Kondo effect in coupled quantum dots with RKKY interaction: Effects of finite temperature and magnetic field

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We study transport through two quantum dots coupled by a Ruderman-Kittel-Kasuya-Yoshida interaction as a function of temperature and magnetic field. By applying the numerical renormalization group method, we obtain the transmission and the linear conductance. At zero temperature and magnetic field, we observe a quantum phase transition between the Kondo screened state and a local spin singlet as the RKKY interaction is tuned. Above the critical RKKY coupling, the Kondo peak is split. However, we find that both finite temperature and magnetic field restore the Kondo resonance. Our results agree well with recent transport experiments on gold grain quantum dots in the presence of magnetic impurities [H. B. Heersche *et al.*, Phys. Rev. Lett. **96**, 017205 (2006)].

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I. INTRODUCTION

In recent years, the Kondo effect[1] in semiconductor quantum dots has gained significant interest both theoretically and experimentally.[2–4] Electronic transport in quantum dots is strongly influenced by the Coulomb blockade[5] due to their small size. In these systems, a single unpaired spin can interact with conduction electrons, leading to screening of the spin and an enhanced conductance at low bias and low temperatures. More recently, due to rapid progress in spintronics and quantum information, it becomes desirable to gain more tunable spin control in double quantum dots where an effective spin-spin interaction known as the Ruderman-Kittel-Kasuya-Yoshida (RKKY)[6] coupling is generated between the two dots via conduction electrons in the lead. The RKKY coupling competes with the Kondo effect in these systems, leading to a quantum phase transition between the Kondo screened phase at weak RKKY coupling and a local spin-singlet state at strong coupling. Part of this rich physics has been studied previously in the two-impurity Kondo[7] and Anderson[8] problems.

Recently, indications for a competition between Kondo screening and the RKKY interaction have been observed experimentally.[9] This experiment stimulated theoretical and experimental efforts on the above-mentioned quantum phase transition in coupled dots. Very recent measurements have been reported to observe the restoring of the Kondo resonance in a gold quantum dot with magnetic impurities at finite temperatures and magnetic fields where an effective RKKY coupling is generated between the dot and the impurities.[10] Though similar systems have been studied theoretically via several approaches,[11–13] little is known about the transport properties at finite temperatures and magnetic fields. Motivated by these recent experiments, here we systematically study transport properties of double quantum dots coupled by a RKKY interaction at finite temperatures and magnetic fields via the numerical renormalization group (NRG) method,[14] a nonperturbative approach to quantum impurity systems. In contrast to other techniques, this method does not rely on any assumptions regarding the ground state or the leading divergent couplings, which is crucial in our analysis.

II. MODEL

We consider a two-impurity Anderson model, as shown in Fig. 1, describing two quantum dots which are separately coupled to two-channel leads and subject to an antiferromagnetic RKKY spin-spin interaction and a local magnetic field. This setup is general enough to describe both experiments mentioned above. The Hamiltonian of the system is given by

$$H = H_D + H_l + H_t + H_J + H_B,$$

$$H_D = \sum_{is}\left(\epsilon_{di} + \frac{U}{2}\right) d^\dagger_{i\sigma} d_{i\sigma} + \frac{U}{2}\sum_i (N_i - \mathcal{N})^2,$$

$$H_l = \sum_{\alpha i k \sigma} \epsilon_{\alpha i k \sigma} c^\dagger_{\alpha i k \sigma} c_{\alpha i k \sigma},$$

$$H_t = \sum_{\alpha i k \sigma} V_{i\alpha} c^\dagger_{\alpha i k \sigma} d_{i\sigma} + \text{H.c.},$$

$$H_J = J\mathbf{S}_1\mathbf{S}_2, \quad H_B = -B(\mathbf{S}_{1z} + \mathbf{S}_{2z}). \tag{1}$$

Here, $\alpha = L/R$ denotes the left/right lead, $i=1,2$ denotes the two dots, $N_i = \Sigma_\sigma d^\dagger_{i\sigma} d_{i\sigma}$ is the number of electrons occu-

