Electron transport in multilevel quantum dots

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What are quantum dots? ...

...... measure current across dot, \( I = I(V_{sd}) \);

and differential conductance:

\[
G_c(V_{sd}) = \frac{dI}{dV_{sd}}
\]

the zero-bias conductance is

\[
G_c(V_{sd} = 0)
\]

(s.t. \( G_c = 1=\mathcal{R} \) if ohmic)

And the dot itself could be e.g....
Semiconductor quantum dot:

GaAs/n-doped GaAs heterostructure (‘top’ view).

- $V_{t1}$
- $V_G$
- $V_{bl}$
- $V_r$

Source lead

Drain lead

e.g. zero-bias conductance vs gate voltage, and its $T$-dependence:

Molecular quantum dot:

Single-molecule transistor, based on di-vanadium complex.

e.g. differential conductance vs $V_{sd}$; and its T-dependence:
Nanotube quantum dot:

\[ V_{\text{source drain}} \quad V_{\text{sd}} \quad V_{\text{gate}} \quad V_{g} \]

\begin{center}
\textbf{SiO}_2 \\
\textbf{doped Si}
\end{center}

\textit{e.g. differential conductance ‘maps’ in the \((V_{g}, V_{sd})\)-plane:}

1. Introduction.

Moreover, however obvious, remember:

The ‘system’ is dot + leads, so:

– this is a $\sim 10^{23}$ electron system.....

.... of *interacting* electrons ....

.... that is not in general in equilibrium (save for zero bias, $V_{sd} \to 0$).
1. Introduction.

**Why study quantum dots? ....**

– central to molecular electronics/device physics: single-electron transistors, molecular rectifiers, transistor arrays and logic gates, spintronics, quantum computation, entanglement etc.

– tunnel-coupled quantum dots provide controlled/tunable realisation of *strongly correlated ‘quantum impurity’ systems*; which embody much of many-body theory in a nutshell, and has led to strong resurgence of interest in Kondo and related physics...

  e.g. the spin-1/2 Kondo effect in a semiconductor QD, manifest in the unitarity limit for the zero-bias conductance ......
Spin-1/2 Kondo effect in a semiconductor QD ...

Odd electron valleys:—

– spin-1/2 Kondo effect;
– unitarity limit in zero-bias conductance for $T \leq T_K$:

– associated in effect with a single dot level, singly occupied.
– Kondo progressively killed by increasing $T$.

**Even electron valleys:**
- no Kondo; suppressed conductance

**Odd electron valleys:**
- spin-1/2 Kondo effect;

This odd/even (or ‘Kondo/non-Kondo’) alternation is common in QDs ……

…. but not ubiquitous:

– if the dot level spacing is sufficiently small, might expect instead to see $S=1$ Kondo physics in an even valley, i.e.

Such behaviour is indeed observed ……. e.g......

Talk about aspects of the $S=1$ and $S=1/2$ Kondo regimes, and the transitions between them ……

Odd valley: spin $-1/2$ Kondo, strongly enhanced zero-bias conductance.

Even valley: also strongly enhanced zero-bias conductance, indicative of (underscreened) spin-1 Kondo.
Outline:

2. Model
   – 2-level dot coupled to two conducting leads.
   – some issues/questions.

Numerical results from Wilson’s numerical renormalization group (NRG)*. Method of choice – non-perturbative RG, providing essentially exact results on low-temperature/energy scales central to the physics and to experiment. + Analytical methods where possible.

3. Results
   – static/thermodynamic properties.
   – evolution of Kondo scale.
   – phase diagram(s).
   – single-particle dynamics, and transport.
   – experiment.

[* use both ‘standard’ NRG and full density matrix/complete Fock space NRG (Peters, Pruschke, Anders; Weichselbaum, von Delft …)]
MODEL:

2-level dot, coupled to two conducting leads.

\[
H_D = \hat{n}_1 \hat{n}_1 + \hat{n}_2 \hat{n}_2 + U (\hat{n}_1^\dagger \hat{n}_1^\# + \hat{n}_2^\dagger \hat{n}_2^\#) + U^0 \hat{n}_1 \hat{n}_2 \quad J_H \quad \hat{s}_1 \cdot \hat{s}_2 \\
\text{ }(J_H > 0 \text{ – ferromagnetic [Hund’s rule] coupling})
\]

\[
H_0 = \begin{pmatrix} X & X \\ X & X \end{pmatrix} \begin{pmatrix} 2 \hat{c}_k^\dagger \hat{c}_k^{3/4} \hat{c}_k^{3/4} \\ \hat{d}_k^\dagger \hat{d}_k^{3/4} \hat{d}_k^{3/4} \end{pmatrix} \quad \text{ – two non-interacting, metallic leads}
\]

\[
H_V = \begin{pmatrix} X & X & X & X \\ X & X & X & X \end{pmatrix} \begin{pmatrix} V_{1L} \quad (\hat{c}_k^\dagger \hat{d}_k^{3/4} + \hat{d}_k^\dagger \hat{c}_k^{3/4}) \end{pmatrix} \quad \text{ – dot/leads tunnel coupling}
\]

