# Diagrammatic Quantum (Quasi-)Monte Carlo Out of equilibrium / in real time 

## Olivier Parcollet

Center for Computational Quantum Physics (CCQ)
Flatiron Institute, Simons Foundation
New York


## Out of equilibrium \& strong correlations

- Many experiments : Pump probe, quantum dots, ultra-cold atoms, cavities.


Pump probe


Nano-electronics


Ultra-cold atoms

- Computational physics challenge :
- Exact methods for out of equilibrium systems, at strong coupling
- Control, speed and precision
- Long time (after quench), steady state. Resolve various energy/time scales.

Early Monte Carlo have sign problem Muelbacher et al. PRB 2009; Werner et al PRB 2009; Schiro PRB 2009.

## Example : a simple model for a quantum dot

- Anderson model with two leads ( $L, R$ ).

$$
\begin{array}{cc}
\text { Bath } & \text { Local orbital } \\
\sum_{\substack{k \sigma \\
\alpha=L, R}} \varepsilon_{k \alpha} c_{k \sigma \alpha}^{\dagger} c_{k \sigma \alpha}+\sum_{\sigma} \varepsilon_{d} d_{\sigma}^{\dagger} d_{\sigma}+U n_{d \uparrow} n_{d \downarrow}+\sum_{\substack{k \sigma \\
\alpha=L, R}} g_{k \sigma \alpha}\left(c_{k \sigma \alpha}^{\dagger} d_{\sigma}+h . c .\right)
\end{array} \begin{gathered}
\text { Hybridization } \\
\text { Level width at } U=0 \\
\Gamma=\pi \rho_{E_{F}} g^{2}
\end{gathered}
$$

- Questions: Spectral function ? Kondo temperature ? Current ?

We want a precise solution, at low temperature, any $V_{b}$, in steady state

## Summary of the approach

- Perturbation theory in interaction U (I0-I5 orders) for physical quantities.

$$
Q(t, U)=\sum_{\substack{\text { Time }}}^{K} Q_{n}(t) U^{n}{ }_{\text {Interaction }}^{n}
$$

I. Works even at long time, even in strong coupling regime (e.g. Kondo effect)
2. How to compute $\mathrm{Q}_{\mathrm{n}}(\mathrm{t})$ ? Cost $\mathrm{O}\left(2^{\mathrm{n}}\right)$.

High dimensional integrals.
Real time "diagrammatic" Quantum Monte Carlo Beyond stochastic methods : Quasi-Monte Carlo (QQMC)
3. How to sum the series ?

- See also : Expansion around atomic limit.
"Inchworm" approach. Cohen, Gull, Reichman, Millis PRL (2015)

Schwinger-Keldysh
I- Notations

## Three diagrammatic techniques.

- $\mathrm{T}=0$ : Ground state
- Matsubara : finite T, in thermal equilibrium
- Schwinger-Keldysh
- General. Equilibrium or out of equilibrium. Real time.
- A bit more complex technically. It is not possible to write diagrams with only one Green function.
- Conceptually simpler. Bath are explicitly included, no hidden relaxation (or Gell-Man Low theorem).


## Notations

- Canonical fermion operator
- $\mathrm{a}, \mathrm{b}=$ multi-index $: \mathrm{k}, \mathrm{x}$, spin,.. everything but time.

$$
\left\{c_{a}, c_{b}^{\dagger}\right\}=\delta_{a b}
$$

- Chronological product

$$
\begin{aligned}
& T A(t) B\left(t^{\prime}\right)=\theta\left(t-t^{\prime}\right) A(t) B\left(t^{\prime}\right)+\zeta_{A B} \theta\left(t^{\prime}-t\right) B\left(t^{\prime}\right) A(t) \\
& \check{T} A(t) B\left(t^{\prime}\right)=\theta\left(t^{\prime}-t\right) A(t) B\left(t^{\prime}\right)+\zeta_{A B} \theta\left(t-t^{\prime}\right) B\left(t^{\prime}\right) A(t)
\end{aligned}
$$

$$
\zeta_{A B}= \pm 1 \quad \text { A }, \mathrm{B} \text { both fermionic } ?-\mathrm{I} \text { else }+\mathrm{I}
$$

