# The density matrix formulation for quantum impurities in steady states out of equilibrium

Based on: [BD, Andrei PRB 06], [BD PRL 07] and Capri Spring School 2009 lecture notes

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Thanks to: Denis Bernard, Édouard Boulat, Hubert Saleur, Dirk Schuricht, ...

**Trieste, July 2009**

## Driven quantum mechanics in a dispersive environment

- Two separate thermal/particle baths can exchange electrons with a quantum mechanical system (impurity).
- The two baths are held at a fixed difference of chemical potential.
- With a steady particle flow, the system is in a “non-equilibrium steady state”.

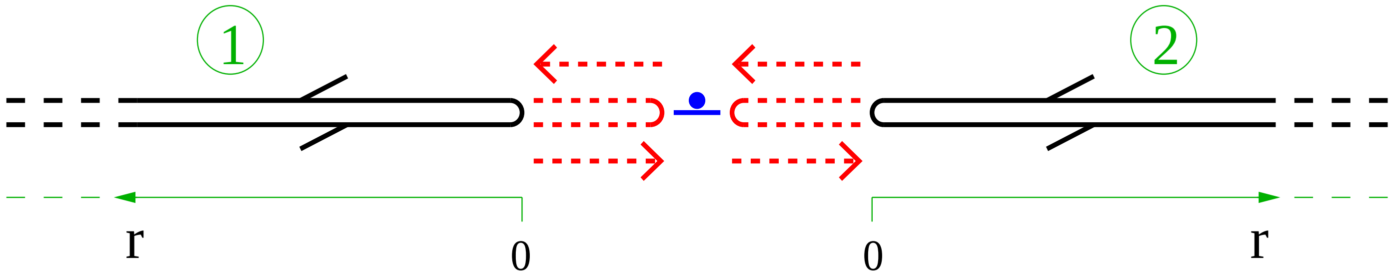
$\Longrightarrow$ Interplay between out-of-equilibrium and quantum mechanics

## Goal of talk

- Show in some detail how the real-time formulation (Keldysh, cf. lectures of A. Kamenev) gives rise to the scattering state formulation (cf. talks of N. Andrei, H. Saleur (next week)).
- Describe the two main, decoupled ingredients of the scattering state formulation: steady state ($Y$-operator) and dynamics ($\mathcal{U}$-operator).
- Specialise these ingredients to various situations: CFT, perturbation theory, integrable models.

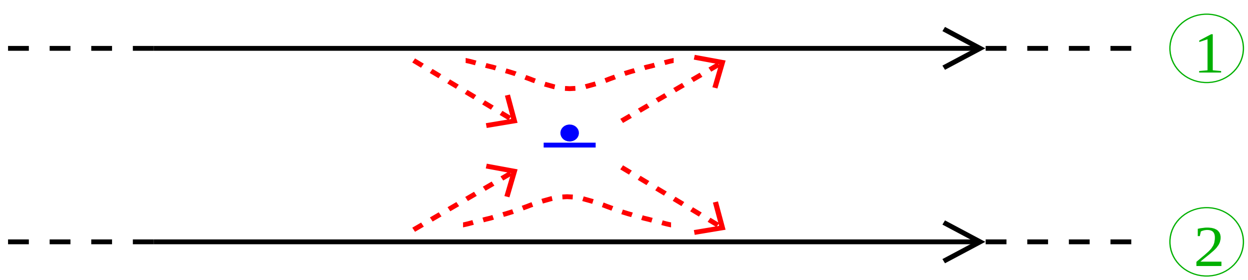
## Pictorial representation

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




CFT + boundary interaction

- Equivalent unfolded representation: right-moving fermions on line




Chiral CFT + impurity

## Dynamics of impurity models: quantum observables

- Fermions of metallic sheets (or electrodes) $\Psi_{1,2}(x)$:

