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Quantum phase transition in coupled quantum dots

Natan Andrei
Physics Department, Rutgers University, Piscataway, New Jersey 08855

Gergely T. Zimányi
Physics Department, University of California, Davis, California 95616

Gerd Schön
Institut für Theoretische Festkörperphysik, Universität Karlsruhe, D-76128 Karlsruhe, Germany

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We study two quantum dots in the limit of strong dot-lead coupling and weak dot-dot tunneling. The model maps on Ising-coupled Kondo impurities. We argue that a new quantum critical fixed point exists at an intermediate value of the mutual capacitance, supporting non-Fermi-liquid behavior. We construct the total conductance across the double dot structure. It exhibits a strongly peaked behavior as a function of the mutual capacitance, gate voltage, and temperature. [S0163-1829(99)50632-2]

Electron tunneling through quantum dots is fundamentally affected by intriguing many-body effects. The Coulomb interaction imposes a prohibitive energy cost E_C on the transfer of electrons, known as Coulomb blockade.[1,2] Fine-tuning of the gate voltage $V_{\rm G}$ is required to reinstate charge flow, manifesting itself in sharp conductance peaks as a function of $V_{\rm G}$.

Remarkably, the charge transfer is accompanied by an orthogonality catastrophe. Single level quantum dots form a well-controlled realization of the Kondo model.[3] For metallic islands the analogy to the Kondo problem was also recognized early,[4] with an exact formulation due to Matveev.[5] The Kondo-type slow rearrangement of the electron states leads to a substantial downward renormalization of E_C,[6] as well as a smoothing of the conductance peaks.[7,8] Additional processes, such as the effect of higher order terms[9] and inelastic cotunneling[10] were also analyzed.

New effects arise when two such systems are allowed to interact. We argue that a robust quantum phase transition takes place in the coupled dot system when their mutual capacitance is varied. It is driven by a change of the degeneracy of the ground state. The total conductance exhibits an inverse power-law temperature dependence at this critical point.

We start by considering a structure of two metallic quantum dots, each coupled to its own lead. Single level dots will be commented on at the end of the paper. The lead-dot barriers are assumed to be narrow such that the tunneling can be modeled as a point contact. Furthermore we assume the presence of a strong enough magnetic field to achieve a fully spin-polarized electron gas. Thus the number of ‘‘flavors,’’ i.e., of additional quantum numbers of transverse momenta and electron spin, is restricted to 1. Extensions to multiple flavors will be studied below. The dot is assumed to be large enough to support a degenerate electron gas with small level spacing. This level spacing serves as a low energy cutoff,below which our scaling arguments do not hold. The Hamiltonian of one lead-dot system can then be written

$$H=\sum_{k\alpha}\epsilon_k c^\dagger_{k\alpha}c_{k\alpha}+J\sum_{kk'\,\alpha\neq\beta}c^\dagger_{k\alpha}c_{k'\beta}+\text{H.c.}+H_{e\text{-}e}, \quad (1)$$

where ϵ_k is the energy of the electrons, J is the tunneling amplitude, and the pseudospin indices α and β take the values 1, when referring to the lead and 2 when describing electrons in the dot, and $H_{e\text{-}e}$ is the electron-electron interaction term that will be discussed below. Many particle tunneling terms are irrelevant and are hence dropped. In the pseudospin notation the tunneling term is proportional to $(\sigma^+_{\alpha\beta}+\sigma^-_{\alpha\beta})$.[5]

Next we discuss the electron-electron interaction. In the lead the interaction only induces a Fermi-liquid-type modification of the parameters, but on the dot its effect is more profound. When the interaction is treated on the Hartree level, it can be represented by a charging energy, the scale of which is $E_C=e^2/2C$, where C is the capacitance of the dot. Experimentally it is also possible to tune the overall potential of the system by a gate voltage $V_{\rm G}$. The electrostatic energy of the dot can then be expressed as $E_Q=(Q-Q_{\rm G})^2/2C$, where (essentially) $Q_{\rm G}=CV_{\rm G}$ and Q is the charge on the dot. Tuning $Q_{\rm G}$ beyond $e/2$ makes it energetically favorable to transfer an electron across the barrier, giving rise to the well-known set of parabolas as the ‘‘band structure’’ of the system. Transport becomes possible when the energies of states with different number of electrons are degenerate. Thus the conductance shows sharp peaks as a function of $Q_{\rm G}$, with maxima at $Q_{\rm G}/e=n+1/2$. In the vicinity of these degeneracy points the energies of the states with n and $n+1$ electrons are much closer to each other than to any other state. It is then reasonable to truncate the Hilbert space to two states. A *second* pseudospin of $S=1/2$ can be introduced to represent this constraint on the allowed states. With this notation H assumes the Kondo type form, as first derived in its entirety by Matveev:[5]

