Quantum impurities in non-equilibrium steady states

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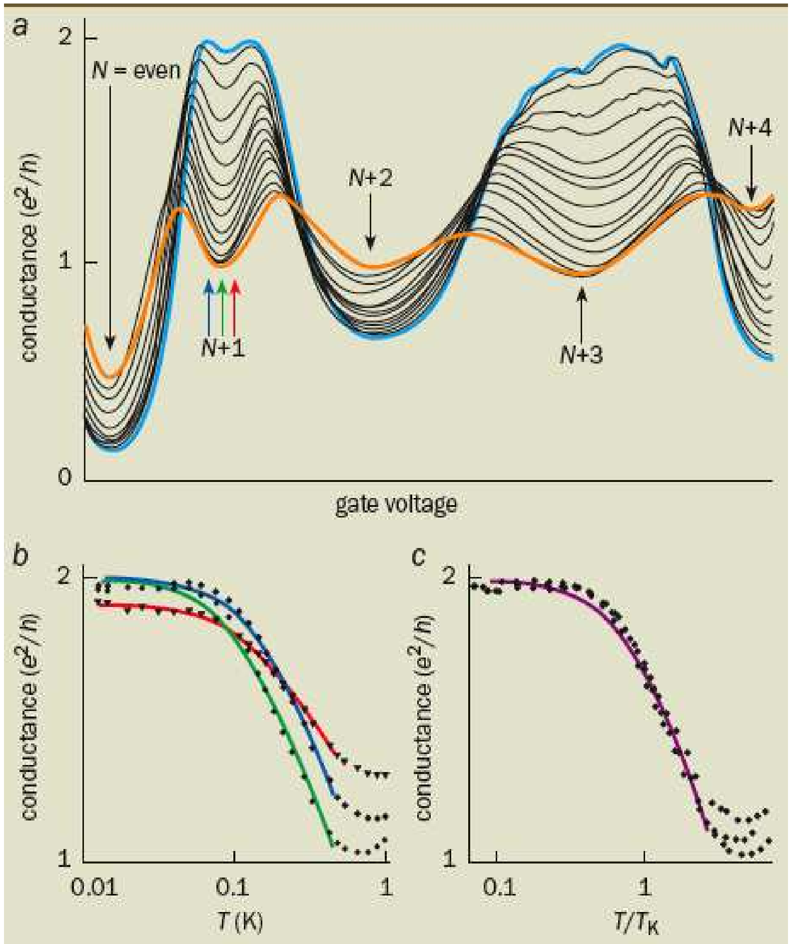
Experiments on quantum dots

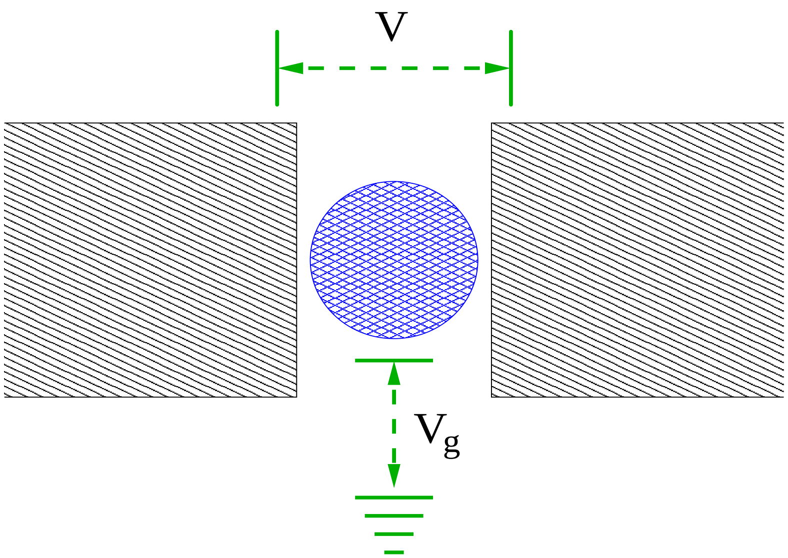
L P Kouwenhoven and C M Marcus 1998 Quantum dots, Physics World, June, 35-39.

D Goldhaber-Gordon et al. 1998 Kondo effect in a single-electron transistor, Nature 391, 156-159.

