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



- 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.



Nano-electronics

Ultra-cold atoms

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).



Questions : Spectral function ? Kondo temperature ? Current ?

We want a precise solution, at low temperature, any V_b, in steady state



Hybridization

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

Level width at U=0 $\Gamma = \pi \rho_{E_E} g^2$





Summary of the approach

Perturbation theory in interaction U (10-15 orders) for physical quantities.

Time

- I. Works even at long time, even in strong coupling regime (e.g. Kondo effect)
- 2. How to compute $Q_n(t)$? Cost $O(2^n)$. 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.

- T=0 : Ground state
- Matsubara : finite T, in thermal equilibrium
- Schwinger-Keldysh
 - <u>General</u>. 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
- a,b = multi-index : k, x, spin, ... everything but time.

 $\{c_a, c_b^{\dagger}\}$

Chronological product

> $TA(t)B(t') = \theta(t - t')A(t')$ $\check{T}A(t)B(t') = \theta(t'-t)A(t')$

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

$$\} = \delta_{ab}$$

$$(t)B(t') + \zeta_{AB}\theta(t'-t)B(t')A(t)$$

$$(t)B(t') + \zeta_{AB}\theta(t-t')B(t')A(t)$$

<u>Total</u> Hamiltonian of the system, e.g.

 $H = H_{dot} + H_{bath} + H_{dot-bath}$

- H(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

 $|\psi(t)\rangle = U_H(t,t_0) |\psi(t_0)\rangle$

Heisenberg representation for operator A

$A(t) \equiv U_H^{\dagger}(t, t_0) A(t_0) U_H(t, t_0)$

Reminder : density matrix

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

$$Tr\rho = 1$$

$$\rho^{\dagger} = \rho$$

$$\rho \ge 0$$

$$i\partial_t \rho(t) = [H(t), \rho(t)]$$

$$\rho(t) = U_H(t, t_0)\rho(t_0)U_H(t_0)$$

$$\langle A(t) \rangle \equiv Tr(\rho(t)A(t_0)) = 0$$

- Out of equilibrium : 2 independents objects. H and ρ .
- Thermal equilibrium :

$$\bar{
ho}$$



 $\bar{\rho} = \frac{1}{Z} e^{-\beta H}, \qquad Z = Tr e^{-\beta H}$ $\bar{\rho} = \frac{1}{Z} e^{-\beta (H - \mu \hat{N})}, \qquad Z = T r e^{-\beta (H - \mu \hat{N})}$

One particle Green functions



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

$$G_{ab}^{++}(t,t') = \theta(t-t')G_{ab}^{>}(t,t') + \theta(t'-t)G_{ab}^{<}(t,t')$$

$$G_{ab}^{--}(t,t') = \theta(t'-t)G_{ab}^{>}(t,t') + \theta(t-t')G_{ab}^{<}(t,t')$$

In equilibrium, only one ! Fluctuation-Dissipation theorem, Kubo-Martin-Schwinger relation

$$\left\langle c_b^{\dagger}(t')c_a(t) \right\rangle = \left\langle c_a(t)c_b^{\dagger}(t'+i\beta) \right\rangle \qquad G_{ab}^{<}(\omega) = -e^{-\beta\omega}G_{ab}^{>}(\omega)$$

$$\begin{aligned} G_{ab}^{++}(t,t') &\equiv -i \left\langle T c_a(t) c_b^{\dagger}(t') \right\rangle \\ G_{ab}^{--}(t,t') &\equiv -i \left\langle \check{T} c_a(t) c_b^{\dagger}(t') \right\rangle \\ G_{ab}^{<}(t,t') &\equiv i \left\langle c_b^{\dagger}(t') c_a(t) \right\rangle \\ G_{ab}^{>}(t,t') &\equiv -i \left\langle c_a(t) c_b^{\dagger}(t') \right\rangle \end{aligned}$$

Schwinger-Keldysh 2- Diagrammatic expansion

- Start at $t = t_0$ (=0 in most slides below)
- With initial condition : $\rho = \rho_0$ at thermal equilibrium with <u>non interacting</u> Hamiltonian H₀ at a temperature β
- NB : it is possible to start with interacting equilibrium. Baym-Kadanoff contour. Not covered here.
- Study the expansion of correlators at finite time.