$$\{\Psi_j(x), \Psi^\dagger_{j'}(x')\} = \mathbf{1}\delta_{j,j'}\delta(x-x')$$

$$H_e = -i\int_{-L}^{L} dx \sum_{j=1,2} \Psi^\dagger_j(x)\frac{d}{dx}\Psi_j(x)$$

$$[H_e, \Psi_j(x)] = i\frac{d}{dx}\Psi_j(x)$$

- Impurity's observables:
  - fermionic $d_\alpha, d_\alpha^\dagger$, annihilation and creation of electrons on the impurity
  - bosonic (hermitian): $D_\beta$, internal observable/change of the impurity states preserving the electron number; hamiltonian $H_i$
- Impurity interaction: tunnelling $T_\alpha, T_\alpha^\dagger$, co-tunnelling $U_\beta^{(0,\pm1)}$:

$$I = \sum_{j,\alpha} \left( \Psi_j^\dagger(0) T_\alpha d_\alpha + d_\alpha^\dagger T_\alpha^\dagger \Psi_j(0) \right) + \sum_{j,k,\beta} \Psi_j^\dagger(0) U_\beta^{(j-k)} \Psi_k(0) D_\beta$$

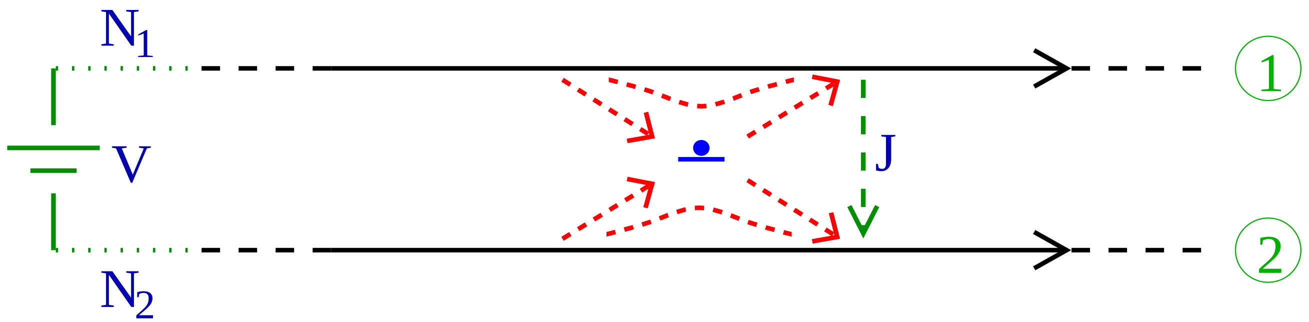
$$\boxed{H = H_e + H_i + I = H_0 + I}$$

## In particular: interacting resonant-level model (IRLM)

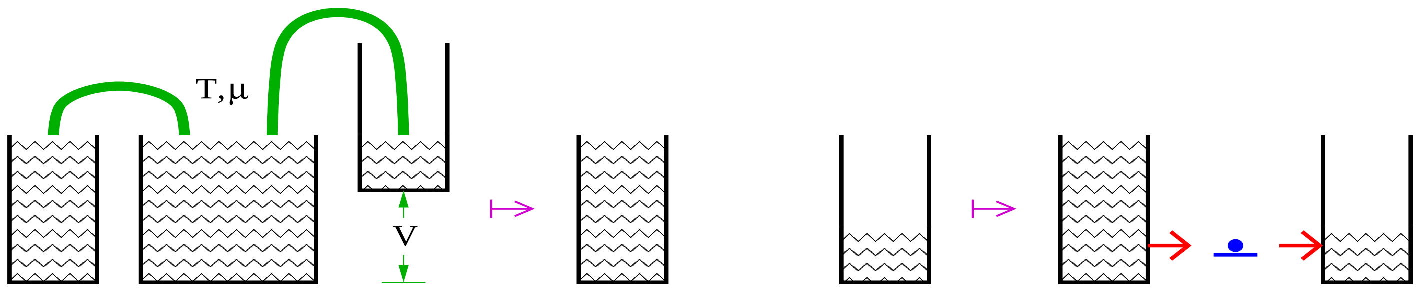
Spinless bulk electrons, two-state impurity degree of freedom:

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

## Applying a voltage: steady-state current



## Constructing the steady in real time: the Schwinger-Keldysh formulation




- Time $t = 0$: leads **isolated from impurity** at **potential difference** $V$, in **equilibrium with thermal and particle bath** $\Rightarrow \rho_0 = e^{-(H_0 - VQ)/T}$ where

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

- Bath disconnected and potential $V$ brought to $0$.
- Connection with impurity: tunnelling strengths turned on (local quantum quench).
- Time $t = \infty$: steady-state reached $\Rightarrow$

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

## Large-time limit

- **Does the limit exist?** In order to reach the steady state: $L \gg t \gg T^{-1}$. Limit exists in IRLM by Caldeira-Leggett: tunnelling allows relaxation by emission of electrons. Limit is proven to exist [BD, Andrei 06] in Kondo by $SU(2)$ symmetry, thanks to large-time factorisation of correlation functions:
  - interaction picture expression

$$\langle J\rangle(t) = \left\langle \mathcal{P}\exp\left[-i\int_t^0 dt'\, I(t')\right]\, J\, \mathcal{P}\exp\left[-i\int_0^t dt'\, I(t')\right]\right\rangle_0$$

  - large-time factorisation

$$\langle I(t_1)I(t_2)I(t_3)J\rangle_0 \quad \rightarrow \quad \langle I(t_1)I(t_2)\rangle_0\, \langle I(t_3)J\rangle_0$$

- **What is the result of the limit?** If $V=0$, one can show [BD, Andrei 06] that it is $e^{-H/T}$. Thermalisation after local quench. Hence for $V\neq 0$, correct non-equilibrium steady state. Note: out of equilibrium, “slowly turning on interaction” does not help. Baths essential not only to obtain steady state, but also to maintain it.
- **Limit of what objects?** The limit exists (correlation functions factorise) only for operators supported on a finite interval. For instance: $Q$ no, but $J$ yes.

  Reduction of allowed observables $\Rightarrow$ loss of information $\Rightarrow$ irreversibility.

## Scattering states and Hershfield's density matrix

- Quantum mechanics: starting with a quantum state looking like a free wave function in a region of order $L$ where the potential is flat, taking the limit $L \gg t \gg a$ where $a$ is some scale in the problem, and looking only around the region where the potential is not flat, one gets a **scattering state**.

- In general, scattering states **are not large-$L$ limits of eigenstates** of $H(L)$. They are eigenstates of $H(L=\infty)$ in a very special sense.

- The limit $L \gg t \gg T^{-1}$ in the Schwinger-Keldysh formulation should be **naturally described by scattering states of $H$**. Initial statistical distribution $e^{-(H_0 - VQ)/T}$ of (finite-$L$) states gives rise to statistical distribution of scattering states of $H$:

$$\langle \mathcal{O} \rangle_{ne} = \frac{\mathrm{Tr}_{scatt.\ states}\,(\rho_{ne}\mathcal{O})}{\mathrm{Tr}_{scatt.\ states}\,(\rho_{ne})}$$

- The operator $\rho_{ne}$ is Hershfield's density matrix for non-equilibrium steady states [Hershfield 93] (although it was introduced in a different way). Usually introducing the $Y$ operator:

$$\rho_{ne} = e^{-(H-VY)/T}$$

A priori, $Y$ may depend on $T$ and $V$!

## Properties of $Y$ operator

[Hershfield 93], [Mehta, Andrei 06], [BD 07], [BD 09]

- Steady-state condition.

  If $\mathcal{O}$ is finitely supported, then also $[H, \mathcal{O}]$ is. Then $\langle [H, \mathcal{O}] \rangle_{ne}$ can be calculated, and it is zero by the fact that the large-time limit exists. Since this holds for any $\mathcal{O}$, this implies

  $$\boxed{[H, Y] = 0}$$

  because finitely supported operators are enough observables to determine scattering states.

- Asymptotic conditions.