Model rather general; and rich. Look first at the dot states arising in the ‘atomic limit’, where dot decouples from leads .......
Atomic limit: dot states

\[ H_D = \hat{n}_1 + \hat{n}_2 + U (\hat{n}_1 \hat{n}_1 + \hat{n}_2 \hat{n}_2) + U^0 \hat{n}_1 \hat{n}_2 i J_{H} \hat{s}_1 \hat{s}_2 \]

effectively a one-level problem; ‘filling level 1’.
Atomic limit: dot states

\[ H_D = \hat{n}_1^2 + \hat{n}_2^2 + U (\hat{n}_1^\dagger \hat{n}_1^# + \hat{n}_2^\dagger \hat{n}_2^#) + U^0 \hat{n}_1 \hat{n}_2 \hat{i} \ J_H \hat{s}_1 \hat{s}_2 \]

effectively a one-level problem; 'filling level 2'.

[Diagram of the dot states with annotations]
Atomic limit: dot states

\[ H_D = \hat{n}_1 + \hat{n}_2 + U (\hat{n}_1\hat{n}_1 + \hat{n}_2\hat{n}_2) + U^0\hat{n}_1\hat{n}_2 \]
Atomic limit: dot states

\[ H_D = ^21\hat{n}_1 + ^22\hat{n}_2 + U (\hat{n}_1^\text{#} + \hat{n}_2^\text{#}) + U^0 \hat{n}_1 \hat{n}_2 i \ J_H \ \hat{s}_1 \hat{s}_2 \]

All states shown are spin S=1/2 or 0.

Finally, there's the S=1 state.
Atomic limit: dot states

\[ H_D = \hat{n}_1^1 + \hat{n}_2^2 + U (\hat{n}_1^1 \hat{n}_1^# + \hat{n}_2^2 \hat{n}_2^#) + U \hat{n}_1 \hat{n}_2 \hat{J}_H \hat{s}_1 \hat{s}_2 \]

Obvious question: what happens on coupling to the leads? ....

– ‘deep’ in the S=1/2 regimes, low-energy model is usual spin-1/2 Kondo.

So ultimate stable fixed point (FP) is usual strong coupling FP: dot spin quenched on scale \( T_K \); strongly enhanced \( T=0 \) zero-bias conductance, \( G_C(0) \approx 2e^2/h \):

System a ‘normal’ Fermi liquid.
Atomic limit: dot states

\[ H_D = 2_1 \hat{n}_1 + 2_2 \hat{n}_2 + U (\hat{n}_1' \hat{n}_1' + \hat{n}_2' \hat{n}_2') + U^0 \hat{n}_1 \hat{n}_2 \hat{J}_H \hat{s}_1 \hat{s}_2 \]

Obvious question: what happens on coupling to the leads? ...

- ‘deep’ in the \( S=1 \) regime, low-energy model will be spin-1 Kondo.

Is it 1-channel or 2-channel spin-1 Kondo? Depends on coupling to leads....

If 2-channel, \( S=1 \) wholly quenched on coupling to leads (strong coupling FP); and strong *suppressed* dc, \( G_c(0) \gg 0 \) (Pustilnik/Glazman).

If 1-channel, \( S=1 \) only partially quenched on coupling to leads (‘underscreened’ \( S=1 \) FP, Nozieres/Blandin); in this case, strongly *enhanced* \( G_c(0) \gg 2e^2/h \): System a ‘singular’ Fermi liquid (Mehta, Andrei *et al*).
Questions contd:

– for S=1 regime, two-channel behaviour is generic. So apparent puzzle (Coleman et al): why do exps see strongly enhanced $G_c(0) \gg 2e^2/h$?

Answer: low-energy model is generically 2-channel spin-1 Kondo with channel anisotropy:

\[ J_i \quad \text{L}^0 \quad J^+ \quad \text{R}^0 \quad : J^+ > J_i \]

2-stage quenching of spin-1:

– on ‘high’ scale $T_{K+} \gg D \exp(i 1/\beta_{+})$, quench spin S=1! S=1/2 by coupling to R $^0$.

