Entanglement entropy and quantum phase transitions in quantum dots coupled to Luttinger liquid wires

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We study a quantum phase transition which occurs in a system composed of two impurities (or quantum dots) each coupled to a different interacting (Luttinger-liquid) lead. While the impurities are coupled electrostatically, there is no tunneling between them. Using a mapping of this system onto a Kondo model, we show analytically that the system undergoes a Berezinskii-Kosterlitz-Thouless quantum phase transition as function of the Luttinger liquid parameter in the leads and the dot-lead interaction. The phase with low values of the Luttinger-liquid parameter is characterized by an abrupt switch of the population between the impurities as function of a common applied gate voltage. However, this behavior is hard to verify numerically since one would have to study extremely long systems. Interestingly though, at the transition the entanglement entropy drops from a finite value of ln(2) to zero. The drop becomes sharp for infinite systems. One can employ finite size scaling to extrapolate the transition point and the behavior in its vicinity from the behavior of the entanglement entropy in moderate size samples. We employ the density matrix renormalization group numerical procedure to calculate the entanglement entropy of systems with lead lengths of up to 480 sites. Using finite size scaling we extract the transition value and show it to be in good agreement with the analytical prediction.

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I. INTRODUCTION

There has been a recent flurry of activity relating entanglement entropy (EE) (known also as the von Neumann entropy in quantum physics, and related to the Shannon entropy in information theory2–4, and the Bekenstein-Hawking entropy in the framework of black holes5,6), to quantum phase transitions (QPTs)7–9 in condensed matter10. The notion of EE for a many-body system in a pure state arises when one divides it into two distinct regions: A and B. The entanglement between the subsystems A and B is measured by the EE $S_{A/B}$ related to $\rho_A$ or $\rho_B$, the reduced density matrix of regions A or B, respectively.

Specifically, using the Schmidt decomposition, one can express any many-body pure state of the entire system, $|\Psi\rangle$, as the sum of two orthonormal basis sets of regions A ($\{|\phi_{A,i}\rangle\}$) and B ($\{|\phi_{B,j}\rangle\}$), such that

$$|\Psi\rangle = \sum_i \alpha_i |\phi_{A,i}\rangle \otimes |\phi_{B,i}\rangle,$$

with real $\alpha_i \geq 0$ obeying $\sum_i \alpha_i^2 = 1$. This basis is closely related to the eigenbasis of the reduced density operators $\hat{\rho}_{A/B} = \text{Tr}_{B/A}|\Psi\rangle\langle\Psi|$, i.e.,

$$\hat{\rho}_{A/B} = \sum_i \alpha_i^2 |\phi_{A/B,i}\rangle\langle\phi_{A/B,i}|.$$

A unique measure of entanglement between the two regions A and B, is the von Neumann entropy of the reduced density matrix:

$$S_{A/B} = -\sum_i \alpha_i^2 \ln(\alpha_i^2),$$

equivalent to the Shannon entropy of the squared Schmidt coefficients $\alpha_i^2$. This measure is also called the EE. Evidently $S_A = S_B$.

Much effort was devoted to establishing the connection between EE and QPTs in many-particle one-dimensional (1D) systems. It has been shown that in the critical regime of these models there are deviations from the celebrated area law3,4,7,13,14, which states that the EE $S_A$ should depend only on the surface area between regions A and B, hence it is constant (i.e., independent of system size) for 1D systems. This is indeed the case when the system has a finite correlation length (when it is gaped16). For cases in which the correlation length is infinite (i.e., in the critical regime) a logarithmic correction appears in the EE with a universal prefactor. Using conformal field theory arguments the EE of an infinite one-dimensional Luttinger Liquid (LL)12 and various corresponding spin chains was calculated, and the universal prefactor was related to the central charge of the underlying conformal field theory12,13,17. Corrections to the EE due to finite size13,14 and the presence of a defect15,16 were also con-
sidered. For example, a static impurity embedded in a spinless LL, no matter how weak it is, will result (for reconsidered. For example, a static impurity embedded in a
tion group (DMRG) for an infinite system.

crossover between the finite value and zero at the critical
are still correlated), and therefore the EE is zero. The

glement between the two parts exists (even though they
is in a ferromagnetic Kondo phase, in which no entan-
noninteracting or weakly interacting (the LL param-
onto an effective Kondo model

to a different external lead, which are intercoupled only
via electrostatic interactions (no inter-impurity tunnel-
ing), undergoes a Berezinskii-Kosterlitz-Thouless (BKT) QPT as function of the LL parameter and the dot-
lead interaction. This transition is similar in nature to
the QPT recently predicted in the case where a quantum
point contact is coupled to one of the impurities. The
QPT manifests itself in the behavior of the population of
both impurities. One of the impurities (corresponding to
a broad level) swaps its population with the second (nar-
row) impurity as a function of a common external gate
voltage applied on the dots. Similar switching in differ-
ent contexts have been studied extensively. By map-
ing this problem onto that of a multiflavored Coulomb
gas we have recently demonstrated that if the leads are
non-interacting (regular Fermi-Liquids) the population
switching is steep but not abrupt, in agreement with
previous studies. Once the external leads are LLs, we
will show that this switching becomes abrupt at a
critical value of the electron interactions in the lead (i.e.,
at a critical value of the LL parameter) or between the
lead and the impurity.

The second goal is to understand the EE behavior in
this system, especially its sensitivity to the QPT. As we
shall see, the system we consider here may be mapped
onto an effective Kondo model. When the leads are
noninteracting or weakly interacting (the LL parameter
is close to one) the system corresponds to a anti-
ferromagnetic Kondo phase, and therefore the two dis-
connected parts of the system are nevertheless entangled,
leading to a finite EE. On the other hand, for stronger in-
teraction (lower values of the LL parameter) the system
is in a ferromagnetic Kondo phase, in which no entan-
glement between the two parts exists (even though they
are still correlated), and therefore the EE is zero. The
crossover between the finite value and zero at the critical
interaction corresponding to the QPT should be sharp
for an infinite system.

