Smearing of charge fluctuations in a grain by spin-flip assisted tunneling

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(Dated: November 10, 2018)

PACS numbers: 75.20.Hr, 71.27.+a, 73.23.Hk

We investigate the charge fluctuations of a grain coupled to a lead via a small quantum dot in the Kondo regime. We show that the strong entanglement of charge and spin flips in this setup can result in a stable SU(4) Kondo fixed point, which considerably smears out the Coulomb staircase behavior already in the weak tunneling limit. This behavior is robust enough to be experimentally observable.

Recently, quantum dots have attracted a considerable interest due to their potential applicability as single electron transistors or as basic building blocks (qubits) in the fabrication of quantum computers. One of their most important features is the Coulomb blockade phenomenon, i.e., as a result of the strong repulsion between electrons, the charge of a quantum dot is quantized in units of the elementary charge e. Even when the quantum dot is weakly-coupled to a bulk lead, so that electrons can hop from the lead to the dot and back, the dot charge remains to a large extent quantized. This quantization has been thoroughly investigated both theoretically and experimentally. The quantity of interest here is the average dot charge as a function of the voltage applied to a back-gate. For a weakly-coupled dot, at low temperatures, this function generally exhibits sharp steps, resulting in the “Coulomb staircase”. We emphasize the fact that a direct measurement of the average dot charge can be performed with sensitivity well below a single charge.

In this Letter, we investigate the shape of the steps of the Coulomb staircase in the presence of spin-flip assisted tunneling. The setup we examine consists of a (large) dot or grain coupled to a reservoir through a smaller dot (Fig.1). We assume that the smaller dot contains an odd number of electrons and acts as an S=1/2 Kondo impurity. A different limit where the small dot rather acts as a resonant level has been partially studied in Ref. 6 where it was shown that the resonant level can smear the Coulomb blockade (nevertheless, for a narrow resonance at the Fermi energy, the effect is weak). Furthermore, the charge of the grain in such a device can be used to measure the occupation of the dot.

In the following analysis, we focus on the regime where the back-gate voltage is such that the charging states of the grain with 0 or 1 electron are degenerate. We show below that in this case, the charge degrees of freedom of the grain become strongly entangled with the spin degrees of freedom of the small dot resulting in a stable fixed point with an SU(4) symmetry. The major consequence of this enlarged symmetry in our setup is that the dot’s capacitance exhibits instead of a logarithmic singularity a strongly reduced peak as a function of the back-gate voltage, smearing charging effects in the grain considerably. The Coulomb staircase behavior becomes smeared out already in the weak tunneling limit due to the prominence of spin-flip assisted tunneling. The possibility of a strongly correlated ground state possessing an SU(4) symmetry has also been discussed very recently in the (very) different context of two small dots coupled with a strong capacitive inter-dot coupling.

The model we consider is described by the Anderson-like Hamiltonian:

\[
H = \sum_k \epsilon_k a_k^\dagger a_k + \sum_p \epsilon_p a_p^\dagger a_p + \frac{\hat{Q}^2}{2C} + \varphi \hat{Q} + \sum_{\sigma} e a_{\sigma}^\dagger a_{\sigma} + Un_{\uparrow}n_{\downarrow} + t \sum_{k\sigma}(a_{k\sigma}^\dagger a_{\sigma} + \text{h.c.}) + t \sum_{p\sigma}(a_{p\sigma}^\dagger a_{\sigma} + \text{h.c.}),
\]

where \(a_{k\sigma}, a_{\sigma}, a_{p\sigma}\) are the annihilation operators for electrons of spin \(\sigma\) in the lead, the small dot, and the grain, respectively, and \(t\) is the tunneling matrix element which is assumed not to depend on \(k\). We assume in the sequel that the junctions are symmetric and narrow enough,
i.e., contain one channel only. The energy spectrum in
the grain is assumed to be continuous, which implies that
the grain is sufficiently large (at the micron scale). \( \hat{Q} \)
denotes the charge operator of the grain, \( C \) is the capa-
ticity between the grain and the gate electrode, and \( \varphi \) is
related to the back-gate voltage \( V_g \) through \( \varphi = -V_g \).
\( \epsilon < 0 \) and \( U \) stand for the energy level and charging en-
ergy of the small dot, and \( n_\sigma = a_\sigma^\dagger a_\sigma \). The inter-dot
capacitive coupling is weak and neglected here. We con-
sider the situation where the small dot is in the Kondo
regime (which requires the last level to be singly occupied
and the condition \( t \ll (-\epsilon, U + \epsilon) \) to be satisfied).