- Build the diagrammatic at finite time.
- If needed, take the limit
- Separate diagrams technique & thermalization/relaxation/bath questions.



 $\operatorname{Tr}(\rho_0 A(t) B(t')...)$

 $t, t' \to \infty$ or $t_0 \to -\infty$

Interaction picture

H = 1

Hamiltonian evolution of whole system (dot + bath)



Non interacting part

- Evolution operator in interaction picture
 - $U(t) \equiv$ $i\partial_t U(t) = \hat{V}(t)U(t)$ U(0) = 1

$$H_0 + V(t)$$

Interaction (U term)

$$^{H_0t}Ae^{-iH_0t}$$

$$e^{iH_0t}U_H(t)$$

$$\rightarrow \quad U(t) = T \exp\left(-i\int_0^t \hat{V}(u)du\right)$$

Time evolution of a physical quantity

• Start at t=0 (t0) from a non-interacting equilibrium density matrix ρ_0

• Average of an operator A

$$\begin{aligned} \langle A(t) \rangle &= \operatorname{Tr} \left(\rho_0 A(t) \right) \\ &= \operatorname{Tr} \left(\rho_0 \left(U(t) \right)^{\dagger} \hat{A}(t) U(t) \right) \\ &= \operatorname{Tr} \left(\rho_0 \check{T} \exp \left(+i \int_0^t V(t) \right) \right) \end{aligned}$$

• Expand the exp.

• Problem : not a T ordered product ! How to use a Wick theorem ?

$$U(t) = T \exp\left(-i \int_0^t \hat{V}(u)\right)$$

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Average in initial state $\hat{V}(u)du \hat{A}(t)T \exp\left(-i\int_{0}^{t} \hat{V}(u)du\right)$



Wick theorem : reminder

- H_0 a quadratic (gaussian) Hamiltonian for fermions $H_0 = c_a^{\dagger} M_{ab} c_b$
 - Then the N body correlator is given by ($\zeta(P)$ is the signature of P) $\left\langle Tc_{a_1}(t_1) \dots c_{a_n}(t_n) c_{a'_n}^{\dagger}(t'_n) \dots c_{a'_1}^{\dagger}(t'_1) \right\rangle$

$$\langle X \rangle_0 \equiv \frac{1}{Z_0} Tr \left(e^{-\beta H_0} X \right)$$
$$Z_0 = Tr \left(e^{-\beta H_0} \right)$$

- Requires a "gaussian" density matrix ρ_0
- Wick theorem is valid on any contour, as long as a time ordering is defined.

n

$$\begin{split} \Big\rangle_{0} &= \sum_{P \in S_{n}} \zeta(P) \prod_{k=1}^{n} \left\langle Tc_{a_{k}}(t_{k})c_{a'_{P(k)}}^{\dagger}(t'_{P(k)}) \right\rangle_{0} \\ &= \det_{1 \leq i,j \leq n} \left[\left\langle Tc_{a_{i}}(t_{i})c_{a'_{j}}^{\dagger}(t'_{j}) \right\rangle_{0} \right] \end{split}$$

Schwinger Keldysh double contour

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

$$\begin{aligned} \mathbf{0} \\ \langle A(t) \rangle &= \operatorname{Tr} \left(\rho_0 \check{T} \exp \left(+i \int_0^t \hat{V} \right) \right) \\ &= \left\langle \mathbf{T}_{\mathcal{C}} \hat{A}(t) \exp \left(-i \int_{\mathcal{C}} \hat{V} \right) \right\rangle \end{aligned}$$

Correlation function

$$\langle T_{\mathcal{C}}A(t,\alpha)B(t',\alpha')\rangle = \langle T_{\mathcal{C}}A(t,\alpha)B(t',\alpha')\rangle$$

Diagrams : expand the exponential.