Finally, as a third goal, we use EE to numerically study
the properties of this QPT. Density matrix renormaliza-
tion group (DMRG) is the most convenient numer-
ical method to calculate the ground state properties of
this interacting system, since EE appears naturally in the
procedure. One might wonder though why not calculate
directly the population of the impurities and see when
population switching becomes discontinuous? This turns
out to be extremely difficult since, in order to distinguish
between a real discontinuity and a sharp transition, one
must exceed length scales of order of the inverse relevant
Kondo temperature. As we shall see, the latter is quite
small even for noninteracting leads, and is further
pressed by LL correlations (until it vanishes at the transition point). One possible solution to this problem
is to use DMRG with soft boundary conditions. Here
we shall show that by combining EE and BKT finite size
scaling it is possible to obtain a reliable estimate of the
critical interactions in the lead for manageable lead sizes.

This paper is organized as follows: In the next sec-
tion we introduce the model. Then in Sec. III we detail
the mapping of our model onto a Kondo model, and il-
strate the appearance of a BKT QPT. An analytical
calculation of the dependence of the transition point on
the parameters of the system is given. In the following
section (Sec. IV), we calculate the EE using the DMRG
numerical method, employing three different finite size
procedures to determine the critical value of the interac-
tion in the lead. All the different procedures give similar
estimates of the critical value, which are in good agree-
ment with theory in the range of parameters for which
the theory is valid. We conclude with a discussion of the
results obtained in the previous sections (Sec. V).

II. MODEL

Here we consider a situation in which two single-state
QDs (impurities) are coupled each to a different 1D wires
in the LL regime (see Fig. I). The two impurities are cou-
pled only by an electrostatic interaction. The spin degree
of freedom is ignored (experimentally this corresponds to
the presence of a strong magnetic field or ferromagnetic
dots and leads which polarization the electron spin). The
system is described by the following Hamiltonian:

\[ H = H_{\text{lead}}^L + H_{\text{lead}}^R + H_{\text{impurities}}, \]

where the Hamiltonian \( H_{\ell}^0 \) of lead \( \ell \) (\( \ell = L, R \) for left, right, respectively) is given by

\[ H_{\text{lead}}^\ell = -t_{\ell} \sum_{j=1}^{N_{\ell}-1} c_{\ell,j}^\dagger c_{\ell,j+1} + \text{H.c.} + U_{\ell} \sum_{j=1}^{N_{\ell}-1} (n_{\ell,j} - \nu_{\ell})(n_{\ell,j+1} - \nu_{\ell}), \]

where \( c_{\ell,j}^\dagger \) is the creation operator of an electron on the \( j \)th site of lead \( \ell \) (whose total length is \( N_\ell \)), \( n_{\ell,j} = c_{\ell,j}^\dagger c_{\ell,j} \) is the population of such a site, and \( t_{\ell} \) (\( U_{\ell} \)) is the hopping ma-
trix element (interaction) between the sites in the lead,
and $\nu_\ell$ is the electronic density in the lead. At half-filling ($\nu_\ell = 1/2$, which we will always use in the numerical calculations) the system is in the LL phase for $-2 < U_\ell/t_\ell < 2\frac{\pi}{21}$ with the LL interaction parameter $g_\ell$ and the velocity of excitations $v_\ell$ given by \[ g_\ell = \frac{\pi}{2 \cos^{-1}(-U_\ell/(2t_\ell))}, \] \[ \frac{v_\ell}{2t_\ell} = \frac{\pi}{2 \cos^{-1}(-U_\ell/(2t_\ell))}. \] (6) (7)

The impurities Hamiltonian is

$$H_{\text{impurities}} = \varepsilon Ln_{L,d} + \varepsilon Rn_{R,d} + U_{LR}(n_{L,d} - \frac{1}{2})(n_{R,d} - \frac{1}{2}) + U'_{L}(n_{L,d} - \frac{1}{2})(n_{L,1} - \nu_{L}) + U'_{R}(n_{R,d} - \frac{1}{2})(n_{R,1} - \nu_{R}) + t'Ld_{L,1}^{\dagger} + t'Rd_{R,1}^{\dagger} + \text{H.c.} \tag{8}$$

where $d_{L,1}^{\dagger}$ is the creation operator of an electron on the left (right) impurity, and $n_{L,d} = d_{L,d}^{\dagger}d_{L,d}$ is the population of the $\ell$-th dot. Here $\varepsilon_{LR}(\ell)$ is the left (right) impurity energy (which may be varied by applying an external gate voltage; we henceforth assume that the latter has equal effect on both impurities, $\varepsilon_{\ell} = \varepsilon_{\ell}^{(0)} - V_g^\ell$), and $U_{LR}$ is the Coulomb coupling between the two impurities. Each impurity is coupled to the corresponding lead by both a local electrostatic interaction of strength $U'_{\ell}$, and a tunneling term parametrized by a hopping matrix elements $t'_{\ell}$. The latter gives rise to level broadenings $\Gamma_\ell = \pi|\hbar'_\ell|^2\rho_0$, with $\rho_0$ being the local density of states on the last site of the lead at the Fermi energy [which is equal to $1/(\pi t_\ell)$] at half filling].

### III. MAPPING ONTO KONDO

Our analytic calculations are based on the Anderson-Yuval mapping to a Coulomb gas\textsuperscript{39–41,45,53–58}. In this approach one expands the partition function to all orders in the dot-lead tunneling matrix elements $t'_L$ and $t'_R$, and evaluates the resulting correlation functions at $t'_\ell = 0$. Thus, the partition function becomes a sum over all possible imaginary time histories of tunneling in and out of each level, and can be cast in the form of a grand-canonical partition function of classical particles (charges) representing these hopping events. Because of the dot-lead interaction, each such process involves Fermi edge singularity physics\textsuperscript{82–83}, hence is associated with a Fermi edge singularity exponent $\kappa_{\text{FES}}$, which is defined through the long-time behavior of the correlation function \[ \langle d_{\ell}^{\dagger}(\tau)c_{\ell,1}(\tau)c_{\ell,1}^{\dagger}(0)\rangle \sim \tau^{-\kappa_{\text{FES}}} \text{ at } t'_\ell = 0. \] In addition, the level width $\Gamma_\ell$ should be replaced by an effective value $\Gamma'_{\text{FES}}$, which includes the prefactors in this correlation function. The value of $\kappa_{\text{FES}}$ plays a crucial role in the following. It has been studied in our previous works\textsuperscript{39–41}; here we will repeat our main findings.

