Population switching and charge sensing in quantum dots: A case for a quantum phase transition

Moshe Goldstein,1 Richard Berkovits,1 and Yuval Gefen2

1 The Minerva Center, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel
2 Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 76100, Israel

A broad and a narrow level of a quantum dot connected to two external leads may swap their respective occupancies as a function of an external gate voltage. By mapping this problem onto that of two coupled classical Coulomb gases we show that such a population switching is not abrupt. However, trying to measure this by adding a third electrostatically coupled lead may render this switching an abrupt first order quantum phase transition. This is related to the interplay of the Mahan mechanism versus the Anderson orthogonality catastrophe, in similitude to the Fermi edge singularity.

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The phenomenon of population switching (PS)1,2,3 occurs in a discrete level quantum dot (QD) — e.g., a QD with one broad and one narrow level. Upon a continuous variation of a plunger gate voltage the occupation numbers of the levels are inverted, cf. Fig. 1. This phenomenon is relevant to a wide range of experimentally observed effects, including the widely used technique of charge sensing1 and, possibly, the occurrence of a large shot noise Fano factor through QD4, as well as correlated lapses of the transmission phase through a QD5,6. One particularly intriguing question in this context is whether or not (at zero temperature) PS is abrupt, hence constitutes a first order quantum phase transition (QPT).

In the following we address this question in the context of a two level QD coupled to leads of spinless noninteracting electrons. This is mapped onto a system of two single level QDs, each coupled to a single lead (cf. Fig. 2). We formulate the problem in terms of two coupled classical Coulomb gases, perform a renormalization group (RG) analysis of this 15 parameter problem, and show that its low temperature behavior is akin to an antiferromagnetic Kondo problem, hence no QPT occurs. This is dramatically changed when a third lead (e.g., a quantum point contact, QPC, serving as a charge sensor) is electrostatically coupled to one of the QDs. The model may then scale to the ferromagnetic Kondo problem, and by tuning the strength of the third lead coupling one induces a QPT.

The problem at hand can be viewed within an even broader context. The features of the Fermi edge singularity are the result of the competition between the Anderson orthogonality catastrophe and the Mahan exciton physics7. The fact that the latter wins gives rise to the divergence at the X-ray absorption edge. Such an interplay is present here too. Turning on the electrostatic coupling to the third lead increases the weight of the orthogonality catastrophe. The latter eventually wins, suppressing transitions between charge configurations before and after PS takes place. This implies a QPT between these two configurations. Our setup then serves as a handy laboratory which allows us to control and tune the relative strengths of two fundamental effects in many-body physics.

The original system of spinless electrons, made of a two (unequal) orbital level quantum dot (QD) connected to two leads (cf. Fig. 2a, is described by the Hamiltonian

\[ H = \hat{H}_{\text{lead}} + \hat{H}_{\text{dot}} + \hat{H}_{\text{dot-lead}}. \]

We assume the leads to be non-interacting, and the dot-lead tunneling matrix elements \( \{ \hat{V}_{\ell} \} \) (i = 1, 2 and l = L, R for left, right) to be real and possess a left-right symmetry, \( |\hat{V}_{\ell L}| = |\hat{V}_{\ell R}| \) (effects of asymmetry are discussed later). We will consider the more intricate case \( s \equiv \text{sign}(\hat{V}_{1L}\hat{V}_{1R}\hat{V}_{2L}\hat{V}_{2R}) = -1 \)7. We now map the original model onto a modified one consisting of two single-level QDs, cf. Fig. 2b. The Fermi operators \( \hat{\psi}_L \) and \( \hat{\psi}_R \) of the new leads are made of symmetric and antisymmetric combinations of the original \( \psi_L \) and \( \psi_R \), respectively. The Hamiltonian is
Here, employing a basis of states spanning the four filling interactions, with $H_{\ell,\text{dot}} = \mathcal{L}_{\ell,\text{lead}} + \mathcal{L}_{\ell,\text{dot}}$, in an obvious notation. Following a Hubbard-Stratonovich transformation, we write:

$$Z = \int \mathcal{D}[\phi] e^{-\int_0^1 \frac{\phi^2(z)}{2} \, dz} \mathcal{Z}_{L}(\phi(\tau)) \mathcal{Z}_{R}(\phi(\tau)),$$