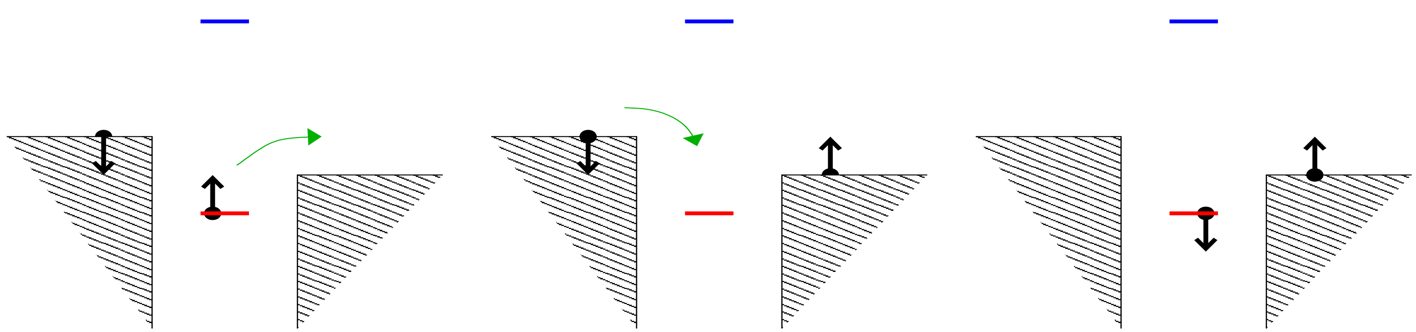


Quantum dot: what happens

see: L P Kouwenhoven and L Glazman 2001 Revival of the Kondo effect, Physics World, January, 33-38



- Quantum dot: mesoscopic object $\Rightarrow$ many electrons, discrete energy levels
- By adjusting V_g: number of electrons fixed on the dot
- Low T: increase of current due to co-tunnelling with spin flip $\Rightarrow$ **Kondo effect**



Kondo effect

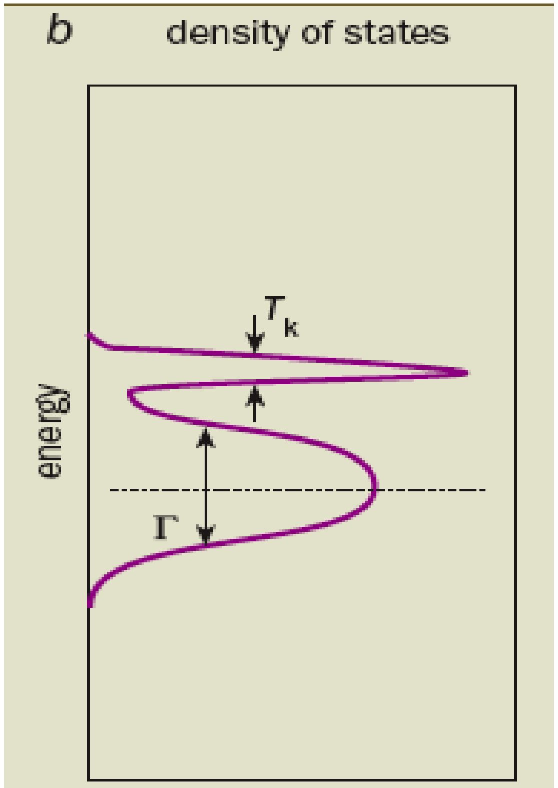
Co-tunelling with spin flip $\Rightarrow$ Heisenberg interaction

$$\vec{S}_{\text{electrons near dot}} \cdot \vec{S}_{\text{dot}}$$

At small temperatures, a **cloud of partially coherent electrons form around the dot**, and the **density of states peaks at the Fermi energy**.

Electrons can use these dot states to go from one side to the other, so **conductivity increases**.

In usual Kondo effect, of magnetic impurities in metals, the Kondo cloud gives more **scattering of electrons' plane waves in different momenta**, thus **reducing conductivity**.



The questions

The system with nonzero bias voltage is **out of equilibrium**: entropy increases. With a steady electric current, we have a **non-equilibrium steady state**. The dynamics that allow the steady state to occur is **purely from quantum mechanics**.