When $g_\ell = 1$ (the lead is noninteracting), we have the usual resonant level model, for which $\kappa_{\text{FES}} = (1 - \frac{2}{\pi}\delta_\ell)^2$ and $\Gamma'_{\text{FES}} = \frac{\pi}{g_\ell\rho_0}\cos(\delta_\ell)$, where $\delta_\ell = \tan^{-1}(\pi\rho_0 U'_\ell/2)$ is the phase shift experienced by the electrons near the Fermi energy in lead $\ell$ due to the corresponding dot-lead interaction\textsuperscript{83}. In the general situation ($g_\ell$ not necessarily equal to unity), standard bosonization treatment yields $\kappa_{\text{FES}} = (1 - g_\ell U'_\ell/(\pi\nu v))\frac{1}{g_\ell}$, and $\nu_\ell$ being the velocity of the bosonic phase excitations in lead $\ell$, and $\Gamma'_{\text{FES}} = \pi|t'_\ell|^2\rho_0$. Taking the limit $g_\ell = 1$ we see that, while within a fermionic description $\kappa_{\text{FES}}$ is expressed in terms of the phase shifts $\delta_\ell$, turning to a bosonized framework these $\delta_\ell$ are replaced by their leading order dependence on $U'_\ell$. This is due to the linearization of the spectrum. Hence, the values of $\kappa_{\text{FES}}$ and $\Gamma'_{\text{FES}}$ in any particular model are renormalized by irrelevant operators not appearing in the Luttinger model. Boundary conformal field theory arguments show that $\kappa_{\text{FES}}$ is related to finite size corrections to the spectrum of the lead with different potentials at its ends, which may be evaluated by analytical or numerical means.

| Non-interacting lead | Bosonization | General expression |
|----------------------|--------------|-------------------|
| $\kappa_{\text{FES}}$ | $(1 - \frac{2}{\pi}\delta_\ell)^2$ | $\frac{1}{g_\ell}(1 - g_\ell U'_\ell/(\pi\nu v))^2$ |
| $\Gamma'_{\text{FES}}$ | $\frac{\pi}{g_\ell}\rho_0\cos(\delta_\ell)$ | $\frac{\pi}{g_\ell}(1 - 2g_\ell\delta_\ell)^2$ |



\[ \delta_\text{eff} = \tan^{-1}\left(\frac{U'_\ell}{\sqrt{(2t'_\ell)^2 - U'_\ell^2}}\right). \tag{9} \]

This discussion is summarized in table I.

The Coulomb gas partition function can then be written in a standard form\textsuperscript{76–78}. The imaginary time history of the system (which is a circle whose circumference is the inverse temperature $1/T$) is divided into intervals in which the system is in one of four possible states of the two dots: $\alpha = 00, 10, 01,$ and 11, corresponding to both dots being empty, only the left dot being occupied, only the right dot being occupied, and both dots being populated, respectively. The state $\alpha$ has a dimensionless energy $h_{\alpha}$, measured in units of $1/\xi$, where $\xi$ is a short-time (high-frequency) cutoff. The intervals are separated by hopping events, which are the classical Coulomb gas particles, as mentioned above. Their minimal separation is limited to $\xi$, which is thus of the order of the inverse bandwidth, $\xi \sim 1/t_\ell$. A transition from configuration $\alpha$ to configuration $\beta$ ($\alpha \neq \beta$) is associated with a fugacity $y_{\alpha\beta} = y_{\beta\alpha}$, and a two-component vector charge $e_{\alpha\beta} = -e_{\beta\alpha}$ (the two components correspond to the left
and right lead, respectively), obeying the triangle rule \( \varepsilon_{\alpha\gamma} + \varepsilon_{\beta\gamma} = \varepsilon_{\alpha\beta} \). Physically, the components of \( \varepsilon_{\alpha\beta} \) represent the effective change in the charge of each lead in the corresponding transition. Values of these parameters for the system discussed are summarized in Table III. The partition function reads:

\[
Z = \sum_{N=0}^{\infty} \sum_{\alpha} y_{\alpha_1\alpha_2} y_{\alpha_2\alpha_3} \cdots y_{\alpha_{N-1}\alpha_N} y_{\alpha_N\alpha_0} \times
\]

\[
\int_{0}^{1/T} \frac{\tau_N}{\xi} d\tau_N \int_{0}^{\tau_N-\xi} \frac{d\tau_{N-1}}{\xi} \cdots \int_{0}^{\tau_{N-1}-\xi} \frac{d\tau_2}{\xi} \int_{0}^{\tau_2-\xi} \frac{d\tau_1}{\xi} e^{-\mathcal{S}(\tau_1, \ldots, \tau_N)},
\]

where \( N + 1 = 1 \), so that \( \tau_{N+1} = 1/T \). The classical Coulomb gas action is:

\[
S(\tau_1, \ldots, \tau_N) = \sum_{i<j=1}^{N} \varepsilon_{\alpha_i\alpha_{i+1}} \varepsilon_{\alpha_j\alpha_{j+1}} \ln \left\{ \frac{\pi \xi T}{\sin[\pi T(\tau_j - \tau_i)]} \right\}
+ \sum_{i=1}^{N} \hbar \alpha_{i+1} \frac{\tau_{i+1} - \tau_i}{\xi},
\]

(11)

One can now write down a set of 15 renormalization group (RG) equations for the Coulomb-gas parameters, which are valid to second order in the fugacities \( y_{\alpha\beta} \) but are otherwise exact:

\[
\frac{dy_{\alpha\beta}}{d\ln \xi} = -\frac{2 - \kappa_{\alpha\beta}}{2} y_{\alpha\beta} + \sum_{\gamma} y_{\alpha\gamma} y_{\beta\gamma} e^{(h_{\alpha} + h_{\beta})/2 - h_{\gamma}} - \sum_{\gamma} y_{\alpha\gamma} y_{\beta\gamma} \kappa_{\alpha\gamma},\]