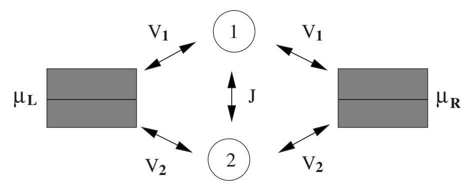

FIG. 1. Two quantum dots (denoted by the two circles) with two-channel lead (chemical potentials μ_L and μ_R). V_1 and V_2 denote the tunneling matrix element between the dots and the lead. There exists a RKKY coupling J between the two dots.

pying dot i, and $\mathbf{S}_i=(1/2)\Sigma_{\sigma\sigma'}d^{\dagger}_{i\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}d_{i\sigma'}$ are the spins of the two levels. Each dot is subject to a charging energy U and J is the RKKY exchange coupling between the two dots which is assumed to be antiferromagnetic ($J>0$). The magnetic field B induces a Zeeman splitting, where we have set $g=1$. Here, we consider the model with particle-hole symmetry, i.e., $\epsilon_{di}=-\frac{U}{2}$, and single occupation for each dot, i.e., $\mathcal{N}=1$. The energies ϵ_{di} of the two dots and their precise position in the Coulomb blockade valley can be tuned experimentally by an external magnetic field and the gate voltage. Here, we neglect the energy dependence of the tunneling matrix elements $V_{i\alpha}$. Without loss of generality, we assume they have left-right symmetry, i.e., $V_{1L}=V_{1R}=V_1$, $V_{2L}=V_{2R}=V_2$, but $V_1\neq V_2$, in general. The intrinsic linewidth of the dot levels due to tunnel coupling to the leads is $\Gamma=\Gamma_L+\Gamma_R$ with $\Gamma_{L/R}=2\pi|V|^2N_{L/R}$, where $N_{L/R}$ is the density of states in the leads.

Since the correct choice of the effective model and the number of leads per dot are important, they deserve some discussion at this point. In both experiments, we refer to Refs. 9 and 10, there are two effective quantum impurities, which interact with conduction electrons in the lead via exchange processes. In Ref. 9, these are two separate quantum dots, while the experiments of Ref. 10 have been interpreted in the sense that a single quantum dot (the gold grain) and a magnetic impurity both interact with conduction electrons. In reality, the antiferromagnetic Kondo coupling and the RKKY coupling between the dots are both generated by interaction with conduction electrons in the lead, the latter due to second-order exchange processes. Essentially, the picture is the following: The two dots couple to different points in the metallic lead, i.e., to different conduction electron modes. These modes are not completely orthogonal (otherwise there would be no RKKY) but they are also not identical. As a result, one obtains a model Hamiltonian where two dots couple to two separate (weakly nonorthogonal) electronic modes. The RKKY coupling depends both on the distance between the dots and on the Fermi wavelength. But both of these quantities are not known accurately enough in the experiments in order to calculate the RKKY coupling microscopically. In that sense, it is a free parameter which has to be inferred from the transport results.

A good approximation to this model—which is much easier to treat computationally—is the situation considered in our work: Each dot couples to its own electronic mode, where the overlap between the modes is neglected. The RKKY coupling is then treated as an additional free parameter, which can be chosen independently of the Kondo exchange couplings. We emphasize that the number of free parameters in this approach is no greater than in the detailed "microscopic" one described above. Moreover, the parameters in our model—the effective Kondo exchange couplings and the RKKY coupling—are much easier extracted from experimental results than, e.g., the distance between the two dots. One, therefore, concludes that for both experiments, the two-channel situation is generic, except for the case where the two dots sit exactly at the same position. In fact, it is much more difficult to realize a double dot coupled to the single-channel lead (one example is a setup very different from the ones considered here: a multilevel dot with single-mode lead close to pinch-off[15]).

