Quantum Quasi-Monte Carlo for non-equilibrium quantum systems

Olivier Parcollet

Center for Computational Quantum Physics (CCQ)

Flatiron Institute, Simons Foundation

New York

FLATIRON INSTITUTE
Center for Computational Quantum Physics

European Research Council
Established by the European Commission

cea

Outline

1. Real time "diagrammatic" Quantum Monte Carlo.

   Solution of the out of equilibrium quantum dot.

C. Bertrand, S. Florens, OP, X. Waintal
Phys. Rev. X *9, 041008 (2019)*

Phys. Rev. B *91, 245154 (2015)*
Phys. Rev. B *100, 125129 (2019)*

2. Quantum Quasi-Monte Carlo.

   How to compute the perturbative expansion faster (x100, x10000) and more precisely.

M. Macek, P. Dumitrescu, C. Bertrand, B.Triggs, OP, X.Waintal
ArXiv:2002.12372

Collaborators

Corentin Bertrand (Flatiron/CCQ)

Cf poster

Philipp Dumitrescu (Flatiron/CCQ)

Cf poster

Marjan Macek (Grenoble, France)

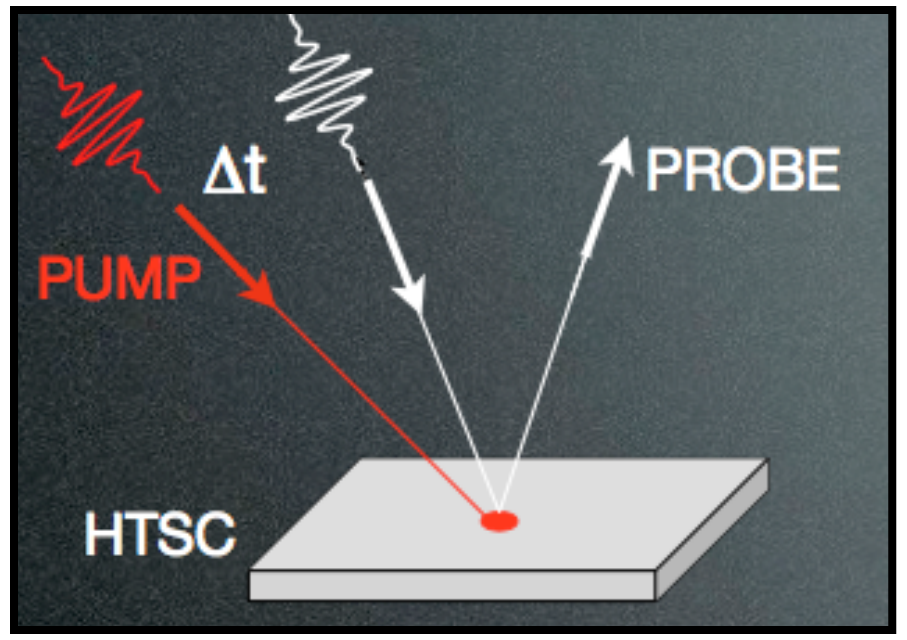
Serge Florens (Grenoble, France)

Bill Triggs (Grenoble, France)

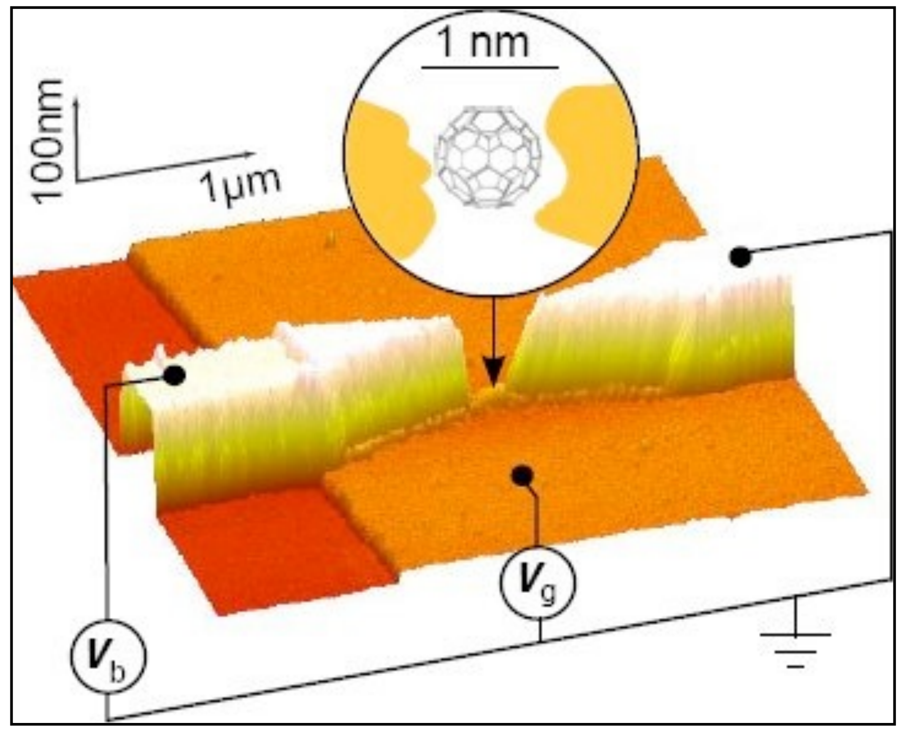
Xavier Waintal (Grenoble, France)

Out of equilibrium & strong correlations

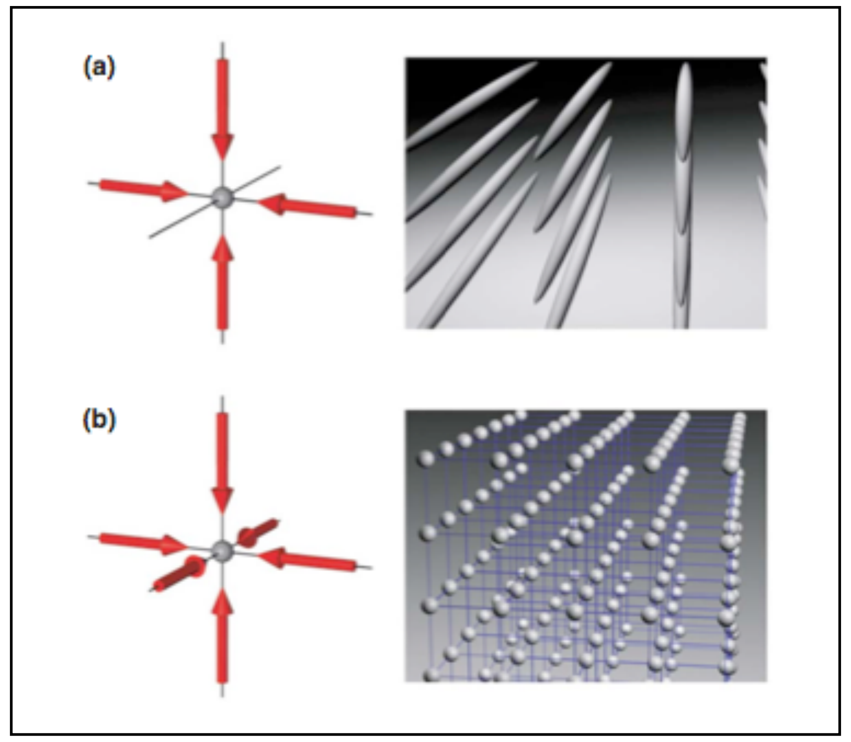
- Many new experiments : Pump probe, quantum dots, ultra-cold atoms, cavities.



Pump probe



Nano-electronics

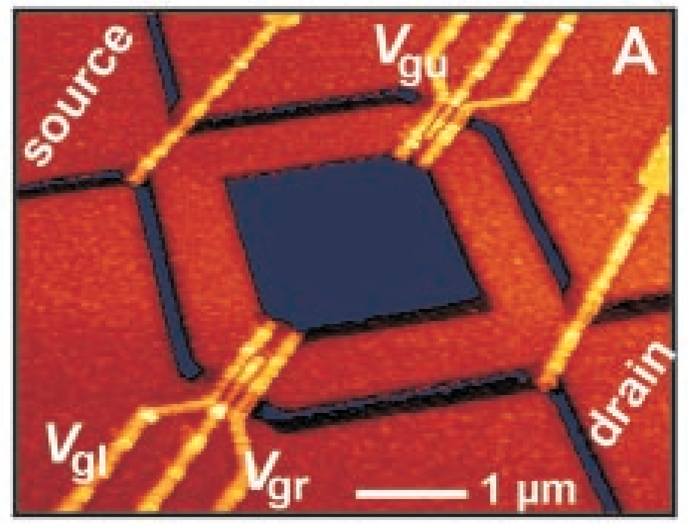


Ultra-cold atoms

- 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.

Road map

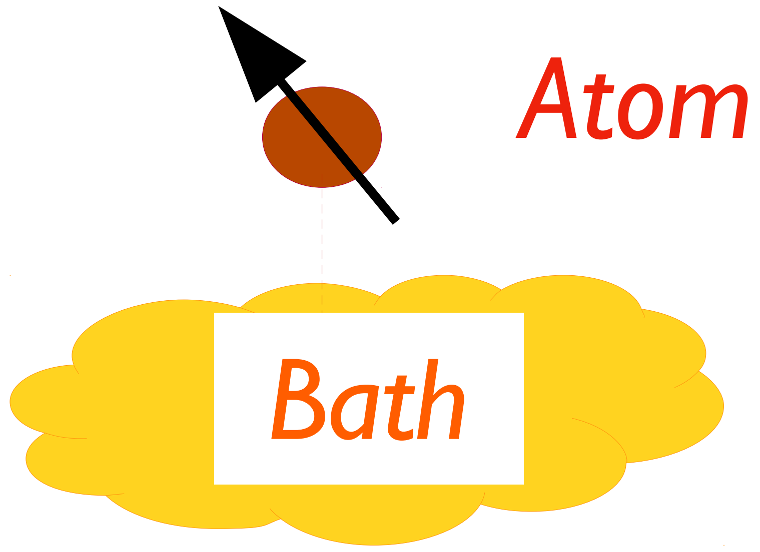
Quantum dots



- Kondo effect.
  L .Glazman et al. 1988, P. Lee 1988.
  D. Goldhaber-Gordon, 1998
- High precision benchmark
  in equilibrium (Bethe Ansatz)

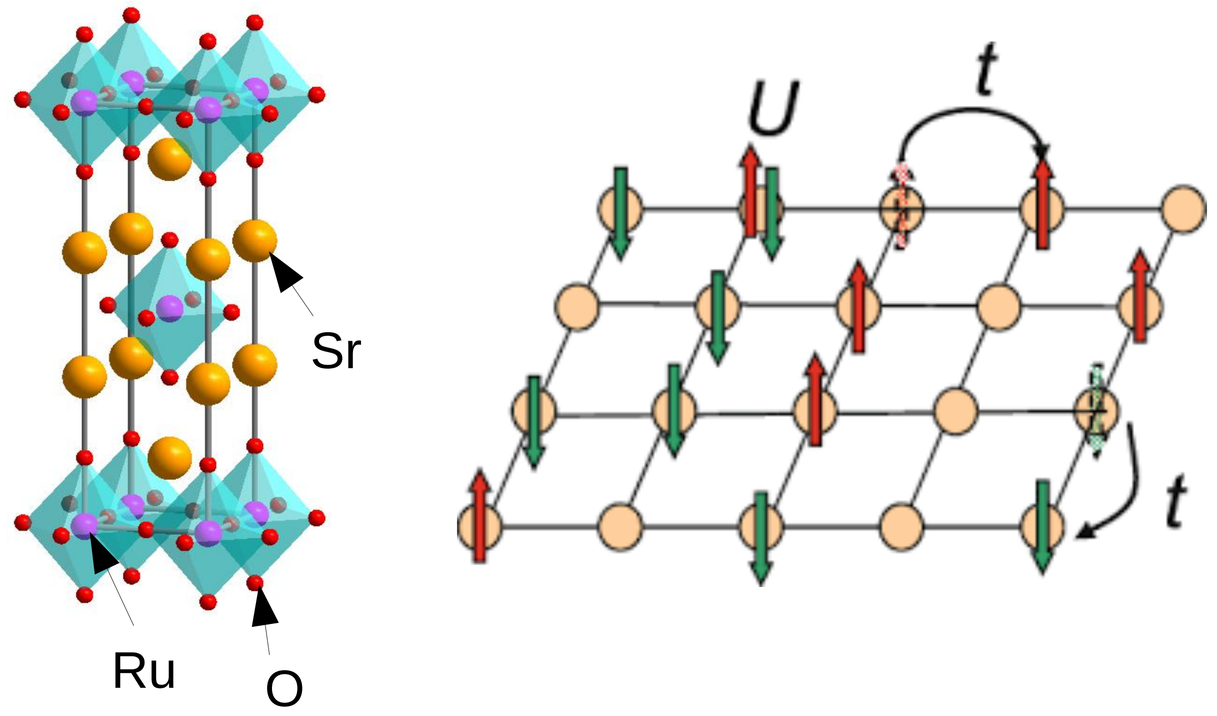
TODAY

Out of equilibrium
DMFT solvers



- 1 atom+ self-consistent bath
- Few exact solvers
  (inchworm *Cf Cohen's talk*,
  our work)

Lattice models
Real solid



- Equilibrium : *cf talk by M. Ferrero*
- Non equilibrium. Transport.

Perturbation theory

$$Q(t) = \sum_{n=0}^{K} Q_n(t) U^n$$

- Use perturbation theory (K=10-15), even deep in strong coupling regime (e.g. Kondo effect).

