Coulomb blockade and non-Fermi-liquid behavior in quantum dots

Frithjof B. Anders,1 Eran Lebanon,2 and Avraham Schiller2
1Department of Physics, Universität Bremen, P.O. Box 330 440, D-28334 Bremen, Germany
2Racah Institute of Physics, The Hebrew University, Jerusalem 91904, Israel

The non-Fermi-liquid properties of an ultrasmall quantum dot coupled to a lead and to a quantum box are investigated. Tuning the ratio of the tunneling amplitudes to the lead and box, we find a line of two-channel Kondo fixed points for arbitrary Coulomb repulsion on the dot, governing the transition between two distinct Fermi-liquid regimes. The Fermi liquids are characterized by different values of the conductance. For an asymmetric dot, spin and charge degrees of freedom are entangled: a continuous transition from a spin to a charge two-channel Kondo effect evolves. The crossover temperature to the two-channel Kondo effect is greatly enhanced away from the box charging energy of the box, thereby generating two independent conduction channels for the local moment formed on the small dot.

In this paper, we explore different regimes of the lead–box device, where charge is not quantized on the quantum dots. We find the following: (i) a line of two-channel fixed points as a function of the gate voltages in the device, extending to the mixed-valent regime of the ultrasmall dot and away from the Coulomb-blockade valleys, charge fluctuations are suppressed on the quantum box. This blocks the interlead exchange coupling at temperatures below the charging energy of the box, thereby generating two independent screening channels for the local moment formed on the small dot. A spin 2CKE then develops on the dot if the effective spin-exchange couplings to the lead and box are tuned to be equal. So far, only the local-moment regime was considered within this scenario.

In this paper, we explore different regimes of the lead–box device, where charge is not quantized on the quantum dots. We find the following: (i) a line of two-channel fixed points as a function of the gate voltages in the device, extending to the mixed-valent regime of the ultrasmall dot and away from the Coulomb-blockade valleys. (ii) Continuous transition from a spin 2CKE to a charge 2CKE for an asymmetric dot; (iii) an intriguing entanglement of spin and charge within the 2CKE that develops in the experimentally relevant case of particle-hole asymmetry, reflected in a simultaneous divergence of the magnetic susceptibility of the dot and the charge capacitance of the box; (iv) an abrupt jump in the $T = 0$ conductance across the two-channel line. Here the Fermi liquids on either side of the critical line are characterized by distinct values of the $T = 0$ conductance.

The setting we consider consists of an ultrasmall quantum dot, modeled by a single energy level $\epsilon_d$, and an on-site repulsion $U$, embedded between a metallic lead and a quantum box. The quantum box is characterized by a finite charging energy, $E_C$, and by a dense set of single-particle levels, which we take to be continuous. Denoting the creation of an electron with spin projection $\sigma$ on the dot by $d_{\sigma}^+$, the corresponding Hamiltonian reads

$$
\mathcal{H} = \sum_{\alpha=L,B} \sum_{k,\sigma} \epsilon_{\alpha k} c_{\alpha k}^\dagger c_{\alpha k\sigma} + E_C (\hat{n}_B - N_B)^2 + \epsilon_d \sum_{\sigma} d_{\sigma}^+ d_{\sigma} + U \hat{n}_{d \uparrow} \hat{n}_{d \downarrow} + \sum_{\alpha, k, \sigma} t_{\alpha} \left\{ c_{\alpha k\sigma}^\dagger d_{\sigma} + \text{H.c.} \right\},
$$

where $c_{Bk\sigma}^\dagger$ creates a lead (box) electron with momentum $k$ and spin projection $\sigma$, $t_L$ ($t_B$) is the tunneling matrix element between the quantum dot and the lead (box), $\epsilon_B (\epsilon_{Lk})$ are the single-particle levels in the lead (box), and $\hat{n}_{d \sigma}$ equals $d_{\sigma}^+ d_{\sigma}$. The excess number of electrons inside the box, $\hat{n}_B = \sum_{k,\sigma} c_{Bk\sigma}^\dagger c_{Bk\sigma} - \theta(\epsilon_{Bk})$, is controlled by the dimensionless gate voltage, $N_B$.