where, after expansion to all orders in the dot-lead coupling terms $\mathcal{L}_{\ell,\text{dot-lead}}$, we obtain:

$$\frac{Z_{\ell,\text{dot-lead}} Z_{\ell,\text{lead}}}{Z_{\ell,\text{lead}} Z_{\ell,\text{dot-lead}}(\phi(\tau))} = \sum_{N_{\ell},N'_{\ell}=0}^{\infty} \frac{(-V_{\ell})^{N_{\ell}}}{N_{\ell}! N'_{\ell}!} \int \frac{d\tau_{\ell}^1}{1/T} \cdots \int \frac{d\tau_{\ell}^N}{1/T} \int \frac{d\tau_{\ell}^1}{1/T} \cdots \int \frac{d\tau_{\ell}^{N'}}{1/T} \langle \tilde{\psi}_{\ell}(0, w_{\ell}^1) \tilde{\psi}_{\ell}(0, \tilde{w}_{\ell}^1) \cdots \tilde{\psi}_{\ell}(0, w_{\ell}^{N_{\ell}}) \tilde{\psi}_{\ell}(0, \tilde{w}_{\ell}^{N_{\ell}}) \rangle. \quad (3)$$

Here $\langle \cdots \rangle_{\ell,0}$ denotes averaging over the bare Lagrangian $\mathcal{L}_{\ell,0} = \mathcal{L}_{\ell,\text{lead}} + \mathcal{L}_{\ell,\text{dot}}(\phi(\tau))$, with $\mathcal{L}_{\ell,\text{dot}}(\phi(\tau)) = \mathcal{L}_{\ell,\text{lead}}(\tilde{\phi}_\ell(\tau)[\tilde{\phi}_\ell(\tau)]^\dagger + \tilde{\phi}_\ell(\tau)], \quad \tilde{\phi}_\ell(\tau) = \tilde{\phi}(\tau) - U/2 + i \phi(\tau); \quad \mathcal{Z}_{\ell,\text{lead}} \text{ and } \mathcal{Z}_{\ell,\text{dot}}(\phi(\tau))$ are the corresponding partition functions. By Wick's theorem $N_{\ell} = N'_{\ell}$, and then this average equals

$$\det \left[ \mathcal{G}_{\ell,\text{lead}}^0(w_p^\ell, w_p'^\ell) \right] \times \det \left[ \mathcal{G}_{\ell,\text{dot}}^0(w_p^\ell, w_p'^\ell) \right],$$

where the lead and dot Green functions are:

$$\mathcal{G}_{\ell,\text{lead}}^0(w, w') = -\frac{\pi T \rho_{\ell}}{\sin[\pi T |w - w'|]}, \quad (4)$$

$$\mathcal{G}_{\ell,\text{dot}}^0(w, w') = e^{-\int_0^1 \tilde{\xi}_\ell(\tau) d\tau} |f[\tilde{\xi}_\ell(\tau) - \theta(w - w')]. \quad (5)$$

Here $\rho_{\ell}$ is the local density of states at the edge of lead $\ell$, $\tilde{\xi}_{\ell,0} = T \int_0^T \tilde{\xi}_\ell(\tau) d\tau$, and $f(\epsilon) = 1/(e^{\epsilon/T} + 1)$. The lead determinants are, as usual, of the Cauchy form, enforcing the Pauli principle. Hence, we will relabel both entry and exit times by $\tau^l_{n_{\ell}}$, with $n_{\ell} = 1, 2, \ldots 2N_{\ell}$, which will be ordered chronologically: $m_{\ell} < n_{\ell}$ implies $\tau^l_{m_{\ell}} < \tau^l_{n_{\ell}}$.