For $J=0$, and $V_{ir}=0$, three triplet configurations $|1,1\rangle=d^{\dagger}_{1\uparrow}d^{\dagger}_{2\uparrow}|0\rangle$, $|1,0\rangle=(1/\sqrt{2})(d^{\dagger}_{1\uparrow}d^{\dagger}_{2\downarrow}+d^{\dagger}_{1\downarrow}d^{\dagger}_{2\uparrow})|0\rangle$, $|1,-1\rangle=d^{\dagger}_{1\downarrow}d^{\dagger}_{2\downarrow}|0\rangle$ and the singlet $|0,0\rangle=(1/\sqrt{2})(d^{\dagger}_{1\uparrow}d^{\dagger}_{2\downarrow}-d^{\dagger}_{1\downarrow}d^{\dagger}_{2\uparrow})|0\rangle$ are degenerate. Finite tunneling V_{ir} leads to independent spin-1/2 Kondo screening in each of the two dots. The corresponding Kondo temperatures T_K^1 and T_K^2 are generally different, and given by $T_K^{1(2)}\propto D\exp(-1/2\rho_c J_{1(2)})$, where D is the bandwidth, ρ_c the density of states of the lead, and $J_{1(2)}=4V^2_{1(2)}/U$ the effective Kondo coupling.[1]

The above degeneracy is lifted at finite RKKY coupling $J>0$: Three triplet states are shifted to energy $E_t=J/4$ and the singlet state to energy $E_s=-3J/4$. There exists competition between Kondo screening and a local spin-singlet ground state: the former is expected to be the ground state for small J, the latter for large J. A quantum phase transition at zero temperature between these two phases occurs as the RKKY coupling is tuned.[7,8] Note that a related singlet-triplet transition in two-level quantum dots was studied both for two-mode[16] and for single-mode leads.[15,17,18] In the latter case, a Kosterlitz-Thouless transition from a local singlet state to a single-channel $S=1$ underscreened Kondo model was observed.[15]

An interesting aspect of the Kondo-to-singlet transition in our setup is the tunability between these two phases since one can get good control over the various parameters in experiments. In particular, as observed in the experiment,[10] the Kondo resonance is restored at finite temperatures and magnetic fields close to the singlet-triplet transition. The goal of our work is to describe this behavior theoretically.

The NRG method is applied here to extract ground state properties of the Anderson impurity model. The key idea introduced by Wilson[14] is the logarithmic discretization of the conduction band via the parameter $\Lambda>1$. After performing a Lanczos transformation, the conduction band can be mapped onto a linear chain of fermions.[14] The transformed model can be solved by iterative diagonalization, keeping in each step only the lowest levels. Here, we iterate 44 times, keep the lowest 600 states, and set $\Lambda=4$.

III. TRANSPORT PROPERTIES

We are interested in calculating electronic transport through the dot close to the transition. To this end, we use the generalized Landauer formula[19]

$$I=\frac{2e}{h}\int d\omega(f(\omega-\mu_L)-f(\omega-\mu_R))T(\omega), \tag{2}$$

with the Fermi function $f(\omega)$ and the transmission coefficient[15]

$$T(\omega)=-\sum_{i,\sigma}\frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}\,\mathrm{Im}\,G_{ii\sigma}(\omega). \tag{3}$$

Here, we have introduced the retarded dot Green's functions $G_{ii'\sigma}(t)=-i\theta(t)\langle\{d_{i\sigma}(t),d^{\dagger}_{i'\sigma}\}\rangle$. In the following, we focus on the low bias regime, where $T(\omega)$ can be evaluated in equilibrium, using the NRG. Using the current formula (2), we determine the behavior of the linear conductance $G(T)$