- Real time "diagrammatic" Quantum Monte Carlo *(Cf talk of N. Prokof'ev, M. Ferrero)*

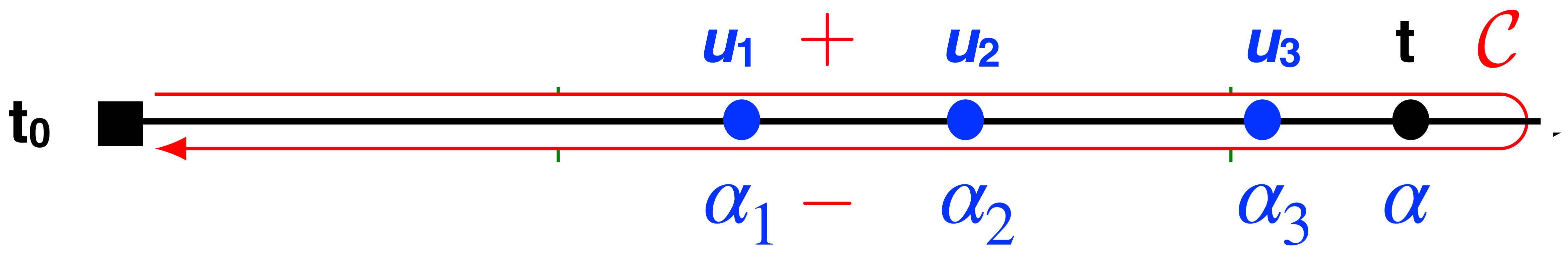
How to compute $Q_n(t)$?

How to sum the series ?

How to compute $Q_n(t)$?

- Schwinger-Keldysh formalism
  Q_n is a n-dimensional integral

Switch on interaction



Vertices. Times u_i.
Keldysh indices α = -1, 1

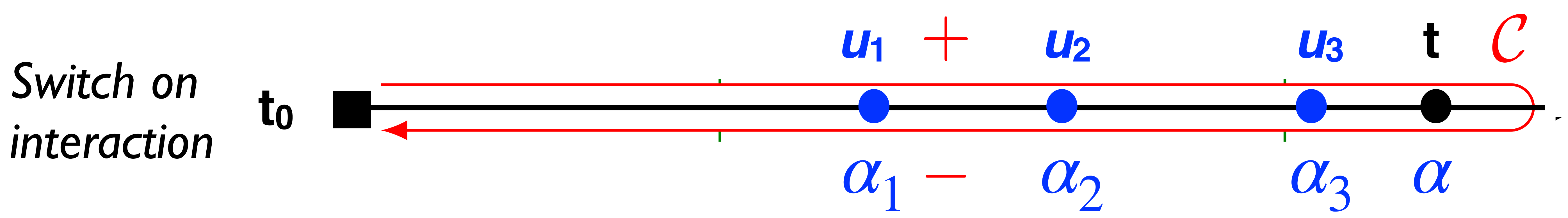
$$Q_n(t) = \frac{1}{n!}\int_{t_0}^{\infty} du_1 \ldots du_n \left(\sum_{\alpha_i=\pm 1} \prod_i \alpha_i \; \det(\ldots) \right)$$

$$\equiv f_n(t, u_1, \ldots, u_n)$$

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

How to compute $Q_n(t)$?

- Schwinger-Keldysh formalism
  Q_n is a n-dimensional integral



Vertices. Times u_i.
Keldysh indices α = -1, 1

$$Q_n(t) = \frac{1}{n!}\int_{t_0}^{\infty} du_1 \dots du_n \left(\sum_{\alpha_i = \pm 1} \prod_i \alpha_i \; \det(\dots) \right)$$

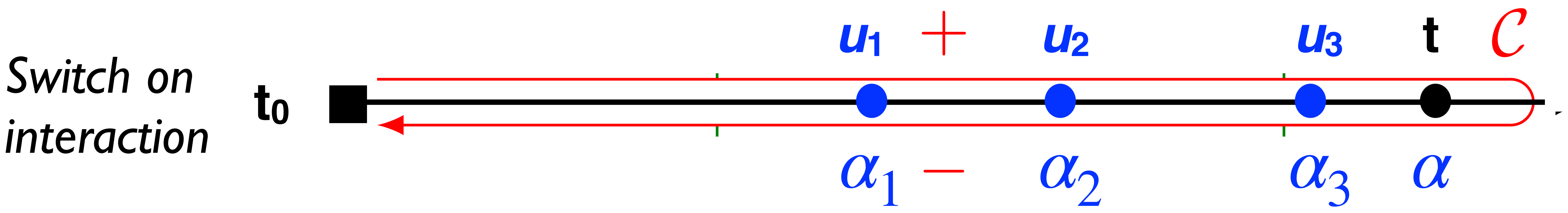
$$\equiv f_n(t, u_1, \dots, u_n)$$

Explicit sum

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

How to compute $Q_n(t)$?

- Schwinger-Keldysh formalism
  Q_n is a n-dimensional integral



Vertices. Times u_i.
Keldysh indices α = -1, 1

$$Q_n(t) = \frac{1}{n!}\int_{t_0}^{\infty} du_1 \ldots du_n \left(\sum_{\alpha_i=\pm 1} \prod_i \alpha_i \ \det(\ldots) \right)$$

$$\equiv f_n(t, u_1, \ldots, u_n)$$

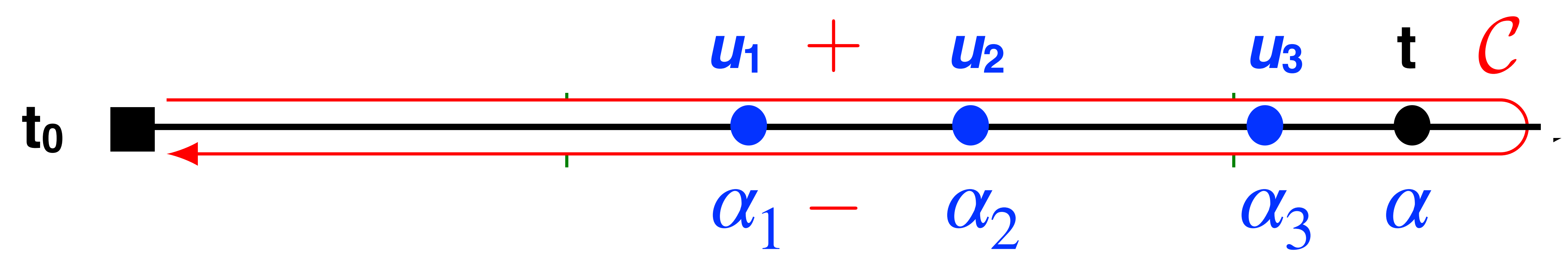
(Quasi) Monte Carlo *Explicit sum*

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

How to compute $Q_n(t)$?

- Schwinger-Keldysh formalism
  Q_n is a n-dimensional integral

Switch on interaction



Vertices. Times u_i.
Keldysh indices α = -1, 1

$$Q_n(t) = \frac{1}{n!}\int_{t_0}^{\infty} du_1 \ldots du_n \left(\sum_{\alpha_i = \pm 1} \prod_i \alpha_i \ \det(\ldots) \right)$$

$$\equiv f_n(t, u_1, \ldots, u_n)$$

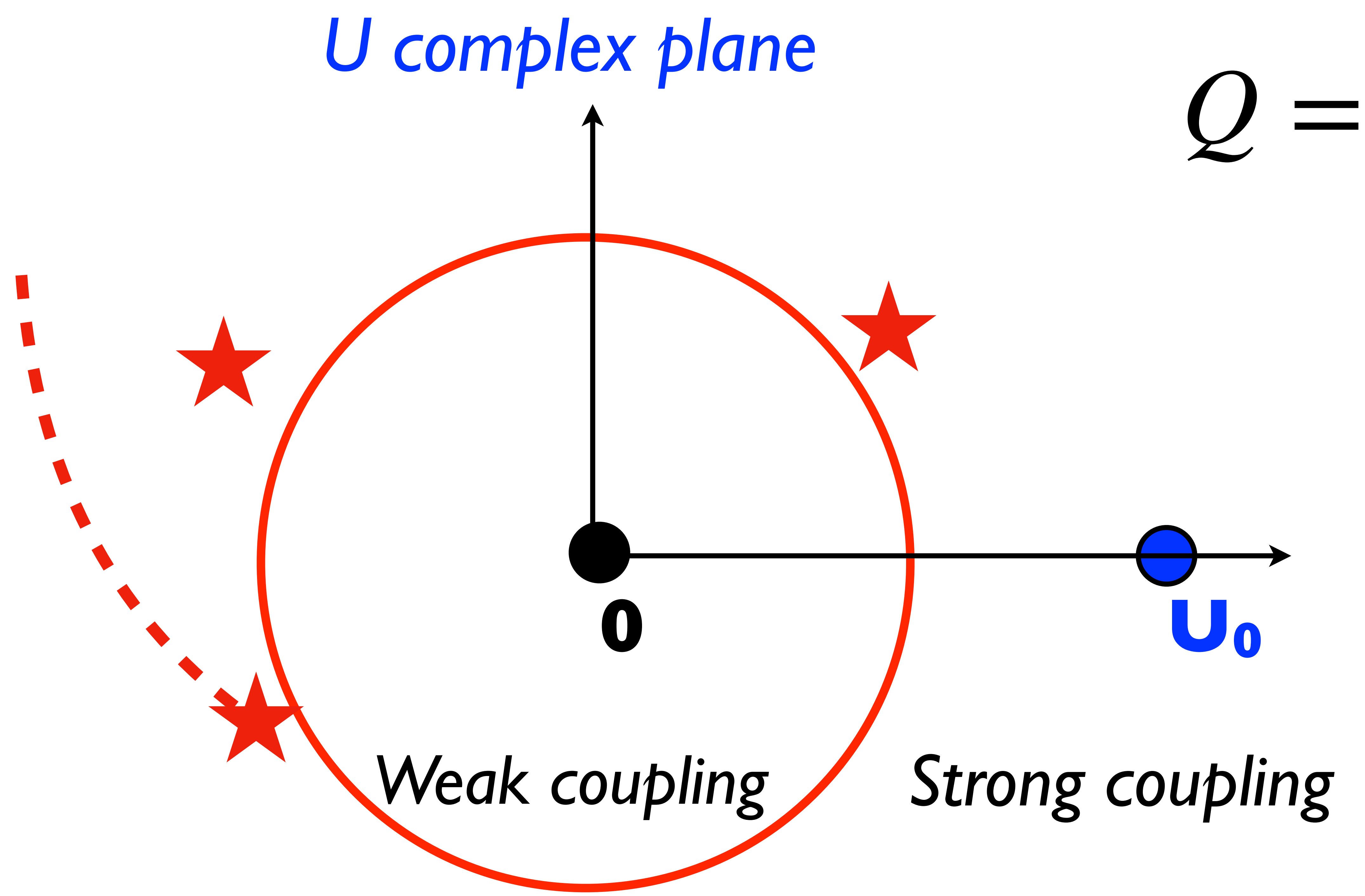
(Quasi) Monte Carlo — *Explicit sum*

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

- Long time limit $t \to \infty$ is easy. f_n is centered around t. Massive cancellations in the sum.
- No "dynamical sign problem" contrary to previous real time QMC, e.g. *P.Werner et al PRB 2009*
- $O(n^3 2^n)$ cost to compute $f_n(u)$. In practice, n = 10-15.

How to sum the series ?

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



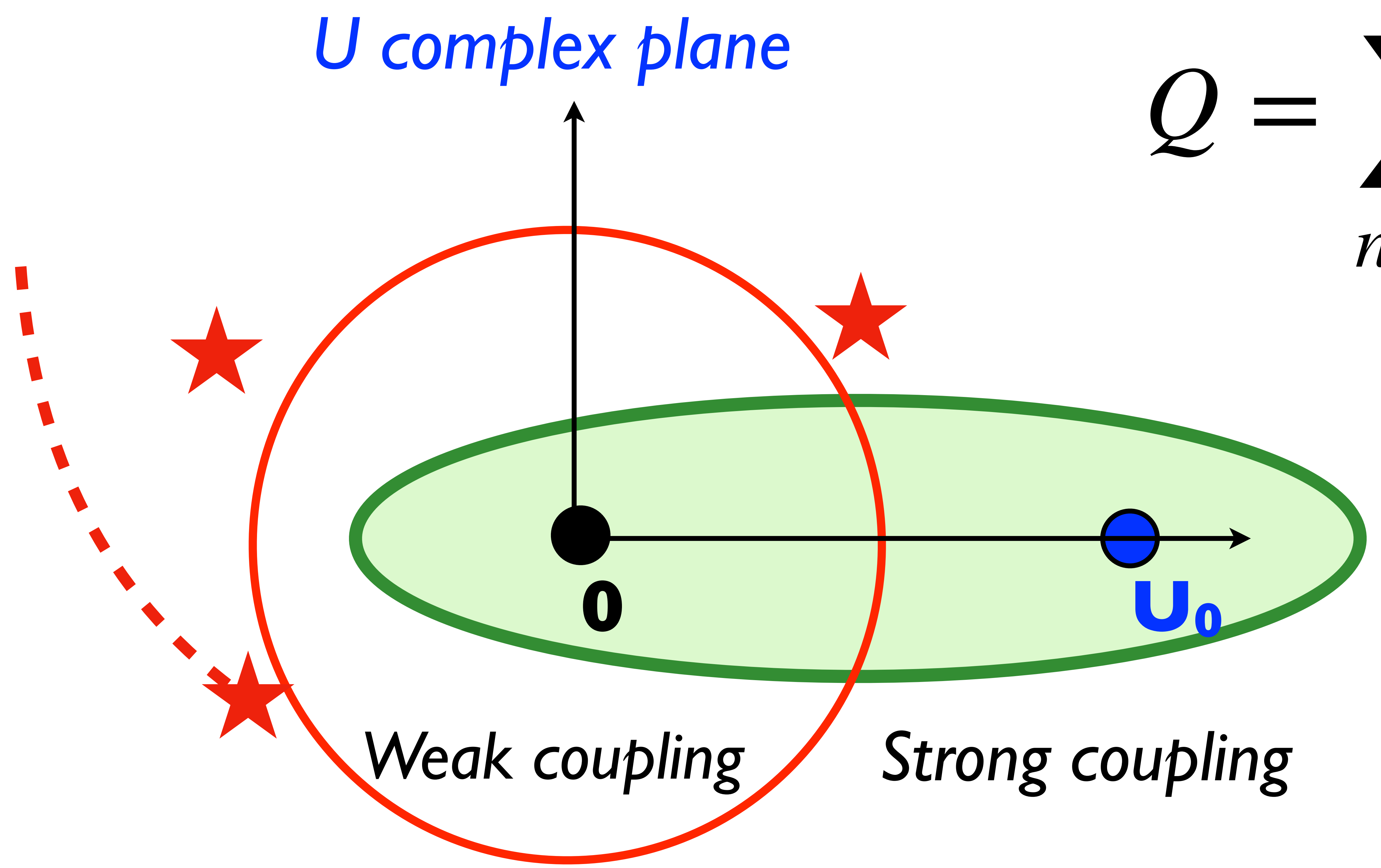
$$Q = \sum_{n\geq 0} Q_n U^n$$

A finite radius of convergence !
Singularities poles, branch cuts

How to sum the series ?