$$H^{\mathrm{K}}=\sum_{k\alpha}\epsilon_k c^{\dagger}_{k\alpha}c_{k\alpha}+J\sum_{kk'\alpha\beta}c^{\dagger}_{k\alpha}(\sigma^{+}_{\alpha\beta}S^{-}+\sigma^{-}_{\alpha\beta}S^{+})c_{k'\beta}-\Delta S^{z}. \qquad (2)$$

Here Δ is the gap between the n and $n+1$ electron states on the dot. The introduction of the two types of pseudospin operators allows a complete mapping of a single dot to the Kondo problem in a magnetic field Δ. Note that the Kondo term is *not* spin-rotationally invariant, it contains only the spin-flip terms. Furthermore, the density of states in general can be different on the lead and the dot. However, in a perturbative analysis only the product of these density of states enters, since every tunneling process connects the lead and the dot. Thus this asymmetry is irrelevant.

We now include the interaction between the two dots caused by their mutual capacitance C_m.[11,12] The generated dot-dot coupling is proportional to $n_{\mathrm{L}}n_{\mathrm{R}}$, where we introduced the L, R notation for the left and right dot, respectively. Here $n_{\mathrm{L,R}}$ denotes the charge of the left or right dot. In pseudospin notation $S^z_{\mathrm{L,R}}=n_{\mathrm{L,R}}-1/2$. The mutual capacitance leads to an antiferromagnetic Ising type coupling: $H^{\mathrm{AF}}_{\mathrm{LR}}=I_zS^z_{\mathrm{L}}S^z_{\mathrm{R}}$, where $I_z\sim E_{C_m}$. The total Hamiltonian then takes the form $H=H^{\mathrm{K}}_{\mathrm{L}}+H^{\mathrm{K}}_{\mathrm{R}}+H^{\mathrm{AF}}_{\mathrm{LR}}$, describing two anisotropic Kondo impurities, coupled by an antiferromagnetic Ising term.

We proceed to analyze the physical content of the model. At $I_z=0$ we have two decoupled Kondo models. At $T=0$ in the magnetic language two independent *isotropic* Kondo singlets are formed with a ‘‘binding energy’’ $\sim T_{\mathrm{K}}$, as the anisotropy of the Kondo coupling is known to be irrelevant around this fixed point. In the charge language, the electrons form strongly hybridized states between the lead and the dot. This hybridization manifests itself by the strong-coupling Kondo phase shift, $\delta=\pi/2$. The key observation is that the ground state is a *singlet*. At finite but small I_z we generalize arguments originally used by Nozieres in the study of the stability of the Kondo fixed points.[16] In our case the dot-dot interaction involves virtual hopping operators to fourth order in the lead-dot hybridization amplitude. The corresponding diagrams contain a large number of fermionic operators, and thus are irrelevant. Alternatively the large number of fermion operators strongly confine the relevant phase space, leading to a positive exponent for the T dependence, again yielding a vanishing effect at $T=0$.

In the opposite limit, $I_z=\infty$, the dot pseudospins are aligned antiferromagnetically. The $(\uparrow,\downarrow)$ and $(\downarrow,\uparrow)$ states are degenerate and form a *doublet*, which is independent of the conduction electrons. In the charge language these states consist of one extra electron being either on the left or on the right dot: (1,0) and (0,1). The energy of forcing on or taking away a dot electron is $\sim I_z$, and is thus prohibited in this limit. Let us recall that the interaction term between the lead electrons and the pseudospin contains only spin raising and lowering terms. Therefore in the allowed Hilbert space the matrix elements of this coupling are zero, and thus the phase shift of the conduction electrons vanishes. The degeneracy of the ground state extends to large but finite I_z couplings as well because dot electrons hybridize only with their corresponding leads. Since the dot-dot coupling does not allow for charge transfer, these fluctuations remain confined to the dot and lead on the same side. Therefore the energies of the doublet’s two states renormalize symmetrically for finite I_z, and thus the degeneracy is preserved. To sum up, the ground state is a singlet for small values of I_z, but changes its symmetry to a doublet at large values of I_z. This change cannot be continuous: the two regions are necessarily separated by a phase transition, describing an Ising type breaking of the symmetry.