At this stage the functional integration over $\phi(\tau)$ can be performed, leading to a two-flavor Coulomb gas grand-canonical partition function: entry (exit) from the dot corresponds to a positive (negative) charge, and the two flavors are correlated due to the interaction $U$ between $L$ and $R$:

$$Z = \sum_{N_{\ell},N_R=0}^{\infty} \left( \frac{\Gamma_{\ell}}{\pi} \right)^{N_{\ell}} \left( \frac{\Gamma_R}{\pi} \right)^{N_R} \int \frac{d\tau_{\ell}^L}{1/T} \cdots \int \frac{d\tau_{\ell}^L}{1/T} \int \frac{d\tau_{\ell}^R}{1/T} \cdots \int \frac{d\tau_{\ell}^R}{1/T} e^{-S(\tau^\ell_{m_{\ell}})} \cdot \cdots \cdot e^{-S(\tau^R_{n_{R}})}. \quad (6)$$

Here $\xi$ is a short-time cutoff, $\Gamma_{\ell} = \pi |V_{\ell}|^2 \rho_{\ell}$ is the width of level $\ell$, and $S(\{\tau^l_{n_{\ell}}\}) = S_L(\{\tau^l_{n_{\ell}}\}) + S_R(\{\tau^R_{n_{R}}\}) + S_U(\{\tau^R_{n_{R}}\})$, with:

$$S_L(\{\tau^l_{m_{\ell}}\}) = \sum_{m_{\ell} < n_{\ell}=1}^{2N_{\ell}} \left( \frac{1}{n_{\ell}} - \frac{1}{m_{\ell}} \right) V_{C}(\tau^l_{m_{\ell}} - \tau^l_{n_{\ell}}) + \epsilon_{\ell} \sum_{n_{\ell}=1}^{2N_{\ell}} (1 - 1/n_{\ell})^2 \epsilon_{R}, \quad \quad (7)$$

$$S_U(\{\tau^R_{n_{R}}\}) = \sum_{n_{R}=1}^{2N_{R}} \sum_{l=1}^{2N_{L}} \left( 1 - 1/n_{L} + n_{R} - 1 \right) |\tau^R_{n_{R}} - \tau^R_{n_{R}}|. \quad (8)$$

The respective fugacities are $\sqrt{\Gamma_{\ell} \xi \Gamma_{\ell}}/\pi$. The different terms in the action $S(\{\tau^\alpha_{n_{\alpha}}\})$ describe species sensitive electric fields, as well as intra-species and inter-species interactions, with $V_{C}(\tau - \tau') = \ln \{\pi T \xi / \sin[\pi T |\tau - \tau'|]\}$.

To facilitate RG analysis, we rewrite the partition function, employing a basis of states spanning the four filling configurations of the two dots: $\alpha = 00, 10, 01, 11$ (cf. Fig. 3). The state $\alpha$ has an energy $h_{\alpha}/\xi$. A fugacity $\gamma_{0,\alpha} = \gamma_{0,\beta}$ corresponds to a transition from configuration $\alpha$ to $\beta$ ($\alpha \neq \beta$), involving a two-component vector charge $e_{\alpha,\beta} = -e_{\beta,\alpha}$ (the two components correspond to the charge removed from the $L$ and $R$ lead, respectively,
Parameters characterizing the Coulomb gas [Eqs. (9)–(10)]: \( h_{\alpha=10,\beta=11} \) is the energy associated with the state \( 11 \); its bare value is \( (\varepsilon_L + \varepsilon_R + U) \). The transition depicted involves the fugacity \( y_{\alpha=10,\beta=11} \) and the charge \( \varepsilon_{\alpha=10,\beta=11} \), whose bare values are \( \sqrt{\Gamma_R \xi / \pi} \) and \( (0, 1) \), respectively (see Table I). Dashed lines indicate couplings generated through RG iterations, e.g., \( y_{10,01} \) (corresponding to \( \rho J_{xy}/2 \)). See the text for further details.

Table I: Parameters appearing in the Coulomb gas model, Eqs. (9)–(10), corresponding to the system depicted in Fig. 2(b). They obey \( \varepsilon_{\alpha \beta} = -\varepsilon_{\beta \alpha} \) and \( y_{\alpha \beta} = y_{\beta \alpha} \). See the text for further details.

