Phase transition, spin-charge separation, and spin filtering in a quantum dot

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We consider low temperature transport through a lateral quantum dot asymmetrically coupled to two conducting leads, and tuned to the mixed-valence region separating two adjacent Coulomb blockade valleys with spin $S = 1/2$ and $S = 1$ on the dot. We demonstrate that this system exhibits a quantum phase transition driven by the gate voltage. In the vicinity of the transition the spin on the dot is quantized, even though the fluctuations of charge are strong. The spin-charge separation leads to an unusual Fano-like dependence of the conductance on the gate voltage and to an almost perfect spin polarization of the current through the dot in the presence of a magnetic field.

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In a single-electron transistor setup\cite{1} the number of electrons $N$ in a quantum dot is controlled by the potential on the capacitively coupled gate electrode. At low temperature $N$ is close to an integer at almost any gate voltage, except narrow mixed-valence regions, where adding a single electron to the dot does not lead to a large penalty in electrostatic energy. The distance between these regions sets the scale for the dependence of measurable quantities on the gate voltage, which makes it convenient to use a dimensionless parameter $N_0$, the gate voltage normalized by this scale. In terms of $N_0$, the mixed-valence regions are narrow intervals of the width

$$\Delta N \sim \Gamma/E_C \ll 1,$$

about half-integer values of $N_0$\cite{2}. Here $E_C$ is the charging energy and $\Gamma$ is the tunneling-induced width of single-particle energy levels in the dot.

In a typical experiment a dot is connected via tunneling junctions to two massive electrodes\cite{3}. At temperatures in the range $\Gamma \lesssim T \ll E_C$, the conductance $G$ is suppressed outside the mixed-valence regions, resulting in a quasiperiodic sequence of well-defined Coulomb blockade peaks in the dependence $G(N_0)$\cite{12}. When $T$ is further lowered, $G(N_0)$ changes dramatically due to the onset of the Kondo effect\cite{2,3}. At $T \to 0$ pairs of adjacent Coulomb blockade peaks merge to form broad maxima at $N \approx$ odd integer, separated by smooth crossovers from the minima at $N \approx$ even integer. Although $G(N_0)$ at $T \gtrsim \Gamma$ is very different from that at $T \ll \Gamma$, in the mixed-valence regions both functions are featureless\cite{2,3}.

The evolution of $G$ towards its low-temperature limit can be rather complicated. Indeed, GaAs quantum dots with odd $N$ usually have spin $S = 1/2$\cite{4,7}. In this case the dependence $G(T)$ is characterized by a single energy scale, the Kondo temperature $T_K$: $G(T)$ increases monotonically with the decrease of $T$ at $T \ll \Gamma$\cite{2}. However, dots with even $N$ often have spin $S = 1$ rather than zero\cite{1,2,4}. Kondo effect then occurs in two stages, controlled by two different energy scales, $T_K$ and $T'_K < T_K$\cite{6}. The resulting $G(T)$ is not monotonic: $G$ first raises, and then drops again when $T$ is lowered\cite{7,8}. The dependence of the conductance on the Zeeman energy $B$ of an applied magnetic field is also non-monotonic and is characterized by the same scales $T_K$ and $T'_K$\cite{6}.

The values of $T_K$ and $T'_K$ depend on $N_0$ and their ratio, in general, is not tunable. A notable exception occurs when the conductances of the dot-lead junctions are very different, i.e. when the width $\Gamma = \Gamma_L + \Gamma_R$ is dominated by the contribution from the lead with the stronger coupling to the dot, say, $\Gamma_L \gg \Gamma_R$. (Note that conductances of the junctions are easily tunable in lateral quantum dot systems such as those studied in\cite{8}). It can be shown\cite{2} that in this limit $T'_K \ll T_K$ for all $N_0$. In particular, in the vicinity of the mixed-valence region $T'_K \sim \Gamma_R$ while $T_K \sim \Gamma_L \gg T'_K$. Accordingly, the second stage of the Kondo effect will not develop if

$$\Gamma_R \ll \max\{T, B\} \ll \Gamma_L.$$

In this paper we show that under these conditions the conductance in the mixed-valence region between the Coulomb blockade valleys with $S = 1/2$ and $S = 1$ on the dot varies with $N_0$ on the scale which is parametrically small compared with $\Delta N$, in striking difference with the conventional smooth dependence described above.