(12)

\[
\frac{d\kappa_{\alpha\beta}}{d\ln \xi} = -\frac{2}{\gamma} \sum_{\alpha\gamma} y_{\alpha\gamma} e^{h_{\alpha} - h_{\gamma}} \kappa_{\beta\gamma} - \sum_{\gamma} y_{\beta\gamma} e^{h_{\beta} - h_{\gamma}} \kappa_{\alpha\gamma},\]

(13)

\[
\frac{dh_{\alpha}}{d\ln \xi} = h_{\alpha} - \sum_{\gamma} y_{\alpha\gamma} e^{h_{\alpha} - h_{\gamma}} + \frac{1}{4} \sum_{\beta,\gamma} y_{\beta\gamma} e^{h_{\beta} - h_{\gamma}},\]

(14)

where \( \kappa_{\alpha\beta} = \varepsilon_{\alpha\beta} \varepsilon_{\beta\alpha} \) and \( \kappa_{\alpha\beta} = \kappa_{\beta\alpha} + \kappa_{\alpha\gamma} - \kappa_{\beta\gamma} \).

We will now concentrate on the Coulomb-blockade valley, i.e., \( |\varepsilon_0|, \varepsilon_0 + U \gg \Gamma_L, \Gamma_R \), where \( \varepsilon_0 = (\varepsilon_L + \varepsilon_R)/2 \), and we assume a small level separation \( \varepsilon_L - \varepsilon_R \) (see below). In this regime only the singly-occupied states are important at low energies. The RG flow is thus divided into three stages: (i) In the first one, \( \xi^{-1} \gg \max(|\varepsilon_0|, \varepsilon_0 + U_{LR}) \), and hence all the four filling configurations of the dots must be treated on equal footing. (ii) Then, as one enters the regime \( \min(|\varepsilon_0|, \varepsilon_0 + U_{LR}) \ll \xi^{-1} \ll \max(|\varepsilon_0|, \varepsilon_0 + U_{LR}) \), the state with higher energy among the unoccupied and doubly-occupied configurations becomes higher than the cutoff and is discarded; (iii) Finally, for \( \xi^{-1} \ll \min(|\varepsilon_0|, \varepsilon_0 + U_{LR}) \), only the singly-occupied states 10 and 01 are left. In this last stage what remains is a Coulomb gas of only a single type of transitions. It is thus equivalent to the one originally derived by Anderson and Yuval for the single-channel anisotropic Kondo model, indicating the equivalence of the two systems. Under this mapping the two states 10 and 01 become, respectively, the up and down states of the spin. The main effect of the two first stages of the flow is to establish the fugacity of the 10 \( \equiv 1 \) transition, which is akin to the spin flip part \( (J_{xy}) \) of the Kondo exchange coupling (via virtual processes through the doubly occupied state 11 and the unoccupied state 00). In addition, these two first stages lead to renormalization of the corresponding Coulomb-gas charge (related to the \( J_z \) part of the Kondo exchange) and the energy difference between these states, which is analogous to a local magnetic field \( B_z \) along the z axis applied on the Kondo spin.

Comparing the two Coulomb gases we can extract the parameters of the equivalent Kondo model. To the leading order in \( \max(\Gamma_{FES}^L, \Gamma_{FES}^R)/\min(|\varepsilon_L|, |\varepsilon_L + U_{LR}|) \) we find:

\[
\rho_0 J_z = 1 - \frac{\kappa_{FES}^L + \kappa_{FES}^R}{2} + \sum_{\ell=L,R} \frac{\kappa_{FES}^\ell \Gamma_{FES}^\ell}{\pi} \left\{ \frac{Q_{2\kappa_{FES}^\ell}(|\varepsilon_0|) |\varepsilon_\ell|}{|\varepsilon_\ell|} + \frac{Q_{2\kappa_{FES}^\ell}(|\varepsilon_\ell + U_{LR}|) |\varepsilon_\ell + U_{LR}|}{|\varepsilon_\ell + U_{LR}|} \right\}
\]

\[
(15)
\]

\[
\rho_0 J_{xy} = 2 \frac{\Gamma_{FES}^L \Gamma_{FES}^R}{\pi} \left\{ \frac{Q_{\kappa_{FES}^L + \kappa_{FES}^R}(|\varepsilon_0|) |\varepsilon_0|}{|\varepsilon_0|} + \frac{Q_{\kappa_{FES}^L + \kappa_{FES}^R}(|\varepsilon_0 + U_{LR}|) |\varepsilon_0 + U_{LR}|}{|\varepsilon_0 + U_{LR}|} \right\}
\]

\[
(16)
\]

where \( P_{\mu}(x) = \Gamma(1 - \mu/2)/x^{1 - \mu/2} \) with \( \Gamma(\varepsilon) \) the gamma function, \( Q_{\mu}(x) = (1 - \mu/2)P_{\mu}(x) \), and all the parameters of the original model refer to their bare values. Without interactions (apart from the Coulomb coupling between
the dots $U_{LR}$) one has $\kappa_{FES}^\ell = 1$, and these expressions reduce to those obtained in previous studies.\textsuperscript{45,61–65}

\begin{align}
\rho_0 J_z &= \frac{\Gamma_L}{\pi} \left( \frac{1}{\varepsilon_L + U_{LR}} + \frac{1}{|\varepsilon_L|} \right) + \frac{\Gamma_R}{\pi} \left( \frac{1}{\varepsilon_R + U_{LR}} + \frac{1}{|\varepsilon_R|} \right) \tag{18}
\end{align}

\begin{align}
\rho_0 J_{xy} &= \frac{2\sqrt{\Gamma_L}}{\pi} \left( \frac{1}{\varepsilon_L + U_{LR}} + \frac{1}{|\varepsilon_L|} \right) \tag{19}
\end{align}

\begin{align}
B_z &= \varepsilon_L - \varepsilon_R - \frac{\Gamma_L}{\pi} \ln \frac{\varepsilon_L + U_{LR}}{|\varepsilon_L|} + \frac{\Gamma_R}{\pi} \ln \frac{\varepsilon_R + U_{LR}}{|\varepsilon_R|} \tag{20}
\end{align}

Since $U_{LR}$ is typically of the order of the bandwidth $\sim t_\ell$, the $Q_\alpha(x)$ and $P_\alpha(x)$ functions only change the corresponding terms by factors of the order of unity with respect to the case $\kappa_{FES}^\ell = 1$. Hence, the main effect of having $\kappa_{FES}^\ell \neq 1$ thus comes through the first term on the right hand side of Eq. (15).