\[
\begin{array}{ccc}
\text{Fugacities} & \text{Charges} & \text{Energies} \\
y_{00,10} & \sqrt{\frac{\Gamma_L \xi}{\pi}} & \varepsilon_{00,10} = (1, 0) & h_{00} = 0 \\
y_{00,01} & \sqrt{\frac{\Gamma_L \xi}{\pi}} & \varepsilon_{00,01} = (0, 1) & h_{10} = \varepsilon_L \xi \\
y_{10,11} & \sqrt{\frac{\Gamma_L \xi}{\pi}} & \varepsilon_{10,11} = (0, 1) & h_{01} = \varepsilon_R \xi \\
y_{10,11} & \sqrt{\frac{\Gamma_L \xi}{\pi}} & \varepsilon_{10,11} = (0, 0) & h_{11} = (\varepsilon_L + \varepsilon_R + U) \xi \\
y_{10,01} & 0 & \varepsilon_{10,01} = (-1, 1) & \\
y_{01,11} & 0 & \varepsilon_{01,01} = (1, 1) & \\
\end{array}
\]

\[
\frac{dh_{\alpha}}{d \ln \xi} = h_{\alpha} - \sum_\gamma y_{\alpha \gamma} e^{h_{\alpha,\gamma} - h_{\gamma}} + \frac{1}{4} \sum_\gamma y_{\beta \gamma} e^{h_{\beta,\gamma} - h_{\gamma}}. \quad (13)
\]

We now address the parameter regime in the vicinity of population switching. This requires a small level separation, \( |\varepsilon_L - \varepsilon_R| < |\Gamma_L - \Gamma_R| \). Defining \( \varepsilon_0 = (\varepsilon_L + \varepsilon_R)/2 \), we have, in the Coulomb-blockade valley, \( |\varepsilon_0|, \varepsilon_0 + U \gg \Gamma_L, \Gamma_R \). The RG flow is then divided into three stages: (i) \( \xi^{-1} \gg \max(|\varepsilon_0|, \varepsilon_0 + U) \), all four filling configurations take equal part in the RG flow; (ii) \( \min(|\varepsilon_0|, \varepsilon_0 + U) \ll \xi^{-1} \ll \max(|\varepsilon_0|, \varepsilon_0 + U) \), the higher energy configuration between 00 and 11 drops out; (iii) \( \xi^{-1} \ll \min(|\varepsilon_0|, \varepsilon_0 + U) \), only configurations 10 and 01 survive. In this last stage we are left with a Coulomb gas of only a single type of transitions. The latter is equivalent to the one obtained for the single channel anisotropic Kondo model [10], with the two (pseudo-)spin states represented by configurations 10 and 01. The main effect of the two first stages of the flow is to establish the fugacity of the 10=01 transition, (via virtual processes through the doubly occupied and unoccupied states, 11 and 00), as well as to renormalize the corresponding charge and the energy difference between these states.

The resulting Kondo model has the following couplings, to leading order in \( \Gamma_\ell \) (all the parameters refer to their bare values) [13]:

\[
\rho J_z = 1 - \frac{\varepsilon_{01,01}}{2} + \left[ \frac{\Gamma_L}{2 \pi} \left( \frac{Q_{2\varepsilon_{00,10}}(|\varepsilon_L|)}{\varepsilon_L} \right) \frac{Q_{2\varepsilon_{01,01}}(|\varepsilon_L|)}{\varepsilon_L + U} \right]_{\varepsilon_{00,10}} + \left( \Gamma_R \right) \left[ Q_{2\varepsilon_{01,11}}(|\varepsilon_L|) - P_{2\varepsilon_{01,11}}(|\varepsilon_L + U|) \right], \quad (14)
\]

\[
\rho J_{xy} = \frac{2 \sqrt{\Gamma_L \Gamma_R}}{\pi} \left( \frac{Q_{2\varepsilon_{00,10}}(|\varepsilon_0|)}{\varepsilon_0} \right) \left[ \frac{Q_{2\varepsilon_{01,11}}(|\varepsilon_0|)}{\varepsilon_0 + U} \right], \quad (15)
\]

\[
H_z = \varepsilon_L - \varepsilon_R - \frac{\Gamma_L}{\pi} \left[ P_{2\varepsilon_{00,10}}(|\varepsilon_L|) - P_{2\varepsilon_{01,11}}(|\varepsilon_L + U|) \right] + \frac{\Gamma_R}{\pi} \left[ P_{2\varepsilon_{01,01}}(|\varepsilon_R|) - P_{2\varepsilon_{01,11}}(|\varepsilon_R + U|) \right], \quad (16)
\]