We treat the Hamiltonian of Eq. (1) using a recent adaptation of Wilson’s numerical renormalization-group (NRG) method to the Coulomb blockade. Introducing three collective charge operators for the box $\hat{N} = \sum_{m=\pm \infty} m \langle m | \hat{N}^\pm = \sum_{m=\pm \infty} m \pm 1 \langle m |$, we replace the tunneling term between the dot and the box in Eq. (1) with $\sum_{k,\sigma} t_B \left\{ \hat{N}_+ c_{Bk\sigma}^\dagger d_{\sigma} + \text{H.c.} \right\}$, while the charging-energy term is converted to $E_C (\hat{N} - N_B)^2$. 
Since the dynamics of $\tilde{N}$ is insensitive to the precise number of conduction electrons in the bands, one can relax the constraint $\tilde{N} = \tilde{n}_B$, and regard $\tilde{N}$ as an independent degree of freedom. The resulting Hamiltonian describes then two noninteracting conduction bands coupled to a complex impurity, composed of both $N$ and the dot degrees of freedom. Taking the two conduction bands to have a common rectangular density of states, $\rho(\epsilon) = \rho_0 |D - |\epsilon||$, we solve the resulting model using the NRG. Here the number $N_s$ of NRG states retained sets a lower bound on the ratio $E_C/D$ one can treat. Throughout the paper we set the NRG discretization parameter $\Lambda$ equal to 2.8, while $N_s = 2000$. We begin with a symmetric dot, $U = -2e_d$, and with a box tuned to the middle of a Coulomb-blockade valley, $N_B = 0$. Fixing $E_C$ and the hybridization strength to the lead, $\Gamma_L = \pi \rho t_B^2$, we varied the hybridization to the box, $\Gamma_B = \pi \rho t_B^2$, in search of a 2CKE. Our results for $E_C = \Gamma_L = 0.1D$ are summarized in Fig. 1. Quite surprisingly, we find a two-channel Kondo point $\Gamma_{B}^{\mathrm{2CK}}$ for all values of $U$, ranging from the local-moment regime $U \gg \Gamma_L$, to the strongly mixed-valent regime $U \approx 0$, to the unrealistic regime of $U > 0$. The development of a 2CKE is reflected in a logarithmic divergence of the dot susceptibility as $T \rightarrow 0$ (see Fig. 1), and in a finite-size spectrum that converges to the conventional two-channel fixed point (i.e., identical energies, degeneracies, and quantum numbers).

The emergence of a spin 2CKE for $U \gg \Gamma_L$ proves the scenario of Ref. 14. Specifically, the associated Kondo temperature decays exponentially with $U$ for $U \gg \Gamma_L$, $E_C$ (inset of Fig. 1), while the ratio $\Gamma_{2CK}/\Gamma_L$ approaches the asymptotic value $1 + 2E_C/U$ (not shown). Here and throughout the paper we define the Kondo temperature $T_K$ according to the Bethe ansatz expression for the slope of the $\ln(T)$ diverging term in the susceptibility of the two-channel Kondo model. 12

$$\chi(T) \sim (\mu_B g)^2 (2k_B T)^{-1} \ln(T_K/T). \quad (2)$$

We emphasize, however, that our NRG calculations go well beyond the Schrieffer-Wolff transformation used in Ref. 12 confirming that no relevant perturbations are generated at higher orders in the tunneling amplitudes.

Contrary to the local-moment regime, the development of a spin 2CKE in the mixed-valent regime (let alone for $U < 0$) is an unexpected feature, with no apparent spin degree of freedom to be overscreened. Moreover, $T_K$ is significantly enhanced for $U \approx 0$, exceeding $E_C$ in Fig. 1. This behavior is reminiscent of the two-channel Anderson model, where the 2CKE likewise persists into the mixed-valent regime. 14 Particularly intriguing is the limit of a noninteracting dot, which reduces to the familiar problem of a quantum box connected to a lead by single-mode tunneling. Although a charge 2CKE was predicted for the latter setting at the degeneracy points of the Coulomb blockade, no spin 2CKE was previously anticipated.