 $\left| \hat{C} \hat{A}(t,\alpha) \hat{B}(t',\alpha') \exp\left(-i \int_{\mathcal{C}} \hat{V}(u) du \right) \right\rangle$

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Fundamental relation

• Connect the notations +/- to the double contour

$$\mathbf{G} \equiv -i \left\langle T_{\mathcal{C}} c_a(t,\alpha) c_b^{\dagger}(t',\alpha') \right\rangle = \begin{pmatrix} G_{ab}^{++}(t,t') & G_{ab}^{+-}(t,t') \\ G_{ab}^{-+}(t,t') & G_{ab}^{--}(t,t') \end{pmatrix}$$



$$G_{ab}^{++}(t,t') \equiv -i \left\langle Tc_a(t)c_b^{\dagger}(t') \right\rangle$$
$$G_{ab}^{--}(t,t') \equiv -i \left\langle \tilde{T}c_a(t)c_b^{\dagger}(t') \right\rangle$$
$$G_{ab}^{+-}(t,t') \equiv i \left\langle c_b^{\dagger}(t')c_a(t) \right\rangle$$
$$G_{ab}^{-+}(t,t') \equiv -i \left\langle c_a(t)c_b^{\dagger}(t') \right\rangle$$

Diagrammatics

- Same diagrams (topology, ...) as ordinary T=0 (or Matsubara) diagrams. But with an additional index α for each time
- T=0 "ordinary formalism"



Any diagrammatic approximation (large N, DMFT,) can be generalized to non equilibrium

Keldysh



$$\begin{split} \langle A(t) \rangle &= \operatorname{Tr} \left(\rho_0 A(t) \right) \\ &= \operatorname{Tr} \left(\rho_0 \left(U(t) \right)^{\dagger} \hat{A}(t) U(t) \right) \\ &= \operatorname{Tr} \left(\rho_0 \check{T} \exp \left(+i \int_0^t \hat{V}(u) du \right) \hat{A}(t) T \exp \left(-i \int_0^t \hat{V}(u) du \right) \right) \end{split}$$

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

Z=1

Schwinger-Keldysh formalism Q_n is a n-dimensional integral

> $Q_n(t) = \frac{1}{n!} \int_{t_0}^{\infty} du_1 \dots du_n \left[\sum_{\alpha_i = \pm 1}^{\infty} \prod_i \alpha_i \det(\dots) \right]$ $\equiv f_n(t, u_1, \dots, u_n)$ (Quasi) Monte Carlo

 f_n is centered around t. Massive cancellations in the sum.



Interaction expansion of the Green function

Integrand cancels except if u_i are close to t = t'

})

 $\begin{bmatrix} g_{\sigma}^{u_n u_1}(u_n, u_1) & g_{\sigma}^{u_n u_2}(u_n, u_2) & \dots & g_{\sigma}^{\sim}(u_1, u_n) \end{bmatrix}$

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 $\det M(\alpha_1, \alpha_2, u_1, u_2)$



Olusterization¹ around time t=t'. Cancellations. Illustration at n = 2



Profumo, Messio, OP, Waintal PRB 91, 245154 (2015)



Z=I Revisited



$$P_{\sigma}(\{u_k\},\{\alpha_k\}) = \begin{bmatrix} g_{\sigma}^{<}(u_1,u_1) & g_{\sigma}^{\alpha_1\alpha_2}(u_1,u_2) & \dots & g_{\sigma}^{\alpha_1\alpha_n}(u_1,u_n) \\ \vdots & & \vdots \\ g_{\sigma}^{\alpha_n\alpha_1}(u_n,u_1) & g_{\sigma}^{\alpha_n\alpha_2}(u_n,u_2) & \dots & g_{\sigma}^{<}(u_1,u_n) \end{bmatrix}$$

$$du_n\left(\prod_{i=1}^n U(u_i)\right) \times$$

 $\sum \prod \alpha_i \det P_{\uparrow}(\{u_i\}, \{\alpha_i\}) \det P_{\downarrow}(\{u_i\}, \{\alpha_i\})$

Z=I Revisited



Proof : For fixed u_i , cancellation. Take u_{max} the largest u_i . $q^{\alpha_i}(u_i, u_{\max}) = q^{\alpha_i}(u_i, u_{\max})$ $g^{+\alpha_i}(u_{\max}, u_i) = g^{-\alpha_i}(u_{\max}, u_i)$

$$G_{ab}^{--}(t,t') = \theta(t'-t)G_{ab}^{-+}(t,t') + \theta(t-t')G_{ab}^{+-}(t,t')$$

• The dets do not depend on α_{max} , so it cancels the sum.

$$du_n\left(\prod_{i=1}^n U(u_i)\right) \times$$

 $\sum \alpha_i \det P_{\uparrow}(\{u_i\},\{\alpha_i\}) \det P_{\downarrow}(\{u_i\},\{\alpha_i\})$

 $\forall i$ $\forall i$ $G_{ab}^{++}(t,t') = \theta(t-t')G_{ab}^{-+}(t,t') + \theta(t'-t)G_{ab}^{+-}(t,t')$

=0

Schwinger-Keldysh formalism Q_n is a n-dimensional integral

> $Q_n(t) = \frac{1}{n!} \int_{t_0}^{\infty} du_1 \dots du_n \left[\sum_{\alpha_i = \pm 1}^{\infty} \prod_i \alpha_i \det(\dots) \right]$ $\equiv f_n(t, u_1, \dots, u_n)$ (Quasi) Monte Carlo

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





How to sum the series ?