## Hamiltonian evolution

- Total Hamiltonian of the system, e.g.

$$
\mathrm{H}=\mathrm{H}_{\text {dot }}+\mathrm{H}_{\text {bath }}+\mathrm{H}_{\text {dot-bath }}
$$

- $\mathrm{H}(\mathrm{t})$ determines the dynamics in real time. Can be time dependent.
- Evolution operator $U_{H}$ : evolves the state of the system from $t_{0}$ to $t$

$$
|\psi(t)\rangle=U_{H}\left(t, t_{0}\right)\left|\psi\left(t_{0}\right)\right\rangle
$$

- Heisenberg representation for operator A

$$
A(t) \equiv U_{H}^{\dagger}\left(t, t_{0}\right) A\left(t_{0}\right) U_{H}\left(t, t_{0}\right)
$$

## Reminder : density matrix

- For the whole system (e.g. dot + baths)
- Describes the occupation of the levels.

$$
\begin{array}{rlr}
\operatorname{Tr} \rho & =1 & \\
\rho^{\dagger} & =\rho & \\
\rho & \geq 0 & \\
i \partial_{t} \rho(t) & =[H(t), \rho(t)] & \\
\rho(t) & =U_{H}\left(t, t_{0}\right) \rho\left(t_{0}\right) U_{H}^{\dagger}\left(t, t_{0}\right) & \\
\langle A(t)\rangle & \equiv \operatorname{Tr}\left(\rho(t) A\left(t_{0}\right)\right)=\operatorname{Tr}\left(\rho\left(t_{0}\right) A(t)\right) & \text { for correlataors } \rho
\end{array}
$$

- Out of equilibrium : 2 independents objects. H and $\rho$.
- Thermal equilibrium :

$$
\begin{aligned}
& \bar{\rho}=\frac{1}{Z} e^{-\beta H}, \quad Z=\operatorname{Tr} e^{-\beta H} \\
& \bar{\rho}=\frac{1}{Z} e^{-\beta(H-\mu \hat{N})}, \quad Z=\operatorname{Tr}^{-\beta(H-\mu \hat{N})}
\end{aligned}
$$

## One particle Green functions

- Definitions
+,- : just notations
for the moment

$$
\begin{aligned}
G_{a b}^{++}\left(t, t^{\prime}\right) & \equiv-i\left\langle T c_{a}(t) c_{b}^{\dagger}\left(t^{\prime}\right)\right\rangle \\
G_{a b}^{--}\left(t, t^{\prime}\right) & \equiv-i\left\langle\check{T} c_{a}(t) c_{b}^{\dagger}\left(t^{\prime}\right)\right\rangle \\
G_{a b}^{+-}\left(t, t^{\prime}\right)=G_{a b}^{<}\left(t, t^{\prime}\right) & \equiv i\left\langle c_{b}^{\dagger}\left(t^{\prime}\right) c_{a}(t)\right\rangle \\
G_{a b}^{-+}\left(t, t^{\prime}\right)=G_{a b}^{>}\left(t, t^{\prime}\right) & \equiv-i\left\langle c_{a}(t) c_{b}^{\dagger}\left(t^{\prime}\right)\right\rangle
\end{aligned}
$$

- Only 2 Green functions are independents (from the definition of T)

$$
\begin{aligned}
& G_{a b}^{++}\left(t, t^{\prime}\right)=\theta\left(t-t^{\prime}\right) G_{a b}^{>}\left(t, t^{\prime}\right)+\theta\left(t^{\prime}-t\right) G_{a b}^{<}\left(t, t^{\prime}\right) \\
& G_{a b}^{--}\left(t, t^{\prime}\right)=\theta\left(t^{\prime}-t\right) G_{a b}^{>}\left(t, t^{\prime}\right)+\theta\left(t-t^{\prime}\right) G_{a b}^{<}\left(t, t^{\prime}\right)
\end{aligned}
$$

- In equilibrium, only one!