To understand the 2CKE for $U = 0$, we revisit the problem of a quantum box connected to a lead by a nearly fully transmitting single-mode point contact. Following Refs. 15 and 16 we model this system by a one-dimensional (1D) geometry, where $x < 0$ ($x > 0$) represents the lead (box), and $x = 0$ corresponds to the noninteracting dot. The deviation from perfect transmission is modeled by weak backscattering at $x = 0$. Extending the bosonization treatment of Ref. 16 to a finite local magnetic field acting on the dot, and carefully accounting for an underlying symmetry of the Hamiltonian 16 we obtain the following linear magnetic susceptibility for $k_B T \ll E_C$:

$$\chi(T) = \chi_0 \left( \frac{\mu_B g}{\hbar v_F} \right)^2 \left[ \ln \left( \frac{D_{\mathrm{eff}}}{2\pi k_B T} \right) - \psi \left( \frac{1}{2} + \frac{\Gamma}{2 k_B T} \right) \right], \quad (3)$$

where $\chi_0 = \Gamma/(4\pi R)$ and $\Gamma = R(8\gamma E_C/\pi^2) \cos^2(\pi N_B)$. Here, $R$ is the reflectance, $v_F$ is the Fermi velocity, $\gamma$ equals $e^C$ with $C \approx 0.5772$, $\psi(x)$ is the digamma function, and $D_{\mathrm{eff}}$ is an effective cutoff of the order of $E_C$.

Equation 3 features a logarithmic temperature dependence down to $k_B T \sim \Gamma$. Hence, $\chi(T)$ diverges logarithmically for perfect transmission, when $\Gamma \propto R$ vanishes. In fact, $\chi(T)$ diverges logarithmically at perfect transmission for all gate voltages, except for half-integer values of $N_B$ where $\chi_0$ vanishes. In particular, Eq. 3 predicts $T_K(N_B) \propto 1/\cos^2(\pi N_B)$.

Equation 3 formally describes the limit $E_C \ll \Gamma_L$, since $\Gamma_L$ serves as the effective bandwidth for the 1D model used (see Ref. 14, Sec. III). Surprisingly, we find
good agreement with the NRG results for $U = 0$ even for $E_C$ as large as $\Gamma_L$. (i) Scanning $N_B$ for fixed $E_C$ and $\Gamma_L$, we find a 2CKE for all gate voltages, with a Kondo temperature that varies by less than 0.2\% for each fixed value of $E_C$. The ratio $T_K(0)/T_K(N_B)$ is well described by $\cos^2(\pi N_B)$ (solid line). Inset: The box charge $\langle N \rangle$ vs $N_B$ for $\Gamma_L = E_C = 0.1D$ and $U = \epsilon_d = 0$. Here $\Gamma_B/\Gamma_L$ equals 1 (squares), 1.72 (filled circles + solid line), and 3.24 (crosses). The Coulomb staircase is completely washed out for $\Gamma_B = \Gamma_B^{2CK}(0) = 1.72T_K$, but is gradually recovered upon departure from $\Gamma_B^{2CK}(0)$.

So far we have considered a symmetric dot, and varied $U = -2\epsilon_d$. In reality, however, $U$ is large and fixed. The experimentally tunable parameters are the dot level $\epsilon_d$, the dimensionless gate voltage $N_B$, and, to a lesser degree, the tunneling rates $\Gamma_L$ and $\Gamma_B$. In Figs. 3 and 4 we explore the 2CKE as a function $\epsilon_d$, for $U/D = 2$ and $\Gamma_L = E_C = 0.1D$. Figure 3(a) shows the two-channel line $\Gamma_B^{2CK}/\Gamma_L$ versus $\epsilon_d$, for $N_B = 0$. The two-channel line separates two distinct Fermi liquids, where the dot is coupled more strongly to the box (for $\Gamma_B$ above the line) or to the lead (below and to the side of the line). Deep in the local-moment regime there is good agreement with the estimate of Ref. 5 based on the Schrieffer-Wolff transformation (dashed line). However, large deviations develop as one approaches the mixed-valent regime.

Fixing $\Gamma_B$ at the $N_B = 0$ value of $\Gamma_B^{2CK}$, the shape of the charge step dramatically changes upon going from the local-moment to the mixed-valent regime [see Fig. 3(b)]. For $\epsilon_d = -U/2$, one recovers a conventional Coulomb-blockade staircase, with charge plateaus at integer units of charge. Upon decreasing $\epsilon_d$, the Coulomb staircase is gradually smeared, until it is essentially washed out for $\epsilon_d/D \approx -1.73$. Upon further decreasing $\epsilon_d$, there is a reentrance of the Coulomb staircase. However, the
Quite remarkably, the degeneracy point where\( H_{\text{spin}} \) is tuned to the corresponding \( \epsilon_d \) is shifted to integer values of \( N_B \), and the charge plateaus occur at half-integer units of charge.

