Quantum phase transition in capacitively coupled double quantum dots

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We investigate two equivalent, capacitively coupled semiconducting quantum dots, each coupled to its own lead, in a regime where there are two electrons on the double dot. With increasing interdot coupling a rich range of behavior is uncovered: first a crossover from spin- to charge-Kondo physics, via an intermediate SU(4) state with entangled spin and charge degrees of freedom; followed by a quantum phase transition of Kosterlitz-Thouless type to a non-Fermi liquid ‘charge-ordered’ phase with finite residual entropy and anomalous transport properties. Physical arguments and numerical renormalization group methods are employed to obtain a detailed understanding of the problem.

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Introduction. – Semiconductor quantum dots provide a beautifully direct, tunable mesoscopic realization of a classic paradigm in many-body theory: the spin-Kondo effect [2], wherein a single spin in an odd-electron dot is quenched by coupling to the conduction electrons of a metallic lead. Recent advances in nanofabrication techniques now also permit the controlled construction of coupled quantum dot systems, the simplest being double dot (DD) devices. Central to the design of circuits for logic and quantum information processing, and widely studied both theoretically [3–9] and experimentally [10–15], spin and orbital degrees of freedom are now relevant, leading to the possibility of creating novel correlated electron states. Recently for example a symmetrical, capacitively coupled semiconducting DD has been studied [5] in a regime with a single electron (n = 1) on the DD, and the lowest energy states (nL, nR) = (1, 0) and (0, 1) near degenerate. The low-energy physics, which determines the conductance at small bias, was shown [5] to be governed by a fixed point with SU(4) symmetry, leading to an unusual strongly correlated Fermi liquid state where the spin and orbital degrees of freedom are entangled.

In this paper we study a capacitively coupled, symmetrical semiconducting DD system, but now in a regime with two electrons on the DD such that (1, 1), (2, 0) and (0, 2) are the relevant low energy states. As shown below, the associated physics is both rich and qualitatively distinct from the n = 1 sector: on increasing the ratio U′/U of inter- and intra-dot coupling strengths, we find that the system first evolves continuously from an SU(2) × SU(2) spin-Kondo state where the dot spins are in essence separately quenched, to an SU(4) Kondo state with entangled charge and spin degrees of freedom when U′/U = 1. Thereafter, for a tiny increase in U′/U, there is then a smooth crossover to a novel charge-Kondo state; followed by suppression of charge-pseudospin tunneling, manifest in collapse of the associated Kondo scale and a Kosterlitz–Thouless (KT) quantum phase transition to a doubly degenerate charge-ordered state — a non-Fermi liquid phase with ln 2 entropy and anomalous low-energy transport and thermodynamic properties. Detailed results for this diverse range of behavior are obtained using the numerical renormalization group (NRG) method [16, 17], preceded by simple physical arguments that enable the essential physics to be understood.

Model and physical picture. – We consider two equivalent, capacitively coupled semiconducting (single-level) dots, each coupled to its own lead. The Anderson-type Hamiltonian is $H = H_0 + H_V + H_D$, where $H_0 = \sum_{i,k,\sigma} \epsilon_i \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} + U \sum_i \hat{n}_{i\sigma} \hat{n}_{i\sigma}$ refers to the leads ($i = L/R$) and $H_V = \sum_{i,k,\sigma} V \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}^\dagger$ to the lead-dot couplings. $H_D$ describes the isolated dots,

$$H_D = \sum_{i=L,R} (\epsilon \hat{n}_i + U \hat{n}_i \hat{n}_{i\downarrow} + U' \hat{n}_L \hat{n}_R)$$

with $\hat{n}_i = \sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$ and $\epsilon$ the intradot Coulomb interaction, $U'$ the interdot (capacitive) coupling. In the isolated DD, increasing $|\epsilon| = -\epsilon$ (via suitable gate voltages) generates the usual Coulomb blockade staircase. For $0 < |\epsilon| < \min(U, U')$ the ground state occupancy is $n = 1$, with degenerate configurations $(n_L, n_R) = (1,0)$ and a ln 4 residual entropy ($k_B \equiv 1$) [3–5]. Coupling to the leads quenches this entropy, and the strongly correlated effective low-energy model is SU(4) Kondo [4, 5]. The underlying physics here is rich, including spin-filtering arising from the continuous crossover to the SU(2) orbital Kondo effect in a strong magnetic field [5]. But no quantum phase transition occurs in this $n = 1$ sector.