- I. At finite time t, the series is convergent Bertrand et al. Phys. Rev. X 9, 041008 (2019)
- models). Need re-summation technique
- Change the starting point, cf M. Ferrero's talk, see also Profumo et al. PRB 91, 245154 (2015) 3.

Using the perturbative series: three possibilities

2. A infinite t (steady state), the series has a finite radius of convergence (for impurity, lattice





A finite radius of convergence ! Singularities poles, branch cuts

Resum with conformal maps

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

W complex plane $Q = \sum Q_n U^n$ *n*≥0 $W_0 \neq W(U_0)$ 0 Riemann Schwartz-Christoffel

Change of variable W(U), with W(0) = 0

$$Q = \sum_{n \ge 0} Q_n U^n = \sum_{p \ge 0} \bar{Q}_p W^p$$

Converges at W_0





Let us end with some results (quantum dot)

I - Equilibrium. Benchmarks.

Reminder : model for the quantum dot

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



Questions : Spectral function ? Kondo temperature ? Current ?

We want a precise solution, at low temperature, any V_b, in steady state



Hybridization

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

Level width at U=0 $\Gamma = \pi \rho_{E_F} g^2$







Kondo effect in equilibrium

 $A(\omega) = -\frac{1}{\pi}ImG^{R}(\omega)$

• Sum the series for each frequency independently

Resumption of the series using conformal maps

Benchmark with NRG (numerical renormalisation group)

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





Kondo Temperature

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

$\omega = 0$

 2Γ

Kondo temperature





Fermi liquid at low energy

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

Self energy (Re)

Self energy (Im)



Phys. Rev. X 9, 041008 (2019)





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.** Phys. Rev. B 103, 155104 (2021)





2-Non equilibrium

Out of equilibrium Bertrand et al. 2019 Spectral function **Phys. Rev. X** 9, 041008 (2019) $V_{\rm b}/\Gamma = 0.6$ $\pi\Gamma A$ 15 - V_b 10 · U/Γ 5 -0 -10 0 -10 ω/Γ

Destruction of the Kondo resonance by voltage bias 1.0••••• $U/\Gamma = 0$ $V_{\rm b}/\Gamma = 0.0$ $U/\Gamma = 5$ $V_{\rm b}/\Gamma = 0.8$ $V_{\rm b}/\Gamma = 1.6$ 0.8 $V_{\rm b}/\Gamma = 2.4$ $V_{\rm b}/\Gamma = 3.2$ $V_{\rm b}/\Gamma = 4.0$ 0.6 $\pi\Gamma A$ 0.40.2********* V_b increases





T = 0

 $T = \Gamma/50$





I-V_b Characteristics

• Particle hole *asymmetric* case



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



Distribution function on the dot

Equilibrium, for all U. Fermi function.

$$f(\omega) = n_F(\omega - \mu_R) = \frac{1}{1 + e^{\beta(\omega - \mu_R)}}$$

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



 μ_L μ_{R}

Illustration at T=0, $g_L = g_R$

$$f(\omega) = \frac{g_L^2 n_F(\omega - \mu_L) + g_R^2 n_F(\omega - \mu_R)}{g_L^2 + g_R^2}$$











- 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.

Conclusion



- Diagrammatic/determinantal QMC in Keldysh Phys. Rev. B 91, 245154 (2015)
- Quantum dot equilibrium/out of equilibrium, resummation with conformal maps Phys. Rev. X 9, 041008 (2019) Phys. Rev. B 100, 125129 (2019)
- Quantum Quasi-Monte Carlo Phys. Rev. Lett. 125, 047702 (2020) Phys. Rev. B 103, 155104 (2021)

References



Thank you for your attention!