Fluctuation-Dissipation theorem, Kubo-Martin-Schwinger relation

$$
\left\langle c_{b}^{\dagger}\left(t^{\prime}\right) c_{a}(t)\right\rangle=\left\langle c_{a}(t) c_{b}^{\dagger}\left(t^{\prime}+i \beta\right)\right\rangle \quad G_{a b}^{<}(\omega)=-e^{-\beta \omega} G_{a b}^{>}(\omega)
$$

Schwinger-Keldysh
2- Diagrammatic expansion

## General strategy

- Start at $\mathrm{t}=\mathrm{t}_{0}$ (=0 in most slides below)
- With initial condition:
$\rho=\rho_{0}$ at thermal equilibrium with non interacting Hamiltonian $\mathrm{H}_{0}$ at a temperature $\beta$
- NB : it is possible to start with interacting equilibrium. Baym-Kadanoff contour. Not covered here.
- Study the expansion of correlators at finite time.

$$
\operatorname{Tr}\left(\rho_{0} A(t) B\left(t^{\prime}\right) \ldots\right)
$$

- Build the diagrammatic at finite time.
- If needed, take the limit

$$
t, t^{\prime} \rightarrow \infty
$$

or $\quad t_{0} \rightarrow-\infty$

- Separate diagrams technique \& thermalization/relaxation/bath questions.


## Interaction picture

- Hamiltonian evolution of whole system (dot + bath)

- Operator in interaction picture ( $\neq$ Heisenberg picture).

$$
\hat{A}(t) \equiv e^{i H_{0} t} A e^{-i H_{0} t}
$$

- Evolution operator in interaction picture

$$
\begin{aligned}
& \quad U(t) \equiv e^{i H_{0} t} U_{H}(t) \\
& i \partial_{t} U(t)=\hat{V}(t) U(t) \longrightarrow U(t)=T \exp \left(-i \int_{0}^{t} \hat{V}(u) d u\right) \\
& U(0) \longrightarrow 1
\end{aligned}
$$

## Time evolution of a physical quantity

- Start at $\mathrm{t}=0(\mathrm{t} 0)$ from a non-interacting equilibrium density matrix $\rho_{0}$
- Average of an operator A

$$
U(t)=T \exp \left(-i \int_{0}^{t} \hat{V}(u) d u\right)
$$

Average in

$$
\begin{aligned}
\langle A(t)\rangle & =\operatorname{Tr}\left(\rho_{0} A(t)\right) \quad \text { initial state } \\
& =\operatorname{Tr}\left(\rho_{0}(U(t))^{\dagger} \hat{A}(t) U(t)\right) \\
& =\operatorname{Tr}\left(\rho_{0} \check{T} \exp \left(+i \int_{0}^{t} \hat{V}(u) d u\right) \hat{A}(t) T \exp \left(-i \int_{0}^{t} \hat{V}(u) d u\right)\right)
\end{aligned}
$$

- Expand the exp.
- Problem : not a T ordered product! How to use a Wick theorem ?


## Wick theorem : reminder

- $\mathrm{H}_{0}$ a quadratic (gaussian) Hamiltonian for fermions

$$
H_{0}=c_{a}^{\dagger} M_{a b} c_{b}
$$

- Then the $N$ body correlator is given by $(\zeta(P)$ is the signature of $P)$

$$
\begin{aligned}
&\left\langle T c_{a_{1}}\left(t_{1}\right) \ldots c_{a_{n}}\left(t_{n}\right) c_{a_{n}^{\prime}}^{\dagger}\left(t_{n}^{\prime}\right) \ldots c_{a_{1}^{\prime}}^{\dagger}\left(t_{1}^{\prime}\right)\right\rangle_{0}=\sum_{P \in S_{n}} \zeta(P) \prod_{k=1}^{n}\left\langle T c_{a_{k}}\left(t_{k}\right) c_{a_{P(k)}^{\prime}}^{\dagger}\left(t_{P(k)}^{\prime}\right)\right\rangle_{0} \\
&=\operatorname{det}_{1 \leq i, j \leq n}\left[\left\langle T c_{a_{i}}\left(t_{i}\right) c_{a_{j}^{\prime}}^{\dagger}\left(t_{j}^{\prime}\right)\right\rangle_{0}\right] \\
&\langle X\rangle_{0} \equiv \frac{1}{Z_{0}} \operatorname{Tr}\left(e^{-\beta H_{0}} X\right) \\
& Z_{0}=\operatorname{Tr}\left(e^{-\beta H_{0}}\right)
\end{aligned}
$$

- Requires a "gaussian" density matrix $\rho_{0}$
- Wick theorem is valid on any contour, as long as a time ordering is defined.