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

$$Q = \sum_{n \geq 0} Q_n U^n$$

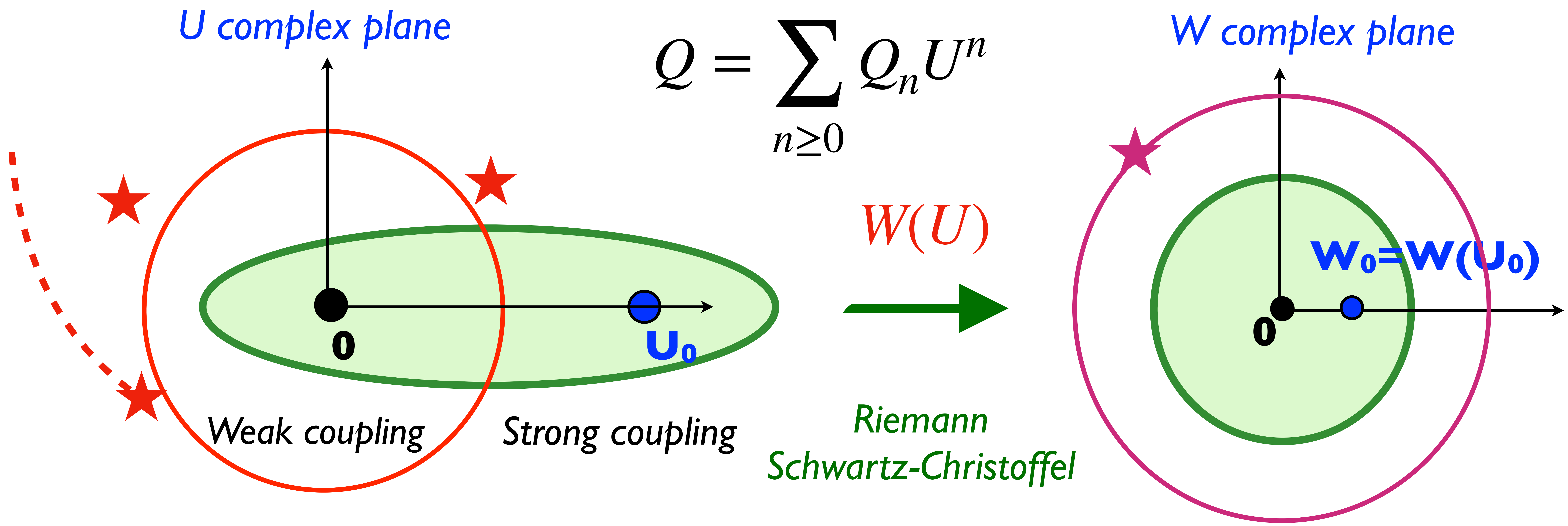


A finite radius of convergence !
Singularities poles, branch cuts

How to sum the series ?

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

$$Q = \sum_{n \geq 0} Q_n U^n$$

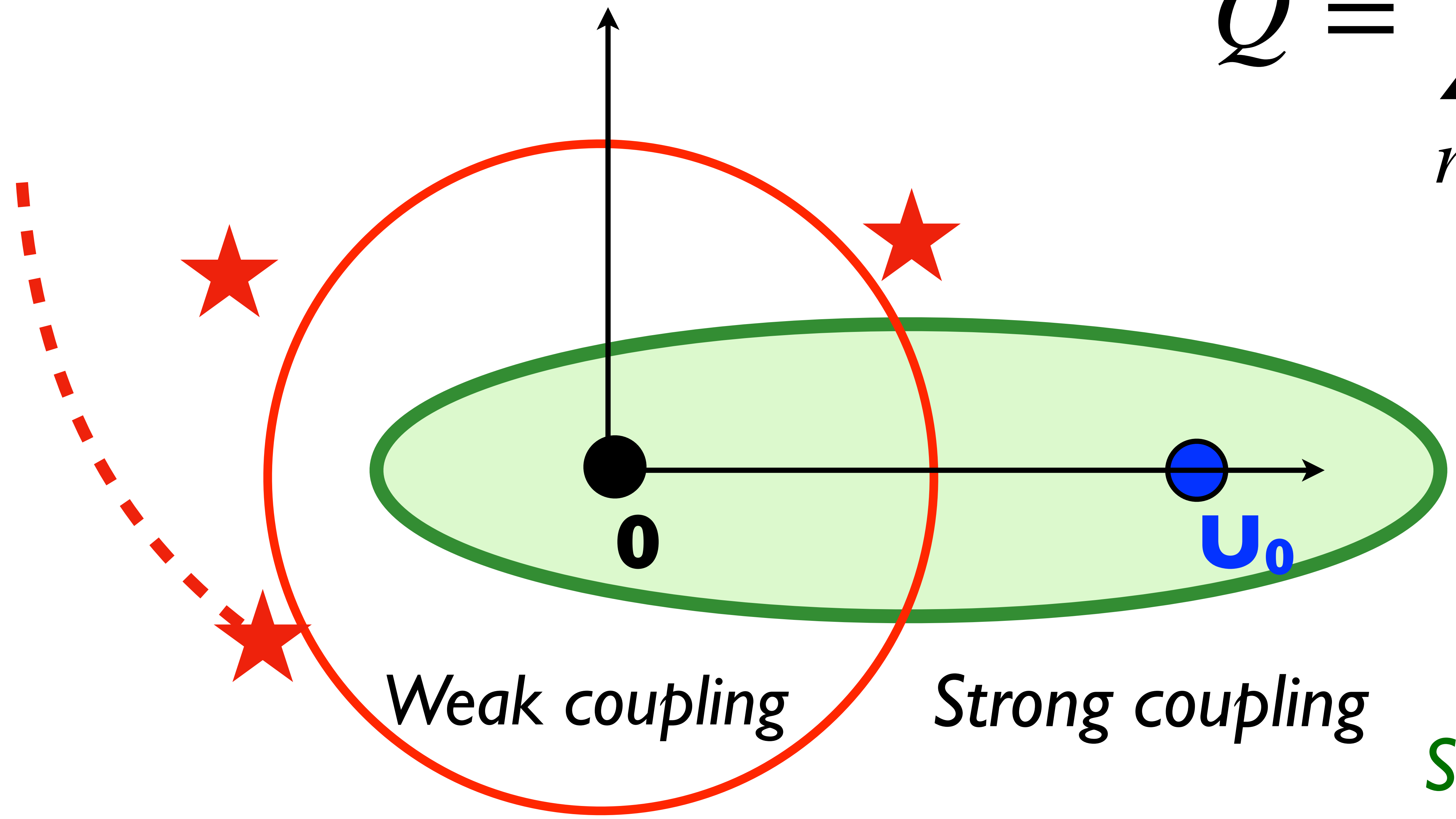


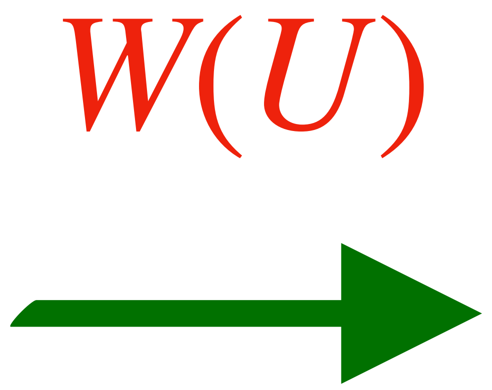
A finite radius of convergence !
Singularities poles, branch cuts

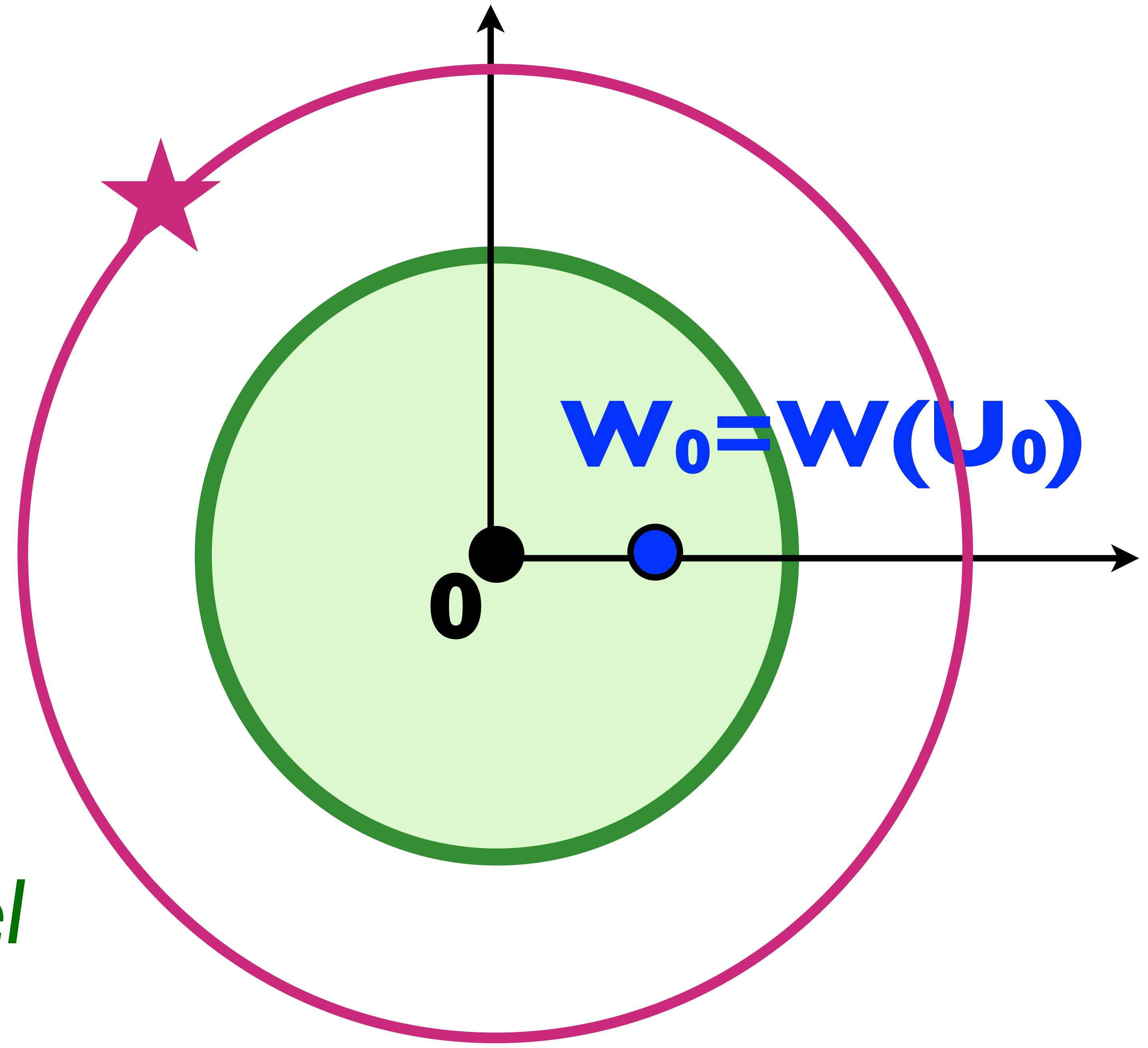
How to sum the series ?

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

$$Q = \sum_{n\geq 0} Q_n U^n$$







A finite radius of convergence !
Singularities poles, branch cuts

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

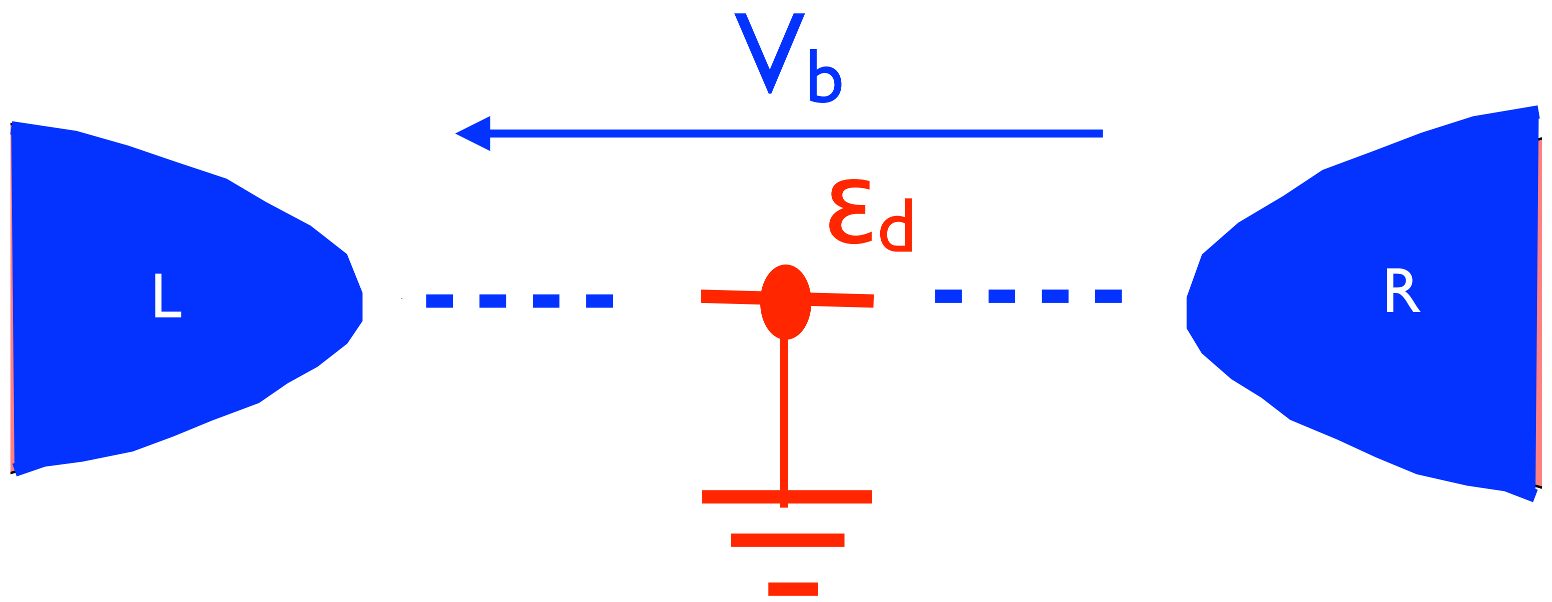
$$Q = \sum_{n\geq 0} Q_n U^n = \sum_{p\geq 0} \bar{Q}_p W^p$$

