# 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.*—Semiconducting quantum dots provide [1] 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 $(n_L, n_R) = (1, 0)$ 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 Letter 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 interdot and intradot coupling strengths, we find that the system first evolves continuously from an $SU(2) \times SU(2)$ 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 the suppression of charge-pseudospin tunneling, manifest in the 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 ln2 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 $H_0 = \sum_{i,\mathbf{k},\sigma} \epsilon_{\mathbf{k}} a^\dagger_{\mathbf{k}i\sigma} a_{\mathbf{k}i\sigma}$ refers to the leads ($i = L/R$) and $H_V = \sum_{i,\mathbf{k},\sigma} V(a^\dagger_{\mathbf{k}i\sigma} c_{i\sigma} + \text{H.c.})$ to the lead-dot couplings. $H_D$ describes the isolated dots,

$$H_D = \sum_{i=L,R} (\epsilon \hat{n}_i + U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}) + U' \hat{n}_L \hat{n}_R \qquad (1)$$

with $\hat{n}_i = \sum_\sigma \hat{n}_{i\sigma} = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma}$. $U$ denotes the intradot Coulomb interaction, and $U'$ 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 $(n_L, n_R) = (1, 0)/(0, 1)$ and a ln4 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 fourfold 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 density of states). 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 ln2 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 into 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 $U$ the 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 nondegenerate *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; moreover, 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 $(1, 1)$ spin states connect *directly* to themselves under $V_R^2$ or $V_L^2$ (as above), quenching of the spin entropy is not inhibited and no transition occurs. Instead, a continuous crossover from the $SU(4)$ Kondo to the 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 $(n_L, n_R) = (2, 0)/(0, 2)$ (hence ln2 residual entropy). The line of FP is obtained by supplementing the free lead Hamiltonians by potential scattering *correlated to dot occupancy*, of the form $H_K = K\sum_{i,\sigma}\sum_{\mathrm{k},\mathrm{k}'} a^\dagger_{\mathrm{k}i\sigma} a_{\mathrm{k}'i\sigma}(\hat{n}_i - 1)$ (cf. [18]). The actual value of $K$ is obtained numerically by matching to the NRG energy levels.

A comparison of the NRG energy level flows for large iteration numbers, with the characteristic energy level structure for the two FP, enables the phase diagram to be

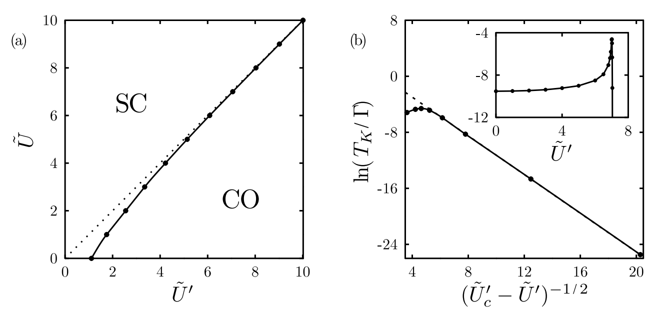


FIG. 1. (a) Phase diagram in the $(\tilde{U}', \tilde{U})$ plane; the $SU(4)$ line $U' = U$ is also shown (dotted line). (b) For $\tilde{U} = 7$ in the SC phase, $\ln(T_K/\Gamma)$ vs $[\tilde{U}'_c - \tilde{U}']^{-1/2}$ close to the transition, showing the exponential vanishing of $T_K$. Inset: $\ln(T_K/\Gamma)$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