Here flow towards underscreened S=1 fixed point.

– then on ‘low’ scale $T_{K-} \gg D \exp(i 1/\beta_{-})$; quench spin S=1/2! S=0 by coupling to L $^0$.

(flowing then to fully screened, strong coupling FP)

But the two scales may be vastly different in magnitude.

And if $T_{K-}$ ‘irrelevantly small’, in practice might as well be 0:

– experiment will then ‘see’ the underscreened spin-1 FP.

We'll take this for granted here; in practice, consider effective 1-channel set-up from beginning.
Atomic limit: dot states

\[ H_D = \hat{n}_1 + \hat{n}_2 + U (\hat{n}_1 \hat{n}_2 + \hat{n}_2 \hat{n}_1) + U_0 \hat{n}_1 \hat{n}_2 | J_H | S_1 \phi S_2 \]

Questions contd:

- where does exp fit in to figure?
- so does there exist a quantum phase transition (QPT) between ‘regular’ spin-1/2 Kondo and spin-1 Kondo (Pustilnik /Borda)?
- If so, what is the nature of the QPT?
- Can exp be explained?
So consider explicitly:

\[
H_D = \hat{n}_1^2 + \hat{n}_2^2 + U (\hat{n}_1 \hat{n}_1^\# + \hat{n}_2 \hat{n}_2^\#) + U^0 \hat{n}_1 \hat{n}_2 \hat{J}_H \mathbf{\hat{s}}_1 \cdot \mathbf{\hat{s}}_2
\]

\[
H_0 = \begin{pmatrix} X & X & X & X \\ X & X & X & X \end{pmatrix}_{=L;R, \ k;3/4}
\]

- two non-interacting, metallic leads

\[
H_V = \begin{pmatrix} V_1 & \ldots & V_2 \\ \ldots & \ldots & \ldots \end{pmatrix}_{=L;R, \ i=1;2, \ k;3/4}
\]

- dot/leads tunnel coupling
Recall discussion of ‘atomic limit’: -

What of the phase boundaries on coupling to leads?

– all phases that were $S=1/2$ or 0 in the atomic limit are continuously connected (as we know..); here the stable fixed point is the usual strong coupling (or frozen impurity) FP.

– but the underscreened triplet state has a distinct FP. So we expect a quantum phase transition; and hence the qualitative behaviour shown. Indeed.
For purposes of illustration here, will now fix $t_1$, and progressively decrease $t_2$ from ‘high up’ in the spin-1/2 Kondo regime, down into the spin-1 Kondo regime, to $t_2 = t_1$:

We’ll chose specifically $t_1 = j \cdot U = 2 \cdot j \cdot U^0$ (‘midpoint’); the point $t_2 = t_1$ is then particle-hole symmetric.

Will consider sequentially:

– static/thermodynamic properties.
– evolution of the Kondo scale.
– phase diagram(s).
– single-particle dynamics.
– transport/differential conductance.
– and experiment.
Screened spin-1/2 Kondo phase.

\[ T_K \]

\[ S_{\text{imp}}(T) \text{ vs } T = D: \]

Fixed \[ \frac{2}{1} = \frac{i}{U = 2}, \text{with } U = 20; J_H = 5; U^0 = 0 \]

(energies i.t.o. ‘hybridization strength’ \[ i = \frac{1}{\sqrt{21/\hbar^2}} \];

\[ 2_2 = +9 \text{ (and } 2_1 = i \text{ 10) } \]

– high \[ 2_2 \approx 0 \]; so essentially

\textit{single}-level S=1/2 Kondo for \( T \).

– intermediate \( \ln(2) \) plateau, characteristic of spin-1/2 local moment FP.

– characteristic Kondo scale \( T_K \); below which dot spin quenched:

\( S_{\text{imp}}(T = 0) = 0; \)

Usual spin-1/2 strong coupling FP.

\[ \frac{2}{1} \]

– and progressively lowering \[ 2_2 \]:
Entropy, $S_{\text{imp}}(T)$ vs $T = D$:

Screened spin-1/2 Kondo phase.

Now decrease $^2T_2$:

$^2T_2 = 5; 4; 3$:

- Kondo scale progressively decreases.
Entropy, $S_{\text{imp}}(T)$ vs $T=D$:

$\ln(2)$

$S_{\text{imp}}(T)$

$T/D$

$\frac{2}{2} = 2:8$

$T_K$ vanishes at a critical $2;_2;_c$ (here $2;_2;_c = 2:775$)

- symptomatic of a QPT to the underscreened triplet phase.