The number of minima of the action is one for small I_z and two for large I_z. *At the transition point* all three minima are degenerate, and separated by barriers: this raises the possibility of the transition being first order. However, the operator(s) $\psi^{\dagger}_{1(2),\uparrow}\psi_{1(2),\downarrow}$, connecting the central minimum with one of the two side minima, have a dimension *one*. Therefore the interminima tunneling, represented by them, scales *up*, destroying the barrier between these two states. This makes the phase transition *second order*. The scaling of this operator away from criticality was cut off by the energy difference of the minima, and hence was ineffective.

In the related system of two *isotropically* coupled Kondo impurities, a quantum phase transition as function of the interaction was predicted long ago. The results of numerical RG studies[13] were confirmed by conformal field theoretical methods,[14] and rationalized by phase-shift arguments.[15] However, in the isotropic case the ground state on both sides of the transition is a singlet, i.e., the symmetries of the ground states are the same. Thus the fixed point needs to be protected by additional particle-hole and spin rotational symmetries.[17] In the present case, since an actual symmetry breaking occurs at criticality, the transition is robust.

We pause to make connection to previous work by reviewing the band structure. The parabolas now have two indices, representing the charge states of the two dots. For $I_z=0$ the (0,0) and (1,1) curves are touching $E_Q=0$, the latter displaced along the gate charge (Q_{G}) axis by e. The (0,1) and (1,0) curves are centered at $Q_{\mathrm{G}}=e/2$, and are also shifted upward such that they go through the intersection of the (0,0) and (1,1) curves. Exactly this degeneracy of states with different number of charges allows for transport across the dots and gives rise to the conductance peak. If we now introduce the mutual capacitance I_z, the upper parabolas are customarily shifted down by an amount $\sim I_z$. This creates two degeneracy points at $Q_{\mathrm{G}}\sim e/2(1\pm I_z/E_C)$. Thus the original degeneracy of the (0,0) and (1,0) states, which allowed for the Kondo effect, seems to have been destroyed.

In contrast we predict that this new quantum critical point *is observable*. The reason for this is that for small I_z the Kondo energy scale T_{K} is bigger than I_z. Therefore one has to *start* by accounting for the formation of the Kondo singlet, a deeply nonperturbative effect. The subsequent inclusion of I_z means only a small perturbation, similar to a fluctuating magnetic field. According to the above reasoning such a field has a vanishing polarizing effect on the Kondo singlet for $I_z<T_{\mathrm{K}}$. Thus the (0,1) and (1,0) parabolas should not be viewed as shifted from their $I_z=0$ location, and their degeneracy is preserved. An analogous situation occurs in single dots:[4] the effect of the Kondo processes is to strongly *collapse* the band structure, sustaining their degeneracy up to some finite I_z. On the other hand, for $I_z>T_{\mathrm{K}}$ it *is* reasonable to account for I_z first and then treat the Kondo coupling as a perturbation. The two regimes are separated by the quantum critical point at $I_z^c \sim T_{\mathrm{K}}$.

Next we determine the total conductance. We add an interdot tunneling term

$$H_{tun}=I_{\pm}\sum_{kk'} c^{\dagger}_{k\mathrm{L}2}c_{k'\mathrm{R}2}S^{+}_{\mathrm{L}}S^{-}_{\mathrm{R}}+\mathrm{H.c.} \tag{3}$$