## Schwinger Keldysh double contour

- Every times is now a couple ( $\mathrm{t}, \mathrm{a}$ ), $\mathrm{a}= \pm \mathrm{I}$ (Keldysh indices)

$$
\begin{aligned}
0 & \xrightarrow[-]{\stackrel{\mathcal{C}}{\rightleftarrows} t} \\
\langle A(t)\rangle & =\operatorname{Tr}\left(\rho_{0} \check{T} \exp \left(+i \int_{0}^{t} \hat{V}(u) d u\right) \hat{A}(t) T \exp \left(-i \int_{0}^{t} \hat{V}(u) d u\right)\right) \\
& =\left\langle T_{\mathcal{C}} \hat{A}(t) \exp \left(-i \int_{\mathcal{C}} \hat{V}(u) d u\right)\right\rangle
\end{aligned}
$$

- Correlation function

$$
\left\langle T_{\mathcal{C}} A(t, \alpha) B\left(t^{\prime}, \alpha^{\prime}\right)\right\rangle=\left\langle T_{\mathcal{C}} \hat{A}(t, \alpha) \hat{B}\left(t^{\prime}, \alpha^{\prime}\right) \exp \left(-i \int_{\mathcal{C}} \hat{V}(u) d u\right)\right\rangle
$$

- Diagrams : expand the exponential.


## Fundamental relation

- Connect the notations + - to the double contour

$$
\mathbf{G} \equiv-i\left\langle T_{\mathcal{C}} c_{a}(t, \alpha) c_{b}^{\dagger}\left(t^{\prime}, \alpha^{\prime}\right)\right\rangle=\left(\begin{array}{cc}
G_{a b}^{++}\left(t, t^{\prime}\right) & G_{a b}^{+-}\left(t, t^{\prime}\right) \\
G_{a b}^{-+}\left(t, t^{\prime}\right) & G_{a b}^{---\left(t, t^{\prime}\right)}
\end{array}\right)
$$



$$
\begin{aligned}
& G_{a b}^{++}\left(t, t^{\prime}\right) \equiv-i\left\langle T c_{a}(t) c_{b}^{\dagger}\left(t^{\prime}\right)\right\rangle \\
& G_{a b}^{--}\left(t, t^{\prime}\right) \equiv-i\left\langle\check{T} c_{a}(t) c_{b}^{\dagger}\left(t^{\prime}\right)\right\rangle \\
& G_{a b}^{+-}\left(t, t^{\prime}\right) \equiv i\left\langle c_{b}^{\dagger}\left(t^{\prime}\right) c_{a}(t)\right\rangle \\
& G_{a b}^{-+}\left(t, t^{\prime}\right) \equiv-i\left\langle c_{a}(t) c_{b}^{\dagger}\left(t^{\prime}\right)\right\rangle
\end{aligned}
$$

## Diagrammatics

- Same diagrams (topology, ...) as ordinary T=0 (or Matsubara) diagrams.

But with an additional index a for each time

- Any diagrammatic approximation (large N, DMFT, ....) can be generalized to non equilibrium
$T=0$ "ordinary formalism"

- Vacuum diagrams canceled by denominator
- NoVacuum diagram Z=I

$$
Z=1
$$

$$
\begin{aligned}
\langle A(t)\rangle & =\operatorname{Tr}\left(\rho_{0} A(t)\right) \\
& =\operatorname{Tr}\left(\rho_{0}(U(t))^{\dagger} \hat{A}(t) U(t)\right) \\
& =\operatorname{Tr}\left(\rho_{0} \check{T} \exp \left(+i \int_{0}^{t} \hat{V}(u) d u\right) \hat{A}(t) T \exp \left(-i \int_{0}^{t} \hat{V}(u) d u\right)\right)
\end{aligned}
$$

- $A=1 .<1>=1$
- No "partition function", no "vacuum diagrams"


## How to compute $\mathrm{Q}_{\mathrm{n}}(\mathrm{t})$ ?

- Schwinger-Keldysh formalism $\mathrm{Q}_{\mathrm{n}}$ is a n -dimensional integral


Vertices.Times $u_{i}$ Keldysh indices $a=-I$,I

Profumo, Messio, OP, Waintal PRB 91, 245 I54 (2015)
(Quasi) Monte Carlo Explicit sum

- $f_{n}$ is centered around $t$. Massive cancellations in the sum.