found, as shown in Fig. 1(a) in the ($\tilde{U}' = U'/\pi\Gamma$, $\tilde{U} = U/\pi\Gamma$) plane [19]. The transition is seen to occur for all $\tilde{U} \geq 0$ on increasing the interdot $\tilde{U}'$. Consistent with the physical arguments above, for $\tilde{U} \gg 1$ the critical $U'_c$ lies exponentially close to the $SU(4)$ line $U' = U$ [specifically we find $(U'_c/U - 1) \simeq 2T_K^{SU(4)}/\Gamma\tilde{U}^{1/2}$]. Figure 1(b) (inset) shows the $\tilde{U}'$ evolution of $T_K$ [19] in the SC phase, for a typical strongly correlated $\tilde{U} = 7$. It is seen to depart little from its $U' = 0$ value $T_K^{SU(2)} \propto \Gamma\tilde{U}^{1/2}\exp(-1/\rho J)$ (with $\rho J = 8/\pi^2\tilde{U}$) [17], indicative of spin-Kondo physics, until very close to $U' = U$ where it increases rapidly to $T_K^{SU(4)} \propto \Gamma\tilde{U}^{3/4}\exp(-1/2\rho J)$; 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 $U$ and entering the charge-Kondo regime, $T_K$ is seen to drop rapidly and vanishes as the SC $\rightarrow$ CO transition is approached. The transition is of the KT type, consistent with the line of CO FP for $U' \geq U'_c$ and (from NRG energy level flows) no evidence for a separate critical FP, and is further evidenced by [20] the $\tilde{U}' \rightarrow \tilde{U}'_c-$ behavior $T_K \propto \exp(-a/[\tilde{U}'_c - \tilde{U}']^{1/2})$, demonstrated in Fig. 1(b) for $\tilde{U} = 7$. This behavior is generic, even for $U = 0$; here the noninteracting $SU(4)$ ($U' = 0$) scale $T_K^{SU(4)} \sim \Gamma$, and $U'_c - U \approx T_K^{SU(4)}$ implies $\tilde{U}'_c \sim \mathcal{O}(1)$, 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 $S$ ($\equiv S_{\rm imp}$): (i) Free orbital (FO) [17], corresponding to $\Gamma = 0 = U = U'$, with ln16 entropy. This is just the high-$T$ limit of $S(T)$, reached in all cases for nonuniversal $T \approx \max(U, U')$. (ii) $SU(4)$ local moment (LM$^{SU(4)}$), corresponding to $\Gamma = 0$ and $U = \infty = U'$, with associated entropy ln6. (iii) $SU(2) \times SU(2)$ local moment (LM$^{SU(2)}$), $\Gamma = 0 = U'$, and $U = \infty$, with ln2$^2$ entropy. Figure 2 shows $S(T)$ vs $T/\Gamma$ for $\tilde{U} = 7$ ($\tilde{U}'_c \simeq 7.046$). Figure 2(a) illustrates the behavior "deep" in the CO and SC phases. In the former $S(T)$ simply crosses directly from its ln2 (CO) residual value to ln16 (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 ln4 (LM$^{SU(2)}$) for $T \simeq T_K$ ($\simeq T_K^{SU(2)}$). Figure 2(b), for $\tilde{U}' = 6.9 < \tilde{U}$, illustrates the crossover from effective uncoupled $SU(2)$ Kondo to $SU(4)$. Here $S(T)$ increases in a two-stage fashion, first to ln4 (LM$^{SU(2)}$) for $T \sim T_K$ and then ln6 (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 ln6 for $T \sim T_K^{SU(4)}$. In the charge-Kondo regime Fig. 2(d) (for $\tilde{U}' = 7.03$) $S(T)$ again shows the two-stage behavior typical of a KT transition [9,21], but here it first crosses from 0 (SC) to ln2 (CO) for $T \sim T_K$ and then to ln6 (LM$^{SU(4)}$) for $T \simeq [U' - U] = E(1, 1) - E(2, 0)$, consistent with the physical discussion given above.

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

Finally and most importantly, the destruction of the Kondo effect as the SC $\rightarrow$ 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 $T = 0$ local single-particle spectrum [$D_i(\omega) = -{\rm Im}G_i(\omega)/\pi$ with $G_i(t) = -i\theta(t)\langle\{c_{i\sigma}(t), c_{i\sigma}^\dagger\}\rangle$ 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 $\tilde{U}'$ spanning the transition. For $\tilde{U}' = \tilde{U}$ a relatively broad Kondo resonance characteristic of the $SU(4)$ point

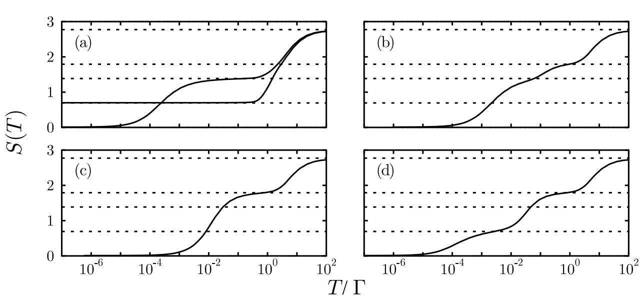


FIG. 2. $S(T)$ vs $T/\Gamma$ for $\tilde{U} = 7$ ($\tilde{U}'_c \simeq 7.046$). (a) $\tilde{U}' = 6$ (SC, "uncoupled spin-Kondo") and 8 (CO); (b) $\tilde{U}' = 6.9$ [crossover to $SU(4)$]; (c) $\tilde{U}' = 7$ [$SU(4)$]; (d) $\tilde{U}' = 7.03$ (charge-Kondo). Dotted lines show ln16, ln6, ln4, and ln2, associated with the FO, LM$^{SU(4)}$, LM$^{SU(2)}$, and CO fixed points, respectively.