where \( P_\alpha(x) = \Gamma(1 - a/2) / x^{1-a/2} \), \( Q_\alpha(x) = (1 - a/2) P_\alpha(x) \). For the system discussed thus far (cf. Table I) the bare values are \( \kappa_{\alpha \beta} = 1 \) for all \( \alpha, \beta \) except...
\[ \kappa_{10,01} = \kappa_{00,11} = 2. \] We then find:
\[ \rho J_{z} = \frac{\Gamma_{L}}{\pi} \left( \frac{1}{\varepsilon_{L} + U} + \frac{1}{|\varepsilon_{L}|} \right) - \frac{\Gamma_{R}}{\pi} \left( \frac{1}{\varepsilon_{R} + U} + \frac{1}{|\varepsilon_{R}|} \right), \] (17)
\[ \rho J_{xy} = \frac{2 \sqrt{\Gamma_{L} \Gamma_{R}}}{\pi} \left( \frac{1}{\varepsilon_{0} + U} + \frac{1}{|\varepsilon_{0}|} \right), \] (18)
\[ H_{z} = \varepsilon_{L} - \varepsilon_{R} - \frac{\Gamma_{L}}{\pi} \ln \frac{\varepsilon_{L} + U}{|\varepsilon_{L}|} + \frac{\Gamma_{R}}{\pi} \ln \frac{\varepsilon_{R} + U}{|\varepsilon_{R}|}, \] (19)

in agreement with the poor man’s scaling of Refs. 8. \( H_{z} \) will change sign as the gate voltage is swept across the Coulomb blockade valley, provided that \(|\varepsilon_{L} - \varepsilon_{R}| < |\Gamma_{L} - \Gamma_{R}|\), hence the spin projection \((S_{z})\) will also change sign, implying a PS. Since \( J_{xy} \) and \( J_{z} \) are antiferromagnetic, they flow to strong coupling, so the PS will be continuous over the scale of the Kondo temperature, \( T_{K} = \frac{\sqrt{U(U+6)}}{\pi} \exp \left[ \frac{\pi (U+5)}{8U(U+4)} \ln \left( \frac{\Gamma_{R}}{\Gamma_{L}} \right) \right] \).

The problem becomes much more intriguing when an electrostatically coupled third lead (e.g., a QPC charge sensor) is introduced, cf. Fig. 2(c). We add to the Hamiltonian a term \( H_{QPC} = H_{lead} + U_{QPC} \psi_{QPC}^{\dagger}(0) \psi_{QPC}(0) :d_{1}^{\dagger}d_{1} - \frac{1}{2} :\), consisting of the Hamiltonian of a free lead plus an interaction term. One may re-employ the Coulomb-gas formalism, but now \( \varepsilon_{\alpha,\beta} \) consists of 3 components \[ 11, 13. \] Denoting the population of dot \( L \) in state \( \alpha \) by \( n_{\alpha L} \), the third component of \( \varepsilon_{\alpha,\beta} \) is given by \( (n_{\alpha,\beta} - n_{\alpha,\alpha})\delta_{QPC}/\pi \), with \( \delta_{QPC} = 2\tan^{-1}(\rho_{QPC}U_{QPC}/2) \) being the change in phase shift of the electronic wave-functions of the QPC caused by a change in the population of dot \( L \), and \( \rho_{QPC} \) the corresponding local density of states. The resulting RG equations [Eqs. (11)-[13]] and their general solution [Eqs. (13)-[16]] are as before. Now, however, the bare valued are \( \kappa_{00,01} = \kappa_{10,11} \) = 1, \( \kappa_{01,10} = \kappa_{01,11} \) = 1 + \( (\delta_{QPC}/\pi)^{2} \), and \( \kappa_{00,10} = \kappa_{01,11} = 2 + (\delta_{QPC}/\pi)^{2} \). At low energies we are still left with an effective Kondo model. The main effect of the QPC would be to reduce \( \rho J_{z} \) by \( (\delta_{QPC}/\pi)^{2}/2 \), through the first term on the r.h.s. of Eq. (14). It may then drive the system to the weak coupling (ferromagnetic Kondo) regime, and render the PS an abrupt first order QPT. For this to happen the QPC charge sensitivity needs not be too high; we require \( \rho_{QPC}U_{QPC} \sim \{ \sum \Gamma_{\ell} \left[ (\varepsilon_{\ell} + U)^{-1} + (|\varepsilon_{\ell}|)^{-1} \right] \}^{1/2} < 1. \)

The transition between the continuous and discontinuous PS regimes, at \( J_{z} = -J_{xy} \), is of the Kosterlitz-Thouless type.