Interaction expansion of the Green function

$$
\begin{aligned}
& G_{\uparrow}^{\alpha, \alpha^{\prime}}\left(t, t^{\prime}\right)=\sum_{n=0}^{\infty} \frac{i^{n}}{n!} \int d u_{1} d u_{2} \ldots d u_{n}\left(\prod_{i=1}^{n} U\left(u_{i}\right)\right) \times \\
& \text { Keldysh indices } \sum_{\alpha_{i}= \pm 1} \prod_{i=1}^{n} \alpha_{i} \operatorname{det} M_{\uparrow}\left(\left\{u_{i}\right\},\left\{\alpha_{i}\right\}\right) \operatorname{det} P_{\downarrow}\left(\left\{u_{i}\right\},\left\{\alpha_{i}\right\}\right) \\
& M_{\sigma}\left(\left\{u_{k}\right\},\left\{\alpha_{k}\right\}\right)=\left[\begin{array}{cccc|c}
g_{\sigma}^{<}\left(u_{1}, u_{1}\right) & g_{\sigma}^{\alpha_{1} \alpha_{2}}\left(u_{1}, u_{2}\right) & \ldots & g_{\sigma}^{\alpha_{1} \alpha_{n}}\left(u_{1}, u_{n}\right) & g_{\sigma}^{\alpha_{1} \alpha^{\prime}}\left(u_{1}, t^{\prime}\right) \\
\vdots & & & \vdots & \vdots \\
g_{\sigma}^{\alpha_{n} \alpha_{1}}\left(u_{n}, u_{1}\right) & g_{\sigma}^{\alpha_{n} \alpha_{2}}\left(u_{n}, u_{2}\right) & \ldots & g_{\sigma}^{<}\left(u_{1}, u_{n}\right) & g_{\sigma}^{\alpha_{n} \alpha^{\prime}}\left(u_{n}, t^{\prime}\right) \\
\hline g_{\sigma}^{\alpha \alpha_{1}}\left(t, u_{1}\right) & g_{\sigma}^{\alpha \alpha_{2}}\left(t, u_{2}\right) & \ldots & g_{\sigma}^{<}\left(t, u_{n}\right) & g_{\sigma}^{\alpha \alpha^{\prime}}\left(t, t^{\prime}\right)
\end{array}\right] \\
& P_{\sigma}\left(\left\{u_{k}\right\},\left\{\alpha_{k}\right\}\right)=\left[\begin{array}{cccc}
g_{\sigma}^{<}\left(u_{1}, u_{1}\right) & g_{\sigma}^{\alpha_{1} \alpha_{2}}\left(u_{1}, u_{2}\right) & \ldots & g_{\sigma}^{\alpha_{1} \alpha_{n}}\left(u_{1}, u_{n}\right) \\
\vdots & & & \vdots \\
g_{\sigma}^{\alpha_{n} \alpha_{1}}\left(u_{n}, u_{1}\right) & g_{\sigma}^{\alpha_{n} \alpha_{2}}\left(u_{n}, u_{2}\right) & \ldots & g_{\sigma}^{<}\left(u_{1}, u_{n}\right)
\end{array}\right]
\end{aligned}
$$

- Integrand cancels except if $u_{i}$ are close to $t=t$ '