For $2;_2 < 2;_2;_c$ have the underscreened spin-1 phase ......

$\frac{2}{2}$

$\frac{1}{1}$
Undercreened spin-1 Kondo phase.

Throughout this phase,
$S_{\text{imp}}(T = 0) = \ln 2$

- characteristic of the USC spin-1 fixed point.

But there is no low-energy scale in this phase that vanishes as transition approached.
Entropy, $S_{imp}(T)$ vs $T=\Delta$:

Undercreened spin-1 Kondo phase.

There is of course a characteristic low-energy scale in the USC phase – $T_K +$:
Entropy, $S_{\text{imp}}(T)$ vs $T=D$: 

Undercreened spin-1 Kondo phase.

$^{2}_{2} = i \ 10 \ (= ^{2}_{1})$

There is of course a characteristic low-energy scale in the USC phase $- T_{K+}$:

But it barely varies throughout the phase.
Spin susceptibility $T \hat{\chi}_{\text{imp}}(T)$; vs $T = D$:

For screened Kondo phase, $T \hat{\chi}_{\text{imp}}(T) \to 0$ as $T \to 0$:

For underseened spin-1 phase, $T \hat{\chi}_{\text{imp}}(T) \to \frac{1}{4}$ as $T \to 0$:

(i.e. $\hat{\chi}_{\text{imp}}(T) \approx \frac{S(S+1)}{3T}$ with $S=1/2$).
“Impurity” charge, $n_{imp}$ ($\hat{n}_1 + \hat{n}_2$): …i.e. the net dot charge

– very boring, evolves smoothly through the transition.

But key re transport (see on)!

– note that transition occurs generally in a ‘mixed valent’ regime of non-integral charge. Implications?
Vanishing of Kondo scale as $^{2}_{2} \log \left(\frac{T_{K}}{\Gamma}\right)$ from screened Kondo phase: -
Vanishing of Kondo scale as $\gamma_2^2 > \gamma_2^2;_c$ from screened Kondo phase:

\[
\frac{T_K}{\exp\left(\frac{i a}{\gamma_2} - \frac{i a}{\gamma_2;_c}\right)}
\]

as $\gamma_2^2 > \gamma_2^2;_c$: ($\gamma_2 = \gamma_2;_c$)

\- QPT of Kosterlitz-Thouless type (consistent with no evidence for a separate critical FP).

[behaviour quite generic........]
Phase transition boundaries in general continuous KT-transitions.

Exception: on the line $y = x$ (as permitted by invariance of $\hat{H}$ under ‘1-2’ transformation $d_{\frac{1}{2}}^{\gamma} \rightarrow d_{\frac{1}{2}}^{\gamma}$)

Phase diagrams:

\[ y = x = z_1 + \frac{1}{2} U + U^0 \]

\[ (U = 20; U^0 = 0; J_H = 5) \]
Can consider the single-particle spectra $D_{ij}(!) = i \frac{1}{\hbar} \text{Im} G_{ij}(!)$
(with i,j referring to dot levels (1 or 2), and $G_{ij}(!) = i \int \theta(t) \text{d}_{i} \phi(t) \text{d}_{j} \phi$);

Equivalently, take even/odd combinations of dot levels, $\text{d}_{i} \phi = \frac{1}{2} \text{d}_{i} \phi \text{d}_{j} \phi$; and work with

$G_{ee}(!) = \frac{1}{2} [ G_{11}(!) + G_{22}(!) \times 2G_{12}(!) ]$ (and $G_{eo}(!) = \frac{1}{2} [ G_{11}(!) \times G_{22}(!) ]$):

Focus here on e-e spectrum $D_{ee}(!) = i \frac{1}{\hbar} \text{Im} G_{ee}(!)$
– which determines the **zero-bias conductance**:

$$G_{c}(T) = G_{0} \int_{1}^{Z} d! i \frac{\partial f(!)}{\partial \phi} 2^{1/4} D_{ee}(!; T) \quad (i = \frac{1}{\sqrt{2^{1/4}}})$$

[where: $G_{0} = \frac{2e^{2}}{h} \sin^{2}2\theta$ and $\sin^{2}2\theta \times \frac{4iL}{iR} = \frac{1}{(1 + iL / iR)^{2}}$ with $i_{L} = i \sin^{2}(\theta)$; $i_{R} = i \cos^{2}(\theta)$;]

s.t. $G_{0} = 2e^{2} \approx h$ for equivalent coupling to leads, $i_{L} = i_{R}$. ]
Single-particle dynamics.  \( (T = 0) \)