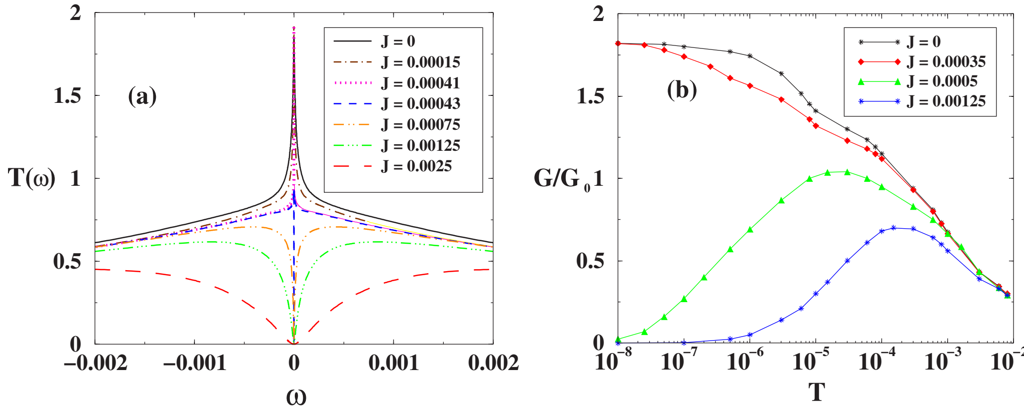

FIG. 2. (Color online) (a) Transmission coefficient at zero temperature for different RKKY interactions. The unit of energy is the half bandwidth $D=1$ of the conduction electrons. Here, $U=1$, $\epsilon_{d1}=\epsilon_{d2}=-0.5$, $\Gamma_{1L}=\Gamma_{1R}=0.05$, $\Gamma_{2L}=\Gamma_{2R}=0.1$, $\Lambda=4$, $T_k^1\approx 0.002$, $T_k^2\approx 0.000\,02$ (for $J=0$). The critical RKKY coupling is $J_c\approx 0.000\,42$. (b) Linear conductance $G(T)$ for different RKKY couplings. Parameters are the same as in (a).

$=\frac{dI}{dV}\big|_{V=0}$ at finite temperatures. Note that the equilibrium transmission $T(\omega)$ also yields a good approximation to the differential conductance dI/dV at finite bias measured in experiments.

IV. QUANTUM PHASE TRANSITION AT ZERO TEMPERATURE FOR ZERO FIELD

In Fig. 2(a), we plot the transmission coefficient $T(w)$ as a function of the RKKY coupling J for zero temperature and zero field. It shows a quantum phase transition between the Kondo screened phase $(J<J_c)$ and the local spin-singlet phase (for $J>J_c$), where $T_K^1<J_c<T_K^2$. The value of J_c is consistent with the previous results by Sakai *et al.*[8] For $J<J_c$, a Kondo peak at $\omega=0$ is observed, where the transmission $T(\omega\to 0)$ tends to reach its unitary limit of 2 (each dot acts as an unitary Kondo channel). Due to systematic numerical errors in the NRG calculation, this limit is underestimated by about 10%. As J is increased, the Kondo peak becomes narrower, indicating a vanishing low-energy scale as the system approaches the critical point. As $J\to J_c$, the transmission reaches the unstable fixed point value $T(\omega\to 0)=1$. For $J>J_c$, the two dots form a local spin-singlet state where the Kondo peak is split and $T(\omega\to 0)=0$. The splitting of the Kondo peak increases as J is increased.

In our analysis, the RKKY coupling J is varied independently, while the two-stage Kondo temperatures T_K^1 and T_K^2 are essentially kept fixed, so that the system remains in the regime $T_K^1<J_c<T_K^2$. Although complete control over the coupling parameters in the experiment is a challenge, one should keep in mind that in Ref. 10—which we mostly refer to—a large number of different samples with different dI/dV traces was considered. Our statement is that among these samples, there are some which have dI/dV characteristics that are well described by our model and parameter choices. In that sense, the regime $T_K^1<J_c<T_K^2$ is not generic, but has been observed experimentally.

Nevertheless, we want to point out that it is still possible to tune the RKKY coupling independently while keeping T_K^1 and T_K^2 approximately fixed. In fact, the experiment[9] is an example, where the RKKY coupling is tuned by varying the couplings between the central big conducting island and each of the two dots on the left and right. While doing so, the Kondo temperatures T_K^1 and T_K^2 can still roughly stay constant, as they are determined mostly by the stronger lead-dot couplings, not the couplings between each dot and the central conducting island.

