The Out-of-Equilibrium Anderson impurity model :
a numerically exact approach whith Diagrammatic Quantum Quasi Monte-Carlo

Calculating Feynman diagrams analytically is impractical beyond the first
few orders. In this talk, I will discuss recent numerical algorithms that allow one to
calculate all diagrams up to order 20 or more. I will show how this technique can be
used to
study the Anderson model, including for parameters deep into the Kondo regime
both at
equilibrium (in precise agreemeent with other techniques) and in out-of-
equilibrium situations
that were not accessible so far.

Correlations and computational quantum transport: automatic calculation of Feynman diagrams at large orders.

While numerical simulations of quantum transport at the mean field level are by now standard, including even the simplest effects of correlations such as Coulomb blockade is a struggle and one almost always has to resort to uncontroled approximations or drastic simplifications to account for more complexe effects such as Kondo physics.
Feynman diagrams are a natural formalism to express correlations and they circonvoluate working at the raw Hilbert space level with many-body wave-functions as is often done numerically (either in quantum Monte-Carlo or tensor network techniques). An immense litterature study different ways to find the most important classes of diagrams and calculate them analytically. In this talk, I will discuss the current effort done in my group to design algorithms that numerically sum all diagrams in a systematic way, order by order up to order 20 or more. I will showcase how this technique can capture out-of-equilibrium effects deep in the Kondo regime.

CORRELATIONS AND COMPUTATIONAL QUANTUM TRANSPORT: AN APPROACH FOR CALCULATING FEYNMAN DIAGRAMS AT LARGE ORDERS

Xavier WAINTAL,
CEA Grenoble, Pheliqs IRIG
With CORENTIN BERTRAND, MARJAN MACEK, PHILIPP DUMITRESCU,
Olivier Parcollet, Bill Triggs and Serge Florens

TOOLS FOR QUANTUM TRANSPORT

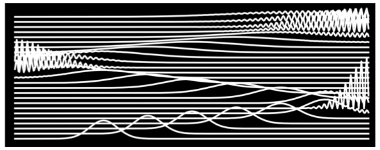
$$\hat{H} = \sum_{ij} H_{ij} c_i^\dagger c_j$$

kwant

HTTP://KWANT-PROJECT.ORG

With TU Delft (Akhmerov, Wimmer et al.)

$$\hat{H}(t) = \sum_{ij} H_{ij}(t) c_i^+ c_j$$



HTTP://TKWANT.KWANT-PROJECT.ORG

$$\hat{\mathbf{H}}(t) = \hat{\mathbf{H}}_0(t) + U\hat{\mathbf{H}}_{\text{int}}(t)$$

$$\hat{\mathbf{H}}_{\text{int}}(t) = \sum_{ijkl} \mathbf{V}_{ijkl}(t) \hat{\mathbf{c}}_i^\dagger \hat{\mathbf{c}}_j^\dagger \hat{\mathbf{c}}_k \hat{\mathbf{c}}_l .$$

?

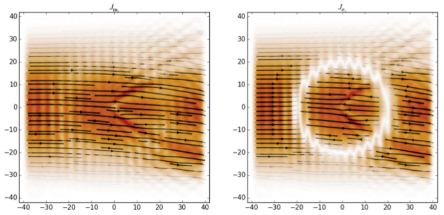
- Kondo physics
- Coulomb blockade, Fermi edge singularity
- 0.7 anomaly
- FQHE
- Quantum computers

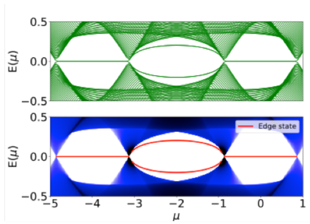
...

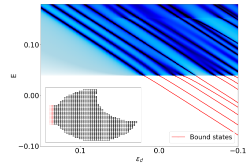
KWANT GALLERY

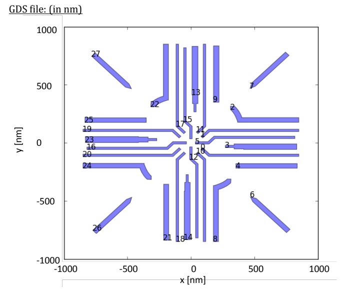
HTTP://KWANT-PROJECT.ORG

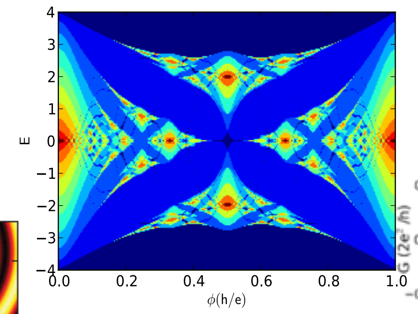
With TU Delft (Akhmerov, Wimmer et al.)

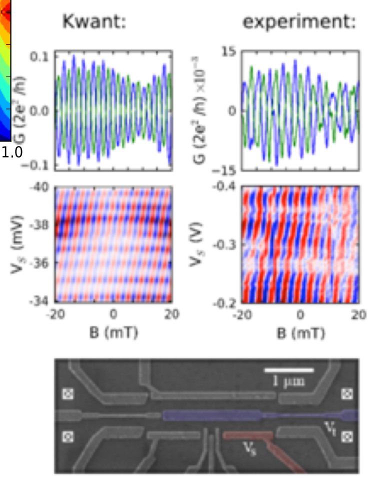


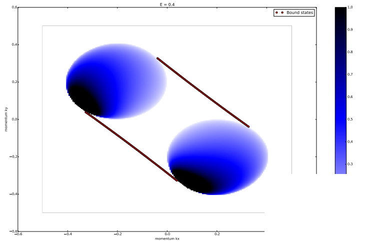


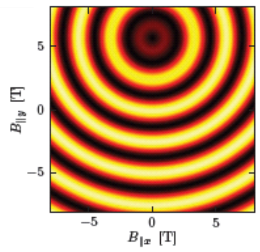


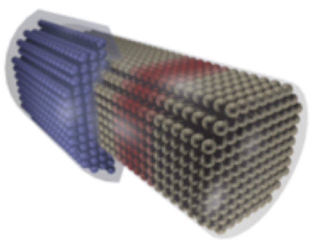


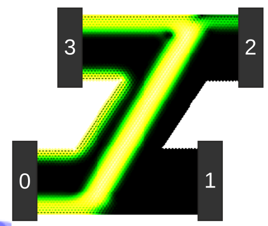


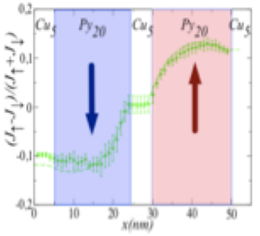


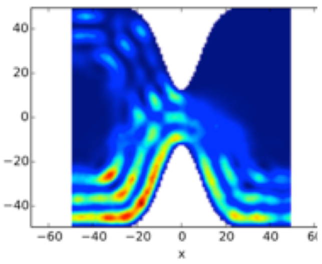


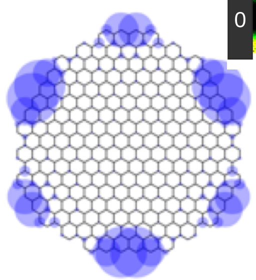


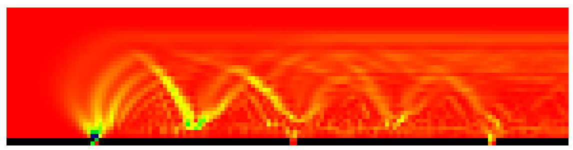




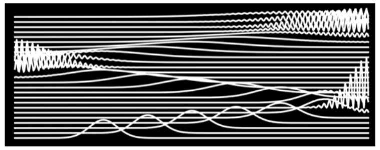








T-KWANT



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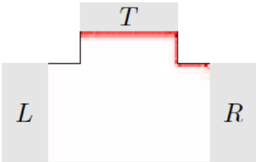
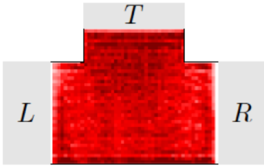
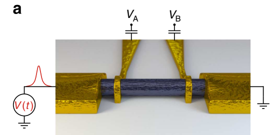
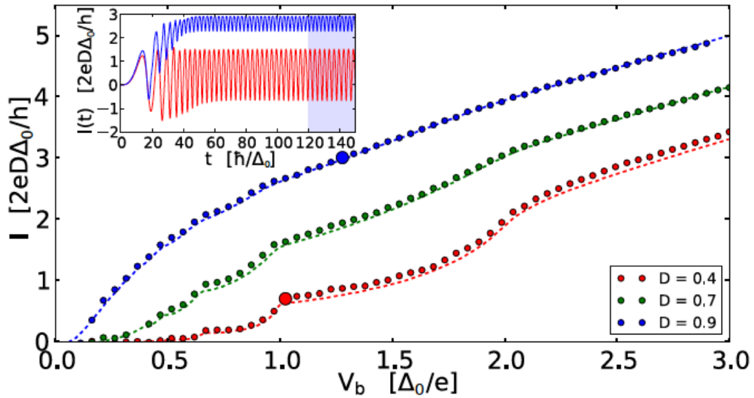
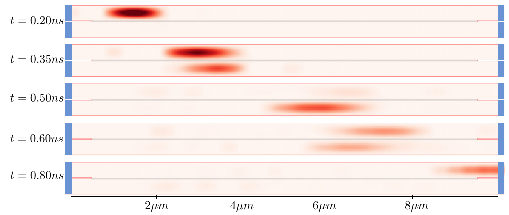
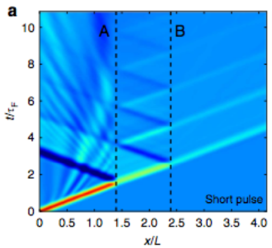