We consider by contrast the $n = 2$ domain of the Coulomb staircase, arising for $\min(U, U') < |\epsilon| < U'+ \max(U, U')$. Two sets of configurations then dominate, according to whether $U' \lessgtr U$: the 4-fold spin-degenerate states $(n_L, n_R) = (1, 1)$, and the degenerate pair $(2, 0)/(0, 2)$, with DD energy difference $E(2, 0) - E(1, 1) = U - U'$. The DD ground state is thus (1, 1) for $U' < U$, and (2, 0)/(0, 2) for $U' > U$; all six states are degenerate at $U' = U$ where the model has SU(4) symmetry. We first give physical arguments for the evolution of
the coupled DD-lead system with increasing $U'$; focusing on the strongly correlated regime of $U'/\Gamma \gg 1$ ($\Gamma = \pi V^2 \rho$ with $\rho$ the lead DoS). Here an effective low-energy Hamiltonian may be obtained from second order perturbation theory (PT) in the lead-dot tunneling $V \equiv V_L = V_R$ (with $V_{L/R}$ denoting coupling to the L/R lead) [18].

For $U' = 0$ the dots are fully decoupled. Only $(1, 1)$ states are relevant. The effective model is obviously two uncoupled spin-$\frac{1}{2}$ Kondo models. The spin entropy is quenched at the normal Kondo scale $T_K^{SU(2)}$, leading to a local singlet ground state (‘$SU(2) \times SU(2)$ spin-Kondo’).

For $U' \gg U$ by contrast the $(2, 0)/(0, 2)$ DD states dominate, and as shown below the ground state is a *doubly degenerate* ‘charge ordered’ (CO) state with $\ln 2$ entropy. Continuity then implies a quantum phase transition at some critical $U'_c$. As discussed below, for $U' = U$ the effective model is $SU(4)$ Kondo (in the $n = 2$ sector) [18], with entangled spin/charge degrees of freedom but a singlet ground state with a larger Kondo scale $T_K^{SU(4)}$; and is connected continuously to the $SU(2) \times SU(2)$ spin-Kondo state arising as $U' \rightarrow 0$. We thus expect $U'_c > U$.

Hence consider increasing $U'$ above $U$. Since the configurations $(1, 1), (2, 0), (0, 2)$ are degenerate for $U' = U$ this full $n = 2$ manifold must be retained for $U' \simeq U$. Virtual excitations to excited states are eliminated via PT, and divide in two classes [18]: (a) $V_L^2$ or $V_R^2$ processes, involving tunneling to one lead alone. *Any* configuration connects to itself via such, e.g. $(1, 1) \leftrightarrow (1, 1)$ under $V_R^2$ via excited states $(1, 0)$ or $(1, 2)$. (b) $V_L V_R$ processes. These necessarily connect different manifold configurations; the full set is clearly $(2, 0) \leftrightarrow (1, 1)$ and $(0, 2) \leftrightarrow (1, 1)$, there being no direct coupling between $(2, 0)$ and $(0, 2)$. As $U'$ increases above $U$ charge and spin states begin to separate: the degenerate charge pair $(2, 0)/(0, 2)$, components of an effective charge pseudospin, lie lower in energy by $U' - U$ than the $(1, 1)$ spin states. For sufficiently small $U' - U > 0$, tunneling between the $(2, 0)/(0, 2)$ states can however still arise, and quench the charge pseudospin (and hence entropy), producing thereby a non-degenerate charge-Kondo state. But, as above, this tunneling is not direct, being mediated by the higher energy $(1, 1)$ states. We thus expect the associated Kondo scale to be diminished compared to $T_K^{SU(4)}$ (the ‘stabilization’ due to dot-lead coupling at the $SU(4)$ point) and to decrease as $U'$ increases; and moreover that the quenching will cease to be viable when the relative energy $U' - U$ of the $(1, 1)$ states exceeds roughly $T_K^{SU(4)}$, leading to a quantum phase transition to the degenerate CO phase when $U'_c - U \approx T_K^{SU(4)}$. Since the latter is exponentially small for strong correlations, this implies a critical $U'_c$ exponentially close to $U$ (as confirmed by NRG below).