V. TRANSPORT AT FINITE TEMPERATURES

We now determine the behavior of the linear conductance $G(T)/G_0$ at finite temperatures where $G_0=2e^2/h$ is the conductance unit. Results are shown in Fig. 2(b). The Kondo screened and local spin-singlet phases are characterized by stable fixed points with $G(T\to 0)\approx 2G_0$ or 0, respectively. In the Kondo regime, upon lowering the temperature, the conductance rises up to the unitary limit with two steplike structures indicating the two crossover Kondo temperatures T_k^1 and T_k^2.

In the local spin-singlet regime, we find a nonmonotonic behavior of the conductance when T is lowered: After an initial rise due to the Kondo effect, $G(T)$ decreases to zero as the temperature is lowered. The broad peak of $G(T)$ at finite temperatures is, in fact, a signature of the reappearance of the Kondo resonance which is also seen in the experiment.[10]

To gain more insight into the finite temperature behavior, we present the plot of transmission $T(\omega)$ at different temperatures (see Fig. 3) when RKKY is strong enough $(J>J_c)$ so that the Kondo peak is split at zero temperature. We find that as temperature increases, $T(\omega)$ inside the dip first increases due to thermal broadening of the split peaks around $\omega\approx\pm J$ until the Kondo resonance reappears. Then the peak height decreases again as T is further increased, similar to the Kondo effect at finite temperatures without RKKY interaction. The transmission $T(\omega=0)$ reaches its maximum value at a temperature $T_{\max}\propto J-J_c$. Note that the NRG data for $T(\omega)$ at $\omega\leqslant T$ are estimated by extrapolating $T(\omega)$ from higher frequencies. The qualitative behavior of

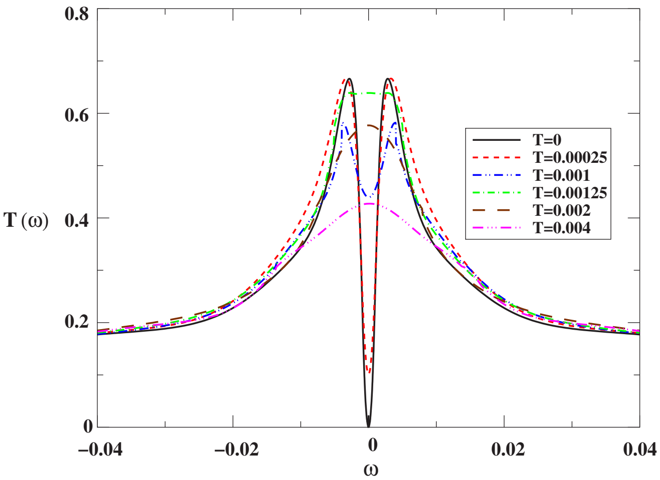

FIG. 3. (Color online) Transmission coefficient $T(\omega)$ for a fixed RKKY coupling $J=0.002$ at finite temperatures. Here, $\Gamma_{1L}=\Gamma_{1R}=0.04$, $\Gamma_{2L}=\Gamma_{2R}=0.08$. The remaining parameters are the same as in Fig. 2.

the transmission—reappearance of the Kondo peak at finite T—agrees well with recent experiments.[10]

VI. EFFECT OF A MAGNETIC FIELD

In the presence of a magnetic field, a singlet-triplet crossover occurs. Here, we discuss the effect of a Zeeman splitting at zero temperature in the presence of a large RKKY coupling J such that the Kondo peak is split in the absence of magnetic fields (see Fig. 4).