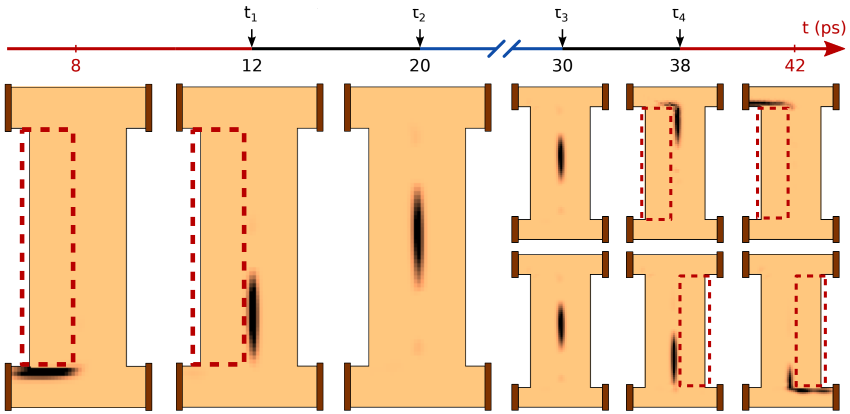


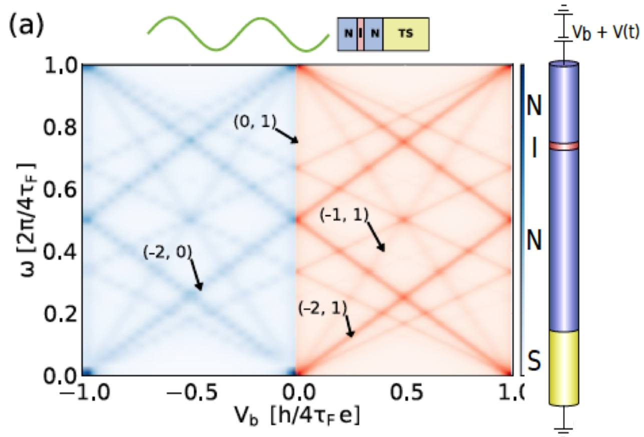






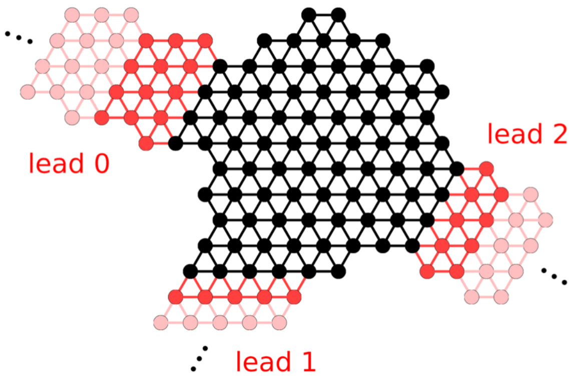




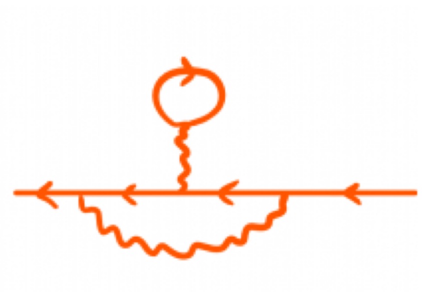


$$\hat{\mathbf{H}}(t) = \hat{\mathbf{H}}_0(t) + U\hat{\mathbf{H}}_{\text{int}}(t)$$

$$\hat{\mathbf{H}}_{\text{int}}(t) = \sum_{ijkl} \mathbf{V}_{ijkl}(t)\hat{\mathbf{c}}_i^\dagger \hat{\mathbf{c}}_j^\dagger \hat{\mathbf{c}}_k \hat{\mathbf{c}}_l .$$

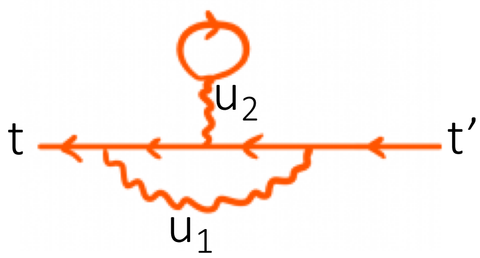


$$Q(U) = \sum_{n=0}^{+\infty} Q_n U^n$$



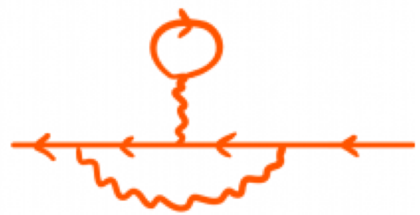
A VERY DIRECT APPROACH:

CALCULATING ALL THE FEYNMAN DIAGRAMS UP TO A GIVEN (LARGE) ORDER



$$\sim U^2 \int du_1 du_2 \;\; g_0(t,u_1)g_0(u_1,u_2)g_0(u_2,u_1)g_0(u_1,t')g_0(u_2,u_2)$$

A VERY DIRECT APPROACH:



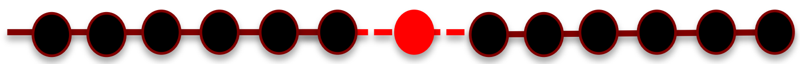
CALCULATING ALL THE FEYNMAN DIAGRAMS UP TO A GIVEN (LARGE) ORDER

$$F(U) = \sum_n F_n U^n$$

- PROBLEM #1: There are n! diagrams.
- PROBLEM #2 How to calculate n dimensional integrals
- PROBLEM #3 How to reconstruct F(U) from the F_n .

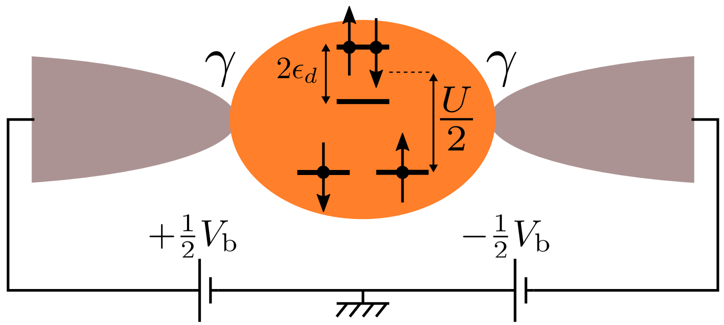
THE OUT-OF-EQUILIBRIUM ANDERSON IMPURITY

=



$$\hat{\mathbf{H}} = \sum_{i=-\infty}^{+\infty} \sum_{\sigma} \gamma_i \hat{\mathbf{c}}^{\dagger}_{i,\sigma} \hat{\mathbf{c}}_{i+1,\sigma} + h.c. + \epsilon_d (\hat{\mathbf{n}}_{\uparrow} + \hat{\mathbf{n}}_{\downarrow}) + U\theta(t) \left(\hat{\mathbf{n}}_{\uparrow} - \frac{1}{2} \right) \left(\hat{\mathbf{n}}_{\downarrow} - \frac{1}{2} \right).$$

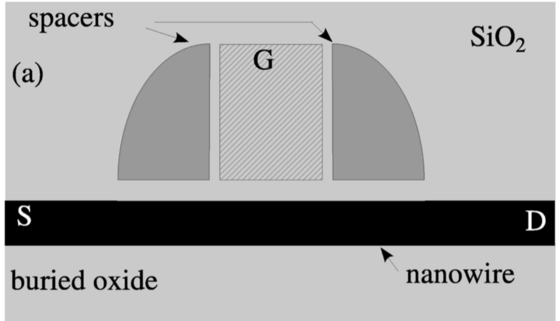
COULOMB BLOCKADE 101

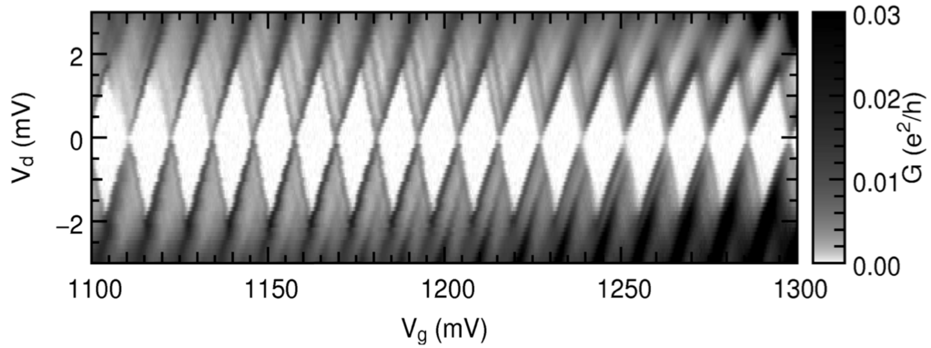


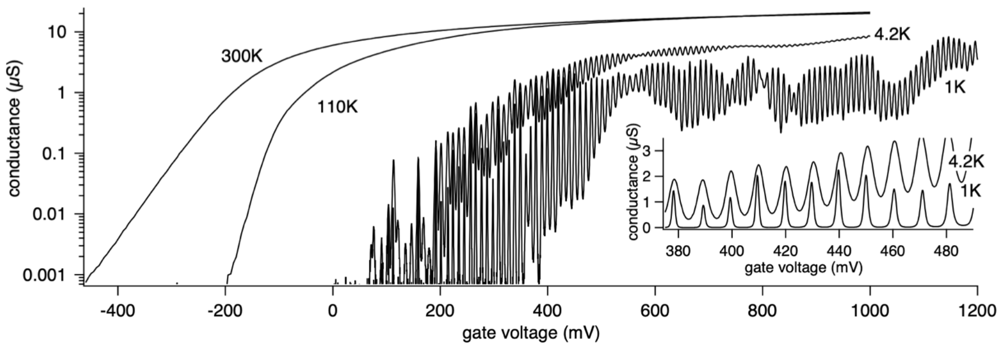
$$E(N) = \frac{U}{2}N^2 + (\epsilon_d - U)N + \frac{U}{2}$$

$$E(N+1) - E(N) = (\epsilon_d - U) + (2N+1)\frac{U}{2}$$

COULOMB BLOCKADE 101

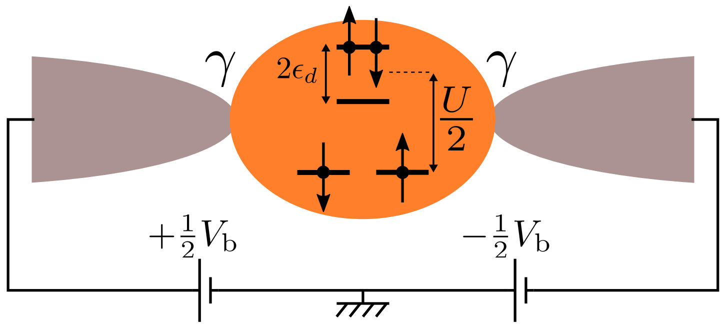






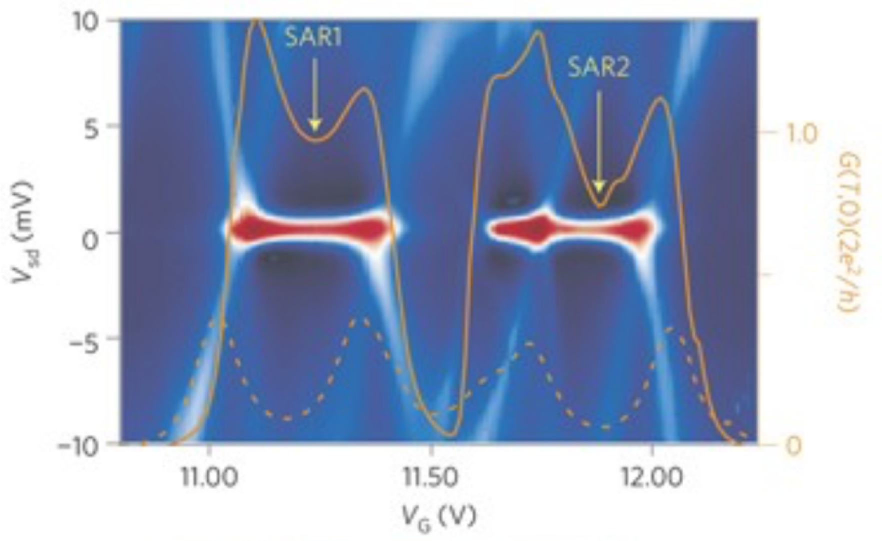
Hofheinz et al. arXiv:cond-mat/0609245

KONDO 101



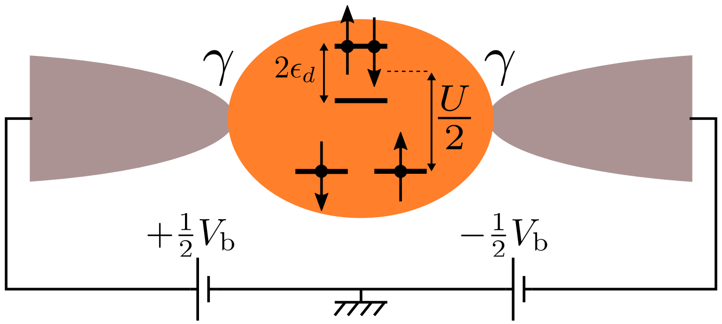
U		γ^2/U		
REPULSIVE INTERACTION	→	ANTIFERROMAGNETIC COUPLING	→	ATTRACTIVE INTERACTION