## Clusterization around time $\mathrm{t}=\mathrm{t}^{\prime}$. Cancellations.

 Illustration at $\mathrm{n}=2$
${ }^{2}$


## Z=| Revisited

- Expand Z

$$
\begin{aligned}
& 1=\sum_{n=0}^{\infty} \frac{i^{n}}{n!} \int d u_{1} d u_{2} \ldots d u_{n}\left(\prod_{i=1}^{n} U\left(u_{i}\right)\right) \times \\
& \underbrace{\sum_{\alpha_{i}= \pm 1} \prod_{i=1}^{n} \alpha_{i} \operatorname{det} P_{\uparrow}\left(\left\{u_{i}\right\},\left\{\alpha_{i}\right\}\right) \operatorname{det} P_{\downarrow}\left(\left\{u_{i}\right\},\left\{\alpha_{i}\right\}\right)}_{=0}
\end{aligned}
$$

$$
P_{\sigma}\left(\left\{u_{k}\right\},\left\{\alpha_{k}\right\}\right)=\left[\begin{array}{cccc}
g_{\sigma}^{<}\left(u_{1}, u_{1}\right) & g_{\sigma}^{\alpha_{1} \alpha_{2}}\left(u_{1}, u_{2}\right) & \ldots & g_{\sigma}^{\alpha_{1} \alpha_{n}}\left(u_{1}, u_{n}\right) \\
\vdots & & & \vdots \\
g_{\sigma}^{\alpha_{n} \alpha_{1}}\left(u_{n}, u_{1}\right) & g_{\sigma}^{\alpha_{n} \alpha_{2}}\left(u_{n}, u_{2}\right) & \ldots & g_{\sigma}^{<}\left(u_{1}, u_{n}\right)
\end{array}\right]
$$

## $Z=\mid$ Revisited

- Expand Z

$$
\begin{aligned}
& 1=\sum_{n=0}^{\infty} \frac{i^{n}}{n!} \int d u_{1} d u_{2} \ldots d u_{n}\left(\prod_{i=1}^{n} U\left(u_{i}\right)\right) \times \\
& \underbrace{\sum_{\alpha_{i}= \pm 1} \prod_{i=1}^{n} \alpha_{i} \operatorname{det} P_{\uparrow}\left(\left\{u_{i}\right\},\left\{\alpha_{i}\right\}\right) \operatorname{det} P_{\downarrow}\left(\left\{u_{i}\right\},\left\{\alpha_{i}\right\}\right)}_{=0}
\end{aligned}
$$

- Proof: For fixed $u_{i}$, cancellation. Take $u_{\text {max }}$ the largest $u_{i}$.

$$
\begin{array}{ll}
g^{\alpha_{i}+}\left(u_{i}, u_{\max }\right)=g^{\alpha_{i}-}\left(u_{i}, u_{\max }\right) & \forall i \\
g^{+\alpha_{i}}\left(u_{\max }, u_{i}\right)=g^{-\alpha_{i}}\left(u_{\max }, u_{i}\right) & \forall i \\
G_{a b}^{++}\left(t, t^{\prime}\right)=\theta\left(t-t^{\prime}\right) G_{a b}^{-+}\left(t, t^{\prime}\right)+\theta\left(t^{\prime}-t\right) G_{a b}^{+-}\left(t, t^{\prime}\right) \\
G_{a b}^{--}\left(t, t^{\prime}\right)=\theta\left(t^{\prime}-t\right) G_{a b}^{-+}\left(t, t^{\prime}\right)+\theta\left(t-t^{\prime}\right) G_{a b}^{+-}\left(t, t^{\prime}\right)
\end{array}
$$

- The dets do not depend on $a_{\text {max }}$ so it cancels the sum.


## How to compute $\mathrm{Q}_{\mathrm{n}}(\mathrm{t})$ ?

- Schwinger-Keldysh formalism $\mathrm{Q}_{\mathrm{n}}$ is a n -dimensional integral


Vertices.Times $u_{i}$. Keldysh indices $a=-1,1$

Profumo, Messio, OP, Waintal PRB 91, 245I54 (2015) (Quasi) Monte Carlo Explicit sum

- Long time limit $\mathrm{t} \rightarrow \infty$ is easy. $f_{n}$ is centered around t . Massive cancellations in the sum.
- $O\left(2^{n}\right)$ cost to compute $f_{n}(u)$. In practice, $n=10-15$.


How to sum the series?