For finite $B<J$, we find an increase of the transmission $T(\omega)$ at $\omega=0$. When B is comparable to the value of the RKKY interaction, $B\approx J$, we observe the reappearance of the Kondo peak where $T(\omega)$ reaches the unitary limit of 1, corresponding to a single-channel $S=1/2$ Kondo effect. When the magnetic field increases further, the Kondo peak splits again. What happens is that due to the Zeeman splitting, one component of the triplet ($|1,1\rangle$) is "pulled down" and eventually becomes degenerate with the singlet $|0,0\rangle$ [see inset (b) of Fig. 4]. At this point, a Kondo effect—analogous to $S=1/2$ Kondo—arises between these two states, which has been discussed previously for a two-level quantum dot within a perturbative scaling approach.[20] Our nonperturbative NRG results confirm this scenario: The transmission $T(\omega=0)$ indeed reaches the unitary limit of the $S=1/2$ Kondo effect. Note that due to tunneling into the lead, degeneracy of the singlet and triplet states occurs at a renormalized value $B\neq J$. Close to the degeneracy point, a four-peak structure emerges in the transmission [see inset (a) of Fig. 4], corresponding to the splitting between the singlet and the lowest (second-lowest) triplet state. Due to NRG broadening effects, the third triplet state is not visible.

In Fig. 5, we present results for the singlet-triplet crossover at smaller RKKY coupling, for different magnetic fields and finite temperature. Compared to the sharp transition in

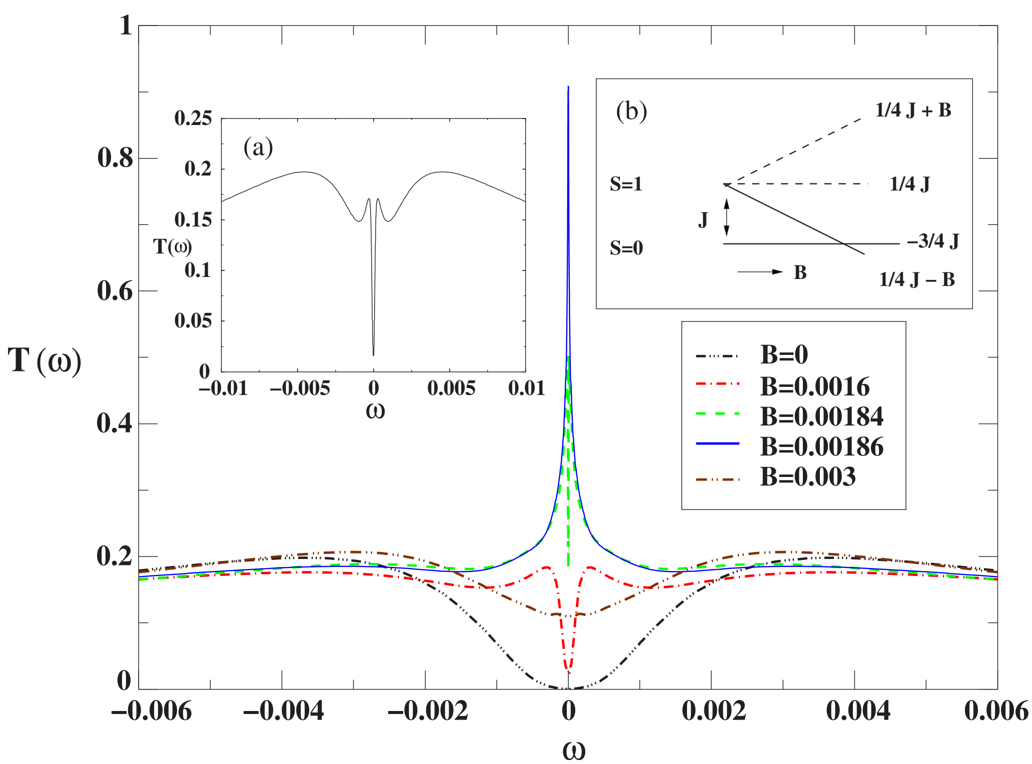

FIG. 4. (Color online) Transmission coefficient $T(\omega)$ of the coupled dots at different magnetic fields. Here, $\Gamma_{1L}=\Gamma_{1R}=\Gamma_{2L}=\Gamma_{2R}=0.06$, $J=0.002$. The remaining parameters are the same as in Fig. 2. Inset (a): the transmission $T(\omega)$ for $B=0.0016$, which clearly shows four peaks in pairs around $\pm(B\pm J)$. Inset (b): The energy levels of the triplet and singlet states in the presence of a finite RKKY coupling J and a magnetic field B. The three triplet states are split into $E_{1,1}=1/4J-B$, $E_{1,0}=1/4J$, and $E_{1,-1}=1/4J+B$. The singlet $|0,0\rangle$ and one of the triplet states $|1,1\rangle$ become degenerate at $B=J$.