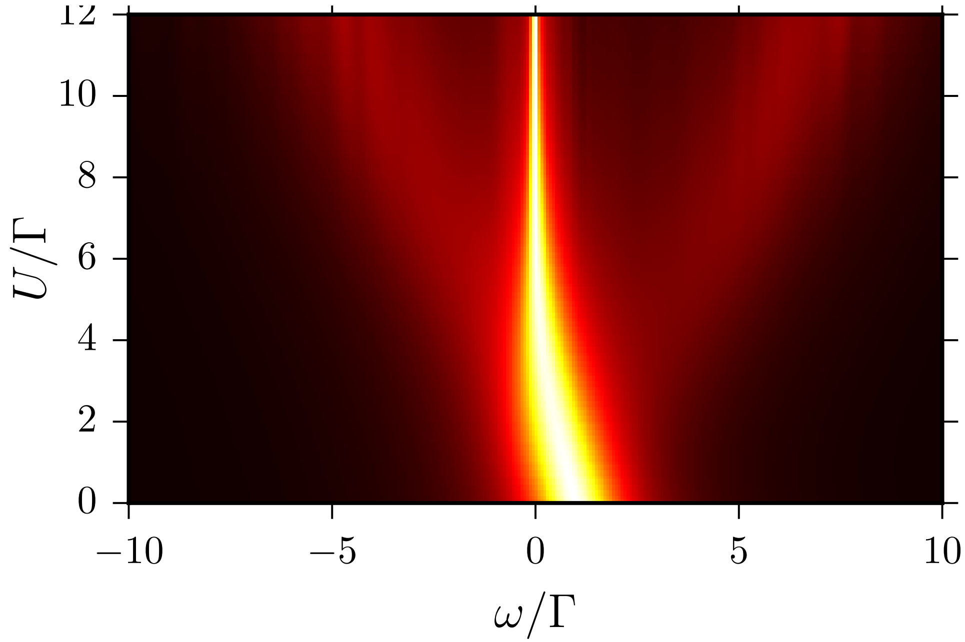
KONDO 101



Nature Physics **5**, 208 (2009)

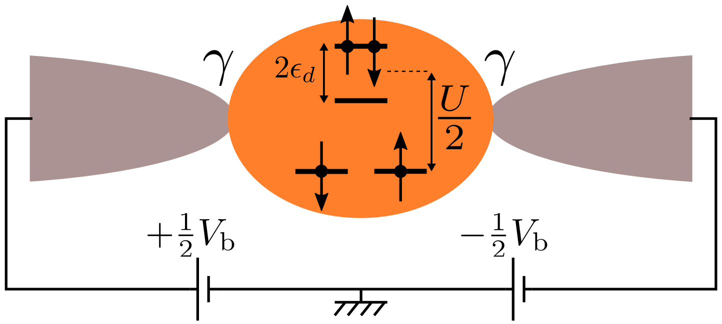
TEASER: AT EQUILIBRIUM

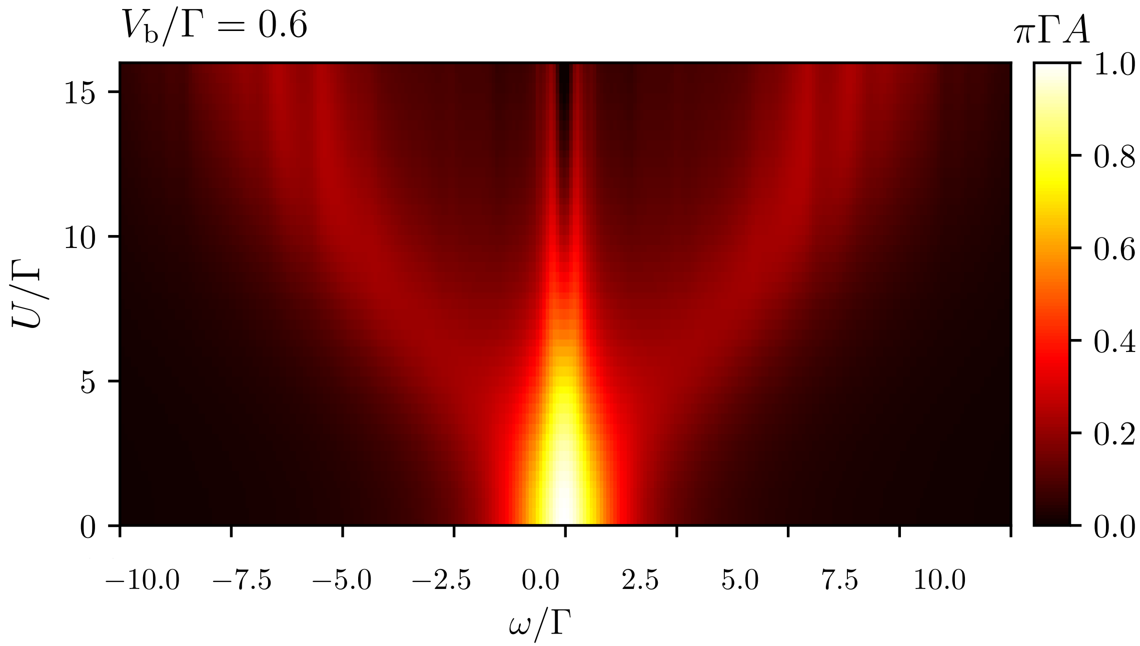




$$\hat{\mathbf{H}} = \sum_{i=-\infty}^{+\infty} \sum_{\sigma} \gamma_i \hat{\mathbf{c}}^{\dagger}_{i,\sigma} \hat{\mathbf{c}}_{i+1,\sigma} + h.c. + \epsilon_d (\hat{\mathbf{n}}_{\uparrow} + \hat{\mathbf{n}}_{\downarrow}) + U\theta(t) \left(\hat{\mathbf{n}}_{\uparrow} - \frac{1}{2} \right) \left(\hat{\mathbf{n}}_{\downarrow} - \frac{1}{2} \right).$$

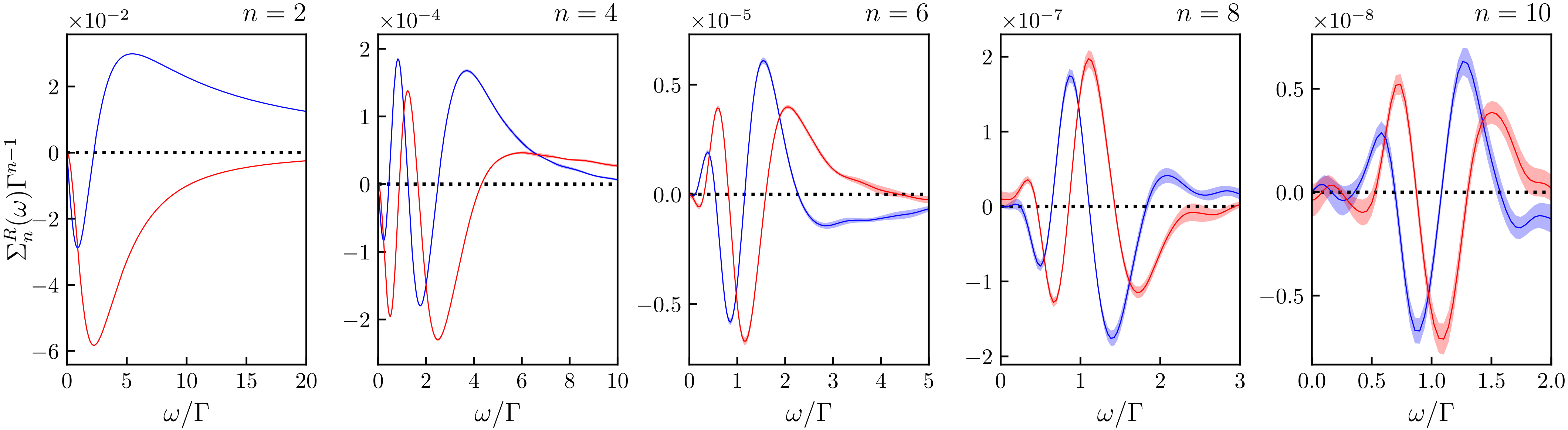
TEASER: OUT-OF-EQUILIBRIUM





$$\hat{\mathbf{H}} = \sum_{i=-\infty}^{+\infty} \sum_{\sigma} \gamma_i \hat{\mathbf{c}}^{\dagger}_{i,\sigma} \hat{\mathbf{c}}_{i+1,\sigma} + h.c. + \epsilon_d(\hat{\mathbf{n}}_{\uparrow} + \hat{\mathbf{n}}_{\downarrow}) + U\theta(t) \left(\hat{\mathbf{n}}_{\uparrow} - \frac{1}{2}\right)\left(\hat{\mathbf{n}}_{\downarrow} - \frac{1}{2}\right).$$

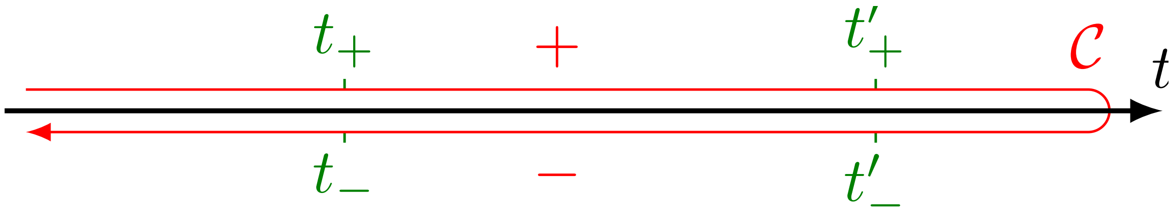
PROBLEM #1: THE N! DIAGRAMS



KELDYSH FORMALISM IN A NUTSHELL

$$\langle \mathcal{O}(t) \rangle = \langle \mathcal{U}^\dagger(t) \mathcal{O} \mathcal{U}(t) \rangle$$