1. Writing $\lim_{t\to\infty} \frac{\mathrm{Tr}(\rho(t)\mathcal{O})}{\mathrm{Tr}(\rho(t))}$ in **interaction picture** with respect to $H_0$, we have

$$\langle \mathcal{O} \rangle_{ne} = \lim_{t\to\infty} \left\langle \mathcal{P} \exp\left[ -i \int_t^0 dt' \, [I(t'), \cdot] \right] \, \mathcal{O} \right\rangle_0$$

   Operators in $I(t)$ are **finitely supported on the right** for $t > 0$. So:

$$\langle \mathcal{O}(x) \cdots \rangle_{ne} \stackrel{x<0,\ldots}{=} \langle \mathcal{O}(x) \rangle_0$$

2. Quasi-periodicity properties under $x \mapsto x + i/T$ for $\mathrm{Re}(x) < 0$ are evaluated using commutators $[H_0 - VQ, \mathcal{O}(x)]$ (r.h.s.) and $[H - VY, \mathcal{O}(x)]$ (l.h.s.). Since $[H, \mathcal{O}(x)] = [H_0, \mathcal{O}(x)]$ for $x \neq 0$, we must have

$$\boxed{[Y, \mathcal{O}(x) \cdots] \stackrel{x<0,\ldots}{=} [Q, \mathcal{O}(x) \cdots]}$$

## From this, formal definition of $Y$ on scattering states

[BD 09]

Scattering states through Lippman-Schwinger equation ($in$ states):

$$|v\rangle = |v\rangle_0 + \frac{1}{E_v - H_0 + i0^+} I |v\rangle$$

where $|v\rangle_0$ is eigenstate of $H_0 = H_e + H_i$, and $|v\rangle$ is eigenstate of $H$, with energy $E_v$.

- **Bare wave function.** For **minimal particles on the impurity**, bare wave function gives

$$\langle 0|\mathcal{O}(x)\cdots|v\rangle \stackrel{x<0,\ldots}{=} \langle 0|\mathcal{O}(x)\cdots|v\rangle_0$$

- **Hybridisation.** Only states $|v\rangle_0$ with minimal particles on impurity give non-zero $|v\rangle$.

$\Rightarrow$ **minimal-particle bare wave functions at negative positions fully determine $|v\rangle$**

- only "one" minimal-particle state thanks to hopping in IRLM
- $SU(2)$ invariance in Kondo model

$\Rightarrow$ $\boxed{Y|v\rangle = q|v\rangle \quad \text{for} \quad Q|v\rangle_0 = q|v\rangle_0}$

## Operator construction

- From hybridisation, we know the quantum numbers of scattering states. Then (IRLM):

$$\{a^\dagger_{p,j}, a_{p',j'}\} = \delta(p-p')\delta_{j,j'}, \quad a_{p,j}|\mathrm{vac}\rangle = 0 \ (p>0), \quad a^\dagger_{p,j}|\mathrm{vac}\rangle = 0 \ (p<0)$$

$$H = \sum_j \int_0^\infty dp\, p \ : a^\dagger_{p,j} a_{p,j} :$$

$$Y = \frac{1}{2}\int dp \left( : a^\dagger_{p,1} a_{p,1} : - : a^\dagger_{p,2} a_{p,2} : \right)$$

- Find a **representation of the canonical commutation relations and the equations of motion** $[H, \psi_j(x)] = \ldots$, $[H, d] = \ldots$, where $H$ is bounded from below.
- For $x \neq 0$, the operators $\psi_j(x)$, $H$ form a closed algebra:

$$[H, \psi_j(x)] = i \frac{d}{dx} \psi_j(x) \quad (x \neq 0)$$

Solution:

$$\psi_j(x) = \int \frac{dp}{\sqrt{2\pi}} e^{ipx} \begin{cases} a_{p,j} & (x < 0) \\ \mathcal{U} a_{p,j} \mathcal{U}^\dagger & (x > 0) \end{cases}$$

The unitary operator $\mathcal{U}$ encodes all the impurity-related dynamics, and in fact defines the impurity model