The dependence of the conductance on $B$ at $B \gg T$ is qualitatively similar to its dependence on $T$ at $T \gg B$\cite{2}. Since $B$-dependence is much easier to understand, we concentrate here on the limit $T \to 0$ (the effect of a finite $T$ is briefly discussed towards the end of the paper).

The first inequality in Eq. (2) allows one to take into account the coupling to the right lead in the lowest non-vanishing order in $\Gamma_R/\Gamma_L$. The conductance at any finite $B$ is then given by\cite{2}

$$g = g_\uparrow + g_\downarrow, \quad g_s = \sin^2 \delta_s.$$ (3)

Here $g = G/G_0$ is the conductance normalized by $G_0 \sim (e^2/h)\Gamma_R/\Gamma_L$, the largest value conductance per spin can reach for strongly asymmetric coupling to the leads; $g_s$ is the conductance (in units of $G_0$) for electrons with spin
induced virtual transitions to states with "wrong"
be "integrated out" with the help of the Schrieffer-Wolff
where
and
with
The first term here describes the electrons in the lead.
For a lateral quantum dot it is sufficient to take into
account only a single propagating mode 2
H₀ = ∑ₖₜξₖψₖψₖ₊,
(5)
and the spectra ξₖ can be linearized near the Fermi level,
which corresponds to a constant density of states ν.

The second term in Eq. (4) describes the tunneling
coupling between the dot and the lead,
Hₜ = ∑ₙₖψₖ₊δₙψₖ + H.c.
(6)
In the following we set τₙ = t, so that all levels in the dot
have the same width Γ = ⰽtv². This assumption is not
essential for the validity of the following consideration.
The last term in Eq. (4) describes an isolated dot,
Hₜ = ∑ₙₚ∥δₚδₚ₊ + Eₜ(−N − N₀)² − EₛṠ² − BS₂, (7)
Here N = ∑ₙₚδₚδₚ₊ and Ṡ = ½ ∑ₙₖ∥δₙδₖ₊, are operators
of the total number of electrons on the dot, and
of the dot’s spin, respectively (σₓ, σᵧ, σᶻ) are Pauli
matrices). For a typical dot the parameters δE (mean
single-particle level spacing), Eₛ (exchange energy), and
Eₜ (charging energy) satisfy Eₛ ≪ δE ≪ Eₜ.

An isolated dot with even N will have S = 1 in the
ground state if the spacing ε between the two single-
particle levels closest to the Fermi level is anomalously
small, 2Eₛ − ε > 0 2, 3, 5. For simplicity, we assume
here that 2Eₛ − ε ≳ Γ. Although this simplification
imposes a stronger restriction on Γ then Γ ≪ δE (this
inequality justifies the tunneling Hamiltonian description
of the dot-late junction 2), it does not affect the results.