It should also be noted that due to renormalization effects, $B_z$ depends not only on the separation between the levels $\varepsilon_L - \varepsilon_R$, but also on their average position $\varepsilon_0$. In particular, for $|\varepsilon_L - \varepsilon_R| < |\Gamma_L - \Gamma_R|$ the sign of $B_z$ will change as a common gate voltage is varied across the Coulomb blockade valley. Correspondingly, the sign of the average spin projection $\langle S_z \rangle$ will also change, i.e., the two levels will swap their population.\textsuperscript{45,61–65}

The famous Kondo renormalization group equations\textsuperscript{66,73} imply that (cf. Fig. 2) for $J_z > -|J_{xy}|$ (including the case $U_\ell = 0$ and $U_\ell' = 0$) the exchange couplings grow under RG flow, and we are in the strong-coupling (antiferromagnetic-like) Kondo phase, where at low energies the Kondo spin is strongly-coupled (entangled) into a singlet with the environment. This behavior sets in at energies below the Kondo temperature, which is parametrically smaller than any other energy scale in the problem, and, in the generic anisotropic case ($J_z > J_{xy}$, where renormalization of $J_z$ is negligible), scales with the exchange couplings as $T_K \xi \sim (\rho_0 |J_{xy}|)^{1/(\rho_0 J_z)}$. The average Kondo magnetization will be a smooth function of $B_z$ (i.e., the population is a continuous function of the gate voltage) with the scale set by the Kondo temperature at low energies ($T \ll T_K$). For $J_z < -|J_{xy}|$ (which may occur only if $\kappa_{FES}^\ell > 1$) we will enter the weak-coupling (ferromagnetic-like) Kondo regime, in which $J_{xy}$ flows to zero under RG, and the Kondo impurity becomes effectively decoupled at low energies, so that the population will be a discontinuous function of the gate voltage at zero temperature. The transition between the strong-coupling and weak coupling regimes (at $J_z = -|J_{xy}|$) is of the BKT type, and the Kondo temperature goes to zero as $\ln(T_K) \sim -(J_z + |J_{xy}|)^{-1/2}$ when approaching the transition from the antiferromagnetic side.

This behavior can be understood in more physical terms. For example, having $g_\ell \neq 1$ would shift $\rho_0 J_z$ by $-1/(g_\ell + 1/g_R)/2$. By the Kondo renormalization group equations this indicates that $J_{xy}$ processes involving tunneling out of one of the leads and into the other are more (less) relevant for $g_\ell > 1$ ($g_\ell < 1$), due to the enhanced (suppressed) tunneling density of states to the endpoint of a LL with attractive (repulsive) interactions\textsuperscript{12,21,22}. In addition, having $U_\ell' \neq 0$ modifies $J_z$. The term linear in $U_\ell'$ in the expression for $\kappa_{FES}^\ell$ represents the Mahan exciton effect\textsuperscript{82,83} and gives a positive (negative) contribution to $J_z$ when $U_\ell' > 0$ ($U_\ell' < 0$): when dot $\ell$ is occupied, then electrons are repelled (attracted) to the end point of lead $\ell$, thus enhancing (suppressing) tunneling by the Pauli principle, and vice-versa. The quadratic term in $U_\ell'$ in the expression for $\kappa_{FES}^\ell$ represents the contribution of the Anderson orthogonality catastrophe\textsuperscript{82,83}, which always suppresses transitions and hence causes a decrease in $J_z$.

In the following numerical calculations we will confine ourselves to the case $U_\ell = U_R = U$ (so that $g_\ell = g_R = g$) and $U_\ell' = U_R' = U'$, i.e., $\kappa_{FES}^\ell = \kappa_{FES}^R = \kappa_{FES}^\ell = \kappa_{FES}^R$. We will also take $N_L = N_R = N$. For $\varepsilon_\ell = \varepsilon_R$ population switching will occur at the point of particle-hole symmetry, $\varepsilon_L = \varepsilon_R = -U_{LR}/2$. The smooth-abrupt transition point will then be:

\begin{equation}
\kappa_{FES}^* = \frac{1 + 8 \frac{\sqrt{\Gamma_{FES}^{LR}}}{U_{LR}} \sum_{\ell, R} Q_{2\kappa_{FES}}(U_{LR} \xi/2)}{1 - 4 \frac{\sqrt{\Gamma_{FES}^{LR}}}{U_{LR}} \sum_{\ell, R} Q_{2\kappa_{FES}}(U_{LR} \xi/2)}, \tag{23}
\end{equation}

These formulas are reliable for $\max(\Gamma_{FES}) \ll U_{LR}$, where the critical $\kappa_{FES}^*$ is close to unity, so that $Q_{2\kappa_{FES}}(U_{LR} \xi/2)$ is also almost equal to one, and $\Gamma_{FES} \approx \Gamma_K$. In addition,
in the vicinity of the population switching we will get

\[ B_z = \frac{\Gamma(2 - \kappa_{\text{FES}})}{(U_{LR}\xi/2)^{1-\kappa_{\text{FES}}}} \frac{4(\Gamma_{\text{FES}}^R - \Gamma_{\text{FES}}^L)(\varepsilon_0 + U_{LR}/2)}{\pi U_{LR}}. \]  

(24)

With the above expressions for \( \kappa_{\text{FES}} \) one may find the critical \( U^* \) and/or \( U^{**} \) for any value of \( \Gamma_{\ell} \) and \( U_{LR} \). One may also test if the critical value \( U^* \) at \( U' = 0 \) and the critical value of \( U^{**} \) at \( U = 0 \) are compatible (i.e., result in the same \( \kappa_{\text{FES}} \)) even if \( \Gamma_{\ell} \) are not small enough with respect to \( U_{LR} \), so that the critical \( \kappa_{\text{FES}} \) itself cannot be calculated analytically (we still need to assume \( \Gamma_{\ell} \approx \Gamma_{\ell} \)).