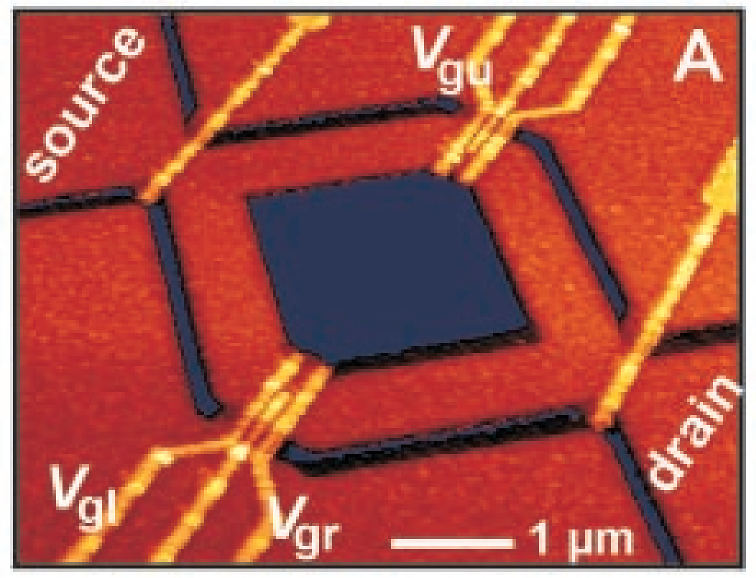
Converges at W_0

A few results
on the quantum dot

A simple model for the quantum dot

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





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

Bath *Dot* *Hybridization*

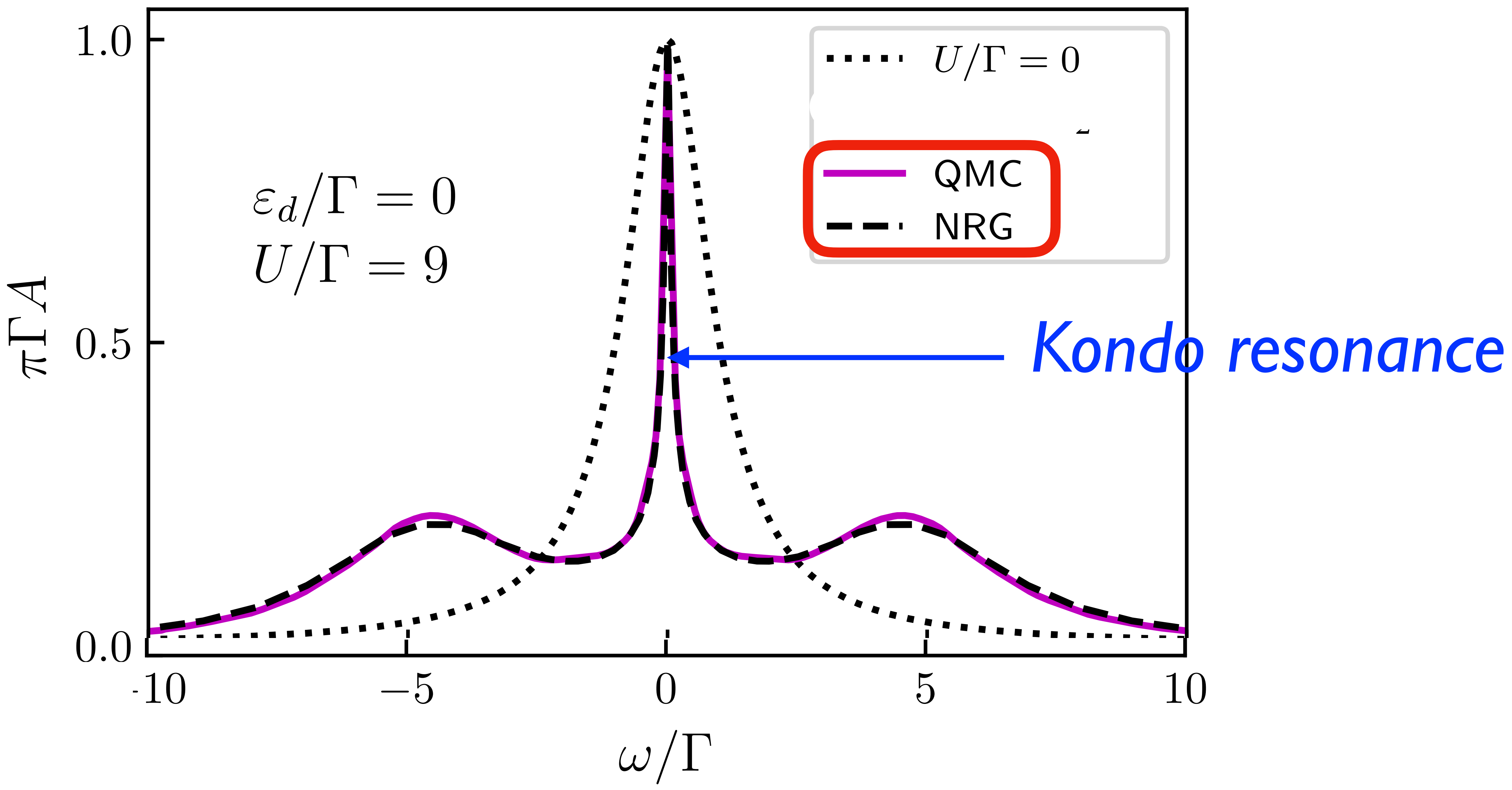
- We want : current I(V_b), spectral function on the dot, Kondo effect, …

Kondo effect in equilibrium

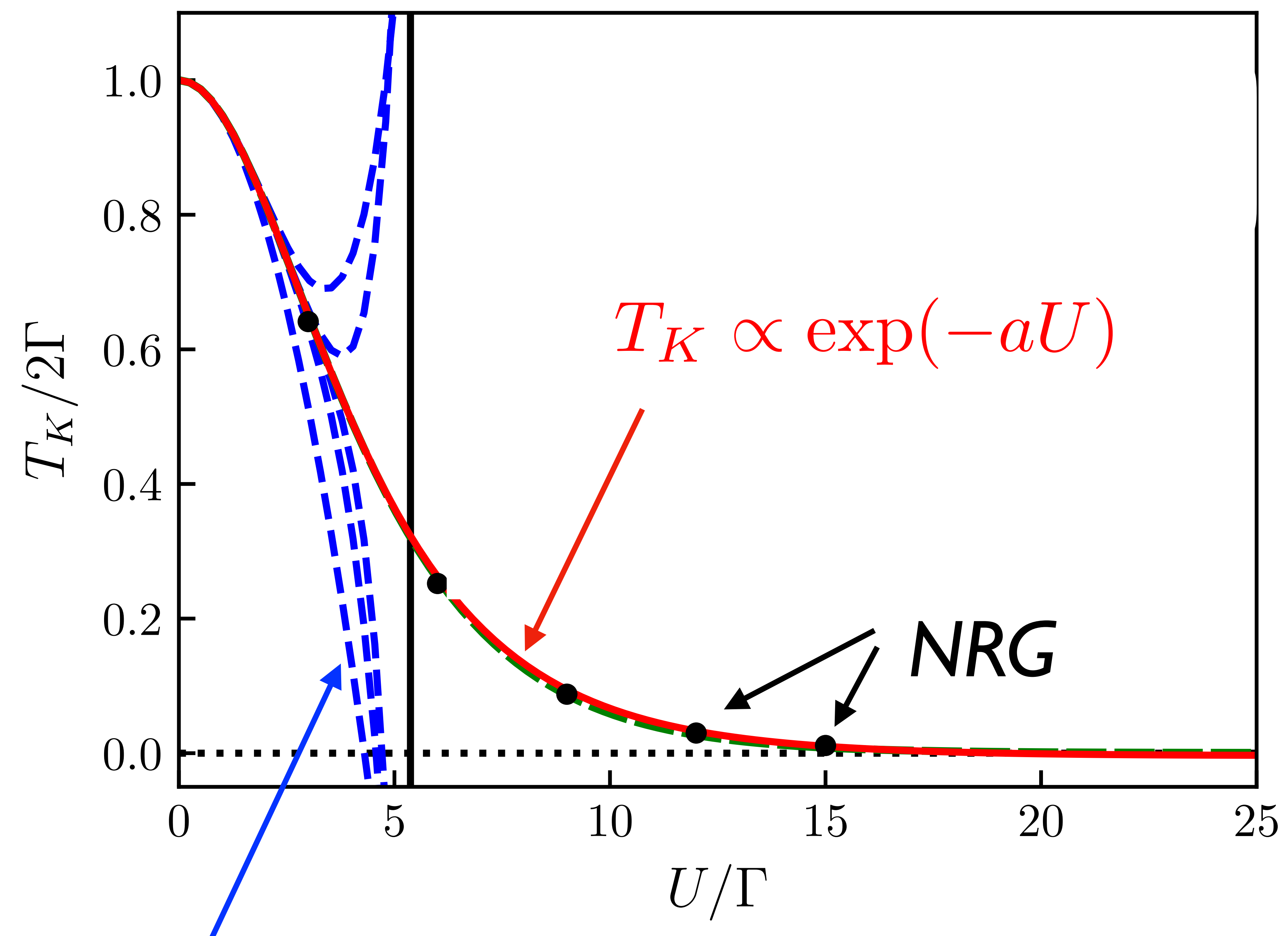
Bertrand et al. 2019
Phys. Rev. X 9, 041008 (2019)

- Benchmark with NRG (numerical renormalisation group)

Spectral function on the dot



Kondo temperature



$$\Gamma = \pi\rho_{E_F}g^2$$

$$T = 0$$

Energy unit (level width at U=0)

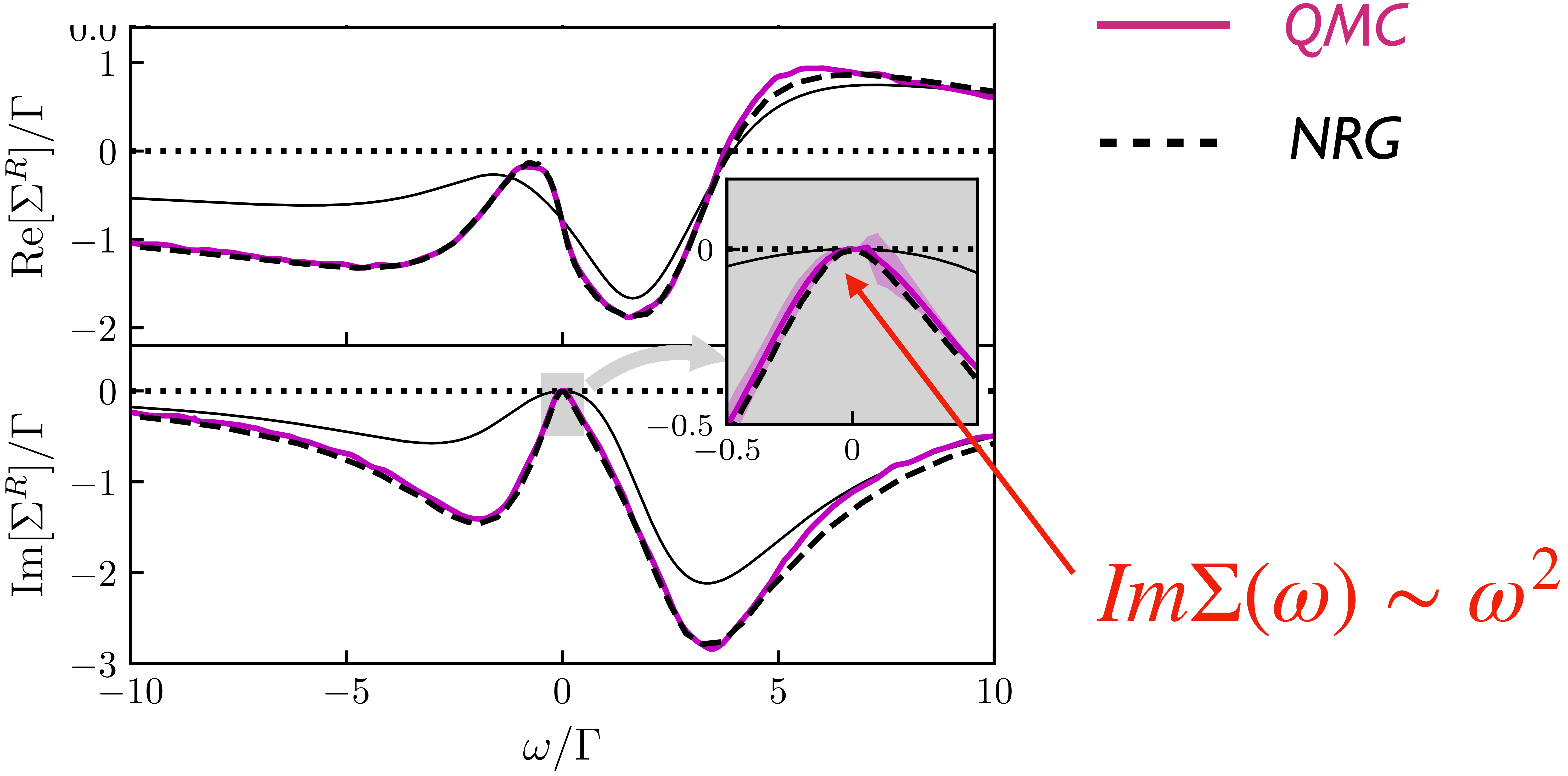
Fermi liquid at low energy

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

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

Self energy (Re)