For the model 4, 5, 6 the phase shifts are given by
δ₁ = (π/2)(N + M), δ₋₁ = (π/2)(N − M), (8)
where N = 〈N〉 is the number of electrons in the dot,
and M = 2(S₂) is the dot’s magnetization 3. We start
with N₀ outside the mixed-valence region,
ΔN ≪ |N₀ − ˜N₀| ≲ 1,  ˜N₀ − 1/2 = odd integer, (9)
Here N ≃ ˜N₀ ± 1/2 is close to an integer. The tunneling-
induced virtual transitions to states with “wrong” N can
be “integrated out” with the help of the Schrieffer-Wolff
transformation, yielding an effective Kondo Hamiltonian
\[ H = H₀ + Vρ + J(s · S) − BS₂, \] 10
where ρ = ∑ₖₜ∥δₖδₖ₊ψₖψₖ₊ and \( s = ½ \sumₖₜ∥δₖδₖ₊σₛδₖδₖ₊ \)
are operators describing the local particle and spin densi-
ties of conduction electrons. The operator S in Eq. (10)
is a projection of ˜S [see Eq. (7)] on the ground state
multiplet of an isolated dot with fixed integer N. The
reduction of the microscopic model (4)-(7) to the Kondo
Hamiltonian (10) is valid only when N₀ is outside the
mixed-valence region and at sufficiently low energies,
\[ |ξₖ| ≲ D = \min\{dₙ, 2E_C|N₀ − ˜N₀|\}, \] 11
where \( dₙ = δE \) (∂E = 2E_C − ε) for odd (even) N. The
parameters V and J in Eq. (10) can be estimated as 2, 3
\[ νV ≃ Δₚ(N₀ − ˜N₀)⁻¹, \quad νJ ≃ |νV|. \] 12
(It should be noted that V and J are subject to strong
mesoscopic fluctuations; the order-of-magnitude estimate
12 is sufficient for our purpose).
The potential scattering term in Eq. (10) is responsible
for the deviations δN of the dot’s occupation from the
corresponding integer values ˜N₀ ± 1/2,
\[ δN = N − (N₀ ± 1/2) ≃ −2νV ≃ Δₚ(N₀ − ˜N₀)⁻¹. \] 13
Note that |δN| is finite and increases with approach to
the mixed-valence region. Also note that a weak mag-
netic field B ≪ Γ does not affect N(N₀).
On the contrary, M(N₀) depends strongly on B. Inde-
\[ \text{Indeed, } M(B) \text{ for a given } N₀ \text{ is controlled by the Kondo}
\text{temperature } T_K(N₀), \text{ which can be estimated from}
\[ \ln(Δ/T_K) ≃ (νJ)² ≃ Δ⁻¹|N₀ − ˜N₀|. \] 14
Accordingly, Tₐ ≃ Γ at |N₀ − ˜N₀| ≃ Δₚ, and decreases
exponentially with the increase of the distance to ˜N₀. A
fixed field B is large compared to Tₐ at |N₀ − ˜N₀| ≫ ΔB, where
ΔB is the distance between N₀ and ˜N₀ at which
B ∼ Tₐ(N₀). In this regime
\[ M/M₀ = 1 − 2\ln(Δ/B/Tₐ) \] 15
where M₀ = 1(2) for N₀ < ˜N₀ (N₀ > ˜N₀). In the oppo-
site limit ΔB ≫ |N₀ − ˜N₀| ≫ Δₚ (note that ΔB ≫ Δₚ
for B ≪ Γ) the system is in the strong coupling regime
B ≪ Tₐ. Here M(N₀) depends strongly on the parity
of N. Indeed, S in Eq. (10) is spin-1/2 operator for odd
N (i.e., for ˜N₀ − N₀ ≫ Δₚ), and spin-1 operator for
even N (N₀ − ˜N₀ ≫ Δₚ). This difference is crucial.
An antiferromagnetic local exchange interaction with a
Indeed, since conclusions regarding this region can be drown as well.

side the mixed-valence region spin is screened, and the ground state is a
Fermi-liquid-like \[11\], and

\[
M \sim B/T_K. \tag{16}
\]

On the contrary, for \(S = 1\) only half of the impurity’s spin is screened, and the ground state is a \textit{doublet} \[11\] \[12\]. The low-energy physics is then described by the ferromagnetic exchange of the conduction electrons with the remaining spin \(S = 1/2\) \[11\] \[12\], and

\[
M = 1 + \left[2 \ln(T_K/B)\right]^{-1}. \tag{17}
\]

Although the above results were obtained for \(N_0\) outside the mixed-valence region \(|N_0 - N_0^*| \lesssim \Delta_N\), some conclusions regarding this region can be drawn as well. Indeed, since \(\delta N\) in Eq. (13) is finite, it is plausible that \(N\) varies continuously with \(N_0\), as sketched in Fig. 1(a).

![Figure 1](image-url)

**FIG. 1:** (a) Number of electrons in the dot \(N\) differs appreciably from an integer in a narrow \textit{mixed-valence} region of the width \(\Delta_N\). (b) At \(B \ll \Gamma\), the width \(\Delta_M\) of the \textit{crossover} region in the dependence of the magnetization \(M\) on the gate voltage \(N_0\) is small compared to \(\Delta_N\). (c) Spin-resolved conductances in the crossover region at \(T \ll B \ll \Gamma\). (d) The total conductance at \(\max\{B, T\} \approx \Gamma\).