These arguments extend readily to $U' < U$, but now the circumstances differ. Spin/charge degrees of freedom do separate on decreasing $U'$ from $U$, $(1, 1)$ states now lying lower by $U - U'$ than $(2, 0)/(0, 2)$. But since the

![FIG. 1: (a) Phase diagram in ($U', \tilde{U}$)-plane; the $SU(4)$ line $U' = U$ is also shown (dotted). (b) For $\tilde{U} = 7$ in the SC phase, $\ln(T_K/\Gamma)$ vs $[U'_c - U']^{-1/2}$ close to the transition, showing the exponential vanishing of $T_K$. Inset: $\ln(T_K/\Gamma)$ vs $U'$](image)

$(1, 1)$-spin-states connect *directly* to themselves under $V_L^2$ or $V_R^2$ (as above), quenching of the spin entropy is not inhibited and no transition occurs. Instead a continuous crossover from $SU(4)$ Kondo to separable $SU(2) \times SU(2)$ spin-Kondo is expected, for $U - U' \approx T_K^{SU(4)}$.

**Results.** – The physical picture is thus clear, and the transition to the degenerate CO phase occurs in the vicinity of the $SU(4)$ point $U' = U$ [18]. We now present NRG results for the DD Anderson model, choosing the midpoint of the $n = 2$ domain, $|\epsilon| = U/2 + U'$. This case is particle-hole (p-h) symmetric, but representative. The physics is wholly robust to departure from p-h symmetry.

The low temperature behavior of the model is governed by two classes of stable fixed points (FP), corresponding to the two zero temperature phases. The first, a strong coupling (SC) fixed point, describes all the singlet ground states; and is reached (as $T \rightarrow 0$ or NRG iteration number $N \rightarrow \infty$) for all $U' < U'_c$. The corresponding FP Hamiltonian is simply a doubled version ($SU(2) \times SU(2)$) of that well known for the spin-1/2 Anderson model [17]. The dot spins and hence entropy are thus quenched at $T = 0$, the system being a Fermi liquid and characterized by a Kondo scale denoted generically as $T_K$. The second, reached for all $U' > U'_c$, is a line (i.e. a one parameter family) of charge ordered (CO) FP. The generic FP Hamiltonian corresponds to setting $\Gamma = 0$ and $U' = \infty$. The DD and leads are then decoupled, but the FP has internal structure reflecting broken symmetry, since dot-states occur in the degenerate pair $(n_L, n_R) = (2, 0)/(0, 2)$ (whence $\ln 2$ residual entropy). The line of FP is obtained by supplementing the free lead Hamiltonians by potential scattering correlated to dot occupancy, of form $H_K = K \sum_{i,\sigma} \sum_{k, k'} a_{k \sigma}^a a_{k' \sigma}^\dagger (\hat{n}_i - 1)$ (cf [18]). The actual value of $K$ is obtained numerically by matching to NRG energy levels.

A comparison of NRG energy level flows for large iteration number, with the characteristic energy level structure for the two FP, enables the phase diagram to be found; as shown in Fig. 1(a) in the $(\tilde{U}', U')/\pi \Gamma, \tilde{U} = \tilde{U}'$.
The transition is seen to occur for all $U \geq 0$ on increasing the interdot $\tilde{U}$. Consistent with the physical arguments above, for $U \gg 1$ the critical $U_c$ indeed lies exponentially close to the $SU(4)$ line $U = U_c$ (specifically we find $(U_c/U - 1) \sim 2T_K^{SU(4)}/\Gamma \tilde{U}^{1/2}$). It is seen to depart lighly from its $U_c = 0$ value $T_K^{SU(2)} \propto \Gamma \tilde{U}^{1/2} \exp(-1/pJ)$ (with $pJ = 8/\pi^2 \tilde{U}$) [17], indicative of spin-Kondo physics, until very close to $U = U_{c}^\prime$ where it increases rapidly to $T_K^{SU(4)} \propto \Gamma \tilde{U}^{3/4} \exp(-1/2pJ)$; i.e. while exponentially small, $T_K^{SU(4)} \propto [T_K^{SU(2)}]^{1/2}$ shows a strong relative enhancement at the $SU(4)$ point [4, 5]. However on increasing $U'$ above $U_{c}^\prime$ and entering the Kondo regime, $T_K$ is seen to drop rapidly and approaches the SC→CO transition is approached. The transition is of KT type, consistent with the line of CO FP for $U' \geq U_{c}^\prime$, and (from NRG energy level flows) no evidence for a separate critical FP; further evidenced by [20] the $U' \to U_{c}^\prime$ behavior $T_K \propto \exp[-a/(U_c' - U')^{1/2}]$, demonstrated in Fig. 1(b) for $U = 7.$ This behavior is generic, even for $U = 0$; here the non-interacting $SU(4)$ ($U' = 0$) scale $T_K^{SU(4)} \propto \Gamma$, and $U_c' - U \approx T_K^{SU(4)}$ implies $U_c' \sim O(1)$, as indeed found (Fig. 1(a)).