After a standard Schrieffer-Wolff transformation, the
system is described by the Hamiltonian:

\[
H = \sum_k \epsilon_k a_k^\dagger a_k + \sum_p \epsilon_p a_p^\dagger a_p + \frac{\hat{Q}^2}{2C} + \varphi \hat{Q}
\]

(2)

To simplify notation, the spin indices have been omitted
and hereafter. \( m,n \) take values in the two sets “lead”
(\( k \)) or “grain” (\( \tau \)). The \( \hat{S} \) is the spin of the small
dot, \( \hat{\sigma} \) are Pauli matrices acting on the spin space of
the electrons and \( J = 2t^2/[1/(\epsilon \gamma) + 1/(U + \epsilon)] \) is the
related Kondo coupling. A direct hopping term \( V =
\sqrt{2}/[1/(\epsilon \gamma) - 1/(U + \epsilon)] \) is also present. We have neglected
the charging energy of the grain \( E_C = e^2/(2C) \ll ((\epsilon \gamma), U) \).

We would like to compute the corrections to the average
charge on the grain due to the \( J \) and \( V \) couplings at zero
temperature bearing in mind that when the tunneling
amplitude \( t \to 0 \), i.e., \( J = 0 \) and \( V = 0 \), the average
grain charge exhibits perfect Coulomb staircase behavior
as a function of \( V_g \). We confine ourselves to values of \( \varphi \)
ine the range \( -\epsilon/(2C) \leq \varphi < \epsilon/(2C) \), which corresponds to
the unperturbed (charge) value \( Q = 0 \). A first intuitive
approach is to assume that \( (J, V) \) are very small
compared to the charging energy \( E_C = e^2/(2C) \) of the grain
and to calculate the corrections to \( Q = 0 \) in perturbation
theory. At second order in perturbation theory, we find

\[
\langle \hat{Q} \rangle = e\left(\frac{3}{8}J^2 + 2V^2\right) \ln \left(\frac{e^2/2C - \varphi}{e^2/2C + \varphi}\right).
\]

(3)

The density of states in the lead and in the grain have
been assumed to be equal and taken to be 1 for sim-
plicity. This result generalizes that of a grain directly
coupled to a lead.

There are two reasons that may suggest this perturba-
tive approach is divergent. Higher-order terms (already
at cubic orders) involve logarithmic divergences associated
with the Kondo coupling, but also other logarithms
indicating the vicinity of a degeneracy point in the charge
sector. Note that the (degeneracy) point where the grain
charging states with \( Q = 0 \) and \( Q = \epsilon \) are degenerate

primarily interested in the situation close to this degen-
eracy point, i.e., in the height of the capacitance peaks
at low temperature, where none of the perturbative argu-
ments above can be applied. The Hamiltonian can be
mapped onto some Kondo Hamiltonian following Ref.
[2]. We introduce the projectors \( \hat{P}_0 \) and \( \hat{P}_1 \) which project
on the states with \( Q = 0 \) and \( Q = \epsilon \) in the grain. The
truncated Hamiltonian then reads:

\[
H = \sum_{k,\tau} \epsilon_k a_k^\dagger a_{k\tau} + \frac{\hat{Q}^2}{2C} + \varphi \hat{Q}
\]

\[
+ \sum_{k,k'} \left[ \sum_\tau \left( \frac{J}{2} \hat{\sigma} \cdot \hat{S} + V \right) a_{k\tau}^\dagger a_{k'\tau} \right]
\]

(4)

where now the index \( \tau = 0 \) indicates the reservoir and
\( \tau = 1 \) indicates the grain. We have also introduced the
small parameter \( h = e/(2C) + \varphi \ll e/C \) which measures
deviations from the degeneracy point. Considering \( \tau \) as
an abstract orbital index, the Hamiltonian can be rewritten
in a more convenient way by introducing another set
of Pauli matrices for the orbital sector:

\[
H = \sum_{k,\tau} \epsilon_k a_k^\dagger a_{k\tau} - e h T^z
\]

\[
+ \sum_{k,k'} \left[ \sum_{\tau,\tau'} \left( \frac{J}{2} \hat{\sigma} \cdot \hat{S} + V \right) a_{k\tau}^\dagger a_{k'\tau'} \right]
\]