Our analysis here can be put in a more general context. Around the point where PS takes place we need to consider only the singly occupied states 10 and 01 (i.e., pseudo-spin up and down, respectively). Let us first ignore the QPC. Processes in which an electron (or a hole) hops in and out of a level (pseudo-spin diagonal, \( J_{z} \)-type processes) give rise to an effective repulsive interaction between the charge of each level and the charge at the edge of the nearby lead, of the form \( \sum_{l} U_{l} \psi_{l}^{\dagger}(0) \psi_{l}(0) \langle d_{l}^{\dagger}d_{l} - \frac{1}{2} \rangle \), \( U_{l} = |V_{l}|^{2} [(\varepsilon_{l} + U)^{-1} + (|\varepsilon_{l}|)^{-1}] \). These correspond [by Eq. (17)] to the usual \( J_{z}S_{z}S_{z}(0) \) coupling generated in the ordinary Anderson model. A process of the type 10\( \leftrightarrow \)01 (pseudo-spin flip, \( J_{xy} \) process) contributes to hybridization of these two configurations, hence (if relevant) to a smearing of the PS. The aforementioned effective repulsion introduces two competing elements into this dynamics. On the one hand, 10\( \leftrightarrow \)01 involves a change in the leads’ state, hence is suppressed by the Anderson orthogonality catastrophe. On the other hand, an electron settling in one of the levels has prepared itself a hole in the lead into which it can hop (a Mahan exciton). This facilitates tunneling out and in (a reduced Pauli-blockade), thus enhancing hybridization of 10\( \leftrightarrow \)01. The overall scaling dimension is given by \( d_{xy} = 1 - (\delta_{L} + \delta_{R})/\pi + (\delta_{L}^{2} + \delta_{R}^{2})/2\pi^{2}, \) where \( \delta_{L} = 2\tan^{-1}(\rho_{0L}U_{l}/2) \) is the phase-shift change in lead \( L \) as a result of the 10\( \leftrightarrow \)01 transition. In this expression for \( d_{xy} \) the linear (quadratic) term in \( \delta_{L} \) denotes the contribution of the Mahan (Anderson) physics [14]. Since \( \delta_{L} < \pi, d_{xy} < 1 \) (relevant), so PS is a continuous crossover. However, when a third lead is added, the scaling dimension is increased by \( (\delta_{QPC}/\pi)^{2}/2, \) the extra orthogonality associated with the QPC [in addition to a less important renormalization of the the other terms, cf. Eqs. (13)-[16]]. This may turn the Anderson effect dominant, and the population switching abrupt [13].

The analysis presented here, while specifically tackling the ubiquitous physics of population switching and charge sensing, is close to earlier studies of QPTs involving two-level systems [10], including Kondo models coupled to Ohmic baths [12-17]. Here we have found that PS is inherently not abrupt, but in attempting to measure it with a third terminal (a QPC) one may induce a QPT. The system at hand is an appealing laboratory to modify and control at will such effects as Mahan exciton, Anderson orthogonality catastrophe and Fermi edge singularity [9]. It also serves to demonstrate the strong effect a measuring device might have on a low-dimensional system.

There are several obvious extensions to our analysis. The absence of left-right symmetry in the original model, implies a finite inter-dot hopping \( t_{LR} \) in the equivalent model, Fig. 2(b) [8]. This additional 10\( \leftrightarrow \)01 coupling renders the analysis more complicated. However, one can show that small \( t_{LR} \) leads to smearing of the PS. Finite temperature will also have a rounding effect. In addition, the abrupt/non-abrupt nature of the PS will have manifestations in measurements of transport through the QD of the original model, Fig. 2(a). All these will be discussed elsewhere [13].

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