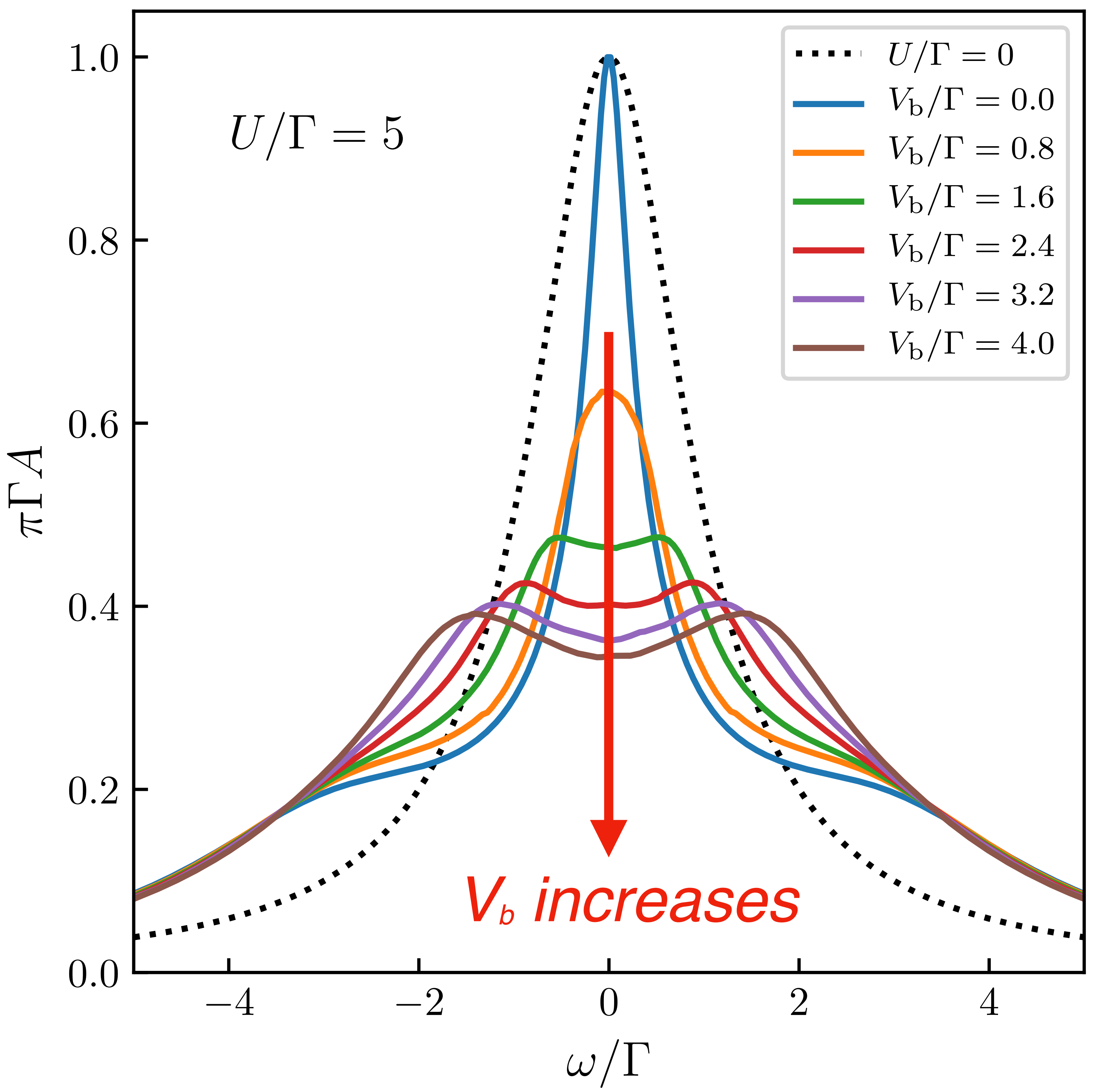
Self energy (Im)

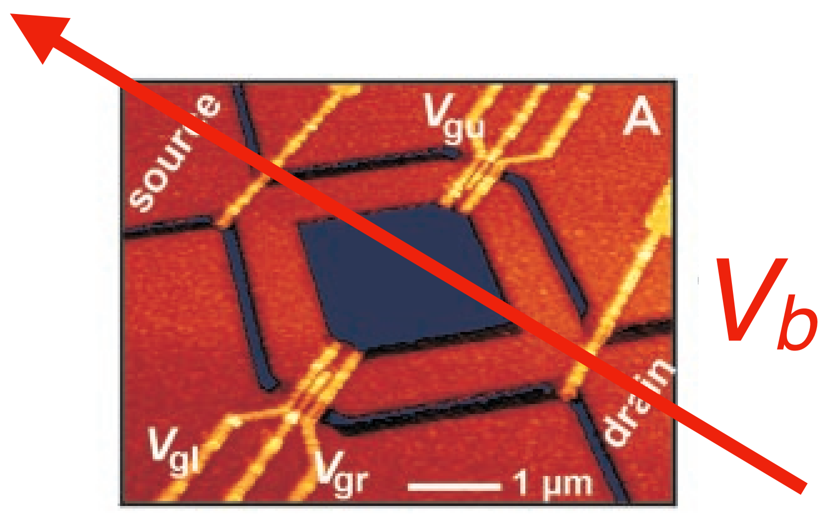


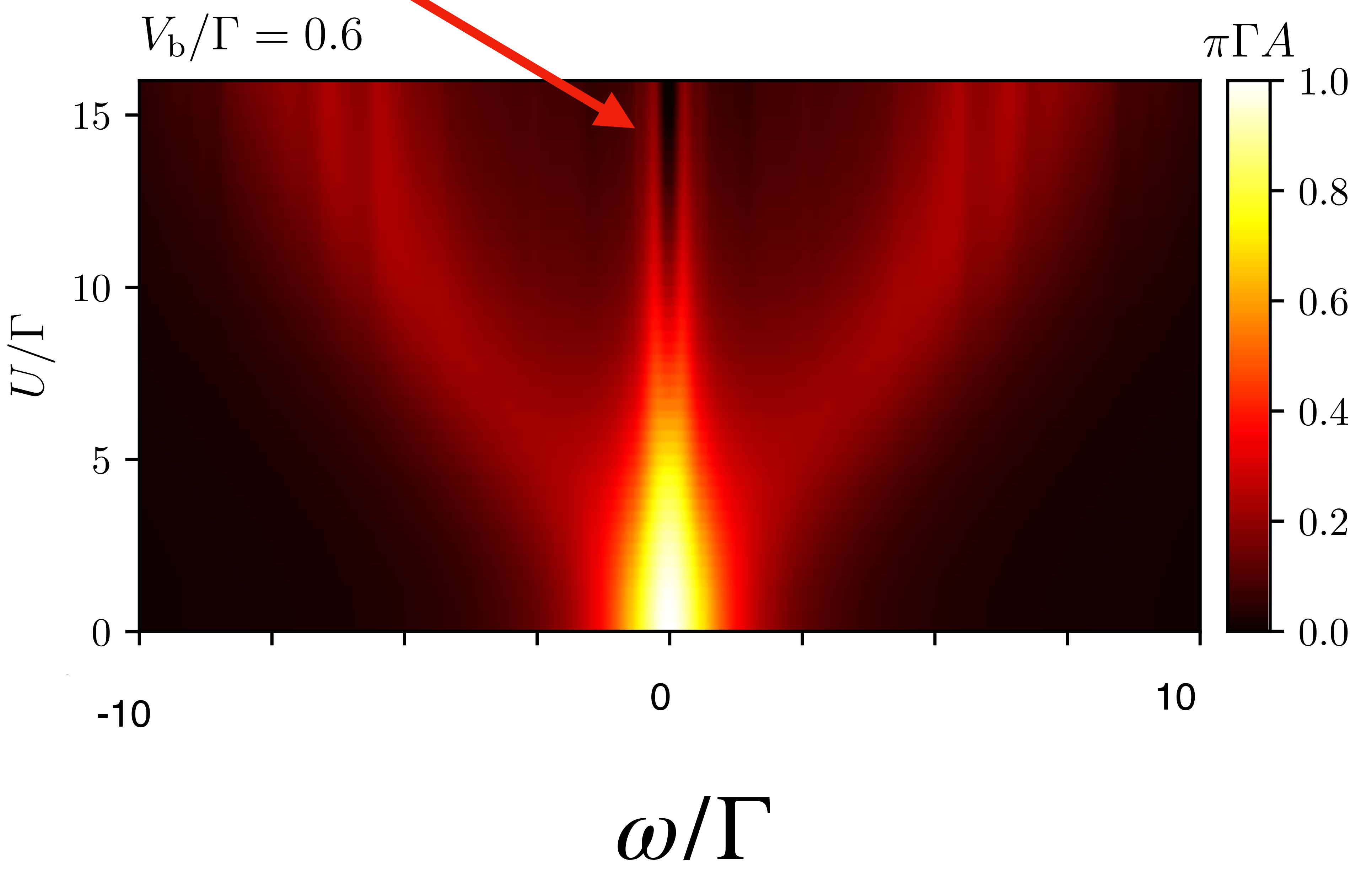
Out of equilibrium

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

- Destruction of the Kondo resonance by voltage bias







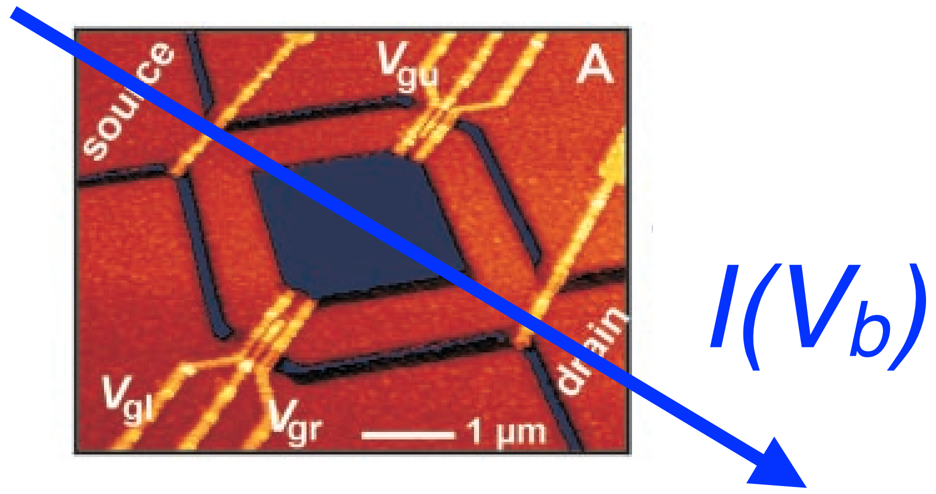
$T = 0$

$T = \Gamma/50$

I-V_b Characteristics

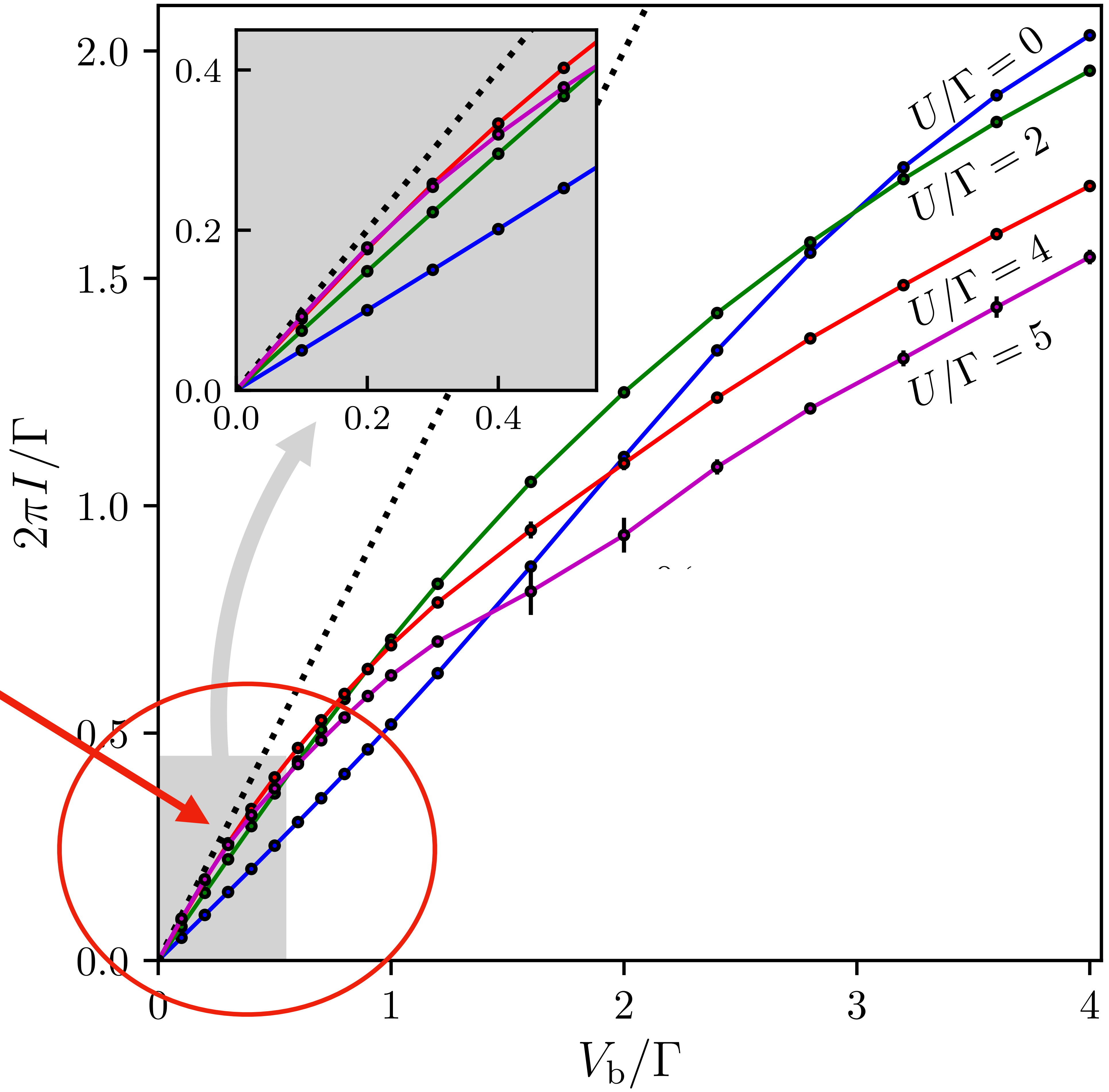
Bertrand et al. 2019
Phys. Rev. X *9, 041008 (2019)*