For screened Kondo phase.

\[ 2^{3/4} D_{ee}(\omega) \text{ vs } \omega \equiv \left( i = 3/4 \sqrt{2^n/2} \right) \quad \text{‘all scales’ overview.} \]

\[ ^2_1 = 10 \quad \text{and} \quad ^2_2 = 4.5, 3.7, 3.5. \]

\( ({}^2_{2; c} = 2:775) \)

Fix \( ^2_1 = i \ U=2, \text{ with } U = 20; J_H = 5; U^0 = 0 \)

– and progressively lower \( ^2_2 \):

\begin{align*}
\text{screened Kondo} \\
\text{USC}
\end{align*}
Single-particle dynamics.

\[ ^{2}_{1} = 10 \text{ and } ^{2}_{2} = 4.5, 3.7, 3.5. \quad (^{2}_{2; c} = 2.775) \]

For screened Kondo phase.

High energy features ...........

\[
\begin{array}{c}
\frac{2}{1} \\
\frac{2}{1} \\
\frac{2}{1} \\
\frac{2}{1}
\end{array}
\quad \rightarrow \quad
\begin{array}{c}
\frac{2}{1} \\
\frac{2}{1} \\
\frac{2}{1} \\
\frac{2}{1}
\end{array}
\]
Single-particle dynamics.

\[ z_1 = 10 \text{ and } z_2 = 4.5, 3.7, 3.5. \ (z_{2,c} = 2.775) \]

Key low-energy feature is of course the Kondo resonance; with characteristic scale \( T_K \):

Kondo resonance progressively narrows as transition approached, and .......

![Graph showing Kondo resonance]
Single-particle dynamics.

\[ I_1 = 10 \text{ and } I_2 = 2.7 \quad (I_{2;C} = 2.775) \]

\[ I_1 = 10 \text{ and } I_2 = 2.7 \quad (I_{2;C} = 2.775) \]

\[ I_2 \] vanishes as the transition to the underscreened spin-1 Kondo phase is crossed.

[Again, there is no low-energy scale in the USC phase that vanishes as transition approached from that side.]
Single-particle dynamics.

\[ \tau_{1} = 10 \quad \text{and} \quad \tau_{2} = 4.5, 3.7, 3.5, 2.7 \quad (\tau_{2; c} = 2.775) \]

How does the Kondo resonance ‘collapse’ as transition approached from screened Kondo phase? ......
Single-particle dynamics.

\[ ^2_1 = \text{i} \times 10 \text{ and } ^2_2 = 4.5, 3.7, 3.5, 2.7 \ (^{2_2; c} = 2.775) \]

How does the Kondo resonance ‘collapse’ as transition approached from screened Kondo phase? ......

– resonance narrows progressively, and vanishes ‘on the spot’.

– and as it does so exhibits scaling in terms of the Kondo scale \( T_K \):
Single-particle dynamics.

$^2_1 = 10$ and $^2_2 = 4.5, 3.7, 3.5$. ($^2_{2,c} = 2.775$)

Scaling spectrum in screened Kondo phase.
Single-particle dynamics.

\[ \gamma_1 = i \, 10 \text{ and } \gamma_2 = 4.5, 3.7, 3.5, 2.7 \ (\gamma_2/c = 2.775) \]

- resonance narrows progressively, and vanishes ‘on the spot’; leaving an incoherent background in underscreened phase (dashed line).

\[ D_{ee}(! = 0), \text{ and hence the (T=0) zero bias conductance } / \ D_{ee}(0); \text{ drops discontinuously across the transition .......} \]
\[ 2^{1/4} D_{ee}(! = 0) \text{ vs } \partial_2 \text{ (for } ^2_1 = i, U = 2 = i 10) \]

\[ \frac{G_c(T = 0)}{G_0} = 2^{1/4} D_{ee}(! = 0) \]

- discontinuity in zero-bias conductance as cross transition

- discontinuity a ‘drop’ from screened \(\Leftrightarrow\) underscreened; as expect from collapsing Kondo resonance.

\[(U = 20; U^0 = 0; J_H = 5)\]
Fix \( \mathbf{2}_1 = i \), \( U=2 \), with \( U = 20; J_H = 5; U^0 = 0 \)
– and progressively lowering \( \mathbf{2}_2 = i \), \( 2; i \), \( 4; i \), \( 6; i \), \( 8; i \), \( 10; i \):

For underscreened Kondo phase.

\[ \mathbf{D}_{ee}(0) \sim \frac{3 \mathbf{b}}{\ln^2 \frac{\mathbf{j}! \mathbf{j}!}{\mathbf{T}_K^2=1}} \]
2^{1/4} D_{ee}(! = 0) \text{ vs } 2^2 \quad (\text{for } 2_1 = i \ U = 2 = i \ 10) \\

\frac{G_c(T = 0)}{G_0} = 2^{1/4} D_{ee}(! = 0)

- discontinuity in zero-bias conductance as cross transition

- discontinuity a ‘drop’ from screened $\leftrightarrow$ underscreened; as expect from collapsing Kondo resonance.