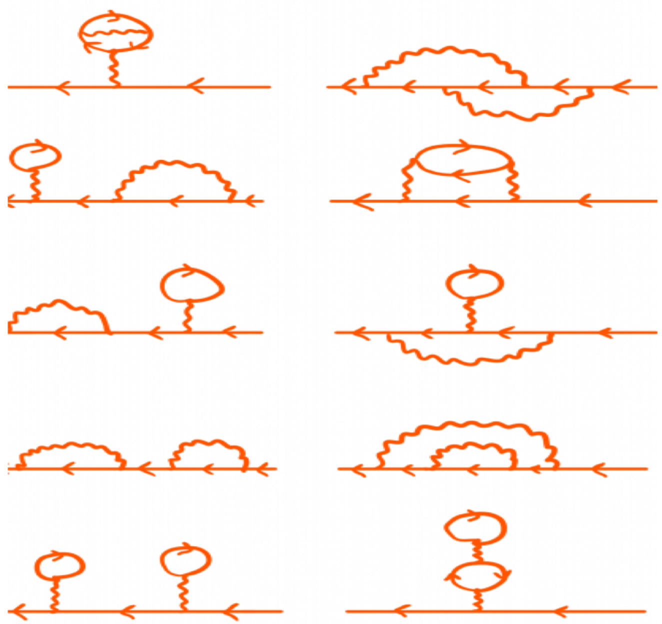
$$\mathcal{U}(t) = T \exp\left(-i \int_0^t \hat{H}_{\text{int}}(u) du \right)$$



$$\langle \mathcal{O}(t) \rangle = \left\langle {\color{red} T_{\mathcal{C}}} \hat{\mathcal{O}}(t) \, \exp\left(-i \int_{\mathcal{C}} \hat{H}_{\text{int}}(u) du \right) \right\rangle$$

WICK DETERMINANTS

$$\left\langle c_1^+ c_1 c_2^+ c_2 c_3^+ c_3 c_4^+ c_4 c_5^+ c_5 \right\rangle = \sum_P (-1)^{|P|} \left\langle c_1^+ c_{P(1)} \right\rangle \left\langle c_2^+ c_{P(2)} \right\rangle \left\langle c_3^+ c_{P(3)} \right\rangle \left\langle c_4^+ c_{P(4)} \right\rangle \left\langle c_5^+ c_{P(5)} \right\rangle$$



WICK DETERMINANTS

$$\left\langle c_1^+ c_1 c_2^+ c_2 c_3^+ c_3 c_4^+ c_4 c_5^+ c_5 \right\rangle = \sum_P (-1)^{|P|} \left\langle c_1^+ c_{P(1)} \right\rangle \left\langle c_2^+ c_{P(2)} \right\rangle \left\langle c_3^+ c_{P(3)} \right\rangle \left\langle c_4^+ c_{P(4)} \right\rangle \left\langle c_5^+ c_{P(5)} \right\rangle$$

$$\left\langle c_1^+ c_1 c_2^+ c_2 c_3^+ c_3 c_4^+ c_4 c_5^+ c_5 \right\rangle = \det \left\langle c_i^+ c_j \right\rangle$$

A « VERY SIMPLE » FORMULA

$$G^c_{ij}(\bar{t},\bar{t}') = \sum_{n=0}^{+\infty} \frac{i^n}{n!} U^n \sum_{\{a_i\}} (-1)^{\sum_i a_i} \int du_1 du_2 \dots du_n \sum_{i_1 j_1 k_1 l_1} V_{i_1 j_1 k_1 l_1}(u_1) \cdots \sum_{i_n j_n k_n l_n} V_{i_n j_n k_n l_n}(u_n) \det \mathbf{M}_n$$

2ⁿ sum cancels disconnected diagrams

$$\mathbf{M}_n = \begin{pmatrix} g^<_{k_1 i_1}(\bar{u}_1,\bar{u}_1) & g^<_{k_1 j_1}(\bar{u}_1,\bar{u}_1) & g^c_{k_1 i_2}(\bar{u}_1,\bar{u}_2) & \dots & g^c_{k_1 j}(\bar{u}_1,\bar{t}') \\ g^<_{l_1 i_1}(\bar{u}_1,\bar{u}_1) & g^<_{l_1 j_1}(\bar{u}_1,\bar{u}_1) & g^c_{l_1 i_2}(\bar{u}_1,\bar{u}_2) & \dots & g^c_{l_1 j}(\bar{u}_1,\bar{t}') \\ g^c_{k_2 i_1}(\bar{u}_2,\bar{u}_1) & g^c_{k_2 j_1}(\bar{u}_2,\bar{u}_1) & g^<_{k_2 i_2}(\bar{u}_2,\bar{u}_2) & \dots & g^c_{k_2 j}(\bar{u}_2,\bar{t}') \\ \dots & \dots & \dots & \dots & \dots \\ g^c_{k_n i_1}(\bar{u}_n,\bar{u}_1) & g^c_{k_n j_1}(\bar{u}_n,\bar{u}_1) & g^c_{k_n i_2}(\bar{u}_n,\bar{u}_2) & \dots & g^c_{k_n j}(\bar{u}_n,\bar{t}') \\ g^c_{l_n i_1}(\bar{u}_n,\bar{u}_1) & g^c_{l_n j_1}(\bar{u}_n,\bar{u}_1) & g^c_{l_n i_2}(\bar{u}_n,\bar{u}_2) & \dots & g^c_{l_n j}(\bar{u}_n,\bar{t}') \\ g^c_{i i_1}(\bar{t},\bar{u}_1) & g^c_{i j_1}(\bar{t},\bar{u}_1) & g^c_{i i_2}(\bar{t},\bar{u}_2) & \dots & g^c_{ij}(\bar{t},\bar{t}') \end{pmatrix}$$

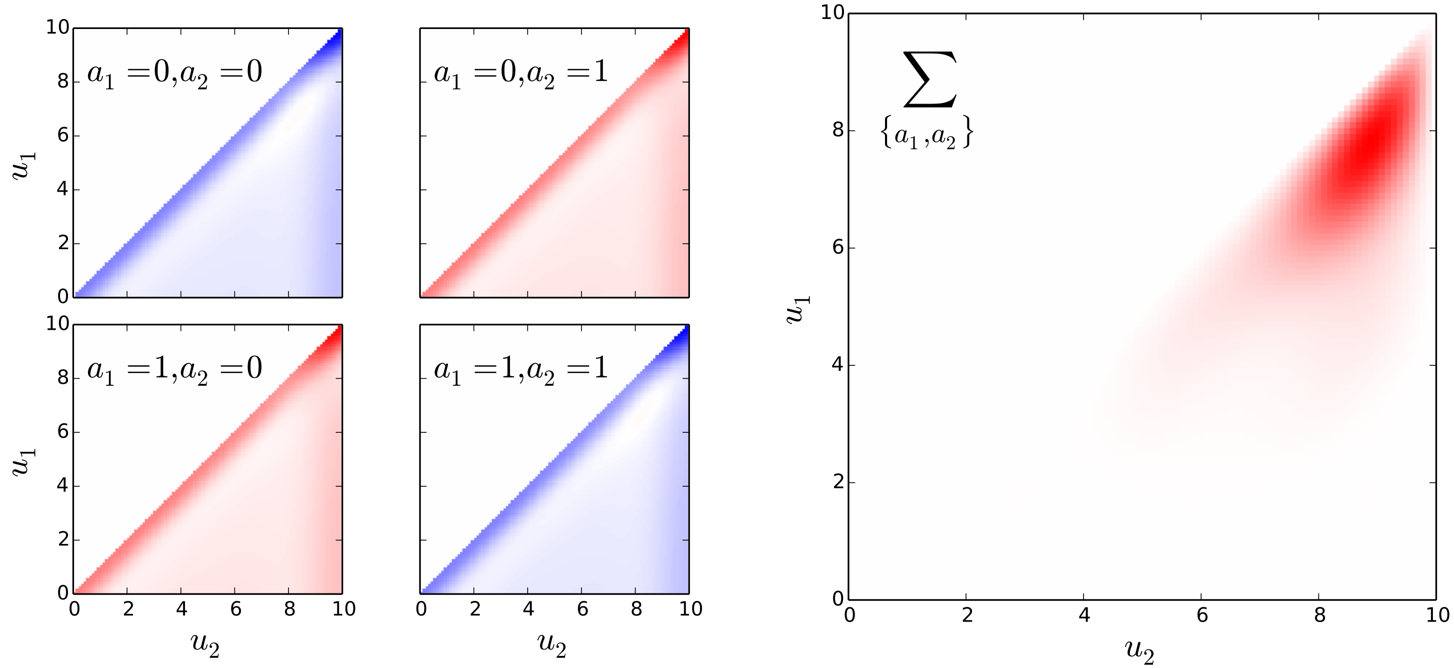
↑

$$g^<_{ij}(t,t') = i \sum_\alpha \int \frac{dE}{2\pi} f_\alpha(E) \Psi_{\alpha E}(t,i) \Psi^*_{\alpha E}(t',j) + i \sum_n f(E_n) \Psi_n(t,i) \Psi^*_n(t',j)$$

Known non-interacting functions.

$$G^c_{ij}(\bar{t},\bar{t}') = \sum_{n=0}^{+\infty} \frac{i^n}{n!} U^n \sum_{\{a_i\}} (-1)^{\sum_i a_i} \int du_1 du_2 \dots du_n \sum_{i_1 j_1 k_1 l_1} V_{i_1 j_1 k_1 l_1}(u_1) \cdots \sum_{i_n j_n k_n l_n} V_{i_n j_n k_n l_n}(u_n) \det \mathbf{M}_n$$