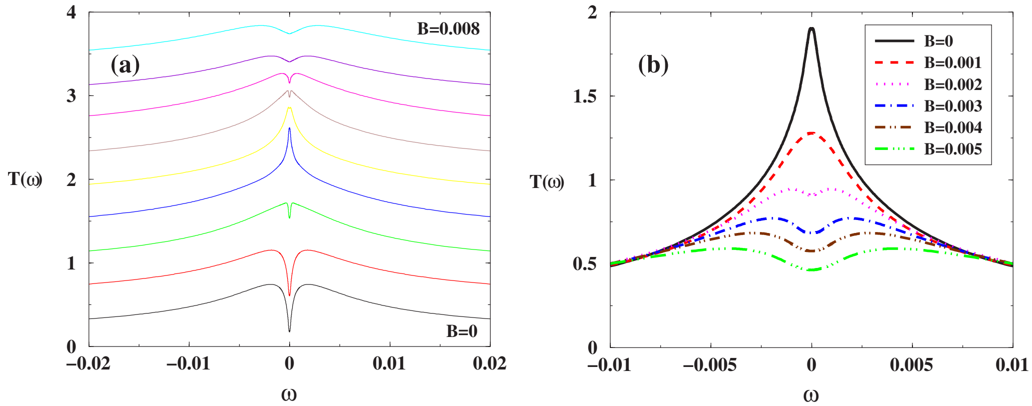

FIG. 5. (Color online) (a) Transmission coefficient $T(\omega)$ of the coupled quantum dots for different magnetic fields. Here, $U=1$, $\epsilon_{d1}=\epsilon_{d2}=-0.5$, $\Gamma_{1L}=\Gamma_{1R}=\Gamma_{2L}=\Gamma_{2R}=0.1$, $\Lambda=4$, $J=0.007$, $T_k\approx 0.0025$ (for $J=0$), $J_c\approx 0.005$, $T=0.000\,01$. The values of B are in steps of 0.001, and the traces of $T(\omega)$ are shifted in steps of $400B$. (b) Transmission vs frequency for ferromagnetic RKKY coupling $J=-0.005$ and different magnetic fields. The remaining parameters are the same as in (a).

Fig. 4 where J is much larger than T_k, the crossover here is smoother and closer to the experimental observation in Ref. 10. Note that due to thermal broadening at a finite temperature, $T(\omega=0)>0$ even in the absence of a magnetic field. For antiferromagnetic RKKY coupling [see Fig. 5(a)], $T(\omega)$ shows the dip-peak-dip structure with increasing magnetic field. For ferromagnetic RKKY [see Fig. 5(b)], the Kondo peak at $B=0$, which is due to complete screening of the triplet, splits monotonically with increasing field due to Zeeman splitting of the triplet levels, as shown in Ref. 10. Both results are qualitatively in good agreement with experiment[10] (for more recent measurements on the magnetic field dependence, see Ref. 21).

VII. CONCLUSIONS

We have studied transport properties of a double quantum dot system with RKKY interaction. Using the numerical renormalization group, we have calculated the transmission at finite frequency as a function of temperature and magnetic field. A quantum phase transition between the Kondo screened phase and a local spin-singlet state is observed. Moreover, we have shown that both finite temperature and a magnetic field can restore the Kondo resonance in the presence of a RKKY coupling. This crossover back into a Kondo screened state is in good agreement with recent measurements.[10] For the differential conductance in a finite magnetic field, we predict a multiple peak structure which is yet to be observed in future experiments.

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