So how do we understand this in general terms?

It’s subtle ......

\((U = 20; U^0 = 0; J_H = 5)\)
"Friedel-Luttinger sum rule"

Recall
\[ G_c(T = 0) = G_0 = 2^{1/2} D_{ee}(! = 0) = \sin^2 \pm \] (1)

with \( \pm = \text{arg} \det G(! = 0) \) the (Fermi level) scattering phase shift.

Can show quite generally – independently of phase (screened/usc) – that
\[ \pm = \frac{1}{\lambda} n_{\text{imp}} + I_L \]
(2)

with \( I_L \) the Luttinger integral:
\[ I_L = \text{Im} \left[ \text{d!} \text{ Tr} \frac{1}{Z_0} \right] G(\lambda) \]

[and \( G(\lambda) \) the 2x2 self-energy matrix, likewise for \( G(\lambda) \);]

For a normal Fermi liquid – the screened phase – Luttinger (integral) theorem holds throughout the phase: \( I_L = 0 \)

So (2) gives \( \pm = \frac{1}{\lambda} n_{\text{imp}} \) – i.e. the Friedel sum rule – and hence from (1):
\[ 2^{1/2} D_{ee}(! = 0) = \sin^2 \frac{1}{\lambda} n_{\text{imp}} \]

: screened Kondo

Well known (+ can check directly from NRG that \( I_L = 0 \)): 
Recall
\[ G_c(T = 0) = G_0 = 2^{1/4} D_{ee}(\epsilon = 0) = \sin^2 \pm \] (1)

with \( \pm = \arg \det G(\epsilon = 0) \) the (Fermi level) scattering phase shift.

Can show quite generally – independently of phase (screened/usc) – that
\[ \pm = \frac{1}{2} n_{\text{imp}} + I_L \] (2)

with \( I_L \) the Luttinger integral:
\[ I_L = \text{Im} \left[ \text{Tr} \left\{ G(\epsilon) \right\} \right] \]

[and \( G(\epsilon) \) the 2x2 self-energy matrix, likewise for \( G(\epsilon) \);]

But the underscreened phase is a ‘singular Fermi liquid’. There is no reason to suppose Luttinger’s theorem \( I_L = 0 \) is satisfied in it. And it isn’t.

So a question arises: in the same way that \( I_L \) has a characteristic value (of zero) for a Fermi liquid phase, regardless of ‘bare’ parameters, might \( I_L \) for the USC phase likewise be an intrinsic characteristic of that phase?

Yes: throughout the USC phase (i.e. regardless of bare parameters \( U, U', J \) etc), find:
\[ jLj = \frac{1/4}{2} : \text{underscreened phase} \]
Recall \[ G_c(T = 0) = G_0 = 2^{1/4} D_{ee}(! = 0) = \sin^2 \pm \] (1)

with \( \pm = \arg \det G(\gamma = 0) \) the (Fermi level) scattering phase shift.

Can show quite generally – independently of phase (screened/usc) – that

\[ \pm = \frac{1}{2} n_{\text{imp}} + I_L \]

(2)

with \( I_L \) the Luttinger integral:

\[ I_L = \text{Im} \left[ Z_0 \right] \frac{1}{2} \text{Tr} \left[ \mathcal{G}(\gamma = 0) \right] G(\gamma) \]

[and \( \mathcal{G}(\gamma) \) the 2x2 self-energy matrix, likewise for \( G(\gamma) \);]

But the underscreened phase is a ‘singular Fermi liquid’. There is no reason to suppose Luttinger’s theorem \( (I_L = 0) \) is satisfied in it. And it isn’t.