2^n sum cancels disconnected diagrams



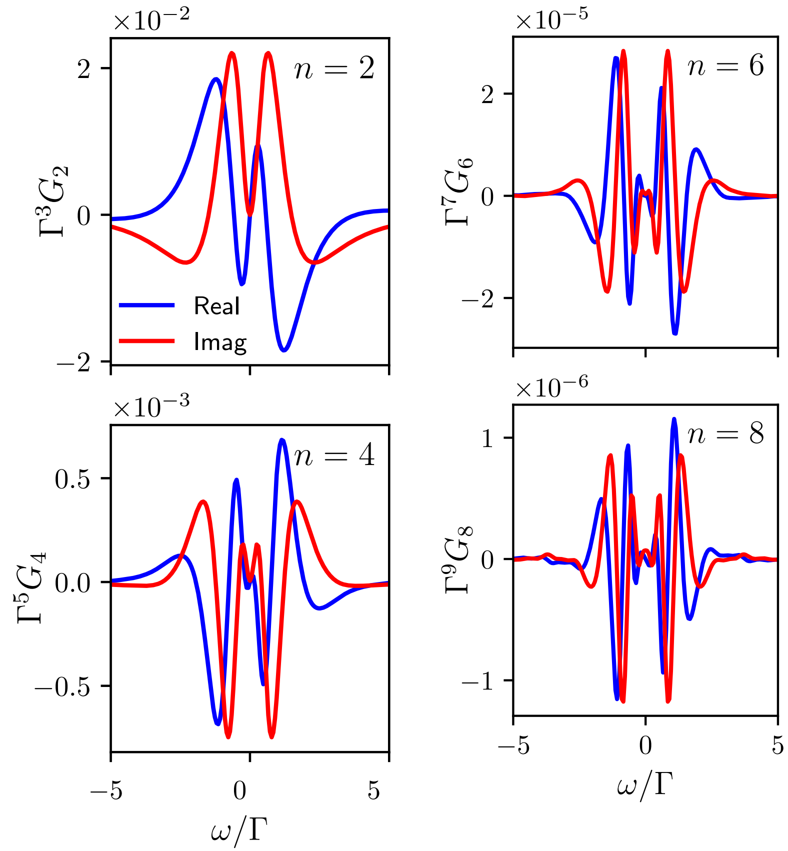
KERNEL EXPANSION

$$\mathbf{M}_n = \begin{pmatrix} g^{<}_{k_1 i_1}(\bar u_1,\bar u_1) & g^{<}_{k_1 j_1}(\bar u_1,\bar u_1) & g^{c}_{k_1 i_2}(\bar u_1,\bar u_2) & \dots & g^{c}_{k_1 j}(\bar u_1,\bar t') \\ g^{<}_{l_1 i_1}(\bar u_1,\bar u_1) & g^{<}_{l_1 j_1}(\bar u_1,\bar u_1) & g^{c}_{l_1 i_2}(\bar u_1,\bar u_2) & \dots & g^{c}_{l_1 j}(\bar u_1,\bar t') \\ g^{c}_{k_2 i_1}(\bar u_2,\bar u_1) & g^{c}_{k_2 j_1}(\bar u_2,\bar u_1) & g^{<}_{k_2 i_2}(\bar u_2,\bar u_2) & \dots & g^{c}_{k_2 j}(\bar u_2,\bar t') \\ \dots & \dots & \dots & \dots & \dots \\ g^{c}_{k_n i_1}(\bar u_n,\bar u_1) & g^{c}_{k_n j_1}(\bar u_n,\bar u_1) & g^{c}_{k_n i_2}(\bar u_n,\bar u_2) & \dots & g^{c}_{k_n j}(\bar u_n,\bar t') \\ g^{c}_{l_n i_1}(\bar u_n,\bar u_1) & g^{c}_{l_n j_1}(\bar u_n,\bar u_1) & g^{c}_{l_n i_2}(\bar u_n,\bar u_2) & \dots & g^{c}_{l_n j}(\bar u_n,\bar t') \\ g^{c}_{i i_1}(\bar t,\bar u_1) & g^{c}_{i j_1}(\bar t,\bar u_1) & g^{c}_{i i_2}(\bar t,\bar u_2) & \dots & g^{c}_{ij}(\bar t,\bar t') \end{pmatrix}$$

→ Expand the determinant over the last raw.
(all times in a single calculation)

$$G^{aa'}_{xx'}(t,t') = g^{aa'}_{xx'}(t,t') + \int du \sum_{b,y} (-1)^b g^{ab}_{xy}(t,u) K^{ba'}_{yx'}(u,t')$$

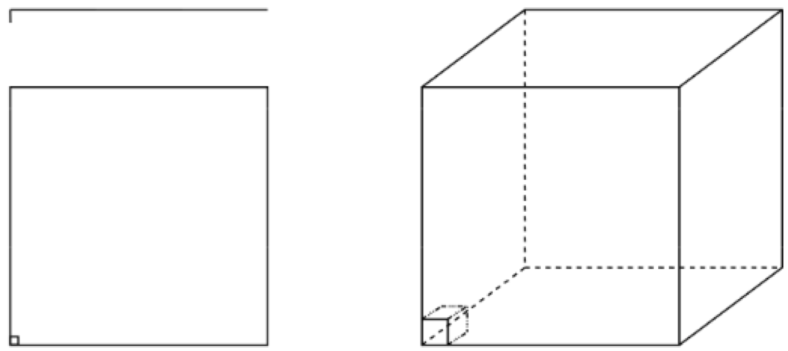
BARE DATA



$\times 10^{-2}$
$n = 2$
$\Gamma^3 G_2$
2
0
−2
Real
Imag
$\times 10^{-5}$
$n = 6$
$\Gamma^7 G_6$
2
0
−2
$\times 10^{-3}$
$n = 4$
$\Gamma^5 G_4$
0.5
0.0
−0.5
−5
0
5
ω/Γ
$\times 10^{-6}$
$n = 8$
$\Gamma^9 G_8$
1
0
−1
−5
0
5
ω/Γ

PROBLEM #2 THE N DIMENSIONAL INTEGRAL

→ The dimensionality curse



$$F(U) = \sum_{n=0}^{\infty} F_n U^n,$$

$$F_n = \int d^n\boldsymbol{u}\, f_n(u_1, u_2, \ldots, u_n).$$

The standard approach: Metropolis Monte-Carlo.

→ Intrinsic very slow convergence $N^{-1/2}$ (in one dimension: $1/N^{15}$or even exponential)

→ We do not build any knowledge of f(u)

MACHINE LEARNING THE INTEGRAND

$$f_n(u_1..u_n) \approx p_n(u_1...u_n)$$

Special class of warper functions that we know how to integrate

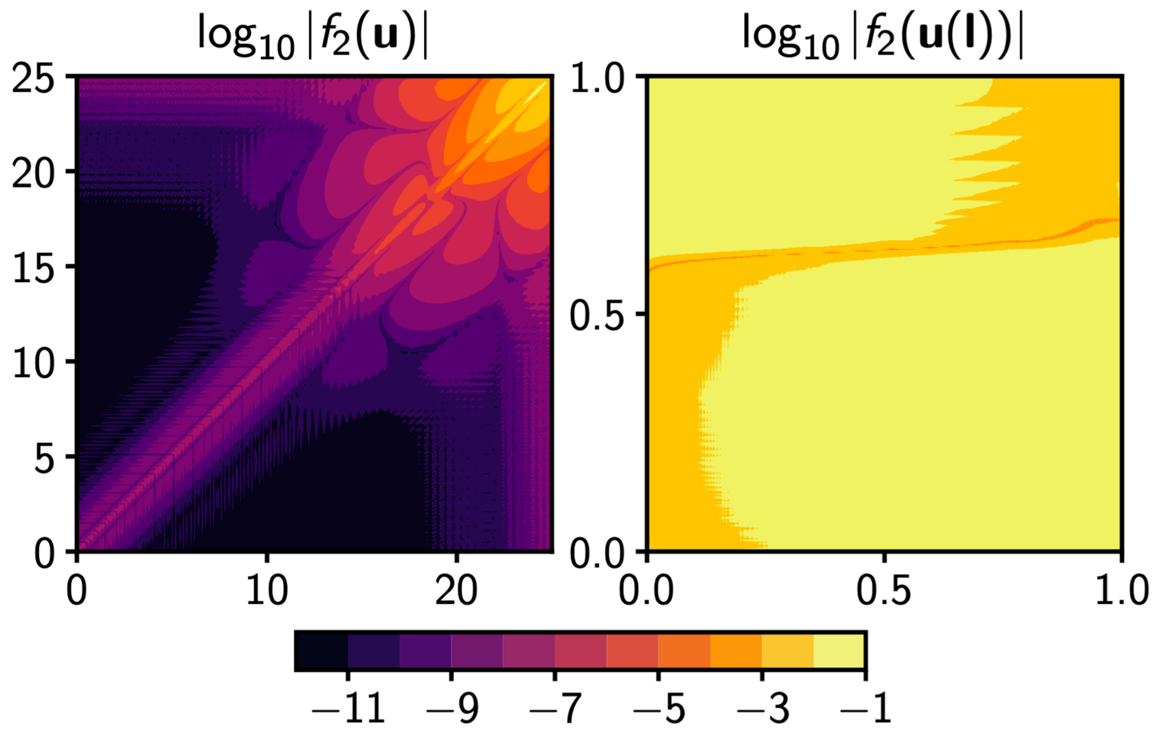
Construct a change of variable $\boldsymbol{u}(\boldsymbol{x})$ such that $\dfrac{\partial \mathbf{u}}{\partial \mathbf{x}} = \dfrac{1}{p_n(u_1...u_n)}$

$$F_n = \int_{[0,1]^n} d^n\boldsymbol{x}\, f_n[\boldsymbol{u}(\boldsymbol{x})] \left| \frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}} \right|$$

And get an almost constant integrand

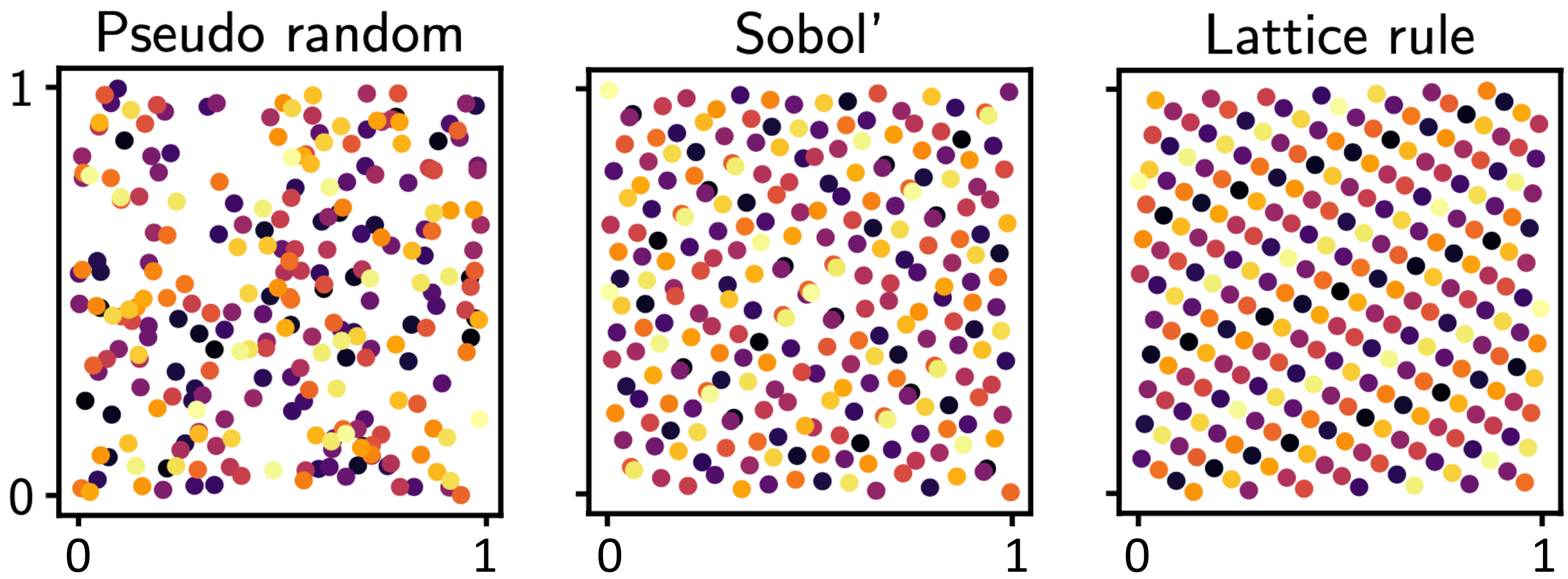
$$p_n(\mathbf{u}) = \prod_{i=1}^{n} h^{(i)}(v_i),$$

