Kittel-Kasuya-Yosida (RKKY) and Kondo physics in two-impurity models.^{15,18} The same mechanism is induced by left/right asymmetries, i.e., for $\Gamma_j^R \neq \Gamma_j^L$. Thirdly, for given left/right symmetry but $\Gamma_1 \neq \Gamma_2$, we obtain an Anderson model with pseudo-spin-dependent tunneling matrix elements t_j . As shown in the right inset of Fig. 3, the Kondo resonance arising at $\Phi = \pi$ is reduced and splits asymmetrically but is well defined even at $\Gamma_2/\Gamma_1 \approx 2$ (we note that the reduction is quite more pronounced for a finite level spacing). As a consequence, the Kondo resonance can be shifted away from the Fermi level by changing the asymmetry of the tunneling matrix elements, an effect also seen in recent experiments.³

Since the conductance is zero for $\delta\epsilon = 0$ and $\phi = \pi$, the Kondo resonance will show up only weakly in the $I(V)$ characteristics by changing the level spacing or the AB flux. However, the crossover to the Kondo effect can, e.g., be measured by the absorption power. Alternatively, in an AB geometry with two dots and one level per dot we expect in equilibrium for $\delta\epsilon = 0$ and $\phi = \pi$ a Kondo resonance in each dot separately. Their effect might be tested by measuring the conductance fluctuations of a parallel quantum wire lying very close to one dot.

Linear conductance. Another fingerprint for the renormalization of the energy levels due to the tunneling splitting Δ is the measurement of the linear conductance. It is calculated by using the renormalized Hamiltonian on the forward and backward propagator according to Eq. (3), including the level broadening (for the backward propagator we take the hermitian conjugate¹³). This effective Hamiltonian is used as an input for the calculation of rates in lowest order in the tunneling coupling.

Figure 4 shows the temperature dependence for $\delta\epsilon = \phi = 0$.¹⁹ At $T = 0$, the spectral density of the f_1 level is a single Lorentzian with width Γ centered at the level position ϵ . The resonance at $\epsilon + U$ is missing for $\epsilon > -U/2$ since the f_2 level is decoupled from the system and is not occupied in the

ground state; see also inset of Fig. 2. Thus, at zero temperature, the conductance is symmetric under a sign change of ϵ , in contrast to the case for spin degenerate levels, where the Kondo effect enhances the conductance for negative ϵ . For finite temperature, the f_2 level starts to become occupied and suppresses the conductance due to the Coulomb repulsion U . This effect is more pronounced for negative ϵ and, therefore, the conductance shows a local maximum for $T \sim \epsilon > 0$ but is nearly monotonic for $\epsilon < 0$. This distinguishes the model from transport through a single level.

The inset of Fig. 4 shows the gate voltage dependence for different AB phases and $\delta\epsilon=0$. The RG predicts Δ to decrease with increasing flux. For $\phi \rightarrow \pi$ the tunnel splitting is small and the level shift by λ leads to a resonance position of the linear conductance near $\epsilon = -\lambda$. In contrast, for $\phi \rightarrow 0$, the tunnel splitting is large and $\tilde{\epsilon}_1 \approx \epsilon$, which leads to a resonance position near $\epsilon = 0$. As a consequence we find that the position of the resonance is strongly influenced by the AB phase and reflects directly the tunnel splitting $|\Delta|$ together with the level renormalization λ .

Finally, we would like to comment on the case when the number of levels is given by $N > 2$. Generalizing the RG equation (3) to this case gives rise to an upward shift of all

particle and hole excitations by approximately $\sim N\Gamma$, while only one level with an equally increased broadening remains approximately at the original position. This means that transport appears to be effectively controlled by single-level physics and may explain recent experiments^{2,3} in the regime $\Gamma \sim \delta\epsilon$ where universal Kondo behavior of single-level dots has been observed.

Summary. We have studied interaction and interference effects in quantum dots with two levels or two quantum dots with one level coupled to reservoirs. We found a new tunnel splitting that changes as a function of an applied magnetic flux and can be measured via the absorption power. As function of the flux, the system can be tuned into an effective model showing Kondo physics. We expect important implications of our results for transport and spectroscopy experiments as well as for the theory of level statistics in quantum dots.

We would like to thank Jürgen König, Teemu Pohjola, and Gerd Schön for valuable discussions. This work is supported by the DFG as part of the Graduiertenkolleg ‘‘Kollektive Phänomene im Festkörper’’ (D.B.), SFB 195 (D.B. and H.S.), and SFB 484 (W.H.).

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