The dependence \(M(N_0)\) is more complicated. Consider the limit \(B \to +0\). In this limit \(M\) is determined solely by the ground state degeneracy. Since the degeneracy can not change continuously, the system must go through a \textit{quantum phase transition} (QPT) at a certain value of \(N_0 = N_0^*\). As shown above, the ground state is either a singlet or a doublet when the charge fluctuations are weak. Therefore, the transition must occur within the mixed-valence region, i.e. \(|N_0^* - N_0^*| \lesssim \Delta_N\). The QPT manifests itself in a singular dependence of the magnetization \(M\) on the gate voltage,

\[
\lim_{B \to +0} M = \theta(N_0 - N_0^*). \tag{18}
\]

Note that in the vicinity of the transition the spin is quantized, even though the fluctuations of charge are very strong, \(N^* = N(N_0^*) \approx \text{half-integer}\) (unlike in the case of transitions that occur at a fixed integer \(N\) \[14\] \[15\]).

Any finite field lifts the degeneracy of the ground state. QPT then turns to a \textit{crossover}, and the sharp step in the dependence of \(M(N_0)\) is smeared. The crossover takes place in a narrow interval of gate voltages \(|N_0 - N_0^*| \lesssim \Delta_M\). We expect that at a sufficiently low field the crossover width \(\Delta_M\) remains to be small compared to \(\Delta_N\), see Fig. 1(b). In order to estimate \(\Delta_M\), we now construct an effective Hamiltonian \(H_{\text{QPT}}\) for the vicinity of the transition.

Such Hamiltonian should be applicable at low energies \((B, T \ll \Gamma)\) and for \(N_0\) in the range \(|N_0 - N_0^*| \ll \Delta_N\), which includes the crossover region. At these energies and gate voltages the number of electrons in the dot is approximately constant, \(N \approx N^*\), while \(M(N_0)\) changes rapidly. It is therefore plausible that \(H_{\text{QPT}}\) acts only on the spin degrees of freedom (spin-charge separation).

At energies below \(\Gamma\) half of the dot’s spin when it is in the triplet state is already screened. The simplest possible model accounting for the interaction of the (still unscreened) spin-1/2 with electrons in the narrow strip of energies \(|\epsilon_k| \lesssim \Gamma\) reads

\[
H_{\text{QPT}} = H_0' + J'(s' \cdot S) - BS^z. \tag{19}
\]

Here \(H_0'\) and \(s'\) [cf. \(H_0\) and \(s\) in Eq. (10)] are defined in terms of the operators \(\psi_{ks}'\) acting in the basis of single-particle states that incorporate an extra scattering phase shift \(\delta^* = \pi N^*/2\).

For \(H_{\text{QPT}}\) to describe the change of the ground state symmetry at \(N_0 = N_0^*\), the exchange constant \(J'\) must change its sign at this point \[11\] \[12\]. Assuming the dependence \(J'(N_0)\) to be analytical, we can write

\[
\nu J'(N_0) \sim \Delta_N^{-1}(N_0^* - N_0). \tag{20}
\]

The coefficient in Eq. (20) has been chosen in such a way that \(\nu J' \sim 1\) for \(N_0^* - N_0 \sim \Delta_N\). This ensures the continuity of \(M(N_0)\) throughout the singlet side of the transition \(N_0 < N_0^*\).

A comment on the status of Eqs. (19), (20) is in order here. The effective low-energy Hamiltonian \(H_{\text{QPT}}\) is in the same relation to the original microscopic model \[11\] \[12\] as, e.g., the effective Fermi-liquid description of strong coupling regime \[11\] is to the Kondo model. As in the latter case, the applicability of \(H_{\text{QPT}}\) can be verified by comparing the predictions of the two models.

The magnetization for the model \[14\] \[20\] is obtained using the standard scaling arguments \[14\]. Very close to the transition (when \(|\nu J'| \ln(\Gamma/B) \ll 1\) the first order perturbation theory in \(\nu J' \ll 1\) yields

\[
M - 1 \approx -\nu J'/2 \sim \Delta_N^{-1}(N_0^* - N_0). \tag{21}
\]

On the doublet side \(M(N_0)\) slowly increases with the distance to the transition, saturating at

\[
M = 1 + \left[2 \ln(\Gamma/B)\right]^{-1}. \tag{22}
\]
Here we defined \( \Delta \) at the border of the mixed-valence region.

On the singlet side of the transition (\( N_0 < N^*_0 \)) the magnetization is given by Eq. (15) (with \( M_0 = 1 \)) for \( B \gg T_K \) and by Eq. (16) for \( B \ll T_K \), where the Kondo temperature \( T_K(N_0) \) satisfies

\[
\ln(\Gamma/T_K) = (\nu J')^{-1} \sim \Delta_N(N_0^* - N_0)^{-1}.
\] (23)

\( T_K \) increases with the distance to the QPT from \( T_K = 0 \) at \( N_0 = N^*_0 \) to \( T_K \sim \Gamma \) at the border of the mixed valence region, where it matches Eq. (14).