$\Rightarrow$ Interplay between out-of-equilibrium and quantum mechanics

- How to study such a situation? The Kondo cloud idea was studied theoretically only at equilibrium.
- What happens with universality? What is the effect of a large voltage?
- The Kondo and Anderson models (and other impurity models) are integrable. What happens with integrability out of equilibrium?

I will try to answer some of these questions with a simpler example: the Interacting resonant level model.

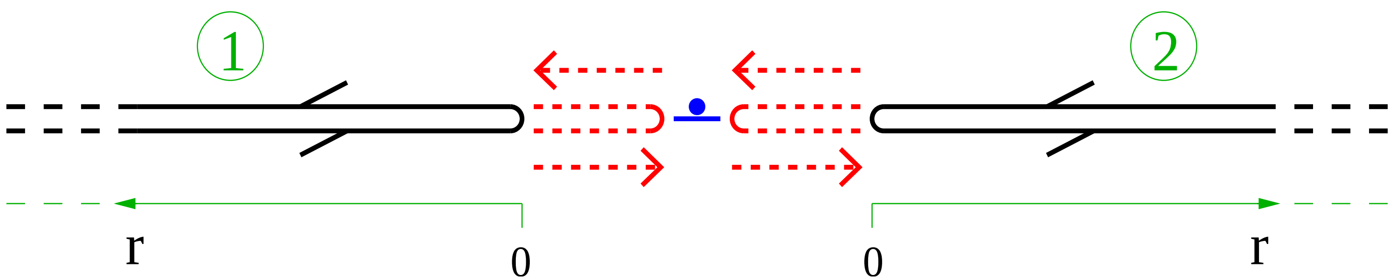
The state of theoretical methods

- Perturbative techniques are very tedious, and real-time perturbation theory presents pathologies in certain cases.
- Universality is still poorly understood in general (Wilson's RG is not directly applicable); and in particular the "large voltage" limit is subject of debates.
- Exact methods (from integrability) apply only when the exact quasi-particles do not couple carriers from both baths.
- New proposed exact method [Mehta, Andrei 2006], on the interacting resonant level model (IRLM), suggest we have a freedom in the choice of exact quasi-particles, and raised many questions [D. 2007; Boulat, Saleur 2007]; there is now some confusion about this model.

I will present a "way of thinking" about non-equilibrium steady states in impurity models that is conceptully clear and simple, gives full perturbative series, gives non-perturbative results with physically motivated truncations, and can explain what integrability means out of equilibrium. In the IRLM, I will discuss the behavior of the current in a certain universal regime.

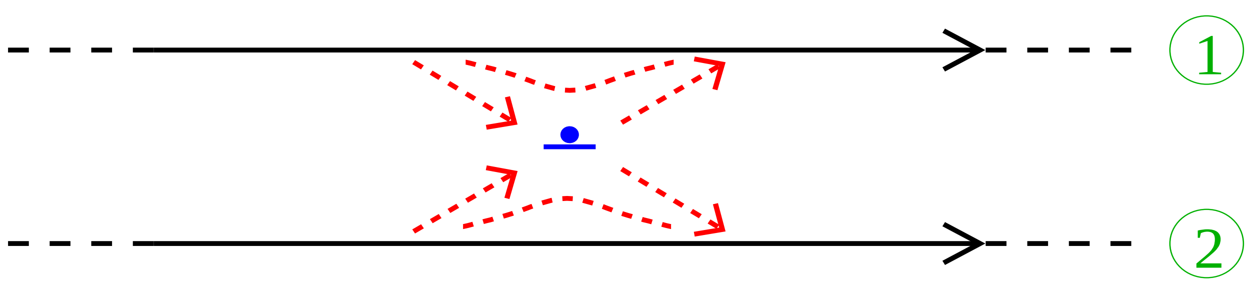
Interacting resonant level model

- “Electrodes”: 1-d massless spinless relativistic free fermions on semi-line $r \geq 0$
- Impurity: “occupied – non-occupied” boundary degree of freedom at $r = 0$