(5)

In this equation, the operators \( \hat{S}, \hat{\sigma} \) act on spin and
the \( (T, \tau) \) act on the (charge) orbital degrees of free-
don. Here, \( h \) mimics a magnetic field acting in orbital
space. An important consequence of this mapping is that
the average grain charge \( \langle \hat{Q} \rangle \) can be identified as
\( \langle \hat{Q} \rangle = e(h - T^z) \). The grain capacitance \( C =
-\partial \langle \hat{Q} \rangle / \partial h \) is thus equivalent to the local suscepti-
bility \( \chi_T = \partial (T^z) / \partial h \). Naturally, to compute the latter,
we have to determine the nature of the Kondo ground state exactly.

Typically, when only “charge flips” are involved
through the \( V \) term, the model can be mapped onto a
two-channel Kondo model, and the capacitance always
exhibits a logarithmic divergence \[2\]. Here, we have a
combination of spin and charge flips. Can we then expect
two distinct energy scales for the spin and orbital
sectors? To answer this question, we perform a pertur-
bative scaling analysis following that of a related model
in Ref. [10]. We first rewrite the interacting part of the
Hamiltonian in real space as:

\[
H_K = \frac{J}{2} \hat{S} \cdot (\psi^\dagger \hat{\sigma} \psi)
\]

\[
+ \frac{V_z}{2} T^z (\psi^\dagger T^z \psi) + \frac{V_z}{2} [T^z (\psi^\dagger T^z \psi) + h.c.]
\]

(6)

\[
+ Q_z T^z \hat{S} \cdot (\psi^\dagger \tau^z \hat{\sigma} \psi) + Q_\perp \hat{S} \cdot [T^z (\psi^\dagger \tau^z \hat{\sigma} \psi) + h.c.],
\]
where \( \psi_{\sigma \tau} = \sum_k a_{k\sigma\tau} \), \( J \) refers to pure spin-flip processes involving the \( S=1/2 \) spin of the small dot, \( V_{\perp} \) to pure charge flips which modify the grain charge, and \( Q_{\perp} \) describes exotic spin-flip assisted tunneling. This Hamiltonian exhibits a structure which is very similar to the one introduced by Borda et al. in order to study a symmetrical double (small) quantum dot structure with strong capacitive coupling \(^7\). However, since the physical situation that led us to this Hamiltonian is very different from Ref. \(^7\), our bare values for the coupling parameters are also very different (for \( J \ll 1 \) and \( V/J \) not too small, i.e., \( 2e + U \) not too close to 0):

\[
V_{\perp} = V, \quad V_z = 0, \quad Q_z = 0, \quad Q_{\perp} = J/4.
\] (7)

We have ignored the potential scattering \( V\psi^\dagger \psi \) which does not renormalize at low energy.

By integrating out conduction electrons with energy larger than an energy scale \( E \ll \Delta_d \) (\( \Delta_d \) being the level spacing of the small dot, i.e., the ultraviolet cutoff), we obtain at second order the following renormalization group (RG) equations for the five dimensionless coupling constants:

\[
\begin{align*}
\frac{dJ}{dl} &= J^2 + Q_z^2 + 2Q_{\perp}^2 \\
\frac{dV_{\perp}}{dl} &= V_{\perp}^2 + 3Q_{\perp}^2 \\
\frac{dV_z}{dl} &= V_z Q_z + 3Q_{\perp} Q_z \\
\frac{dV_{\perp}}{dl} &= 2JQ_z + 2V_z Q_{\perp} \\
\frac{dQ_z}{dl} &= 2JQ_{\perp} + V_z Q_{\perp} + V_{\perp} Q_z ,
\end{align*}
\] (8)