Throughout the USC phase (i.e. regardless of bare parameters U, J etc), we find: \( |I_L| = \frac{1}{4} \)

So (1),(2) give directly that:

\[ 2^{1/4} D_{ee}(\gamma = 0) = \sin^2 i \frac{1}{2} [n_{\text{imp}} i 1]^{\dagger} : \text{underscreened phase} \]

So overall we have:
Can test independently, since can determine $D_{ee}(!)$ and $n_{imp}$ separately via NRG …..
\(2^{1/4} \, D_{ee}(! = 0) = \begin{cases} 
\sin^2 \left( \frac{i}{2} n_{imp} \right) & : \text{screened phase} \\
\cos^2 \left( \frac{1}{2} n_{imp} \right) & : \text{underscreened phase} 
\end{cases}\)
But wait:

$$2^{1/4} D_{ee}(! = 0) = \begin{cases} 
\sin^2 i \frac{1}{2} n_{\text{imp}} & : \text{screened} \\
\cos^2(\frac{1}{2} n_{\text{imp}}) & : \text{underscreened}
\end{cases}$$

– so if $n_{\text{imp}} \in [\frac{3}{2}; 2]$ or $[0; \frac{1}{2}]$ then the conductance should increase (rather than decrease), on passing from the screened to the USC phase.

Since a decrease in the conductance at the transition is naturally associated with a ‘collapsing’ Kondo resonance in the spectrum, this might suggest that an increase in conductance is associated with a collapsing Kondo antiresonance.

Indeed it is: to illustrate, consider line $y = -x$; along which $n_{\text{imp}} = 2$ by symmetry.
Line $y = -x$; along which $n_{\text{imp}} = 2$:

$$2^{1/4} D_{ee}(! = 0) = \begin{cases} 
\sin^2 i \frac{\nu}{2} n_{\text{imp}} \phi &= 0 \\
\cos^2(\frac{\nu}{2} n_{\text{imp}}) &= 1
\end{cases} : \text{screened}$$

Clear Kondo antiresonance in screened Fermi liquid phase;

Again ‘collapses on spot’ as approach transition …..

… jumping discontinuously as enter USC phase.

… and again scaling in terms of (vanishing) Kondo $T_K$ as it does so.
**EXPERIMENT:**


Even valley: also strongly enhanced differential conductance, indicative of spin-1 Kondo effect.

Odd valley: spin $-\frac{1}{2}$ Kondo, strongly enhanced diff con.

For zero-bias conductance take cut along $V_{ds} = 0$
\[ y = \frac{1}{2} U + U^0 \]

Expt 'trajectory' on varying $\xi V_g$:

\[ y = x + \pm^2 \]

i.e. $\frac{1}{2} = \frac{1}{2} + \pm^2$

with level separation $\pm^2$ fixed, and $\frac{1}{2} / \xi V_g$

And can show zero-bias conductance is symmetric f'n of $\xi V_g$ about 'midpoint' (●) of trajectory in USC phase; which lies on $y=-x$ line with $n_{imp} = 2$. 

\[ x = \frac{1}{2} U + U^0 \]

The graph shows the differential conductance $dl/dV / 2e^2h^{-1}$ as a function of gate voltage $\Delta V_G$ and source-drain voltage $V_{ds}$. For zero-bias conductance, take the cut along $V_{ds} = 0$. The color bar indicates the range from 0.0 to 0.9.
EXPERIMENT:

Experimental $T' = 30$ mK:

![Graph](image_url)
EXPERIMENT:

\[ G_c = \frac{(2e^2}{h} \right) \]

Experimental \( T' \) 30 mK:
EXPERIMENT:

Experimental $T' \sim 30 \text{ mK}$:
Comparison to theory (T=0):

Not entirely trivial: need ….

\[ \begin{align*}
\frac{U}{i} + \frac{U^0}{i} + \frac{J_H}{i} + \mathbf{R} &= \left[ \begin{array}{c}
\mathbf{2}_2 \\
\mathbf{2}_1 \\
\mathbf{2}_1 \\
\mathbf{2}_1
\end{array} \right] \\
\end{align*} \]

plus proportionality ('c') between gate voltage and level energy:

\[ \frac{\mathcal{V}_g}{\mathcal{V}_{g;mid}} \frac{\mathcal{V}_{g;mid}}{\text{mV}} = \mathcal{C} \left[ \begin{array}{c}
\mathbf{2}_1 \\
\mathbf{2}_1 \\
\mathbf{2}_1 \\
\mathbf{2}_1 \\
\end{array} \right] \]

and hybridization strength itself.
Comparison to theory (T=0):

\[ G_c(0) = G_0 = \begin{cases} 
\sin^2 i \frac{\sqrt{4} n_{\text{imp}}}{2} & : \text{screened} \\
\sin^2 i \frac{\sqrt{4} [n_{\text{imp}} i]_{\text{imp}}}{2} & : \text{underscreened}
\end{cases} \]