## Local current vs scattering formalism

$$J = -i[H, Q] = -\frac{it}{\sqrt{2}} d^\dagger \psi_o(0) + h.c.$$

But also

$$Q = \int_{-\infty}^{\infty} dx\, q(x) = \int_{-\infty}^{0^-} dx\, q(x) + \int_{0^+}^{\infty} dx\, q(x)$$

so that

$$J = q(0^-) - q(0^+)$$

$$
\begin{aligned}
\langle J \rangle &= \langle q(0^-) - q(0^+) \rangle \\
&= \frac{1}{L} \langle \int_{-L/2}^{L/2} dx \, (q_{in}(x) - \mathcal{U} q_{in}(x) \mathcal{U}^{-1}) \rangle \\
&= \frac{1}{L} \langle Q_{in} - \mathcal{U} Q_{in} \mathcal{U}^{-1} \rangle \\
&= \frac{1}{L} \sum_{in} \rho_{in} \langle in | Q_{in} - \mathcal{U} Q_{in} \mathcal{U}^{-1} | in \rangle \\
&= \frac{1}{L} \sum_{in,\, out} \rho_{in} \langle in | Q_{in} - \mathcal{U} Q_{in} \mathcal{U}^{-1} | out \rangle \langle out | in \rangle \\
&= \frac{1}{L} \sum_{in,\, out} \rho_{in} \langle in | Q_{in} - Q_{out} | out \rangle \langle out | in \rangle
\end{aligned}
$$

$$
\boxed{\langle J \rangle = \frac{1}{L} \sum_{in,\, out} \rho_{in} (Q_{in} - Q_{out}) | \langle in | out \rangle |^2}
$$

## Current noise from $Y$ operator

A careful evaluation of the large-time limit [BD, Andrei 06] shows that

$$Y = \lim_{t \to \infty} e^{-iHt} Q e^{iHt} = Q + \int_{-\infty}^{0} J(t)$$

Current noise (with $\delta J = J - \langle J \rangle_{ne}$):

$$2 \int_{-\infty}^{0} dt \, \langle \{ J(t), \delta J \} \rangle_{ne} = 2 \langle \{ Y - Q, \delta J \} \rangle_{ne} = 4T \frac{d}{dV} \langle J \rangle_{ne} - 2 \langle \{ Q, \delta J \} \rangle_{ne}$$

[Fujii 08]

## How to construct the $\mathcal{U}$ operator?

- CFT: conformal boundary state $\sum_{i,j} B_{i,j} |i\rangle_R \otimes |j\rangle_L$ gives rise to $\mathcal{U}$ operator.
- Free theory (RLM, $U = 0$): use even and odd sectors: $\psi_{e,o} = (\psi_1 \pm \psi_2)/\sqrt{2}$. Operators $H$, $\psi_e$ and $d$ form a closed algebra. Solve.

$$\boxed{\mathcal{U} = e^{-i\int dp\, \phi_p a^\dagger_{p,e} a_{p,e}}, \quad e^{i\phi_p} = \frac{\epsilon_d - p + it^2}{\epsilon_d - p - it^2}}$$

Continuity conditions through the impurity [BD 07]:

$$-i\sqrt{2}td = \psi_e(0^+) - \psi_e(0^-) \qquad \left(\text{note also: } \{\psi_e(0^\pm), d^\dagger\} = \mp it/\sqrt{2}\right)$$

Resolution of the impurity and consistency of operator algebra [BD 07, 09]:

$$\psi_e(0) = \frac{\psi_e(0^+) + \psi_e(0^-)}{2}$$

## Non-locality

In the free case $U = 0$, we find, after inverse Fourier transform,

$$Y - Q =$$

$$-\frac{1}{2}\int_0^\infty dx\, e^{-\left(t^2+i\epsilon\right)x}\left(i\sqrt{2}td^\dagger\psi_o(x) + 2t^2\int_0^\infty dx'\psi_e^\dagger(x')\psi_o(x+x')\right) + h.c.$$

- **Non-locality:** not integral over $x$ of local density at $x$. Related to the fact that $Y$ describes a non-equilibrium state.
- But **weak** non-locality: the non-locality is exponentially vanishing. Related to the fact that there is relaxation at large times, which is essential for the steady state to be reached and to exist.