As \( N_0 \) is tuned through the mixed-valence region \( M \) grows monotonically from \( B \sim B/\Gamma \ll 1 \) to the value given by Eq. (22). The increase takes place mainly in a narrow interval on the singlet side of the transition where \( B \sim T_K(N_0) \). Eq. (23) then yields the estimate

\[
\Delta_M \sim \frac{\Delta_N}{\ln(\Gamma/B)}.
\] (24)

The evolution of the phase shifts with \( N_0 \) can now be deduced from Eq. (5). To the left of the crossover [see Fig. 1(b)] both phase shifts are given by \( \delta_s \approx \pi N^*/2 \) with \( N^* \approx \tilde{N}_0 \), see Eq. (9). As \( N_0 \) is tuned through the crossover, \( \delta_s \) raises, while \( \delta_s \) drops by approximately \( \pi/2 \). Therefore the phase shifts necessarily pass through, respectively, the anti-resonance \( \delta_s = 0 \) (mod \( \pi \)) and resonance \( \delta_s = \pi/2 \) (mod \( \pi \)). Hence, within the crossover region the conductances \( g_s \) satisfy \( g_s/g_\uparrow \ll 1 \), and \( g_\uparrow \) vanishes identically at some value of \( N_0 \). In other words, the system acts as a perfect spin filter.

Details of the dependencies \( g_s(N_0) \) are sensitive to the dot’s occupation at the transition \( N^* \). While \( N^* \) is close to a half-integer, it’s precise value is obviously non-universal. For example, \( N^* \) depends on the values of \( t_n \) for all \( n \) in Eq. (7). In Fig. 1(c) we sketch \( g_s(N_0) \) for \( 0 < \alpha \ll 1 \), where \( \alpha = N^* - \tilde{N}_0 \). The dependence of the total conductance \( g \) on \( N_0 \) in this case has a characteristic Fano-like shape, see Fig. 1(d).

In order to verify the applicability of the effective Hamiltonian (19), we performed extensive numerical renormalization group (NRG) (12) simulations. For this purpose, we truncated the dot’s Hamiltonian (7) to that of a two-level system (13) with

\[
\epsilon_n = n\varepsilon/2, \quad n = \pm 1.
\] (25)

The NRG data, see Fig. 2, are indeed in an excellent agreement with the behavior expected from Eq. (19). The sharpening of the step in the dependence \( M(N_0) \) with the decrease of \( B \), obvious in Fig. 2(a), is described very well by \( \Delta_M/\Delta_N = a[\ln^{-1}(\Gamma/B) + b\ln^{-2}(\Gamma/B)] \) with \( a = 3.0 \) and \( b = 9.5 \); at low field this agrees with Eq. (24).

Here we defined \( \Delta_M \) as the distance in \( N_0 \) between the points where \( M = 0.5 \) and 1, and \( \Delta_N \) as the distance between the points in Fig. 2(b) where \( N = 1.25 \) and 1.75.

So far, we considered the conductance at \( T = 0 \). The above results are valid as long as \( T \ll B \); corrections to \( g_s \) in this case are of the order of \( (T/B)^2 \), and the spin-filtering property remains intact: \( \min(g_\downarrow/g_\uparrow) \sim (T/B)^2 \ll 1 \). At \( T \approx B \) the field has a negligible effect. The dependence \( g(N_0) \) in this limit is very similar to that at \( B \gg T \), see Fig. 1(d) and 2(c), with \( T \) replacing \( B \) in the crossover width Eq. (24). This peculiar dependence will be observable already at moderately low temperatures \( T \ll \Gamma \) (note that the observability of the conventional Kondo effect requires \( T \ll \min\{T_K \} \ll \Gamma \)).

To conclude, we studied a lateral quantum dot asymmetrically coupled to two conducting leads, and tuned to the mixed-valence region between the Coulomb blockade valleys with \( S = 1/2 \) and \( S = 1 \) on the dot. This regime can be realized in devices such as those studied in 3. We predict that, contrary to naive expectations, the conductance varies with the gate voltage on the scale which is parametrically small compared with the width of the mixed-valence region.

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