$$v_i = u_{i-1} - u_i,$$

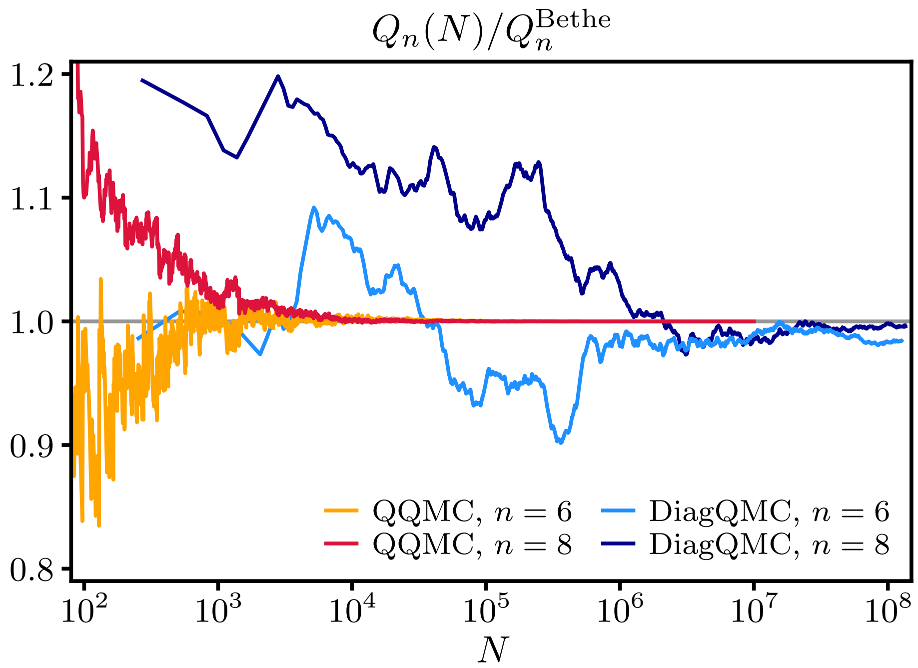


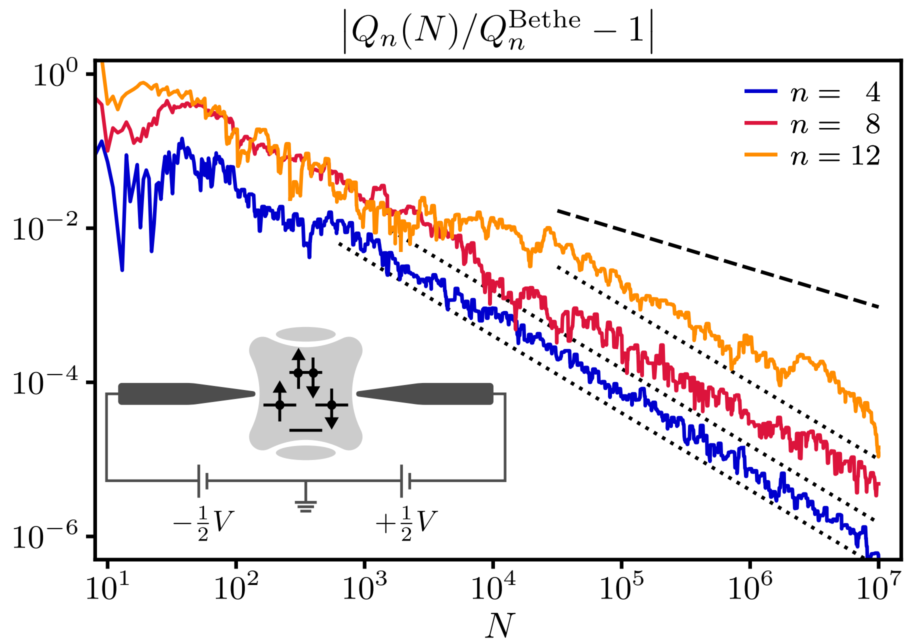
Coming up soon: $$p_n(\boldsymbol{u}) = h_a^{(1)}(v_1)h_{ab}^{(2)}(v_2)\cdots h_{cd}^{(n-1)}(v_{n-1})h_d^{(n)}(v_n)$$

USE QUASI RANDOM NUMBERS TO ESTIMATE THE INTEGRAL



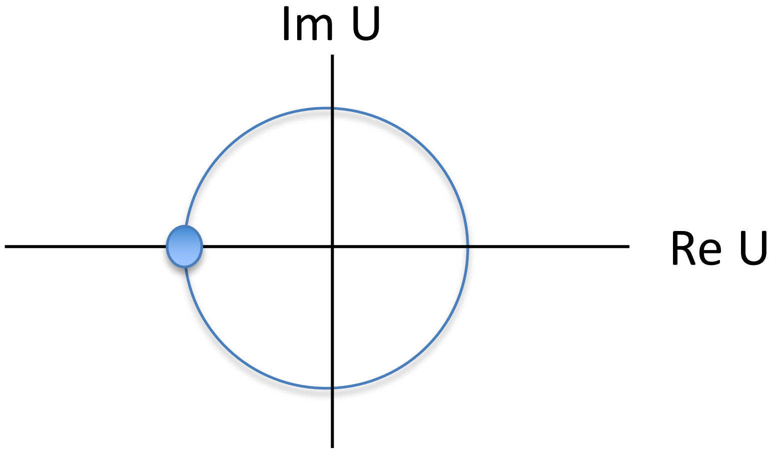
ENJOY THE SPEED-UP

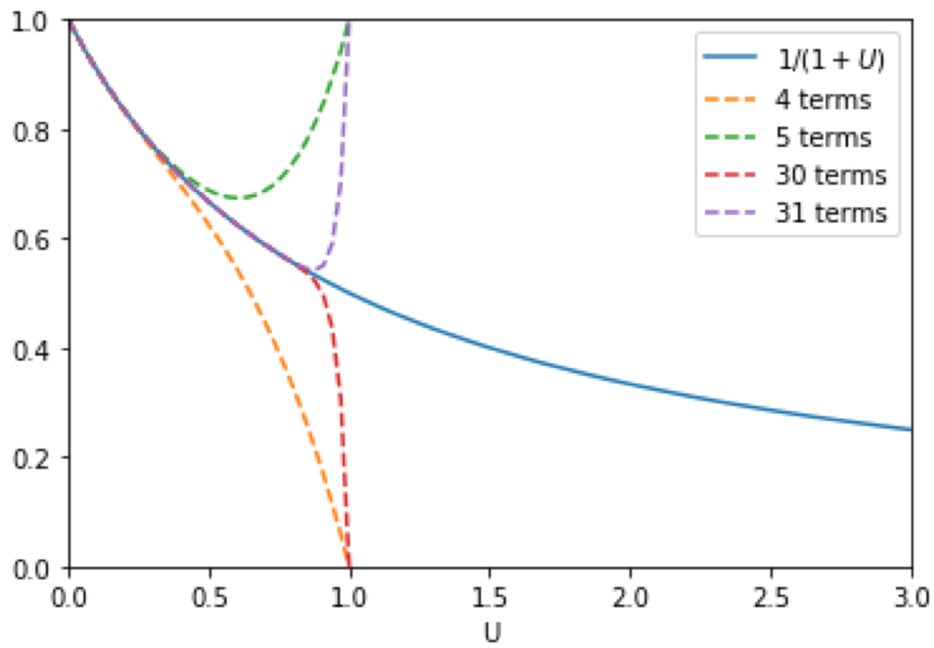




PROBLEM #3: RECONSTRUCTION.