## Interacting case, IRLM $U \neq 0$

- General perturbative form of solution:

$$\mathcal{U} a_{p,e} \mathcal{U}^\dagger = e^{i\phi_p} a_{p,e} + U \int dp_1 dp_2 \, f_{p_1,p_2} \; : a^\dagger_{p_1+p_2-p,e/o} a_{p_1,e/o} a_{p_2,e/o} : + \ldots$$

- A systematic approach for impurity operators [BD 07]: using

$$\left(1 + \frac{iU}{2} d^\dagger d\right) \psi_e(0^+) - \left(1 - \frac{iU}{2} d^\dagger d\right) \psi_e(0^-) = -i\sqrt{2} t d$$

we find

$$(\, d \,,\; d^\dagger \,,\; d^\dagger d) = i \int_0^\infty dx \, c^T_{in}(x) \, \mathcal{P} \exp\left[\int_x^0 dx' (-iE_{in}(x') + A)\right]$$

## Integrability

- Bare construction:

$$\int [dx] \left( \prod e^{i\phi_p(x)+ipx} \psi_e^\dagger(x) \,|\, e^{ipx} \psi_o^\dagger(x) \,|\, \delta(x) d^\dagger \right) \left( \prod S_{p,q}^{e|o,e|o}(x-y) \right) |0\rangle$$

with $S_{p,q}^{v,w}(x>0) = S_{p,q}^{v,w}$ and $S_{p,q}^{v,w}(x<0) = 1$, similarly for $e^{i\phi_p(x)}$.

- ZF operators: new basis for CFT, $\prod A_{p,v}^\dagger |0\rangle$ with

$$A_{p,v} A_{q,w} = -S_{p,q}^{v,w} A_{q,w} A_{p,v}$$

- Exact expression for $\mathcal{U}$:

$$\boxed{\mathcal{U} = e^{-i \int dp\, \phi_p A_{p,e}^\dagger A_{p,e}}}$$

- Local conserved charges:

$$H_{n,v} = \int dp\, p^n A_{p,v}^\dagger A_{p,v}, \quad \mathcal{U} = e^{-i \sum_{n=0}^\infty u_n H_{n,e}}$$

## Integrability out of equilibrium

- The operator $Y$ must preserve the set of momenta, but may interchange the particle types

$$[Y, \sum_v H_{n,v}] = 0 \quad \Rightarrow \quad Y \text{ must act on one-particle subspaces}$$

- Is the IRLM integrable out of equilibrium? Continuity conditions lead to [BD 07, 09]

$$S^{e,e}_{p,q} = \frac{4\epsilon_d - 2(p+q) + i(p-q+2it^2)U}{4\epsilon_d - 2(p+q) - i(p-q+2it^2)U},\ S^{e,o}_{p,q} = \frac{1+iU/2}{1-iU/2},\ S^{o,e}_{p,q} = \frac{1-iU/2}{1+iU/2}$$

$$\Rightarrow \quad [Y, \sum_v H_{n,v}] \neq 0$$

- Mehta and Andrei: same $S^{e,e}$ but $S^{e,o} = S^{o,e} = S^{o,o} = S^{e,e}$.

$$\Rightarrow \quad [Y, \sum_v H_{n,v}] = 0, \quad \text{same universal} \quad \mathcal{U}?$$

## Conclusions and perspectives

We showed how the scattering state formulation naturally arises from the the real-time formulation, and showed how using scattering states and Hershfield $Y$ operator one can essentially separate the dynamical part, with standard perturbative or exact descriptions, from the “non-equilibrium state” part.

Some questions:

- Can we prove that the steady state corresponds to the maximal current? (extremisation of entropy production?)
- Can we develop an efficient diagramatic method from the operator construction?
- Can we unify the various exact constructions of $\mathcal{U}$? (“mine”, Mehta Andrei, Boulat Saleur)
- Can we perturb the $\mathcal{U}$ operator about non-trivial exact points?