bulk CFT + boundary interaction

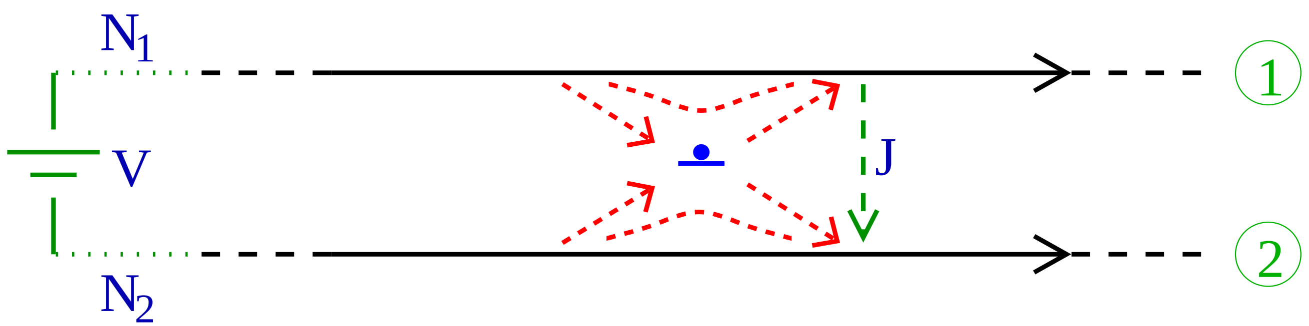
- Equivalent unfolded representation: right-moving fermions on line (with hamiltonian H_0)



Chiral CFT + impurity

$$H = H_0 + t(\psi_1^\dagger(0)d + \psi_2^\dagger(0)d + h.c.) + U(\psi_1^\dagger\psi_1(0) + \psi_2^\dagger\psi_2(0))d^\dagger d + \epsilon_d d^\dagger d$$

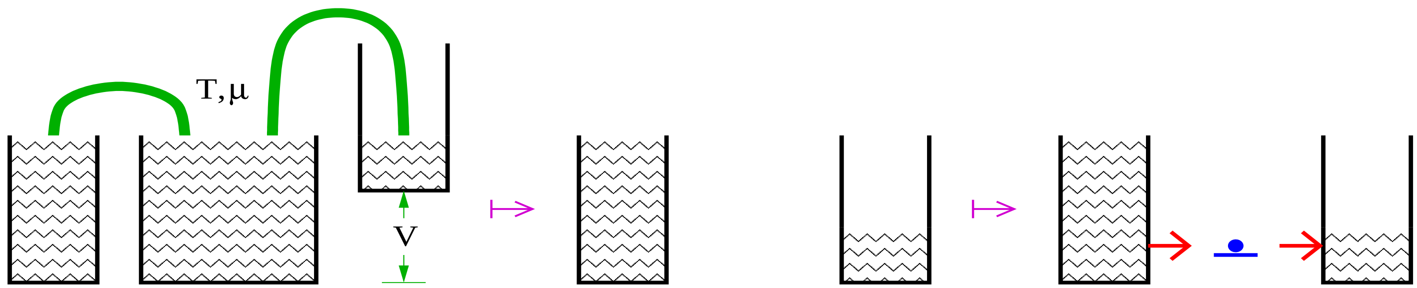
Applying a voltage: steady-state current



Out of equilibrium $V \neq 0$: non-equilibrium steady state

- Equilibrium: usual density matrix $\rho_{\rm eq} = e^{-\beta(H+\mu N+\ldots)}$
- Non-equilibrium steady state:
  - different density matrix $\rho_{\rm non-eq} \neq e^{-\beta(H+\mu N+\ldots)}$
  - entropy production
- Questions about non-equilibrium steady states:
  - Formulation?
  - Density matrix $\rho_{\rm non-eq}$?
  - Universality?
  - Integrability?

Schwinger-Keldysh formulation



- Time t_0: leads **isolated from impurity** at **potential difference** V, in **equilibrium with thermal and particle bath** $\Rightarrow \rho_0 = e^{-\beta(H_0 - VQ)}$ where $\beta = T^{-1}$ and

$$Q = \frac{1}{2}\int dx\,(\psi_2^\dagger\psi_2 - \psi_1^\dagger\psi_1) = \frac{1}{2}(N_2 - N_1)$$

- Bath disconnected and potential V brought to 0.
- Connection with impurity: tunnelling strengths turned on
- Time 0: steady-state reached $\Rightarrow$

$$\rho = e^{iHt_0}\rho_0 e^{-iHt_0}\,, \quad \langle J\rangle_{s.s.} = \lim_{t_0\to-\infty}\frac{\mathrm{Tr}\,(\rho J)}{\mathrm{Tr}\,(\rho)}\,, \quad J = -i[H,Q]$$

Potential problems with Schwinger-Keldysh formulation

- In marginally renormalisable models, it is hard to obtain the full perturbative series;
- It is far from potential exact formulations, based on scatterings and exact steady states;
- There may be problems with reaching a non-equilibrium steady state, associated to an expression for the current that is not perturbative in the tunelling strengths.