IV. NUMERICAL CALCULATION OF ENTANGLEMENT ENTROPY

As discussed above, there are two possible phases for the system. One corresponds to the Kondo antiferromagnetic phase, while the other to the ferromagnetic phase of the Kondo model.

In order to calculate the EE we shall cut the system depicted in Fig. 4 into two parts, L and R. The left region (L) includes the left lead and the corresponding single-level QD (impurity), while the right region (R) includes the right lead and impurity. This is the most natural way to divide the system into two equal parts and has the great advantage of being very natural in the context of numerical DMRG calculations. Particle transfer between the two regions is prohibited. Nevertheless, since the two regions are coupled electrostatically, they are correlated and possibly also entangled. In the anti-ferromagnetic Kondo phase the ground state of the system is a singlet, i.e., an equal superposition of two states (one in which the left impurity is approximately full, while the right one is approximately empty, and vice-versa), resulting in two Schmidt coefficients \( \alpha_1^2 = 1/2 \) and \( \alpha_2^2 = 1/2 \), leading to \( S = S_{LR} = -\ln(1/2) = \ln(2) \). On the other hand, for the ground state of the ferromagnetic Kondo phase, the system is described by a single product many-body state, resulting in \( S = 0 \). The transition will thus manifest itself in a change of the EE between these two values. In the following we will utilize this change to facilitate the identification of the critical transition point.

A. Dot-Lead Interactions

We shall first consider the simplest case for which the leads are a Fermi liquid (i.e., \( U = 0 \) hence \( g = 1 \)) and the only interactions are the interdot interactions \( U_{LR} \) and the dot (impurity)-lead interactions \( U' \). From now on we take the value of the hopping matrix element \( t \) in the leads as our unit of energy. We set \( t'_L = 0.1\sqrt{2} \) and \( t'_R = 0.01\sqrt{2} \), resulting in \( \Gamma_L = 0.02 \) and \( \Gamma_R = 0.0002 \), and vary \( U_{LR} \) and \( U' \). Hereafter in this paper we tune the gate voltage to \( \varepsilon_L = \varepsilon_R = -U_{LR}/2 - 0.0001 \), i.e., slightly above the expected population switching point at half filling. In all forthcoming calculations up to 320 target states were kept for the longer systems. As detailed above, the mapping onto the Kondo model essentially depends only on \( \Gamma_{\text{FES}}^L \), \( \Gamma_{\text{FES}}^R \), and \( \kappa_{\text{FES}} \), which, for the present case, may be simplified to \( \kappa_{\text{FES}} = [1 - 2 \tan^{-1}(U'/2)/\pi]^2 \). As depicted in Fig. 5, varying \( U' \) for a given value of \( U_{LR} \) will result in a modest increase in the EE as \( U' \) becomes more negative, up to a point where a sharp drop in the EE occurs. The larger the interdot interaction \( U_{LR} \) is, the smaller the absolute value of \( U' \) for which this drop occurs. As can be seen in the inset, this drop in the EE occurs for the same value of \( U' \) for which the ground state energy shows a downturn typical of a crossing between two distinct ground-states, as expected from a QPT.

According to the analysis in the previous section, the transition should occur at [see Eq. (23)]

\[ U'^* = 2 \tan \left( \frac{\pi}{2} \left[ 1 - \left( \frac{\pi U_{LR} + 8\sqrt{\Gamma_L \Gamma_R}}{\pi U_{LR} - 4(\Gamma_L + \Gamma_R)} \right)^{1/2} \right] \right). \]  

(25)

Comparing this prediction depicted in the upper inset of Fig. 5 by the curve to the numerical results for the tran-
The system size considered in Fig. 3 is rather small ($N_L = N_R = N = 40$). Nevertheless, one would not expect strong finite-size effects on the critical dot-lead interaction $U^*$, since the mechanism by which tunneling is blocked (the Mahan exciton) is local, i.e., attraction of an electron in the lead to the vicinity of the occupied impurity due to the attractive lead-impurity coupling, as explained in the previous section. Indeed, as can be seen in Fig. 3, the main influence of increasing $N$ is to bring the EE for $-U' < -U^*$ closer to its expected infinite size value of $\ln(2)$, while the estimation of the infinite length dot-lead critical interaction $U^*$ as well as the sharpness of the transition do not seem to depend on $N$. It is also interesting to note that $S$ increases with $|U'|$ for $-U' < -U^*$ (a trend which also appears in Fig. 3). This behavior could be understood as a result of the suppression of the effective $\Gamma_{\text{FES}}$ by the dot-lead interaction (cf. Table 1), consistent with the general trend observed in Fig. 3.

### B. Interactions in the Lead

What happens if we consider a case with no dot-lead interaction (i.e., $U' = 0$), but instead with nearest-neighbor interactions in the leads ($U \neq 0$)? Since, as previously discussed, the phase transition does not depend on the details of the different interactions in the system, but rather on their combined contribution to the Fermi edge singularity exponent $\kappa_{\text{FES}}$, one expects that knowing the critical value of $U^*$ one is able to predict the critical value of $U'$. Thus, using Table I and Eq. (4) one can deduce that the critical LL parameter $g'$ in the absence of dot-lead interaction will be connected to the critical value of $U^*$ in the absence of interactions in the lead ($U = 0, g = 1$) via $g' = (1 - 2 \tan(U^*/2)/\pi)^{-2}$, from which we could find $U^*$ employing Eq. (6). This relation should hold even for $\Gamma_{R,L}/U_{LR} \sim 1$, for which Eq. (25) no longer holds. Thus, for the parameters used in Fig. 3, for which $U'^* = -0.47$, one expects $g'^* \approx 0.75$, resulting in $U^* \approx 1$.