$$\frac{1}{1+U} = \sum_n (-1)^n U^n$$

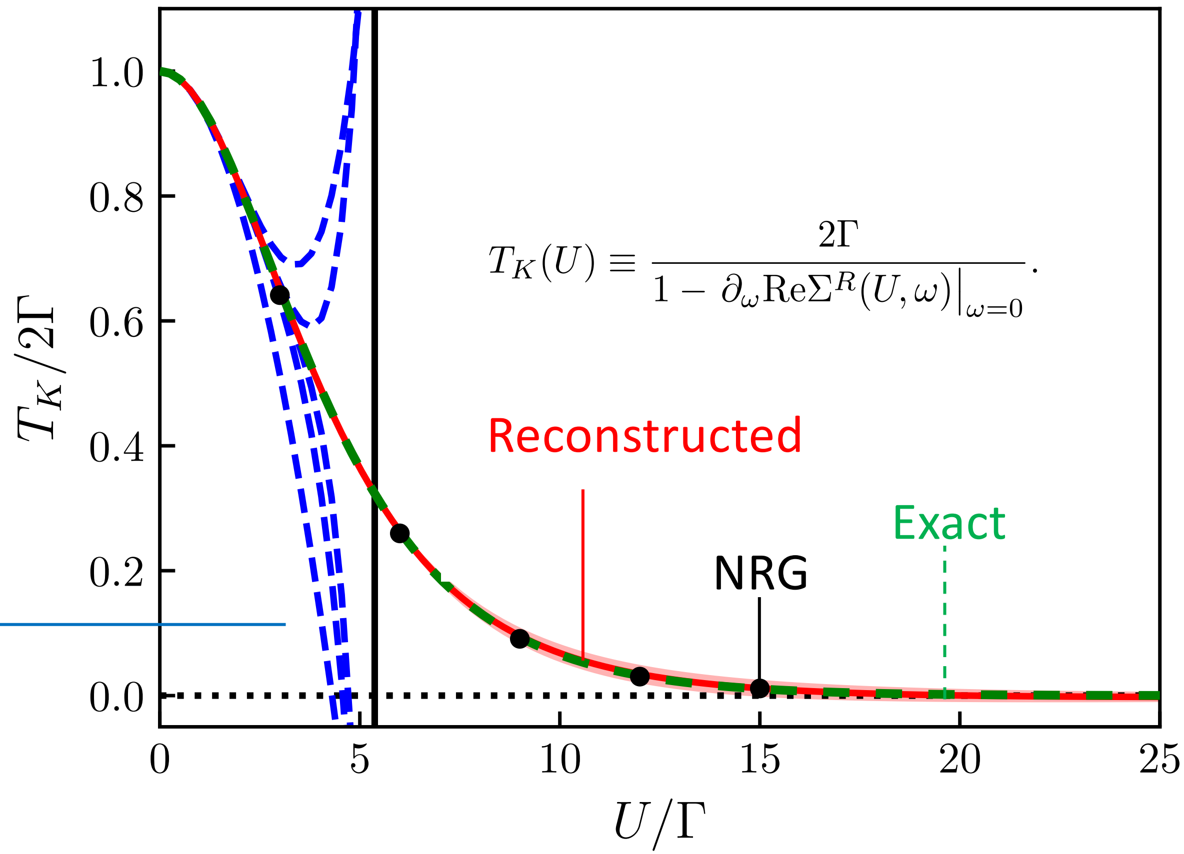




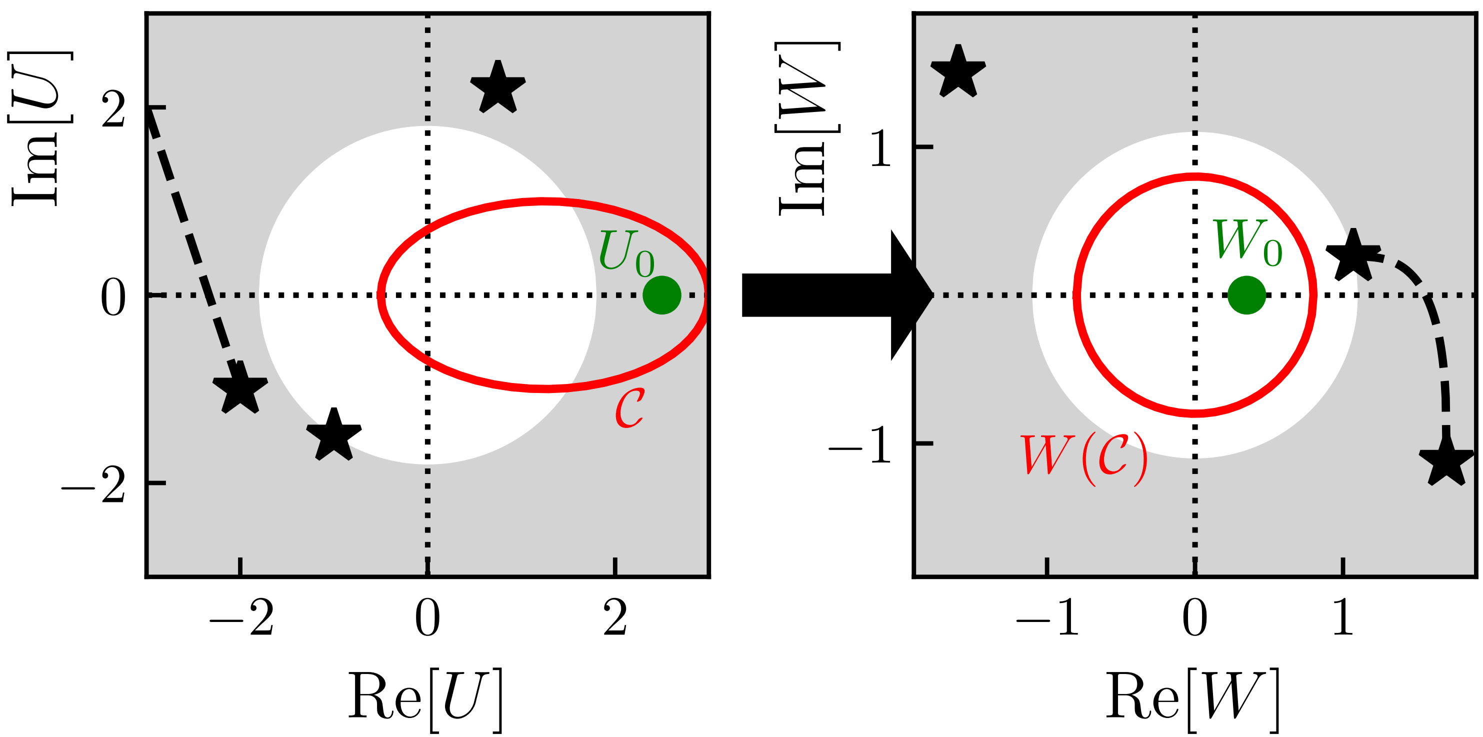
PROBLEM #3: RECONSTRUCTRING F(U) FROM F_N

$$F(U) = \sum_n F_n U^n$$

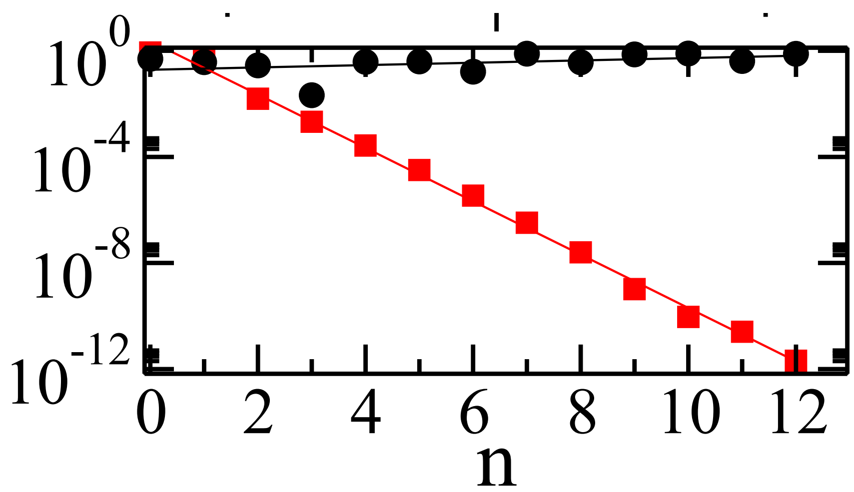
Truncated sum

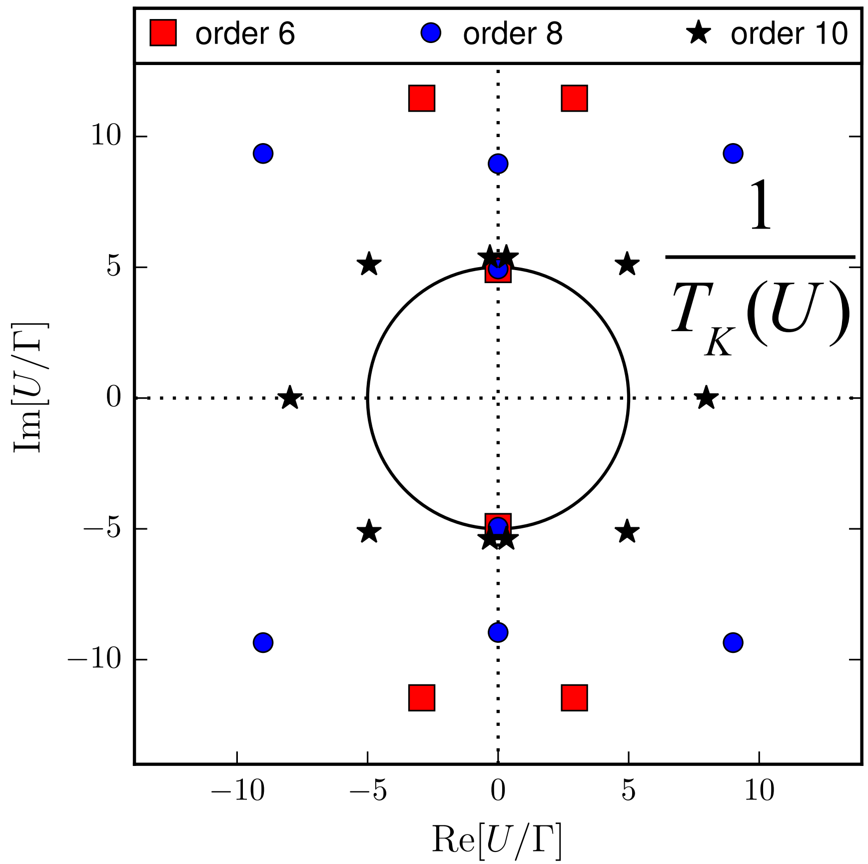


SEPARATION PROPERTY HYPOTHESIS

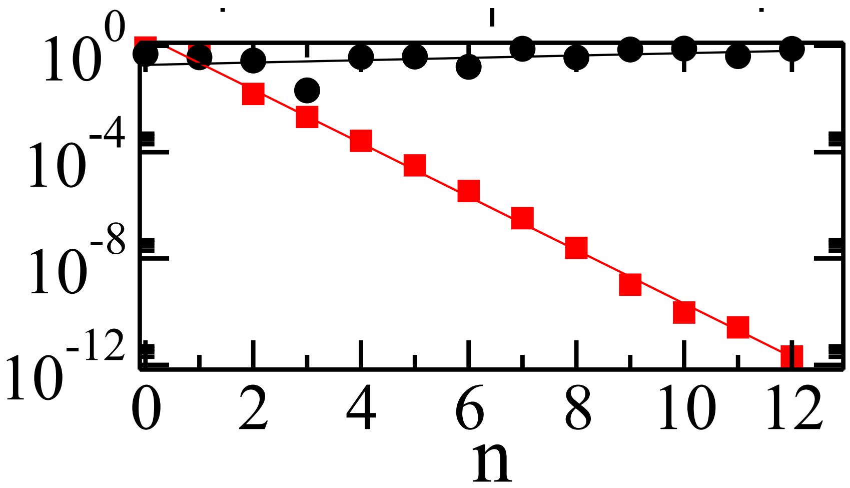


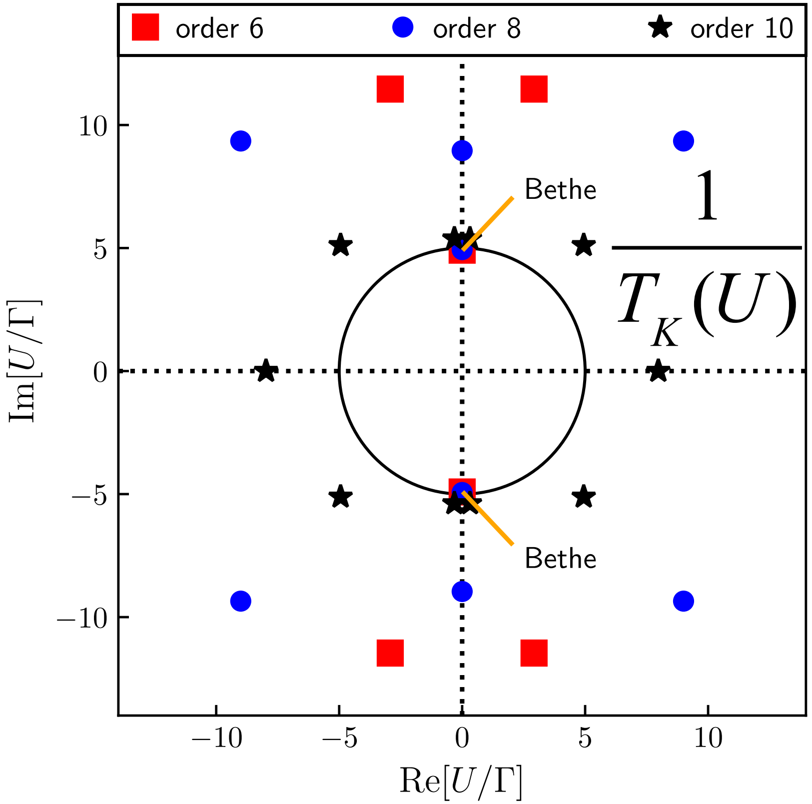
1) FIND THE POLES / ZEROS OF THE INVERSE