(Here, \( n_{\text{imp}} \) 1:9 and 2:1 at transitions.)
$G_c = (2e^2/h)$

Comparison to theory ($T=0$):

- Screened (S)
- USC
- $\log (T_K/T)$
Comparison to theory ($T>0$):

\[
\begin{align*}
G_c &= (2e^2/h) \\
T \equiv &= 0.005 \\
i.e. \ T' &= 30\text{mK with} \quad i' &= 0.5\text{meV}
\end{align*}
\]
In zero-bias limit,
\[
\frac{G_c(T; V_{sd} = 0)}{G_0} = Z_1 \frac{1}{d!} \int_1 \frac{\partial^n \Omega(\tau)}{\partial \tau} \cdot 2^{1/2} D_{ee}(\tau) \quad (f(\tau) = [e^{\tau} = T + 1]^1)
\]

is exact. At finite bias, cannot say anything exact. But if neglect explicit \(V_{sd}\) dependence of self-energies,
\[
\frac{G_c(T; V_{sd})}{G_0} = Z_1 \frac{1}{d!} \int_1 \frac{\partial^n \Omega_L(\tau)}{\partial \tau} + \frac{\partial^n \Omega_R(\tau)}{\partial \tau} \cdot 2^{1/2} D_{ee}(\tau)
\]

with \(f_0(\tau) = f(\tau \frac{1}{2} eV_{sd})\) for \(\tau = L, R\) lead. Calculable; and
\[
\frac{G_c(T = 0; V_{sd})}{G_0} = \frac{1}{4} [D_{ee}(\tau) = + \frac{1}{2} eV_{sd} + D_{ee}(\tau) = i \frac{1}{2} eV_{sd})]
\]

‘symmetrised spectral sum’.
**EXPERIMENT / THEORY: non-zero bias.**

Differential conductance maps in $(V_G; V_{sd})$-plane:

**Theory**

- Differential conductance in a 2D map with $V_{ds}$ on the y-axis and $\Delta V_G$ on the x-axis.

**Experiment**

- Similar map as Theory.

$T = 30 \text{ mK}$

Not bad at all – what can we learn from it? ….
**EXPERIMENT / THEORY: non-zero bias.**

Take cuts through maps at different fixed values of gate voltage; to show conductance as function of $V_{sd}$.

For $\varphi V_g = i \, 10\text{mV}$

-- see single maximum at zero-bias (ie Kondo resonance for USC phase).
EXPERIMENT / THEORY: non-zero bias.

Now increase gate voltage to

\[ V_g = 6 \text{mV} \]

– just entering screened FL phase.

Resonance beginning to split.
EXPERIMENT / THEORY: non-zero bias.

Increase further to

\[ \varphi V_g = 5 \text{ mV} \]

moving further into screened phase.
EXPERIMENT / THEORY: non-zero bias.

And further ....

\( V_g = 3 \text{mV} \)

– seeing clear development of antiresonance (arising from the Kondo antires in \( D_{ee} \)).
EXPERIMENT / THEORY: non-zero bias.

\[ G_c = 2e^2/h \]

\[ V_g = +2 \text{mV} \]
EXPERIMENT / THEORY: non-zero bias.

So ‘vanishing Kondo antiresonance’ case seems in this case to explain experiment rather decently.
...... and what you’ll see if you just ‘miss’ the transition:

Theory

Experiment
...... and what you’ll see if you just ‘miss’ the transition:

Theory

\[ V_{sd} = mV \]

Experiment

\[ V_{sd} = mV \]
Concluding remarks.

Considered a ‘simple’ but rather general two-level quantum dot:

\[ H_D = {^2}_1 \hat{n}_1 + {^2}_2 \hat{n}_2 + U (\hat{n}_1 \hat{n}_1^\# + \hat{n}_2 \hat{n}_2^\#) + U^0 \hat{n}_1 \hat{n}_2 \ i \ J_H \ \hat{s}_1 \hat{s}_2 \]

Continuous line of QPTs in \((^{2}_1;^{2}_2)\)-plane separating an underscreened spin-1 phase from the usual screened phases:

- QPT usually of KT type, with a vanishing Kondo scale as approach transition from screened side.

- rich range of behaviour in static & dynamic properties.

- zero-bias conductance explicable i.t.o. “Luttinger-Friedel sum rules” for two phases; including anomalous transport as transition crossed (+ generalisation of ‘Luttinger integral theorem’ to USC phase).

- both phases seen experimentally; and appear explicable by theory.

.... so models aren’t purely ‘paradigmatic’.
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