- Particle hole ***asymmetric*** case



$$G \sim \frac{e^2}{h}$$

Kondo effect
Unitary limit

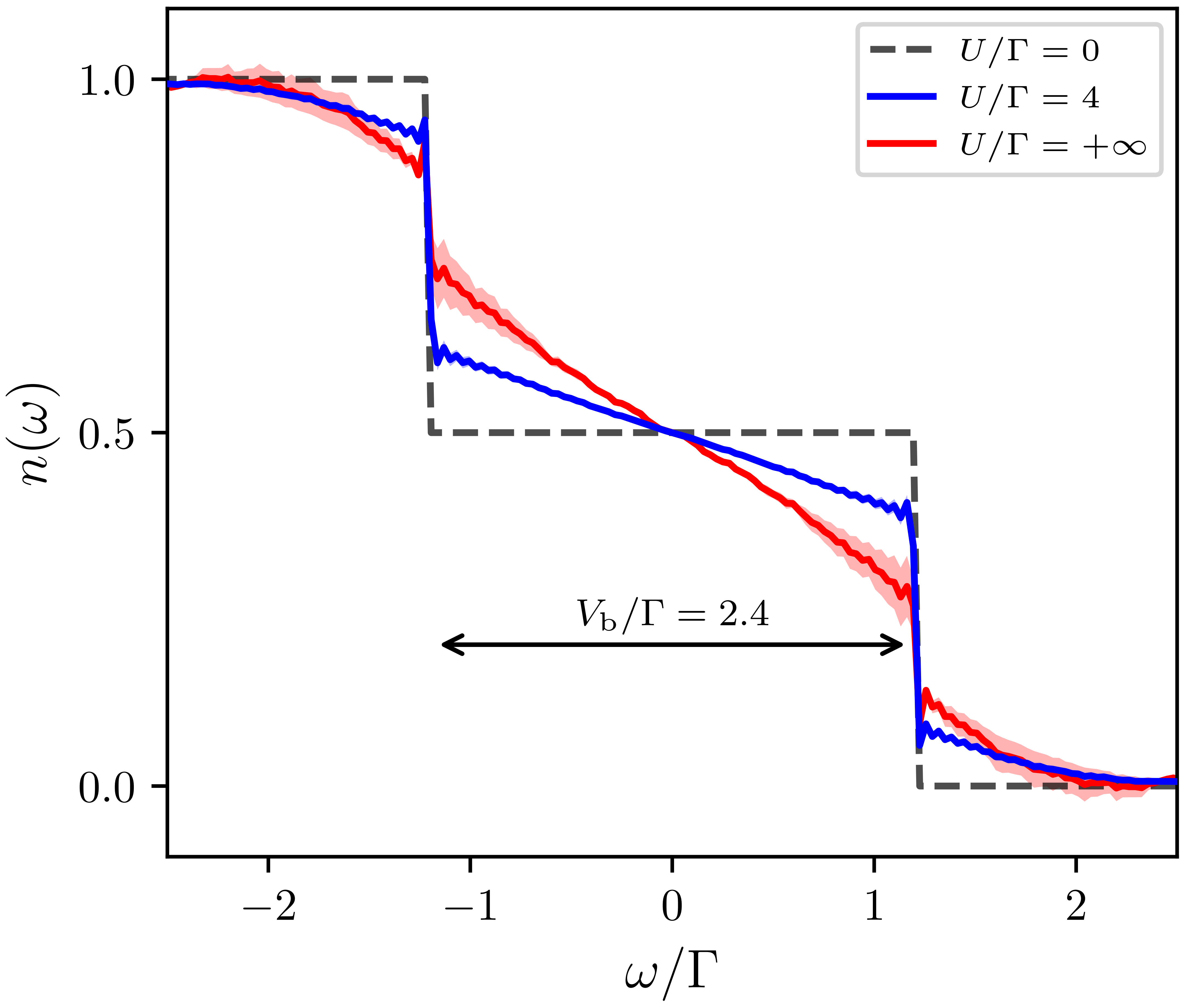


Out of equilibrium distribution function of the dot

- Not a Fermi function
- At U = 0 double step, due to the 2 Fermi leads.
- Finite U, T=0
- Experiments ?

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

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



Quantum Quasi-Monte Carlo

$Q_n(t)$: a n-dimensional integral

$$Q_n(t) = \frac{1}{n!} \int_{t_0}^{\infty} du_1 \ldots du_n \;\; f_n(t, u_1, \ldots, u_n)$$

- How to integrate in large dimensions ?
- Using a minimal number of evaluations of f_n which costs $O(2^n)$

Integration in large dimensions

	Quadratures	*Monte Carlo*
Error scaling	e^{-aN}	$\frac{1}{\sqrt{N}}$

N = *Number of computed points of the integrand*

Integration in large dimensions

J. Dick, F.Y. Kuo, I.H. Sloan "High-dimensional integration: The Quasi-Monte Carlo way," Acta Numerica 22, 133 (2013).

	Quadratures	Quasi-Monte Carlo	Monte Carlo
Error scaling	e^{-aN}	$\frac{1}{N}$	$\frac{1}{\sqrt{N}}$

N = *Number of computed points of the integrand*

Quasi-Monte Carlo

J. Dick, F.Y. Kuo, I.H. Sloan
"High-dimensional integration: The Quasi-Monte Carlo way,"
Acta Numerica 22, 133 (2013).

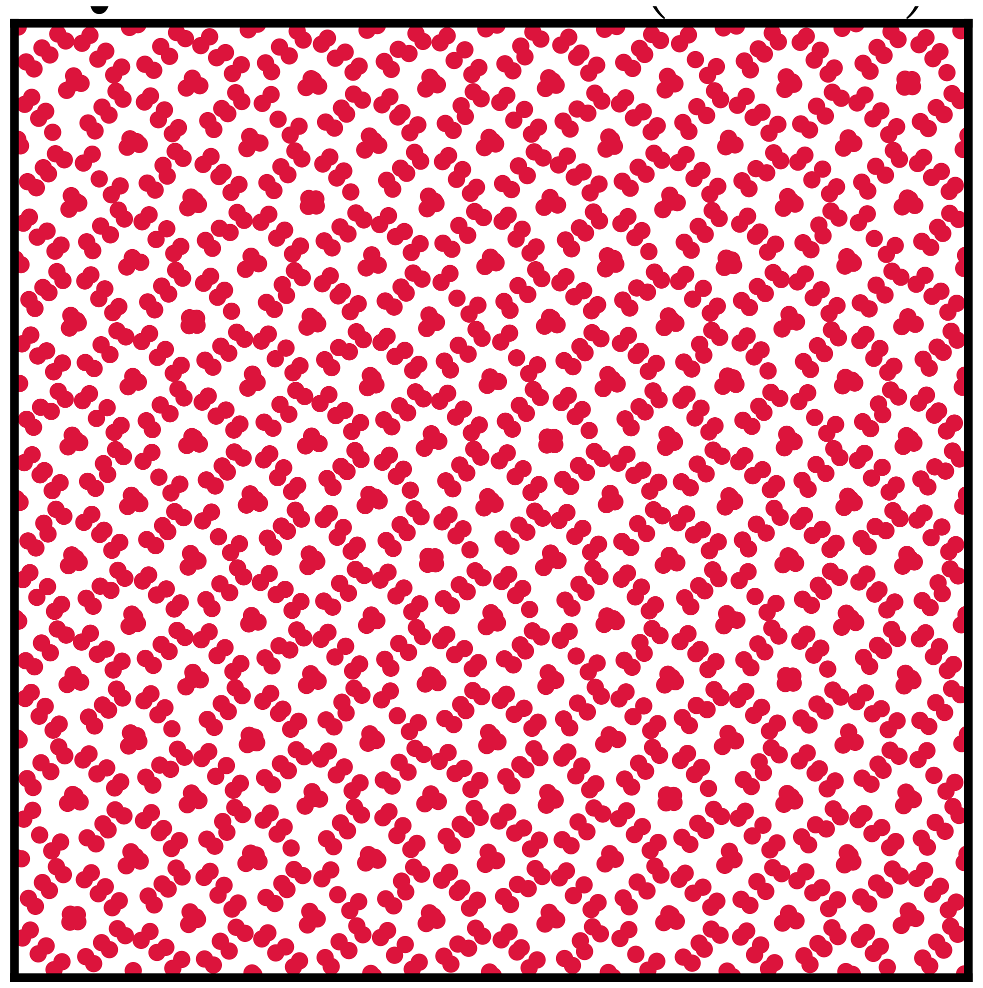
- Evaluate the function on some special points. Low discrepancy sequences, e.g. Sobol'.
- Theorems
  If the function f is "smooth enough" (i.e. proper functional space), then

$$\left| \int d^n x\, f(x) - \frac{1}{N} \sum_{n=1}^{N} f(\bar{x}_i) \right| \leq C(f) \frac{\log(N)^n}{N}$$

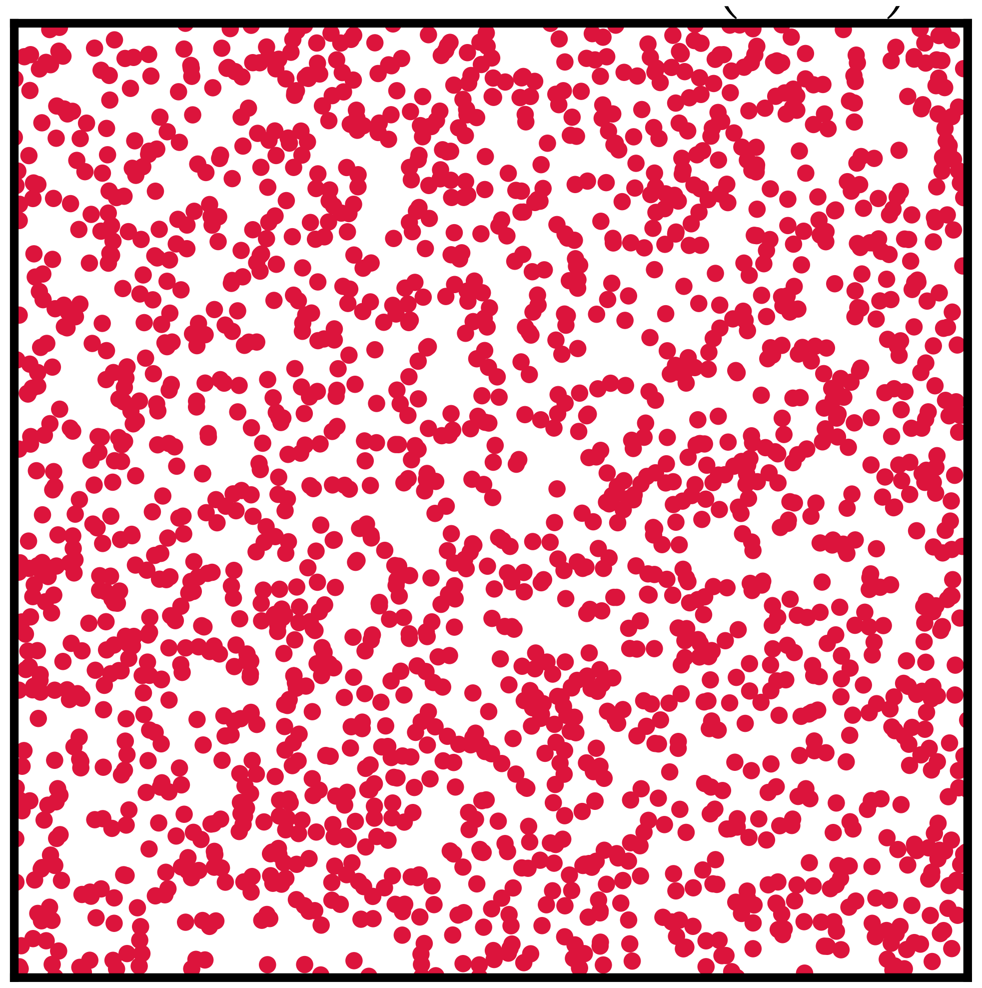
Sobol' sequence

Mathematical bound
In practice O(1/N)

Sobol'



Pseudo Random
Mersenne twister



Quasi-Monte Carlo IS NOT Monte Carlo.
No random numbers.

Is our function smooth enough ?

No, but …

Warp the integral

- Change of variable ***u(x)*** in *n* dimensions.
- Goal : make the function flat/smooth

$$Q_n = \int d^n\boldsymbol{u}\ f_n(u_1, \ldots, u_n) \longrightarrow Q_n = \int_{[0,1]^n} d^n\boldsymbol{x}\ f_n\left[\boldsymbol{u}(\boldsymbol{x})\right] \left|\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}\right|$$

- *u*(*x*) constructed from a *model function $p_n(\boldsymbol{u})$* such that

$$\left|\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}}\right| = \frac{\mathcal{C}}{p_n(\boldsymbol{u})}$$

- Then use quasi-Monte Carlo in new variable *x*.

$$Q_n \approx Q_n(N) = \frac{\mathcal{C}}{N} \sum_{i=0}^{N} \frac{f_n\left[\boldsymbol{u}(\bar{\boldsymbol{x}}_i)\right]}{p_n\left[\boldsymbol{u}(\bar{\boldsymbol{x}}_i)\right]}$$

← *Sobol' sequence*

Model function

- Model function : approximation of the integrand in *n* dimensions.
  Optimized for quicker convergence.

- Machine learning problem.