Indeed this can be demonstrated by the calculation of the EE depicted in Fig. 4 where the finite-size behavior of the same system considered in Fig. 3 (i.e., $U_{LR} = 1.2$, $t_L' = 0.4\sqrt{2}$, and $t_R' = 0.03\sqrt{2}$, resulting in $\Gamma_L = 0.32$ and $\Gamma_R = 0.0018$) is presented. A transition of $S$ from values...
close to $\ln(2)$ to values approaching zero as $U$ increases is apparent. Nevertheless, the transition is much more gradual than for the dot-lead interaction (see Fig. 4), which makes sense since the LL character of the lead will be fully developed only for large sample sizes. A crossing between the curves corresponding to different sizes is apparent. While for small values of $U$ larger system sizes correspond to larger values of $S$; the opposite occurs for large values of $U$, which is a hallmark of finite-size scaling of phase transitions.

It is important to emphasize that since we are dealing with a BKT phase transition, the finite-size scaling differs from that of a traditional second order phase transition. While for a second order transition all the curves are expected to cross at the same point, for a BKT transition the crossing point will drift as function of size and only at the limit of $N \to \infty$ will the crossing point correspond to the critical value $U^*$ of the lead nearest-neighbor interaction. The drift in the crossing point can be seen clearly in the inset to Fig. 5, where the crossing between the $N = 30$ and $N = 40$ curves occurs at $U_c \approx 1.5$, while between $N = 400$ and $N = 480$ $U_c \approx 1.05$.

Unlike for finite size scaling for second order transitions, there is no consensus on the optimal method to extract the transition point $U^*$. Therefore, we shall employ three different methods to identify the critical interaction for which the transition occurs: (I) extrapolation of the crossing point at $N \to \infty$ in the spirit of the phenomenological renormalization group (PRG) procedure, (II) extrapolation of the transition point using a scaling ansatz inspired by the homogeneity condition method, (III) identification of the transition point by an heuristic scaling function. All these procedures give a similar estimate of $U^*$, which is in good agreement with the correspondence between $U^*$ and $U_c^*$.

For the PRG inspired (for details of the PRG procedure see Ref. [84]) extrapolation of the crossing point as $N \to \infty$, one defines $U_c(N_1, N_2)$, which is the value of the crossing between the curve corresponding to length $N_1$ and the curve corresponding to $N_2$, where $N_1$ and $N_2$ are two successive (or next to successive) length values. We then extrapolate the behavior of the crossing points by the formula:

$$U_c(N_1, N_2) = U^* + \frac{C}{N_1 + N_2}, \quad (26)$$

where $C$ is a constant, and the value of the crossing point at infinite length is assumed to correspond to the transition point $U^*$. As can be seen in Fig. 5, Eq. (26) works well for the entire range leading to $U^* = 1.02$. When one examines more carefully the large $N$ region (see the inset) the estimation of the critical point shifts a bit to $U^* = 0.96$. Both values are consistent with the expectations based on the dot-lead interaction data ($U^* = 1 \pm 0.1$).

The second method is inspired by the homogeneity condition method proposed and described in detail in Ref. [86]. In this method a function $b(U, N)$ is constructed from the expectation value of the term in the Hamiltonian driving the transition (in our case the interactions in the lead). Then the transition point is determined by the condition $B(U^*, N) = \partial_N [N^3 \partial_N b(U^*, N)] = 0$. Here we shall replace the expectation value $b(U, N)$ by the EE $S(U, N)$, and rewrite the function $B(U, N)$ as a discrete differentiation:

$$B(U, N) = N^3 S''(U, N) + [3N^2 - (\delta N)^2] S'(U, N), \quad (27)$$
where \( S' \) (\( S'' \)) is the first (second) order discrete differentiation of \( S(U, N) \) \{i.e., \( S'(U, N) = [S(U, N + \delta N) - S(U, N - \delta N)]/(2\delta N) \) and \( S''(U, N) = [S(U, N + \delta N) + S(U, N - \delta N) - 2S(U, N)]/\delta N^2 \}\, and \( \delta N \) is the differentiation step. In Fig. 7 (dashed curve) \( B(U, N) \) is plotted for the larger system sizes \((N = 160, 240, 320, 400)\) with \( \delta N = 80 \). Since for higher values of \( U \) there is strong scatter in the data (as indeed has been noticed in other applications of the HMC, see cf. Ref. 86), we have interpolated \( B(U, N) \) over the whole range by a fit to a 6th degree polynomial (continuous curves), and in the vicinity of \( B(U, N) = 0 \) by a fit to a cubic polynomial (dashed curve). The transition point for each size is determined by \( B(U, N) = 0 \), i.e., the point in which the curve crosses the \( x \)-axis. This point is found to be insensitive to the degree of the interpolation polynomial used. Extrapolating the critical value \( U^* \) from the finite size values corresponding to \( B(U, N) = 0 \) (see inset of Fig. 7) results in \( U^* = 0.94 \).

The third method we shall use in order to determine the critical value of \( U^* \) involves a heuristic scaling function of the different curves appearing in Fig. 5. This scaling is based on the observation that the maximum entropy for all system sizes seems to appear at the same value of \( U \approx 0.55 \), and that the general form of \( S(U, N) \) around this value shifts in a rigid manner as function of \( N \). Thus, we postulate that for \( U < U^* \) one may collapse all the different curves onto a single curve by the following heuristic scaling function:

\[
\tilde{S}(U) = \frac{S_{\text{max}}(N)}{S(U, N)},
\]

where \( S_{\text{max}}(N) = S(U = 0.55, N) \) is the maximum value of the EE for a given length \( N \) of the system. As can be seen in Fig. 8 applying this heuristic function collapses all the different curves on a single one up-to a certain value of \( U \), while for larger values the curves diverge. This is somewhat similar to the situation one encounters for the PRG scaling of the energy gap in the BKT transition. Identifying the point for which the curves begin to diverge with the critical point (as is done in the PRG procedure) results in \( U^* \approx 0.95 \), in agreement with the other methods we employed here for identifying the critical point.