In addition to the two stable (low-temperature) FP, three unstable FP play an important role at finite-$T$, and are seen clearly in the impurity entropy $S = S_{imp}$: (i) free orbital (FO) [17], corresponding to $\Gamma = 0 = U = U'$, with ln 16 entropy. This is just the high-$T$ limit of $S(T)$, reached in all cases for non-universal $T \approx \max(U, U_c')$. (ii) $SU(4)$ local moment (LM$^{SU(4)}$), corresponding to $\Gamma = 0$ and $U = \infty = U'$, with associated entropy ln 6; and (iii) $SU(2) \times SU(2)$ local moment (LM$^{SU(2)}$), $\Gamma = 0 = U'$ and $U = \infty$, with ln 2 entropy. Fig. 2 shows $S(T)$ vs $T/T_\phi$ for $\tilde{U} = 7$ ($U_c' \approx 7.046$). Fig. 2(a) illustrates the behavior ‘deep’ in the CO and SC phases. In the former $S(T)$ simply crosses directly from its ln 2 (CO) residual value to ln 16 (FO) on the scale $T \sim U'$; while in the latter, consistent with the effective underlying spin-1/2 Kondo physics, there is first a crossover from $S(0) = 0$ (SC) to ln 4 (LM$^{SU(2)}$) for $T \sim T_K$ ($\sim T_K^{SU(2)}$). Figure 2(b), for $U' = 6.9 < U$, illustrates the crossover from effective uncoupled SU(2) Kondo to SU(4). Here $S(T)$ increases in a two-stage fashion, first to ln 4 (LM$^{SU(2)}$) for $T \sim T_K$ and then ln 6 (LM$^{SU(4)}$) for $T \sim [U' - U]$ ($= E(2, 0) - E(1, 1)$). This behavior is naturally absent at the $SU(4)$ point, Fig. 2(c): $S(T)$ crosses directly to ln 6 for $T \sim T_K^{SU(4)}$. In the charge-Kondo regime Fig. 2(d) for $U' = 7.03$ $S(T)$ again shows the two-stage behavior typical of a KT transition [9, 21], but here it first crosses from 0 (SC) to ln 2 (CO) for $T \sim T_K$ and then to ln 6 (LM$^{SU(4)}$) for $T \sim [U' - U] = E(1, 1) - E(2, 0)$; consistent with the physical discussion given above.

The physics discussed above naturally shows up also in various thermodynamic susceptibilities. For example, as $U'$ is increased past $U$ into the charge-Kondo regime, we find the ‘impurity’ spin susceptibility $\chi_s$ decreases monotonically; but its charge pseudospin analogue the staggered charge susceptibility $\chi_c^\prime$, given by $\chi_c^\prime \sim 1/T_K$, diverges as $U' \to U_c'$ reflecting the collapse of the charge-Kondo state and the quantum phase transition. For $U' > U_c'$ the ($T = 0$) $\chi_c^\prime$ remains infinite, symptomatic of the broken symmetry CO phase, with $\chi_c^\prime(T) \propto 1/T$ as $T \to 0$. Further details will be given in subsequent work.