Hershfield density matrix for Lippman-Schwinger steady states

In quantum systems, **steady state = quantum state**. Density matrix

$$\rho = \exp[-\beta(H - VY)]$$

where Y [Hershfield 1993] has properties:

- it is diagonalisable and conserved by the dynamics $[H, Y] = 0$;
- its eigenvalues y on any eigenstate $|v\rangle$ of H, $Y|v\rangle = y|v\rangle$ is equal to the eigenvalue of Q on the eigenstate $|v\rangle^0$ that interpolates to $|v\rangle$ when the impurity is added, $Q|v\rangle^0 = y|v\rangle^0$.

That is, quantum averages are

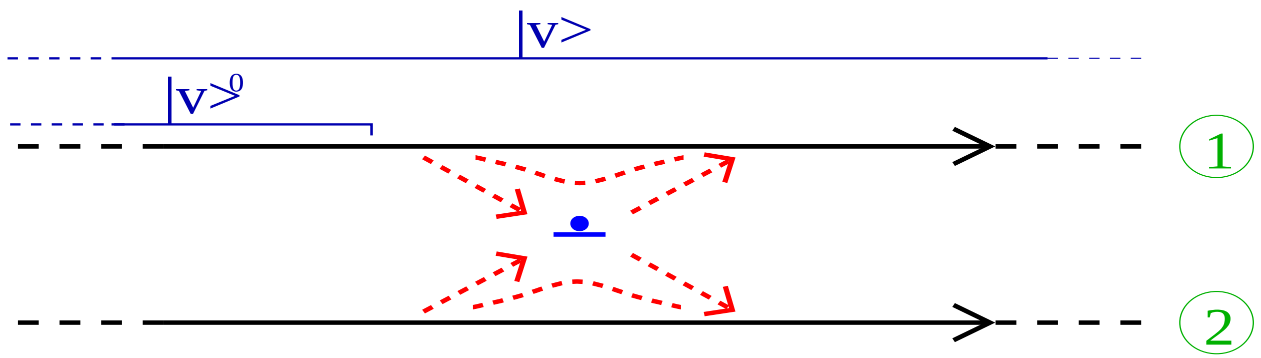
$$\langle\cdots\rangle = \frac{\mathrm{Tr}\,(\rho\cdots)}{\mathrm{Tr}\,(\rho)}\ .$$

and the definition of Y means that

$$\langle\mathcal{O}_1(x_1)\mathcal{O}_2(x_2)\cdots\rangle \stackrel{x_1<0,\,x_2<0,\,\ldots}{=} \frac{\mathrm{Tr}\,(\exp\,[-\beta(H_0 - VQ)]\,\mathcal{O}_1(x_1)\mathcal{O}_2(x_2)\cdots)}{\mathrm{Tr}\,(\exp\,[-\beta(H_0 - VQ)])}$$

Interpolating states:

Pictorially:



In equation:

$$ {}^{0}\langle v|\mathcal{O}_1(x_1)\mathcal{O}_2(x_2)\cdots|w\rangle^{0} \overset{x_1<0,\, x_2<0,\,\ldots}{=} \langle v|\mathcal{O}_1(x_1)\mathcal{O}_2(x_2)\cdots|w\rangle \,. $$

Special cases of Y

- If Q is still conserved by H, then $Y = Q$;
- If Q has a corresponding local conserved charge in the dynamics H (like in integrable models), then it is Y;
- Otherwise Y is a non-local conserved charge. A property of non-equilibrium steady states?