- In general, a large class of possible functions, e.g. functional tensor trains / MPS

$$p_n(\boldsymbol{u}) = h_a^{(1)}(t-u_1)h_{ab}^{(2)}(u_1-u_2)\cdots h_{cd}^{(n-1)}(u_{n-2}-u_{n-1})h_d^{(n)}(u_{n-1}-u_n),$$

- Here, even the simplest case, without any optimization, already gives excellent results.

$$p_n(\boldsymbol{u}) = \prod_{i=1}^{n} h^{(i)}\left(u_{i-1}-u_i\right) \qquad h^{(i)}(u) = e^{-u/\tau}$$

Quantum Quasi-Monte Carlo (QQMC)

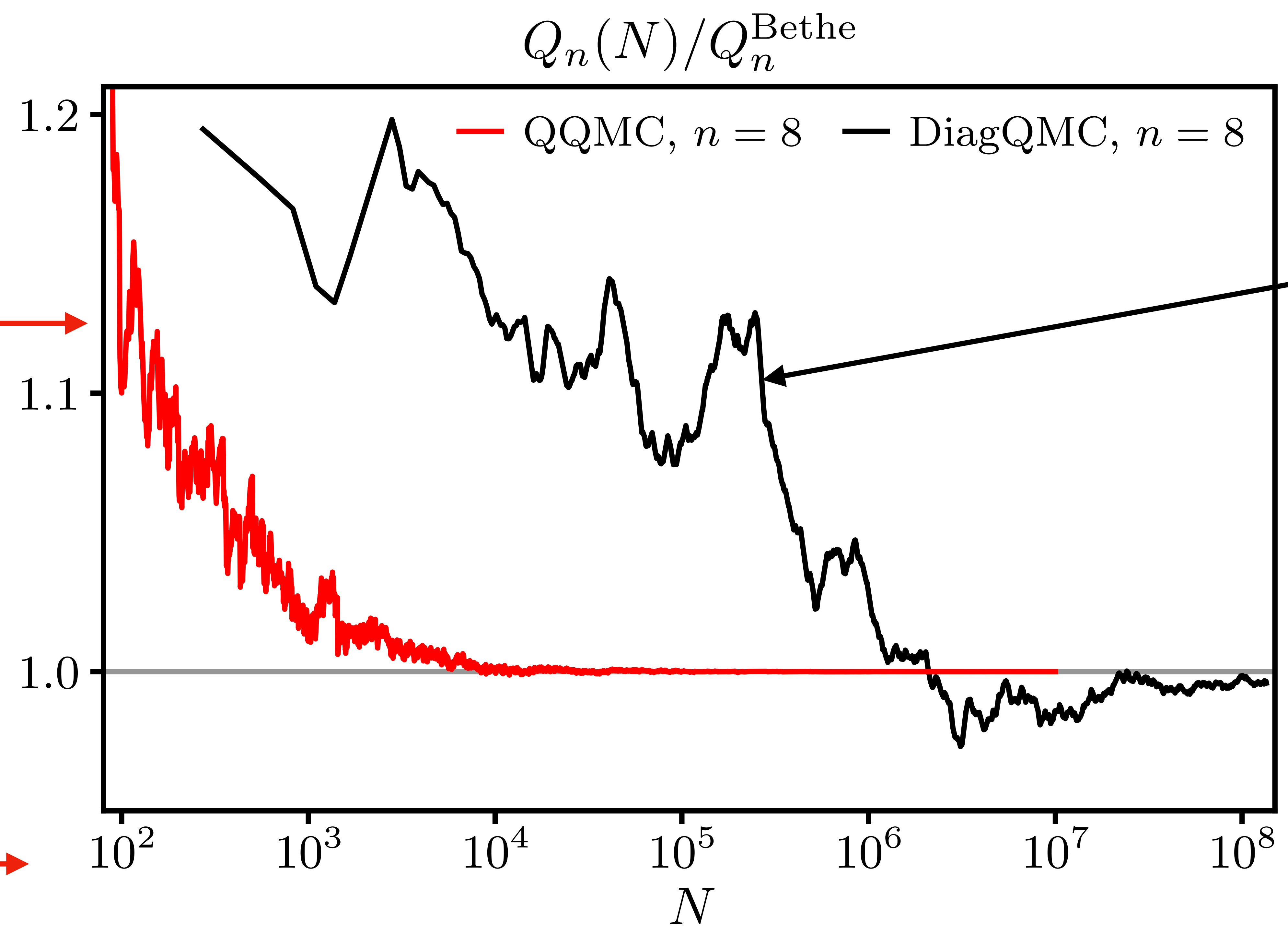
ArXiv:2002.12372

- Compute the integral of the quantum problem with *Quasi-Monte Carlo*

Dot occupation, equilibrium normalized by Bethe Ansatz solution vs number of sampling points

$$Q = \sum_{n \geq 0} Q_n U^n$$

Quantum Quasi-Monte Carlo (QQMC)



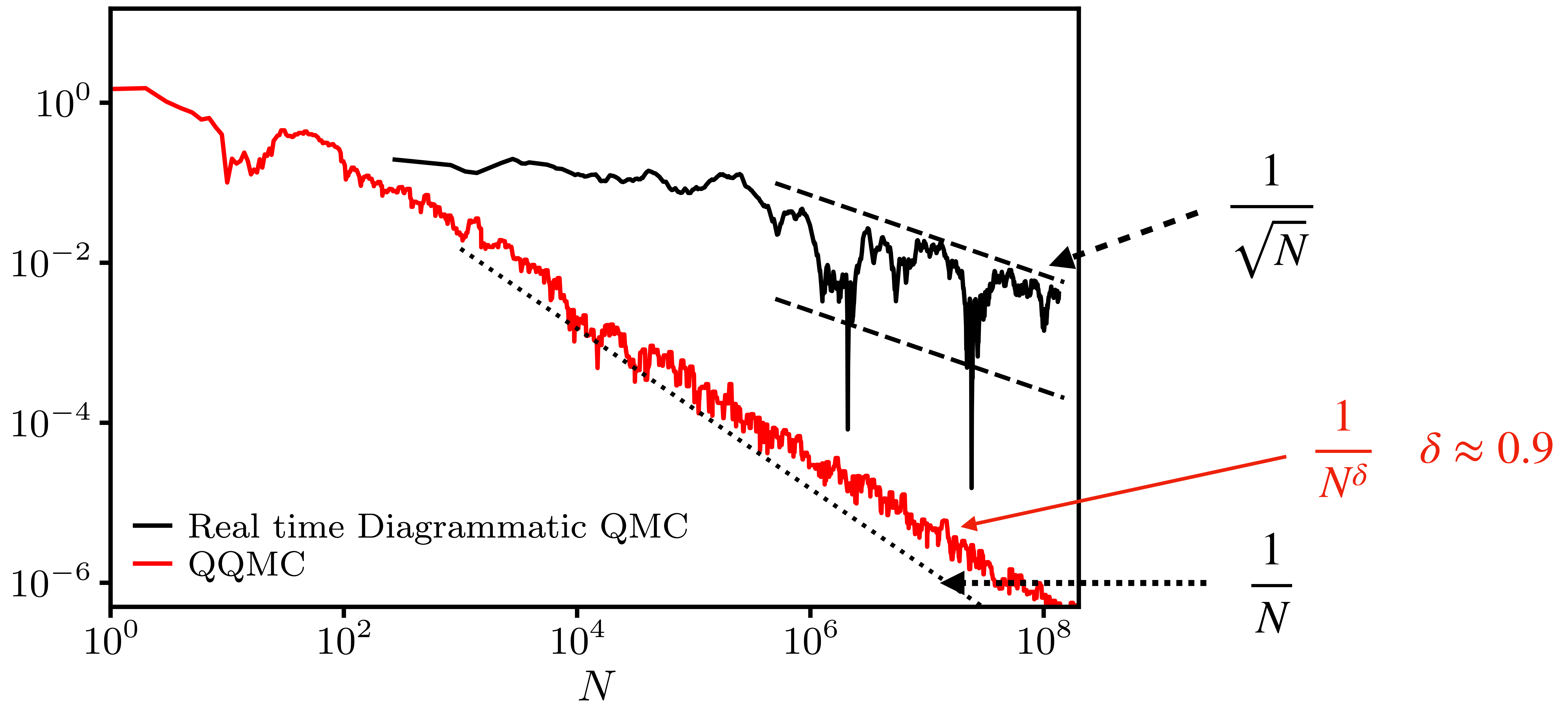
Real time Diagrammatic QMC

Log scale !

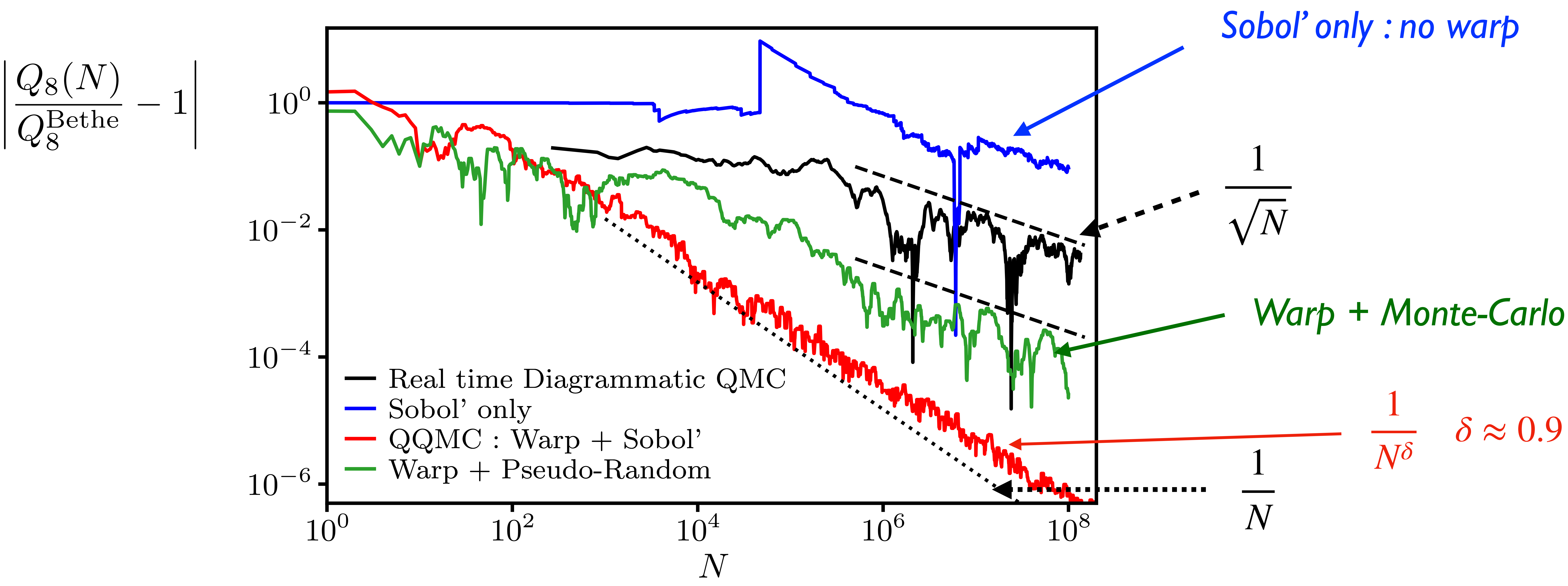
Error scaling with N

- Same curve in log-log

$$\left|\frac{Q_8(N)}{Q_8^{\mathrm{Bethe}}} - 1\right|$$



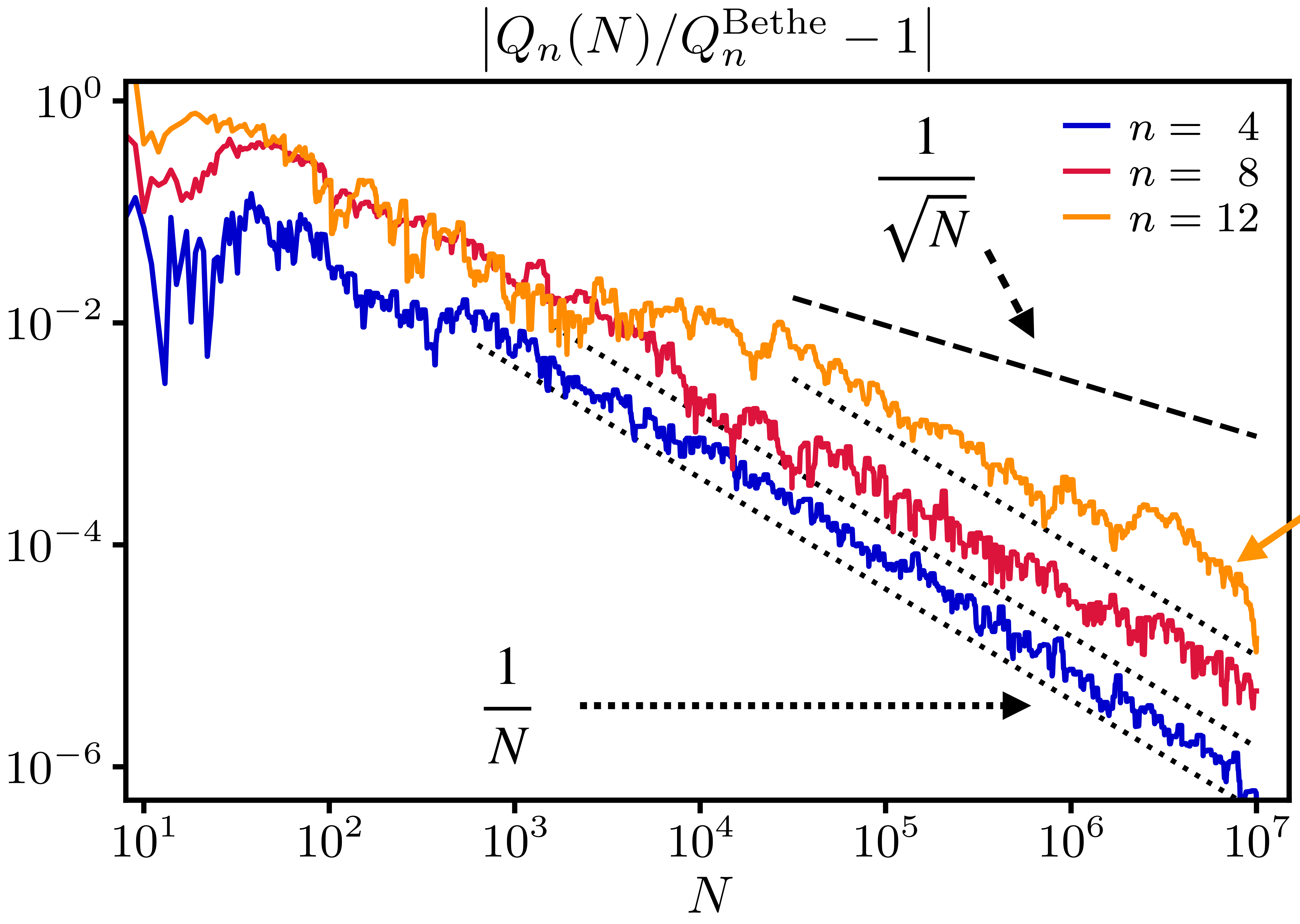
Warping the integral is crucial



- Model function + quasi-MC = best method

Large orders

- Error vs analytical Bethe Ansatz result, vs the number of sampling points ***N***