The pseudospin index 2 appears explicitly, as we are considering dot-dot tunneling. This term breaks the conservation of electrons on each side, and is a relevant perturbation at the quantum critical point. One then expects that the low-temperature behavior of the renormalized tunneling *at criticality* exhibits a singularity: $I_{\pm}(T)\sim T^{-\gamma}$. In the $I_{\pm}\ll J$ limit the bottleneck for the total conductance G is the dot-dot tunneling:

$$G(I_z=I_z^c,T)\sim(I_{\pm}(T))^2\sim T^{-2\gamma}. \tag{4}$$

This is *only a crossover behavior*. As T is further lowered, $I_{\pm}$ grows large and flows to an attractive fixed point, controlling its asymptotic behavior. The structure of the $I_{\pm}$ term is the same as that of the particle-hole symmetry breaking operator, thus it is plausible that its dimension is the same as well. However, the actual value of γ still needs to be determined.[18]

What happens away from criticality? For $I_z<I_z^c$ the Kondo singlets inhibit the transport. At $T=0$ the binding is complete, thus $G(T=0)=0$. Concentrating once again on the bottleneck dot-dot tunneling we compute the scaling dimensions of the involved operators. The fermion operators carry dimension 1/2, the spin raising operator has dimension 1. The current operator is constructed from the $[N,H]$ commutator. Collecting the terms the current-current correlator decays with the sixth power of time. Substituting this into the Kubo formula finally yields $G(T)\sim T^4$. The lead-dot process occurs via the Kondo coupling, which scaled to its unitarity limit, thus it does not give rise to additional powers of T.

In the regime $I_z>I_z^c$ electrons have to break an Ising bond. Thus at zero temperature again $G(T=0)=0$, and at finite T the temperature dependence takes an activated form, $G(T)\sim\exp(-W/T)$, where $W\sim I_z$. To sum it up, the conductance as a function of I_z at zero temperature is zero nearly everywhere, and exhibits a resolution and size limited peak *at* $I_z=I_z^c$. At finite temperatures the peak of $G(T,I_z)$ develops asymmetric, T dependent wings. The different regimes are shown qualitatively in Fig. 1. Finally we examine the effect of tuning the gate charge away from its special value $Q_{\mathrm{G}}=e/2$, considered so far. In the Kondo language this gives a finite value to the magnetic field Δ. For $I_z<I_z^c$ the Kondo singlet is protected by the largest energy scale, T_K at $T=0$. For $0<\Delta<T_{\mathrm{K}}$ the singlet is somewhat polarized, and weak transport is possible. This manifests itself in two small-amplitude ''shadow bands'' in a V shape determined by $|\Delta|=I_z$. This is the locus of the crossing points of the ''shifted parabolas.'' An important transport channel in this region is cotunneling, which only virtually breaks the Kondo singlet. For $I_z=I_z^c$ the pronounced conductance peak of the quantum critical point is present *at* $\Delta=0$. This peak continues out to finite Δ, forming a parabolalike ridge, which smoothly connects to the usual split conductance peaks at $|\Delta|=I_z$ for $I_z>I_z^c$. In this region $I_z>T_K$ is the largest energy scale and constructing the band structure first is appropriate.

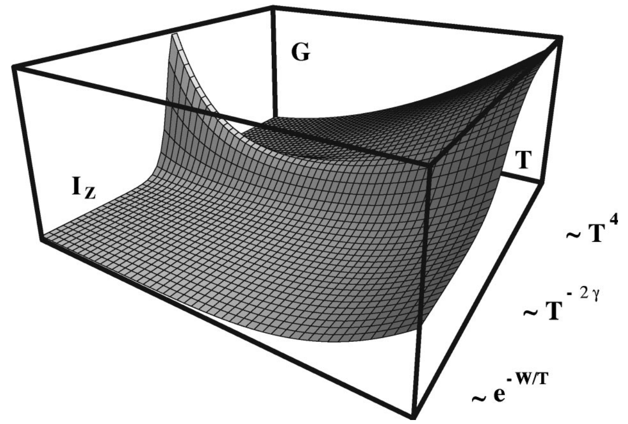

FIG. 1. The qualitative behavior of the conductance G as a function of T and I_z.

Constructing the picture from the large I_z side, the magnetic field Δ is trying to induce a spin-flip transition in the antiferromagnetic singlet. It is competing with the singlet binding energy, so the spin flip can only occur when the binding energy equals the Zeeman energy: $|\Delta|\sim I_z$, forming the usual V locus for the split peaks. Approaching the quantum critical point, however, the binding energy *collapses to zero*, hence the V becomes rounded, and closes at I_z^c, as shown qualitatively in Fig. 2.