with \( l = \ln[\Delta_d/E] \) being the scaling variable. This RG analysis is applicable only very close to the degeneracy point \( \varphi = -e/(2C) \) where the effective Coulomb energy in the grain or \( h \) vanishes and obviously only when all coupling constants stay \( \leq 1 \). Higher orders in the RG have been neglected. We have integrated the RG equations \(^8\) numerically. It is noteworthy that even though we started with completely asymmetric bare values of the coupling constants, due to the presence of the spin-flip assisted tunneling terms \( Q_z \) and \( Q_{\perp} \), all couplings diverge at the same Kondo temperature scale (again, assuming the bare ratio \( V/J \) not too small) \( T_K \sim \Delta_d^{-1/4} \). For example, we have checked numerically that all coupling ratios converge to one in the low energy limit provided the RG equations can be extrapolated in this regime. Therefore, this RG analysis suggests that, as in Ref. \(^7\), our model becomes equivalent at low energy to an SU(4) symmetrical exchange model \((J \gg 1)\):

\[
H_K = J \sum_A \psi^\dagger A \left[ \sum_{\alpha\beta} (S^\alpha + \frac{1}{2})(T^\beta + \frac{1}{2}) \right]^A \psi
\] (9)

where we have introduced the “hyper-spin” \( M^A \in \{2S^\alpha, 2T^\alpha, 4S^\alpha T^\beta\} \) for \( \alpha, \beta = x, y, z \). The operators \( M^A \) can be regarded as the 15 generators of the SU(4) group. Moreover, this conclusion is reinforced by the numerical renormalization group analysis (whose range of validity is broader than Eqs. \(^6\)) of a model analogous to Eq. \(^9\) developed in Ref. \(^7\). Notice that the irreducible representation of SU(4) written in Eq. \(^9\) has been used previously for spin systems with orbital degeneracy \(^11\).

The electron operator \( \psi \) now transforms under the fundamental representation of the SU(4) group, with generators \( t^{\alpha \mu}_\nu \) \((A = 1, ..., 15)\), and the index \( \mu \) labels the four combinations of possible spin and orbital indices. The emergence of such a strongly-correlated SU(4) ground state here clearly reflects the strong entanglement between the charge degrees of freedom of the grain and the spin degrees of freedom of the small dot at low energy due to the prominence of spin-flip assisted tunneling.

The (one-channel) SU(N) Kondo model has been extensively studied in the literature (see, e.g., Ref.\(^12\)). Mostly, the strong coupling regime corresponds to a dominant Fermi liquid fixed point induced by the complete screening of the hyper-spin \( M^A \), implying that all the generators of SU(4) yield a local susceptibility with a behavior in \( \sim 1/T_K \) \(^{13, 14}\). \( T^z \) being one of these generators, we deduce that \( \chi_T = -\partial \langle Q^z \rangle / \partial h \) and then the capacitance of the grain \( C = -\partial \langle Q \rangle / \partial h \) evolve as \( 1/T_K \) \(^{13, 14}\). Consequently, for \( h \ll e/C \), we obtain a linear dependence of the average grain charge as a function of \( V_g = -\varphi \):

\[
\langle Q \rangle - e/2 = -eh/T_K = -e(\frac{e}{2C} + \varphi)/T_K.
\] (10)

This is the main result of this paper. The hallmark of the formation of the SU(4) Fermi liquid in our setup is clear. The (grain) capacitance peaks are completely smeared out by the mixing of spin and charge flips and Matveev’s logarithmic singularity \(^2\) has been completely destroyed.

We now discuss the robustness of our SU(4) liquid. First, \( S^z \) and \( T^z \) are marginal operators which guarantees the stability of the SU(4) fixed point at finite magnetic field \( B \ll T_K \) and not too close to the degeneracy point \( h \ll T_K \) \(^7\). The SU(4) symmetry should be still robust for wider junctions characterized by \( n > 1 \) transverse channels \(^13, 14\); even when the transmission amplitudes for the \( n \) modes are equal (extending results of Ref. \(^7\), an SU(4) Kondo singlet would occur at the renormalized Kondo temperature scale \( T_K[n] \approx \Delta_d^{-1/4} e^{-n[e^{-1/4}]} \)).

Applying a strong magnetic field \( B \gg T_K \) inevitably destroys the SU(4) symmetry. However, we expect the behavior of charge fluctuations close to the degeneracy points to remain qualitatively similar. Indeed, in a large magnetic field spin flips are suppressed, i.e., \( Q_x = Q_y = J = 0 \), and the orbital degrees of freedom, through \( V_{\perp} \) and \( V_z \), develop a standard one-channel Kondo model (the electrons have only spin-up or spin down), which also results in a Fermi-liquid ground state with a linear de-
pendence of the average grain charge as in Eq. (10). Yet, the emerging Kondo temperature will be much smaller, $T_K[B = \infty] \approx \Delta_d e^{-1/2V}$, which affects the slope in (10). Finally, for $h \gg T_K$, the orbital Kondo effect is destroyed and the results of ref. [6] should apply [14].