Equations of motion (in a wide sense)

Equations coming from **stationarity of the action** (in the action formalism)

$$\delta S = 0 \Rightarrow \begin{cases} \textbf{e.o.m.:} \text{ how operators evolve in time} \\ \textbf{impurity conditions:} \text{ relation amongst operators at the boundary / impurity} \end{cases}$$

Impurity conditions in the operator formalism

- General form of eigenstates of H (pseudo-vacuum $|0\rangle$ with $\psi(x)|0\rangle = 0,\ d|0\rangle = 0$):

$$\sum_{\substack{j=0,1;\\ k,k',\ldots=1,2}} \int dx dx' \cdots\ g_{j,k,k',\ldots}(x,x',\ldots)\psi_k^\dagger(x)\psi_{k'}^\dagger(x')\cdots\ (d^\dagger)^j|0\rangle$$

- Wave functions $g_{j,k,k',\ldots}(x,x',\ldots)$ do not have delta-function: finite jumps at $x=0$.
- The following equation holds (where $|v\rangle$ and $|w\rangle$ are states in the Hilbert space):

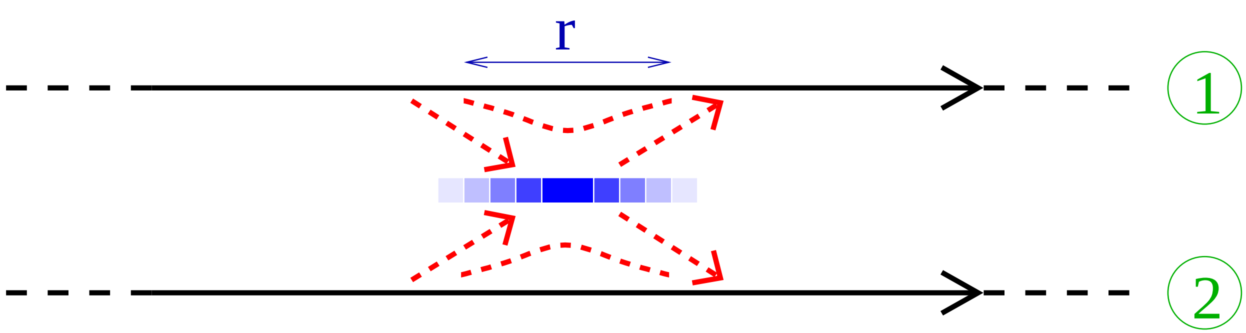
$$\langle v|\int_a^b dx\,[H,\psi_k(x)]\,|w\rangle = \lim_{\eta\to 0^+}\langle v|\int_a^{-\eta} dx\,[H,\psi_k(x)] + \int_\eta^b dx\,[H,\psi_k(x)]\,|w\rangle$$

- This becomes (with $H = H_0 + H_I$)

$$\psi_k(0^+) - \psi_k(0^-) \stackrel{\langle v|\cdot|w\rangle}{=} i\int_a^b dx[H_I,\psi_k(x)]$$

Spreading the impurity

- **Problem:** $\psi_k(0)$ appears but $\psi_k(x)$ has a jump at $x = 0$!
- **Solution:** spreading the impurity:



$$H_I^{(r)} = \int d\mu_r(x) t(\psi_1^\dagger(x)d + \psi_2^\dagger(x)d + h.c.) + $$
$$+U \int d\mu_r(x_1) d\mu_r(x_2)(\psi_1^\dagger(x_1)\psi_1(x_2) + \psi_2^\dagger(x_1)\psi_2(x_2))d^\dagger d + \epsilon_d d^\dagger d$$

- Equivalent to naïve condition $\psi_k(0) = (\psi_k(0^+) + \psi_k(0^-))/2$.

The impurity conditions

With $\psi_e = (\psi_1 + \psi_2)/\sqrt{2}$,

$$\left(1 + \frac{iU}{2} d^\dagger d\right) \psi_e(0^+) - \left(1 - \frac{iU}{2} d^\dagger d\right) \psi_e(0^-) \stackrel{|w\rangle}{=} -itd$$

- Works more generally as an equation for linear maps $\mathcal{H} \longrightarrow \mathcal{F} \otimes \mathcal{I}$;
- Fixes bare scattering matrix of coordinate Bethe ansatz construction;
- Bethe ansatz construction of [Mehta, Andrei 2006] does not satisfy it.