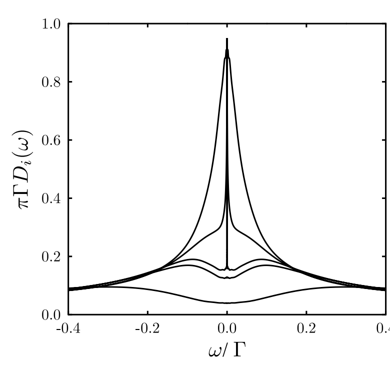


FIG. 3. Transmission $\pi\Gamma D_i(\omega)$ vs $\omega/\Gamma$, for $\tilde{U} = 7$ and (top to bottom) $\tilde{U}' = 7, 7.03, 7.044$ (SC) and $7.048, 7.1$ (CO).

is apparent, with width $\propto T_K = T_K^{SU(4)}$. On increasing $\tilde{U}'$ into the charge-Kondo regime the Kondo resonance, now residing on top of an incoherent continuum, remains intact with $T_i(0) = 1$ throughout the SC phase reflecting the unitarity limit [23]. But it narrows progressively as $T_K$ diminishes, and as $\tilde{U}' \to \tilde{U}'_c-$ the Kondo resonance vanishes "on the spot" such that for $\tilde{U}' > \tilde{U}'_c$ 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 multilevel 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 or 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 $T_i(0) = 1/[1 + (\Sigma^{\mathrm{I}}(0)/\Gamma)]$ in terms of the imaginary part of the dot self-energy, where $T_i(0) < 1$ in the CO phase implies a nonzero $\Sigma^{\mathrm{I}}(\omega = 0)$ and thus a non-FL state (as also manifest, e.g., 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 symmetric case. For a DD device described by the effective model to be realizable, the physics should be suitably robust for breaking these symmetries. As mentioned previously, that is entirely so for departure from the p-h symmetry. $L/R$ symmetry can be broken by detuning, e.g., the dot levels, $\epsilon_{R/L} = \epsilon \pm \delta\epsilon$, or coupling to the leads, $\Gamma_R \neq \Gamma_L$. In that case it is readily shown that the SC FP remains stable, no new corrections to the FP being generated. For the CO FP by contrast, additional relevant perturbations arise. This FP is thus unstable, and flows in its vicinity ultimately cross over to the SC FP under renormalization, with the crossover scale determined by $\delta\epsilon$. We find, however, that for small but finite $\delta\epsilon \ll T_K^{SU(4)}$, the thermodynamics above are essentially unaffected for $T \gtrsim \delta\epsilon$ and that the abrupt drop in the linear conductance at the transition is simply replaced by a continuous but nonetheless sharp crossover over a $U'$ interval on the order of $T_K^{SU(4)}$. In that sense the physics described here is thus also robust to $L/R$ symmetry breaking.

*Conclusion.*—Motivated by extensive recent interest in capacitively coupled DD systems [3–15], we have analyzed a symmetrical, capacitively coupled semiconducting DD in the two-electron regime, using the NRG technique. We have shown that on increasing the interdot coupling the system evolves continuously through a progression of Fermi liquid states from a purely *spin-Kondo* state, via the $SU(4)$ point where charge and spin degrees of freedom are wholly entangled, to a *charge-Kondo* state with a quenched charge pseudospin, before undergoing a quantum phase transition of the Kosterlitz-Thouless type to a non-Fermi liquid, doubly degenerate charge-ordered phase. This provides a striking example of the subtle and many-sided interplay between spin and charge degrees of freedom in small quantum dots.


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[18] $H_{\mathrm{eff}}$ in the $n = 2$ manifold is $H_{\mathrm{eff}} - H_0 = H_\delta + H'$ where $H_\delta = [U - U'] \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$, vanishing at the $SU(4)$ point, and $H' = \frac{J}{2} \sum_{\mathrm{k,k'}} \sum_{i,\sigma} \sum_{j,\sigma'} a^\dagger_{\mathrm{k'}j\sigma'} a_{\mathrm{k}i\sigma} c^\dagger_{i\sigma} c_{j\sigma'}$ with an antiferromagnetic exchange $J$. Terms with $j \neq i$ in $H'$ arise from $V_L V_R$ processes, interconnecting $(2, 0)/(0, 2)$ and $(1, 1)$ states. Those with $j = i$ come from the $V_R^2$ or $V_L^2$ 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 the form $\frac{J}{4} \sum_{i,\sigma} \sum_{\mathrm{k,k'}} a^\dagger_{\mathrm{k}i\sigma} a_{\mathrm{k'}i\sigma} (\hat{n}_i - 1)$, equal and opposite for $n_i = 0$ and 2.

[19] Results are typically shown for an NRG discretization parameter [17] $\Lambda = 3$ keeping $\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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