In the following paragraph, we briefly analyze the conductance of the Kondo dot-grain (KDG) system by connecting a lead to the right of the grain in Fig 1. We therefore add the following term to the Hamiltonian (1):

$$\hat{H} = \sum_{k'} \epsilon_{k'} a_{k'\sigma}^\dagger a_{k\sigma} + t' \sum_{k'\sigma} (a_{k'\sigma}^\dagger a_{k\sigma}^\dagger + h.c.),$$

where $a_{k\sigma}$ are the annihilation operators for electrons in the right lead. For a realistic geometry the charge flips between the right lead and the grain are inevitably the most prominent ones (since $J \propto t^2 \ll t'$ and $\Delta_d \leq \langle \hat{Q}^2 \rangle /2C$). This leads to the complete screening of the orbital spin $T^z$ already at a temperature scale $T^z_K \sim E_c e^{-1/t'} \gg T_K$ [2], and to an underlying two-channel Kondo model:

$$\hat{H}_K^c = \frac{1}{2} t' \hat{T} \cdot \hat{\psi}^\dagger \hat{\tau} \hat{\psi}.$$  \hspace{2cm} (12)

The two orbital states here correspond to $\tau = 1$ for the grain and $\tau = 2$ for the right lead. The transmission between the grain and the right lead becomes perfect and the associated conductance is $2e^2/h$. As a result, the renormalization of the charge flip term $V_\perp$ between the grain and the left lead becomes completely cut off by the screening of the orbital impurity. Therefore, the direct hopping term between the left lead and the grain remains small implying that even for $\varphi = -e/2C$, the conductance through the KDG structure should be (very small) proportional to $2V^2e^2/h$ [10]. Nevertheless, the spin flip term $J$ will continue to flow to strong coupling, making the ratio $Q_\perp (l)/J (l) \ll 1$ at low energy. As a consequence, another non trivial two-channel Kondo model appears in the spin sector and the SU(4) symmetry is explicitly broken. This emergence of two distinct two-channel Kondo models, both in the orbital and in the spin sectors deserves further investigation [17].

To summarize, we have determined exactly the shape of the steps of the Coulomb staircase for a grain coupled to a bulk lead through a small quantum dot in the Kondo regime. We have shed light on the possibility of a stable SU(4) Fermi liquid fixed point, where a Kondo effect appears simultaneously both in the spin and the orbital sectors. This requires the condition $2e + U \neq 0$ on the small dot so that the bare $V_\perp / J$ is not too small. In fact, due to the importance of spin-flip assisted tunneling, charge degrees of freedom of the grain become entangled with the spin degrees of freedom of the small dot, which explains this enlarged symmetry (see Eq. (1)). This implies the destruction of the logarithmic peak present in the Coulomb blockade already in the weak-tunneling limit. Such unusual behavior of charge fluctuations in the grain close to the degeneracy points should be observable via capacitance measurements assuming the level spacing of the grain $\Delta_g$ is small enough, i.e., $\Delta_g / E_c \rightarrow 0$. $T_K$ should not be too far from the Kondo scale in the conductance experiments through a single small quantum dot ($\sim 1K$ [17]), and capacitance measurements can be performed much below 100$mK$ [4]. Clearly, this effect is far more pronounced than the smearing of the Coulomb blockade by a resonant impurity level (e.g., when $e \rightarrow 0$, which can be tuned via the gate voltage $V_g$ of the small dot) which remains weak even if the transmission through the impurity at the Fermi energy is perfect [4]. This should be even more striking by measuring the charge of the grain as a function of the two gate voltages $V_g$ and $V_d$ [18].

More generally, as in Ref. [7], these results bring novel insight on the realization of Kondo ground states with SU(N) ($N \gg 2$) symmetry at the mesoscopic scale.

The authors acknowledge D. Sénéchal, A.-M. Tremblay, and G. Zarand for useful discussions and B. Coish for a careful reading of the manuscript. K.L.H. is supported by NSERC and P.S. by the Swiss NSF, NCCR, and the EU RTN Spintronics No HPRN-CT-2002-00302.

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