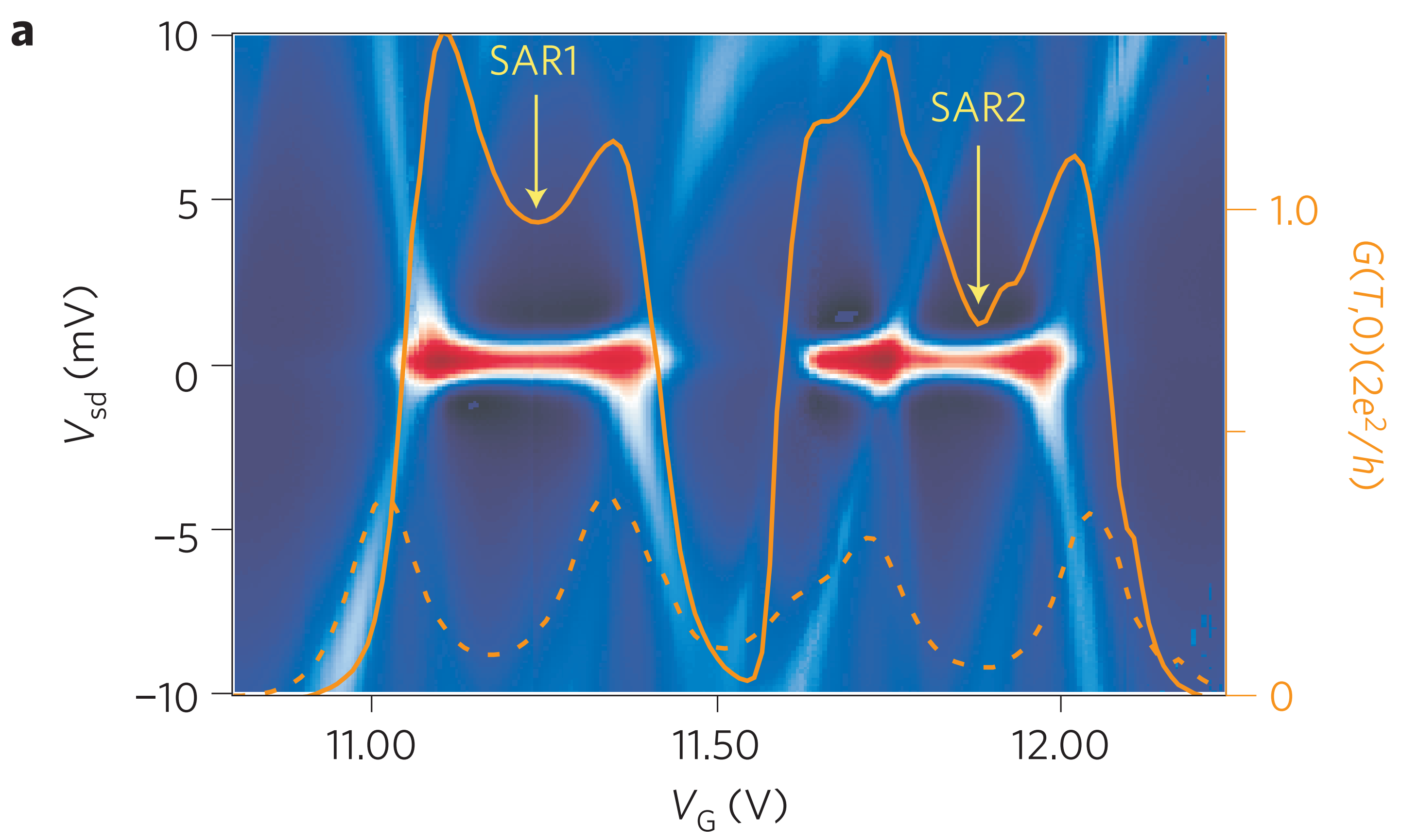


- Precision with N = 10^7 points

$$Q_{12} = \frac{13749310575}{\pi^{12}} - \frac{2505809831525}{1458\pi^{10}} + \frac{90628717412233}{2531250\pi^8} - \frac{84543422632097}{283618125\pi^6} + \frac{131145705977}{100018800\pi^4} - \frac{83711}{27720\pi^2} \approx 0.00048443(7)$$

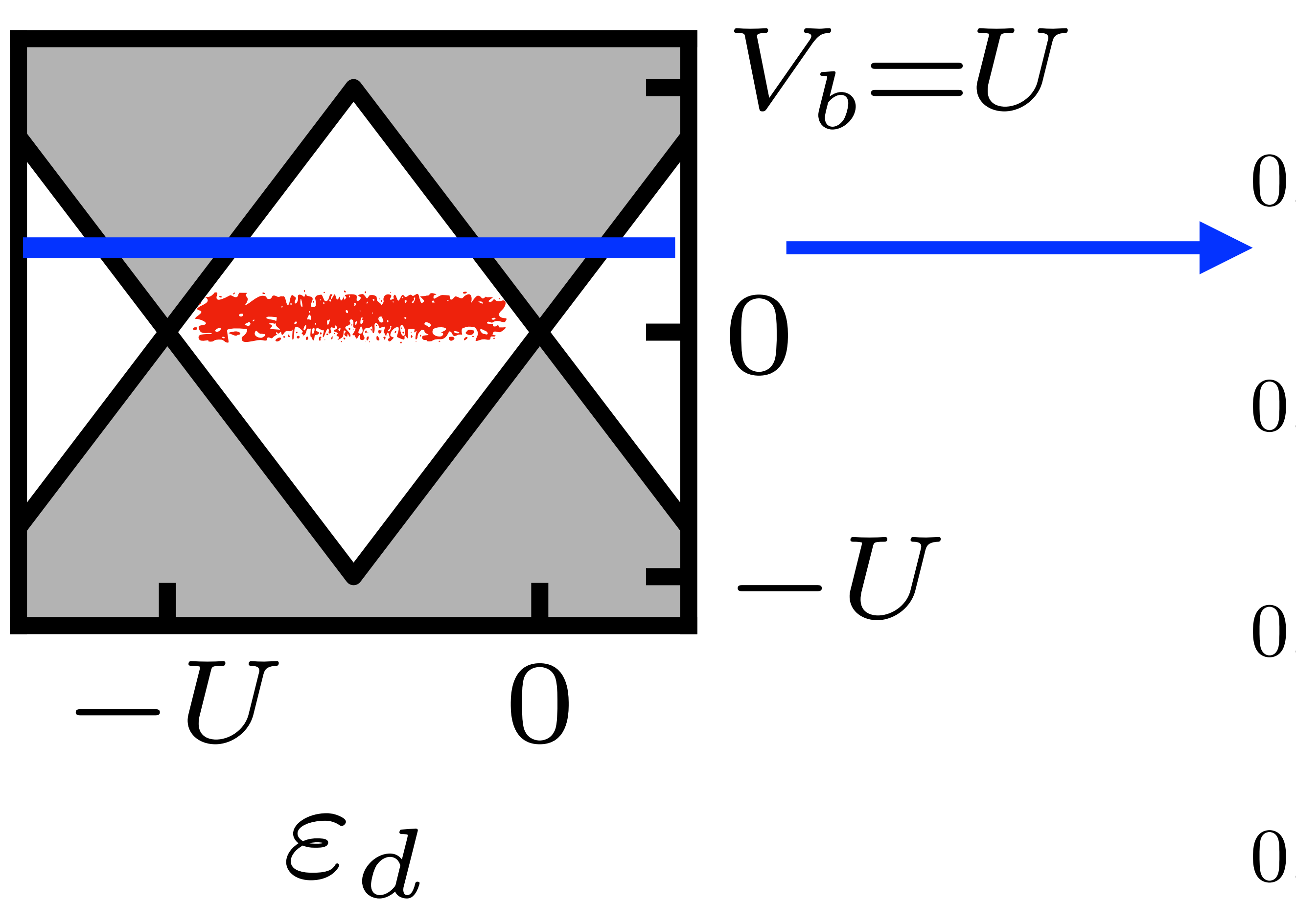
Kondo ridge

Experiment

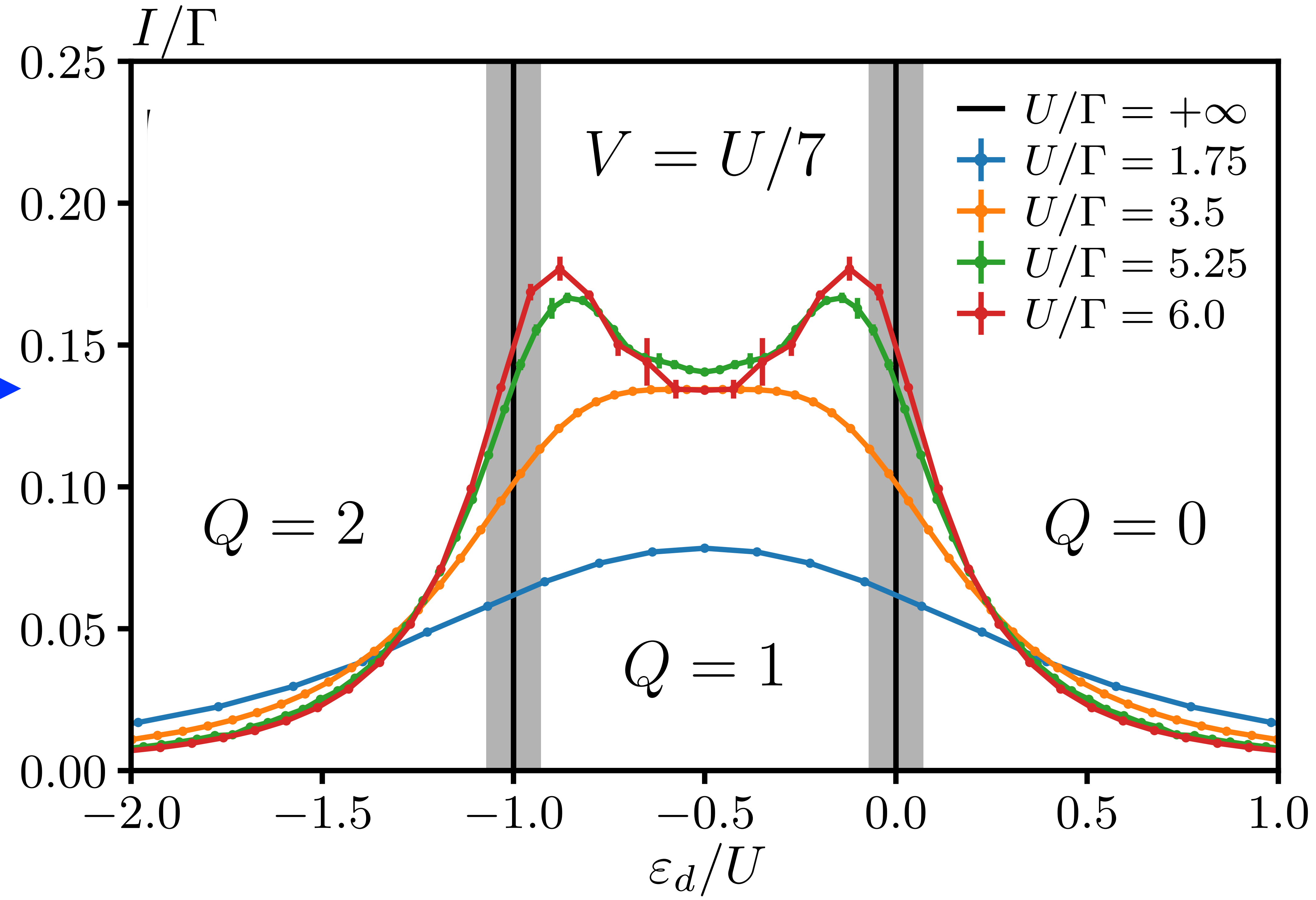


T. Delattre et al.
Nat. Phys. 208 (2009)

Coulomb diamond
T=0, vs U and ε_d



Current vs ε_d for various U, fixed V_b



M. Macek, P. Dumitrescu, C. Bertrand, B. Triggs, OP, X. Waintal
ArXiv:2002.12372

- Many calculations ("parametric runs"), for various U and ε_d.
  About 25 cpu hours/point for order 10.

Conclusion

- Solution of the out of equilibrium quantum dot.
- Perturbation theory even at strong coupling (with resummation)
- Quantum Quasi-Monte Carlo

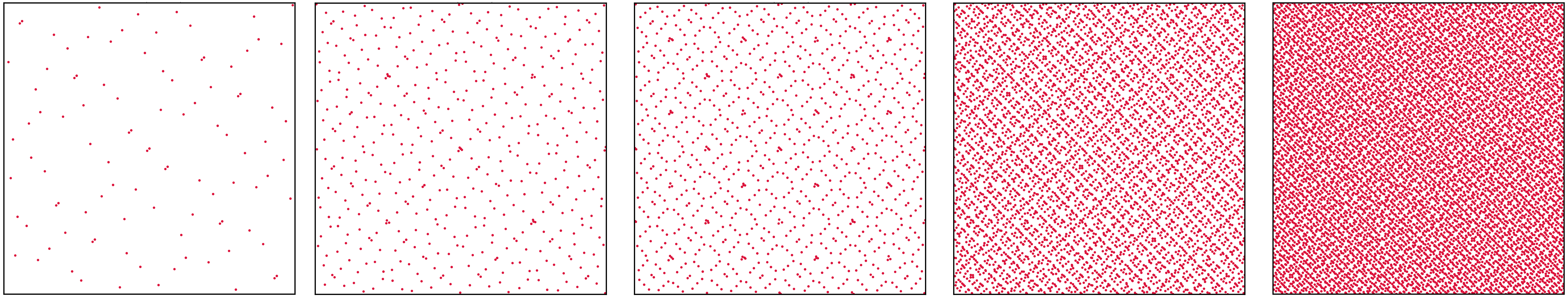
- Roadmap : DMFT solvers, lattice problems …

Thank you for your attention!

Sobol' points

- Illustration in d = 2

N = 100 *N = 500* *N = 1000* *N = 5000* *N = 10000*



Learning the model function

- Optimization of model function from the data
- Proof of concepts : gain speed factor x2, using a projection technique