This implies

$$\psi_e(0^+) \overset{|w\rangle}{=} -itd + \left(1 + \frac{2U}{2i - U} d^\dagger d\right) \psi_e(0^-)$$

$\Rightarrow$ Local operator on the right is written as impurity operators and local operator on the left

The steady-state conditions

Stationarity of averages $\langle [H, b_j \mathcal{O}(x)] \rangle = 0$ and
passing operators at 0^+ to operators at 0^- using impurity conditions gives ($x < 0$):

$$
\begin{aligned}
-i\partial_x \langle b_j \mathcal{O}(x) \rangle &= iA_j \langle b_j \mathcal{O}(x) \rangle + \langle \left(c_j + \sum_i b_i E_{i,j}(0^-) \right) \mathcal{O}(x) \rangle \\
A_j &= \left(\frac{t^2}{2} + i\epsilon_d, \frac{t^2}{2} - i\epsilon_d, t^2 \right)_j \\
c_j &= \left(-t\psi_e(0^-), t\psi_e^\dagger(0^-), 0 \right)_j \\
E_{i,j}(x) &= \begin{pmatrix} -un(x) & 0 & -t\psi_e^\dagger(x) \\ 0 & \bar{u}n(x) & -t\psi_e(x) \\ itu\psi_e(x) & it\bar{u}\psi_e^\dagger(x) & 0 \end{pmatrix}_{i,j}
\end{aligned}
$$

with $b_1 = d,\ b_2 = d^\dagger,\ b_3 = d^\dagger d,\ u = \dfrac{2iU}{2i - U},\ n = \psi_e^\dagger \psi_e + \psi_o^\dagger \psi_o$

Solving in the free case $U = 0$ (and $U = \infty$)

- Integrating:

$$\langle b_j \mathcal{O}(x) \rangle = i e^{-A_j x} \int_{-\infty}^{x} dx' e^{A_j x'} \langle \left(c_j + \sum_i b_i E_{i,j}(0^-) \right) \mathcal{O}(x') \rangle \,.$$

  Choice of integration constant: the limit $x \to -\infty$ of $\langle b_j \mathcal{O}(x) \rangle$ exists.

- The part with c_j contains only operators on the left of the impurity: **averages can be evaluated using impurity-less theory by the steady-state definition**

- For average of current operator

$$\langle J \rangle = -i \langle [H, Q] \rangle = -\frac{it}{2} \langle \psi_o^\dagger(0) d - d^\dagger \psi_o(0) \rangle = -\frac{it}{2} \langle \psi_o^\dagger(0^-) d - d^\dagger \psi_o(0^-) \rangle$$

  this gives at $U = 0$ and $T = 0$

$$\langle J \rangle = \frac{t^2}{4\pi} \left(\arctan \frac{V + 2\epsilon_d}{t^2} + \arctan \frac{V - 2\epsilon_d}{t^2} \right)$$

The general case: perturbative expansion

- Solving perturbatively the integral equation:

$$\sum_{j=1}^{3}\langle b_j \mathcal{O}_j(0^-)\rangle = \sum_{n=0}^{\infty} i^{n+1}\int_{-\infty}^{0} dx_0 \cdots dx_n \times$$
$$\times \langle c^T e^{Ax_n} E(x_n)\cdots e^{Ax_1} E(x_1+\ldots+x_n) e^{Ax_0}\bar{\mathcal{O}}(x_0+\ldots+x_n)\rangle^0$$

- Formally resums into

$$i\int_{-\infty}^{0} dx\,\langle c^T \mathcal{P}\exp\left[\int_0^x dx'\,(E(x')+A)\right]\bar{\mathcal{O}}(x)\rangle^0$$

- Regularisation: use $\varepsilon > 0$ (with $\varepsilon \sim 1/D$ where D is bandwidth) and

$$\int_{-\infty}^{0} \mapsto \int_{-\infty}^{-\varepsilon}$$

Results to order U

- Callan-Symanzik equation (with $m \equiv t^2/2$)

$$\left(\frac{U}{\pi} m \frac{\partial}{\partial m} + \varepsilon \frac{\partial}{\partial \varepsilon}\right) \langle J \rangle = 0$$