To understand this surprising shift of the Coulomb staircase, we note that it happens for \( \Gamma^2_{2\text{CK}} \) several times larger than \( \Gamma_L \) and \( E_C \). We therefore diagonalize first the local problem is a strong admixture of spin and charge within the 2CKE and different values of \( \epsilon_d \). The tunneling rates \( \Gamma_l \) and \( \Gamma_r \) are kept fixed in all curves, with \( \Gamma_l + \Gamma_r = 0.1 D \). Here \( G_0h/2e^2 \) equals \( 4\Gamma_l\Gamma_r/(\Gamma_l + \Gamma_r)^2 \).

The most striking feature of particle-hole asymmetry is the entanglement of spin and charge within the 2CKE that develops. As demonstrated in Fig. 4 for \( N_B = 0 \) and different values of \( \epsilon_d \neq -U/2 \), there is a simultaneous ln(\( T \)) divergence of the dot susceptibility \( \chi(T) \) and the box capacitance \( C(T) = (e^2/2E_C)d\langle N \rangle/dN_B \), when \( \Gamma_B \) is tuned to the corresponding \( N_B = 0 \) value of \( \Gamma^2_{2\text{CK}} \). Hence, the resulting 2CKE is neither of pure spin nor of pure charge character, but rather involves both sectors.

Quite remarkably, the degeneracy point where \( C(T \rightarrow 0) \) diverges is pinned at \( N_B = 0 \) for all \( \epsilon_d \), although the charge curves of Fig. 5(b) show no particular symmetry about this point. Moreover, there are two distinct Kondo scales, \( T_{\text{K}}^{sp} \) and \( T_{\text{K}}^{ch} \), extracted from the slopes of the ln(\( T \)) diverging terms in \( \chi(T) \) and \( C(T) \). Upon decreasing \( \epsilon_d \) from \( -U/2 \) to \( -U \), \( T_{\text{K}}^{sp} \) monotonically increases while \( T_{\text{K}}^{ch} \) monotonically decreases. This marks a continuous transition from a predominantly spin 2CKE deep in the local-moment regime, to a predominantly charge 2CKE, reminiscent of Matveev’s scenario in the strongly mixed-valent regime.

Experimentally, the relevant temperature scale is the crossover temperature \( T_0 \), below which the 2CKE sets in. Estimating \( T_0 \) from the NRG level flow, we find that it roughly traces \( T_{\text{min}} = \min(T_{K}^{sp}, T_{K}^{ch}) \). The latter scale is greatly enhanced when spin and charge are strongly entangled, reaching a maximum of \( k_B T_{\text{min}} \sim 0.4 E_C \) for the model parameters of Fig. 4. Hence, the conditions for observing the 2CKE in realistic quantum-dot devices are most favorable when the spin and charge degrees of freedom are strongly entangled.

The dot susceptibility is very useful theoretically for analyzing the 2CKE, but difficult to measure for a single dot. In Fig. 5 we depict the \( T = 0 \) conductance, \( G(0) \), for the two-lead device proposed in Ref. 2. Here the single lead is replaced with two separate leads, characterized by the tunneling rates \( \Gamma_l \) and \( \Gamma_r \). In equilibrium, this setting is equivalent to a single lead with \( \Gamma_l = \Gamma_l + \Gamma_r \). At \( T = 0 \), the conductance is proportional to the dot spectral function at the Fermi energy, which we calculate using the NRG. Fixing \( \Gamma_l \) and \( \Gamma_r \), \( G(0) \) drops abruptly as \( \Gamma_B \) crosses \( \Gamma^2_{2\text{CK}} \). However, in contrast to the treatment of Ref. 2, the height of the conductance step is not fixed.

In summary, we found a line of two-channel fixed points in a double-dot device, characterized by the number of excess electrons in the box and by the ratio of the tunneling rates. These fixed points govern the crossover from one Fermi liquid to another, and are experimentally detectable by a sharp drop in the conductance. Charge and spin degrees of freedom are generally entangled, and decouple only at special particle-hole symmetry points such as \( N_B = 0 \) and \( \epsilon_d = -U/2 \). The crossover temperature to the two-channel Kondo effect is greatly enhanced away from the local-moment regime, making this exotic effect accessible in realistic quantum-dot devices.

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Details of the calculation will be published elsewhere.