To summarize, the key predictions of our work are as follows. (i) For a gate voltage fixed at $Q_{\mathrm{G}}=e/2$ and tuning I_z, a pronounced conductance peak has to be observed at a critical value $I_z=I_z^c\sim T_{\mathrm{K}}$. (ii) Staying at $Q_{\mathrm{G}}=e/2$, $I_z=I_z^c$, the conductance $G(T)$ should exhibit a power-law singularity in its temperature dependence. (iii) The amplitude of the split conductance peaks at $Q\neq e/2$ should exhibit a marked collapse as $I_z\rightarrow I_z^c$ from above. Experimentally these predictions can be observed by tuning I_z while keeping $I_{\pm}$ fixed,

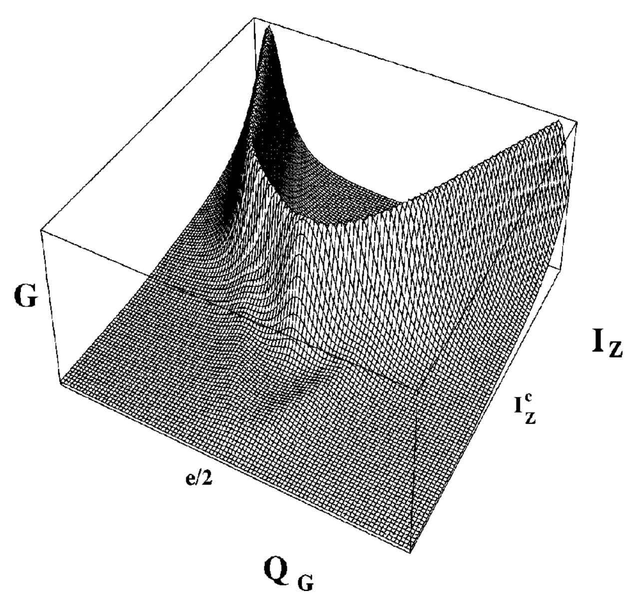

FIG. 2. The conductance peak as a function of I_z and the gate voltage at $T=0$.

whereas previous experiments[19] typically held I_z fixed, and described the evolution of the peak structure with the tuning of $I_\pm$. Also, as I_z/T_K is the controlling dimensionless ratio, experimentally it might be easier to keep I_z fixed and tune T_K instead by varying the lead-dot tunneling.

The above results apply to two coupled metallic islands, each with a large density of states. In the case of two coupled *semiconductor quantum dots* a single level is active on each of them. As the Coulomb repulsion allows only for their single occupancy, a true ''impurity spin'' is formed on each dot, making the mapping to the Kondo problem exact. Then the Varma-Jones analysis establishes the existence of the analogous quantum critical point.[13] The main difference is that this transition has to be protected by more delicate tuning, such as maintaining the particle-hole symmetry. When the tuning is incomplete, we expect the same peak features to be present, but somewhat smeared.

The above theory strictly applies only for the case of a single channel. This requires a narrow, long constriction between the leads and the dot, similar to the case considered in.[20] We expect important changes when the number of flavors of the electrons is increased. Switching off the magnetic field doubles the number of channels. It can be shown[18] that the Ising term is marginal around the ''decoupled'' fixed point, leading to a line of fixed points which terminates at some intermediate value. In the related two Kondo impurities model the one channel critical fixed point expands into a very unusual *area of fixed points*.[21] If such a structure emerges in our case, then a broadened conductance peak will form as a function of I_z at $T=0$, and the finite temperature conductance should exhibit singular temperature dependence with I_z dependent exponents. The case of even larger number of channels has been investigated for single scatterers in relation to the physics of two level systems.[22] It has been shown that a two-dimensional subspace of the flavor indices emerges to dominate exponentially over the others in the course of scaling. Therefore we expect the basic picture of two distinct phases and a well defined quantum phase transition in between to carry over, but obviously further calculations are called for.

In sum we studied the system of two coupled quantum dots. We established the existence of an intriguing quantum critical point. The experimental predictions include a conductance peak at $Q_G=e/2$, an inverse power law T dependence of the conductivity at this same point, and a marked collapse of the split conductance peaks, when the experimental parameters are in the suitable range.

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