Finally and most importantly, the destruction of the Kondo effect as the SC→CO transition is approached is seen vividly in electronic transport, notably the transmission coefficient $T_i(\omega) = \pi \Gamma D_i(\omega)$ with $D_i(\omega)$ the $0$ local single-particle spectrum $D_i(\omega) = -\text{Im} G_i(\omega)/\pi$ with $G_i(t) = -i \theta(t) \langle \{ c_{i\sigma}^\dagger(t), c_{i\sigma}^\dagger \} \rangle$ the retarded dot Green function). At the Fermi level in particular ($\omega = 0$), $T_i(0)$ gives the linear differential conductance across one (either) dot in units of the conductance quantum $2e^2/h$ [22]; and at finite, low bias voltage $V$, the equilibrium $T_i(\omega = eV)$ provides an approximation to the conductance [22]. The low-energy behavior of $T_i(\omega)$ is shown in Fig. 3 for a range of $U'$ spanning the transition.
For $\tilde{U}' = \tilde{U}$ a relatively broad Kondo resonance characteristic of the $SU(4)$ point is apparent, with width $\propto T_K = T_{SU(4)}^K$. On increasing $\tilde{U}'$ into the charge-Kondo regime the Kondo resonance, now residing on top of an incoherent continuum, remains intact with $T_1(0) = 1$ throughout the SC phase reflecting the unitarity limit [23]. But it narrows progressively as $T_K$ diminishes, and as $U' \rightarrow \tilde{U}'$, the Kondo resonance vanishes ‘on the spot’, such that for $\tilde{U}' > U'$ in the CO phase only the background continuum remains. The linear conductance in particular thus drops abruptly at the transition. This appears to be a general signature of an underlying KT transition, it being found also for a multi-level small dot close to a singlet-triplet degeneracy point [21]; and in recent work [9] on two Ising-coupled Kondo impurities, onto which maps the problem of spinless, capacitively coupled metallic islands/large dots close to the degeneracy point between $N$ and $N+1$ electron states [8]. The non-Fermi liquid nature of the CO phase is also seen clearly here, because $T_1(0) = 1 / [1 + (\Sigma^I(0)/\Gamma)]$ in terms of the imaginary part of the dot self-energy; whence $T_1(0) < 1$ in the CO phase implies a non-zero $\Sigma^I(\omega = 0)$ and thus a non-FL state (as also manifest eg in anomalous exponents for the subleading $T$-dependence of thermodynamic properties, although the latter effects are quantitatively minor).

We have considered an equivalent (L/R symmetric) DD system, with specific results shown for the p-h symmetry case. For a DD device described by the effective Hamiltonian, 

$$H_{\text{eff}} = [U - \tilde{U}']\sum_{i,\sigma}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

vanishing at the SU(4) point; and

$$H' = \frac{J}{4}\sum_{k,\k'}\sum_{i,\sigma}\sum_{j,\sigma'}a_{k,i\sigma}^\dagger a_{k',j\sigma'}^\dagger a_{k',j\sigma'} a_{k,i\sigma}$$

with an antiferromagnetic exchange $J$. Terms with $j \neq i$ in $H'$ arise from $V_{\sigma}V_{\gamma}$ processes, interconnecting $(2,0)/(0,2)$ and $(1,1)$ states. Those with $j = i$ come from the $V^2_{\sigma}$ or $V^2_{\gamma}$ processes: acting on $(1,1)$ states gives rise per se to $SU(2) \times SU(2)$ spin-1/2 Kondo; while the $(2,0)/(0,2)$ states generate potential scattering of form

$$\frac{J}{4}\sum_{i,\sigma}\sum_{j,\sigma'}a_{k,i\sigma}^\dagger a_{k',j\sigma'}^\dagger (\hat{n}_{i\sigma} - 1),$$

equal and opposite for $\hat{\sigma}_z = 0$ and $2$.

Results are typically shown for an NRG discretization parameter [17] $\Lambda = 3$ keeping $N \sim 20,000$ states (excluding spin degeneracy) per NRG step. $T_K$ is defined in practice by

$$T_K = 1/\gamma,$$

with $\gamma$ the usual $T = 0$ linear specific heat coefficient [17].

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equal and opposite for $\hat{\sigma}_z = 0$ and $2$.

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