## Using the perturbative series: three possibilities

I. At finite time t, the series is convergent Bertrand et al. Phys. Rev. X 9, 041008 (2019)
2. A infinite $\boldsymbol{t}$ (steady state), the series has a finite radius of convergence (for impurity, lattice models). Need re-summation technique
3. Change the starting point, cf M. Ferrero's talk, see also Profumo et al. PRB 91, 245154 (2015)

## Resum with conformal maps

Profumo et al. PRB 91, 245154 (2015)
Bertrand et al. Phys. Rev. X 9, 041008 (2019)


A finite radius of convergence ! Singularities poles, branch cuts

- Change of variable $\mathrm{W}(\mathrm{U})$, with $\mathrm{W}(0)=0$

$$
Q=\sum_{n \geq 0} Q_{n} U^{n}=\sum_{p \geq 0} \bar{Q}_{p} W^{p}
$$

Let us end with some results (quantum dot)

I- Equilibrium. Benchmarks.

## Reminder : model for the quantum dot

- Anderson model with two leads (L, R).

$$
H=\sum_{\substack{\text { Bath } \\ \alpha=L, R}} \varepsilon_{k \alpha} c_{k \sigma \alpha}^{\dagger} c_{k \sigma \alpha}+\sum_{\sigma} \varepsilon_{d} d_{\sigma}^{\dagger} d_{\sigma}+U n_{d \uparrow} n_{d \downarrow}+\sum_{\substack{k \sigma \\ \alpha=L, R}} g_{k \sigma \alpha}\left(c_{k \sigma \alpha}^{\dagger} d_{\sigma}+h . c .\right)
$$

- Questions: Spectral function ? Kondo temperature ? Current ?

We want a precise solution, at low temperature, any $V_{b}$, in steady state

## Kondo effect in equilibrium

Spectral function on the dot

$$
A(\omega)=-\frac{1}{\pi} \operatorname{Im} G^{R}(\omega)
$$



- Sum the series for each frequency independently
- Resumption of the series using conformal maps
- Benchmark with NRG (numerical renormalisation group)

$$
\begin{array}{cc}
T=10^{-4} \Gamma & \text { C. Bertrand et al. } \\
\text { Phys. Rev. X 9,041008 (2019) }
\end{array}
$$

## Kondo Temperature

$$
T_{K}(U) \equiv \frac{2 \Gamma}{1-\left.\partial_{\omega} \operatorname{Re} \Sigma^{R}(U, \omega)\right|_{\omega=0}}
$$

Kondo temperature


Naive sum
of the series


## Fermi liquid at low energy

- Equilibrium. Self-energy, away from particle-hole symmetry

Self energy (Re)

Self energy (Im)


## Benchmarks

- Steady state inchworm by A. Erpenbeck et al.


Figure from A. Erpenbeck

- Tensor network (MPS) + time evolution

C. Bertrand, D. Bauernfeind, P. Dumitrescu, M. Maček, X.Waintal, O.P.

2-Non equilibrium

## Out of equilibrium

- Destruction of the Kondo resonance by voltage bias



$$
T=0
$$

$$
T=\Gamma / 50
$$

- Particle hole asymmetric case



## Distribution function on the dot

- Equilibrium, for all U. Fermi function.

$$
f(\omega)=n_{F}\left(\omega-\mu_{R}\right)=\frac{1}{1+e^{\beta\left(\omega-\mu_{R}\right)}}
$$

- Out of equilibrium for $U=0$ (in the small g limit). Not a Fermi function



## Out of equilibrium distribution function of the dot

- Finite $\mathrm{U}, \mathrm{T}=0$

$$
n(\omega) \equiv \frac{G^{<}(\omega)}{2 \pi i A(\omega)}
$$

Bertrand et al. 2019
Phys. Rev. X 9, 041008 (2019)


## Conclusion

- Perturbation theory for real time/out of equilibrium systems.
- Success in quantum dots/nano-electronic systems.
- Beyond Monte-Carlo ...
- Next steps : lattice, DMFT solver out of equilibrium.


## References

- Diagrammatic/determinantal QMC in Keldysh Phys. Rev. B 9I, 245I54 (2015)
- Quantum dot equilibrium/out of equilibrium, resummation with conformal maps Phys. Rev. X 9, 041008 (2019) Phys. Rev. B 100, I25I29 (2019)
- Quantum Quasi-Monte Carlo Phys. Rev. Lett. I25, 047702 (2020)
Phys. Rev. B I03, I55I04 (202I)

Thank you for your attention!