- Universal renormalised results:

$$D \gg V, T, \epsilon_d, T_B \text{ with } (T_B/D)^{1+U/\pi} = m/D$$

- Physical infrared cutoffs:

$$T,\ \Delta_\pm \equiv |V/2 \pm \epsilon_d|$$

- For $D \gg V \gg T_B \gg T, |\epsilon_d|$, we have

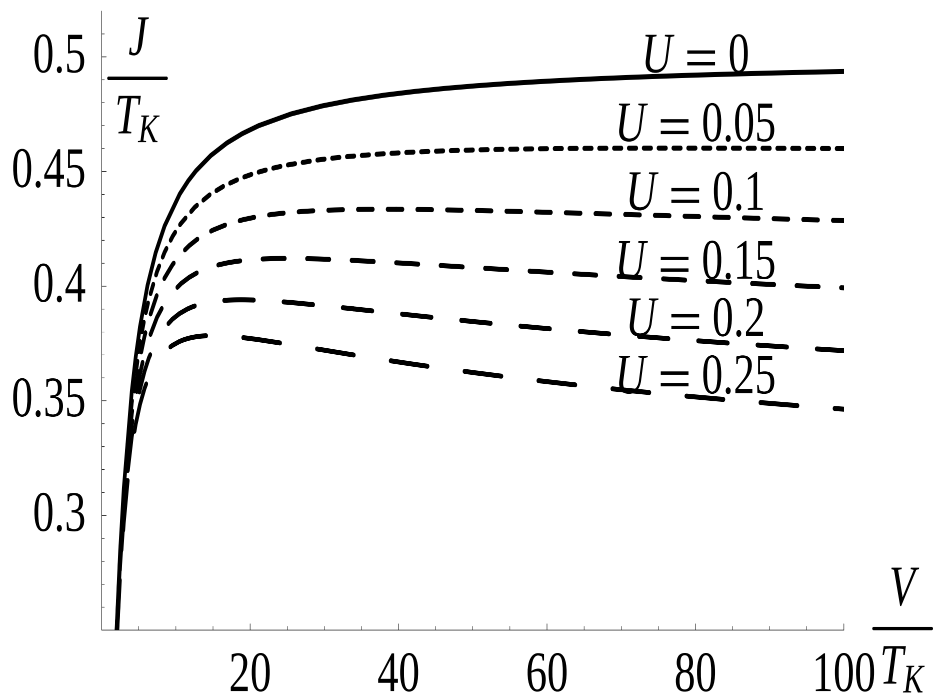
$$\langle J \rangle \sim \frac{1}{2} T_B \left(8 e^{\Psi(1/2)} \frac{T_B}{V} \right)^{\frac{U}{\pi}} \left(1 + O(U^2)\right)$$

- We have at $D \gg T_B \gg T, V, |\epsilon_d|$, in an expansion in $\bar{T} \equiv \pi T / T_B$,

$$\frac{\langle J \rangle}{V} \sim \frac{1}{2\pi} \left(1 + g_2 \bar{T}^2 + g_4 \bar{T}^4 + O(U^2, \bar{T}^6)\right)$$

with

$$\frac{g_4}{g_2^2} = \frac{21}{5} - \frac{U}{\pi}$$



$\frac{J}{T_K}$
0.5
0.45
0.4
0.35
0.3
$U = 0$
$U = 0.05$
$U = 0.1$
$U = 0.15$
$U = 0.2$
$U = 0.25$
20
40
60
80
100
$\frac{V}{T_K}$

Conclusions and perspectives

We have developed an efficient method for obtaining perturbative series and some non-perturbative results in certain models of quantum impurities, that works as easily both in and out of equilibrium.

- Results agree with
  - low-T expansion from conformal perturbation theory of Boulat and Saleur (2007)
  - large-V power law observe by Boulat and Saleur (2007) at a particular value of U
  - infinite-U limit of proposed exact results of Mehta and Andrei (2006)
- Results disagree with
  - small-U expansion of proposed exact results of Mehta and Andrei (2006)

- Integrability
  - there are arguments from definition of Y for non-integrability of the non-equilibrium steady state at generic values of U
  - impurity conditions allow re-construction of conserved charges
- Questions
  - is the non-equilibrium steady state represented by Y integrable?
  - what are the consequences of conservation of higher local conserved charges (e.g. for form factors)?
  - does the method take care of the pathologies found in doing Schwinger-Keldysh real-time perturbation theory for Kondo/Anderson models?
  - how can we use the “re-summed” perturbative expansion?