### C. Both Dot-Lead and Intra-Lead Interactions

Now we shall discuss the behavior for the case where both \( U' \) and \( U \) are nonzero. We will consider the case where both \( U' > 0 \) and \( U > 0 \), which is the case expected to be encountered in realistic experimental devices. We shall set the dot-lead tunneling matrix elements \( t_L = 0.2\sqrt{2} \) and \( t_R = 0.02\sqrt{2} \), corresponding to \( \Gamma_L = 0.08 \) and \( \Gamma_R = 0.0008 \), while retaining \( U_{LR} = 1.2 \). For these parameters \( \max(\Gamma_l)/U_{LR} \ll 1 \) and we expect the determination of the critical point which depends on the parameter \( \kappa_{\text{FES}} \) given in Eq. 28 to hold. Setting \( U' = 0.3 \) and using the relationship given in Eq. (9), the transition is expected to occur at \( U^* \) obeying the following relation:

\[
U' = \sqrt{4 - (U^*)^2},
\]

\[
\tan \left[ \cos^{-1} \left( -\frac{U^*}{2} \right) \right] = 1 - \frac{\pi \kappa_{\text{FES}}^*}{2 \cos(-U^*/2)}.
\]

The right hand side, for a given value of \( \Gamma_L, \Gamma_R, \) and \( U_{LR} \), depends only on \( U^* \). Thus by plotting the right side of Eq. (29) and determining where it crosses the value of \( U' \), it is possible to evaluate \( U^* \). For the parameters considered here, the critical value corresponds to \( U^* = 0.96 \). There is an additional crossing at \( U^* = 1.95 \), but since this is very close to the LL-charge density wave phase transition point (at \( U = 2 \)) it would be extremely hard to observe it numerically for reasonable system sizes.

One may wonder why in the previous sub-section we did not consider also the case of \( \max(\Gamma_l)/U_{LR} \ll 1 \), which would facilitate a direct comparison between \( U^* \) and theory, instead of discussing a case for which \( \Gamma_l \) are comparable to \( U_{LR} \), leaving only the possibility to compare between the numerically computed \( U^* \) and \( U^*_0 \)? The reason is that for \( \max(\Gamma_l)/U_{LR} \ll 1 \) and \( U' = 0, U^* \) tends to be close to zero, i.e., \( g \approx 1 \). For values of the LL close to the non-interacting case, one must go to very large systems to see the LL behavior developing, which is beyond our current capabilities.

Returning to the case at hand, it can be clearly seen in Fig. 8 that as in the previous cases, a typical BKT crossing of the \( S \) as function of \( U \) for the different lengths is observed. Using the extrapolation of the crossing point...
FIG. 9: (Color online) The numerically computed EE $S$ as function of the interactions in the lead $U$, for a constant dot-lead interaction $U' = 0.3$ and different lengths $N$ of the lead. The hopping matrix elements between each lead and the corresponding dot are given by $t_L' = 0.2\sqrt{2}$ and $t_R' = 0.02\sqrt{2}$ ($\Gamma_L = 0.08$ and $\Gamma_R = 0.0008$), while $U_{LR} = 1.2$, corresponding to a Kondo temperature of $T_K \approx 10^{-13}$ at $U = 0.26\, \text{[45]}$. The transition between values of the EE close to $\ln(2)$ (indicated by dashed line) and to zero is steeper than in Fig. 5, although the typical BKT transition crossing are still clearly evident. Inset: An extrapolation of the critical $U^*$ in the same manner as in Fig. 6. The symbols depict the crossing point between the curves in the main figure corresponding to $N_1$ and $N_2$, where successive and next to successive lengths are taken. The line represents a fit to Eq. 26.

at $N \to \infty$ following the PRG procedure, and fitting it to Eq. 26 (see inset), an extrapolated value of $U^* = 0.98$ is obtained, in good agreement with the analytical prediction.

V. DISCUSSION

We have shown that in the presence of repulsive interaction in the lead ($U > 0$, $g < 1$), the system depicted in Fig. 1 may show an abrupt population switching, i.e., an abrupt swap of the left dot-right dot population as function of the applied gate voltage. The nature of the population switching has a clear signature in the behavior of the EE. For smooth switching the system can be mapped on the antiferromagnetic Kondo model, resulting in a finite entanglement between the left and right sub-systems. On the other hand, for abrupt switching the system corresponds to a ferromagnetic Kondo model, for which there is no entanglement between the sub-systems.

Using this behavior of the EE, and the fact that it lends itself to straightforward calculation within the framework of numerical DMRG, we were able to use finite size scaling to identify the QPT between the smooth and abrupt switching phases. We have found that using the signature of the QPT on the EE behavior indeed gives an accurate method to study the transition properties. This reproduces the analytical results obtained by mapping the the system onto a Kondo model. One may expect that the EE could be used in a similar fashion to identify and study different QPTs related to dynamical impurities.

Finally, it should be noted that according to Eq. (23), in the absence of dot-lead interactions ($U' = 0$), and for strong interdot interactions $U_{LR} \gg \max(\Gamma_L)$, the abrupt population switching will occur at values of the LL parameter smaller than a critical value which is quite close to unity

$$1 - g^* \sim \frac{\max(\Gamma_L)}{U_{LR}}.$$  

Thus, for large interdot interaction $U_{LR} \gg \max(\Gamma_L)$, even a weak interaction in the leads will result in an abrupt population switching. Once dot-lead interactions are taken in account, the critical $g^*$ will be further decreased by $2U'/(\pi t)$. Since $t$ is essentially the band width and the dot-lead interaction is parametrically much smaller, the abrupt population switching phase will appear for values of $g \approx 1$ even when repulsive dot-lead interactions are included, and should thus be accessible experimentally. The population switching can be probed using a quantum point contact as a charge sensor.

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