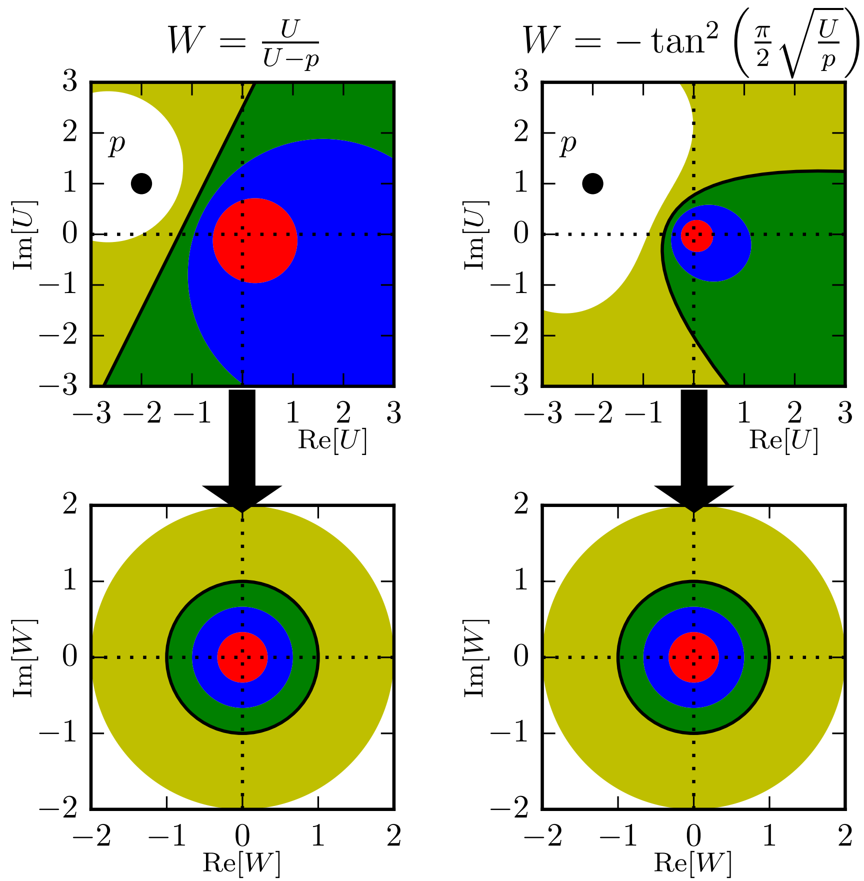


1) FIND THE POLES / ZEROS OF THE INVERSE





2) DESIGN THE CONFORMAL TRANSFORM



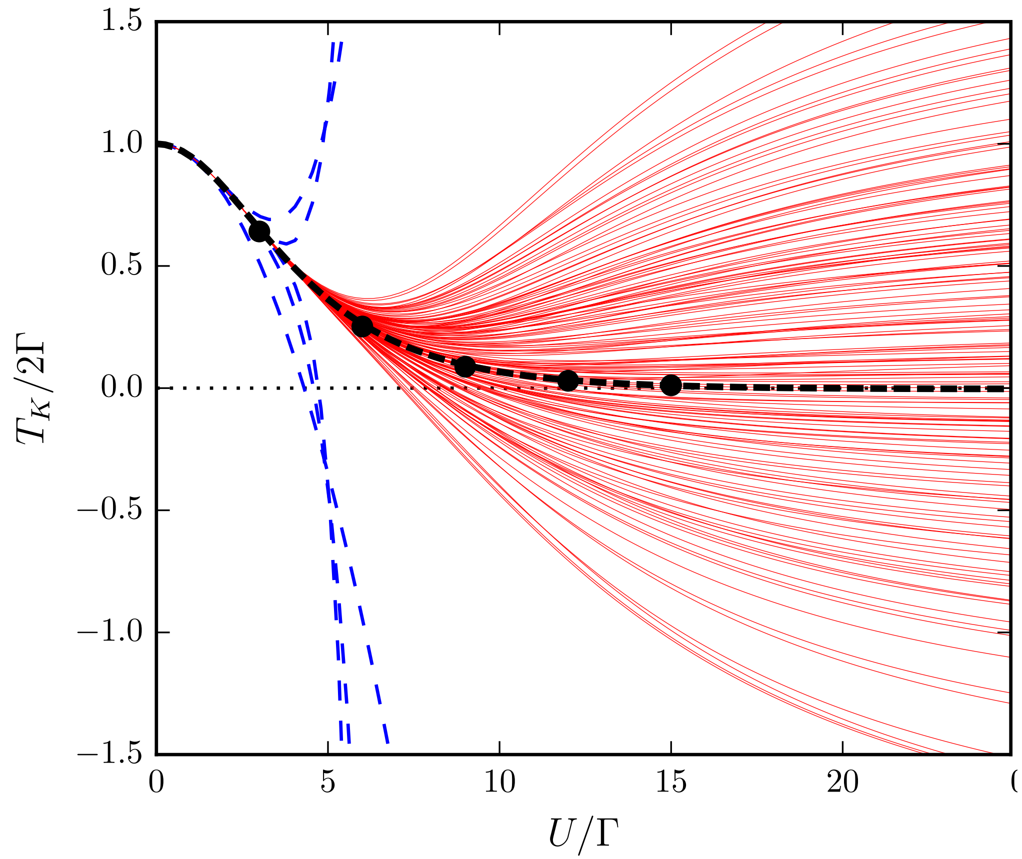
$$F(U(W)) = \sum_n \bar{F}_n W^n$$

W(U): exact

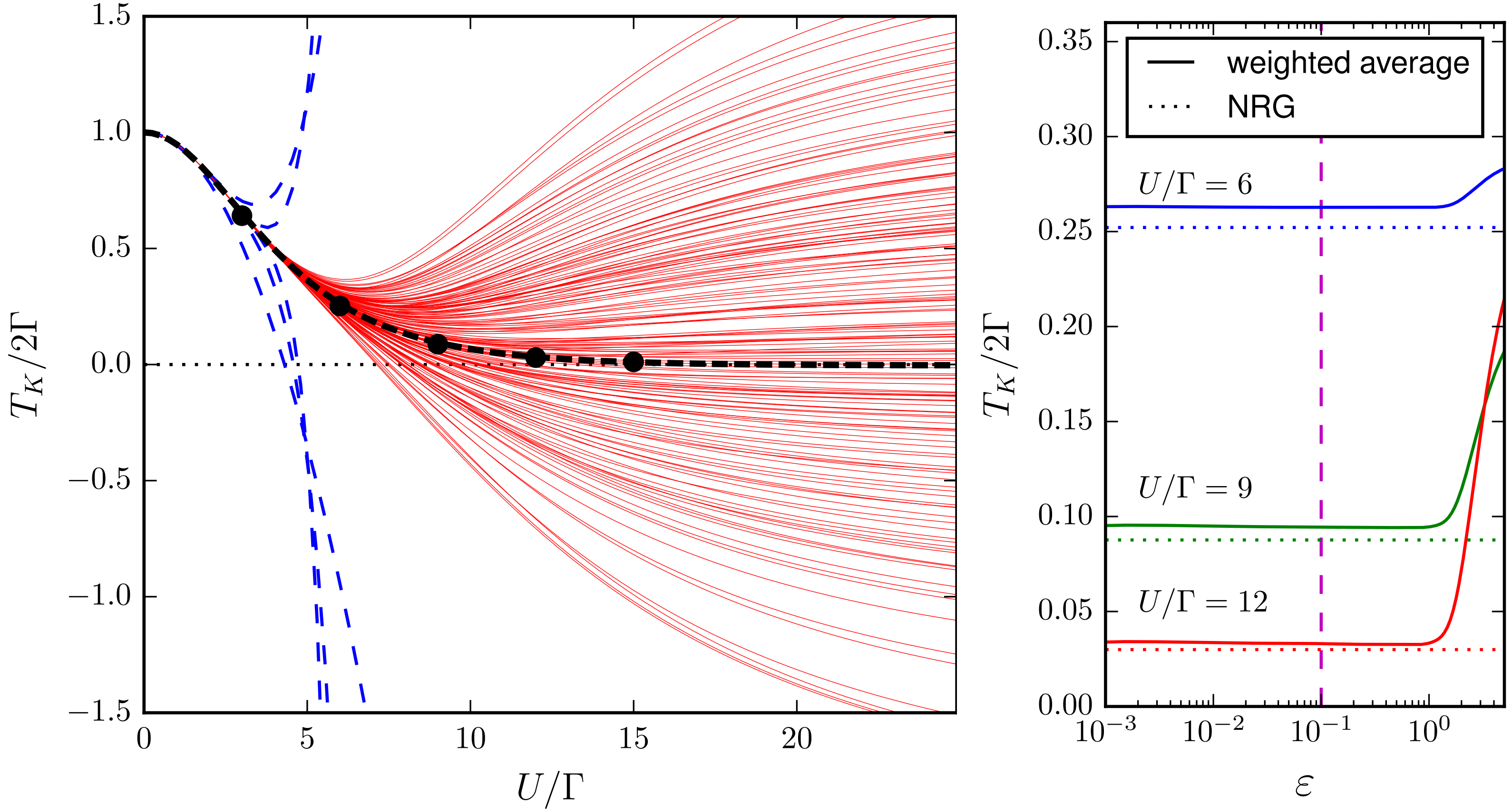
U(W): truncated

$$F(U) = \sum_n \bar{F}_n [W(U)]^n$$

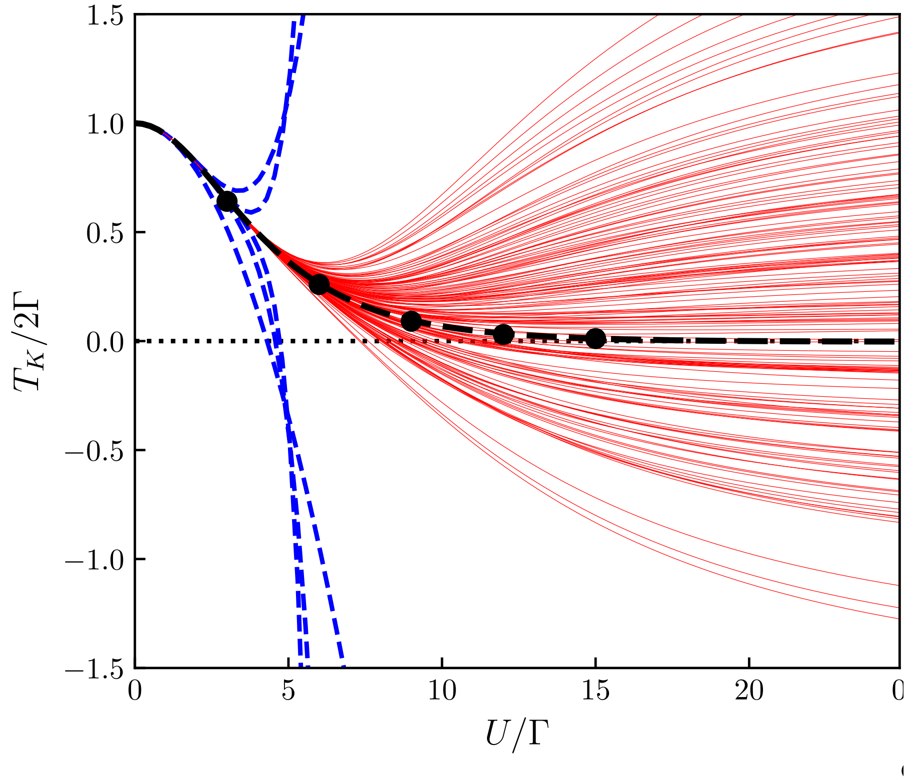
3) ADD BAYESIAN INFERENCE

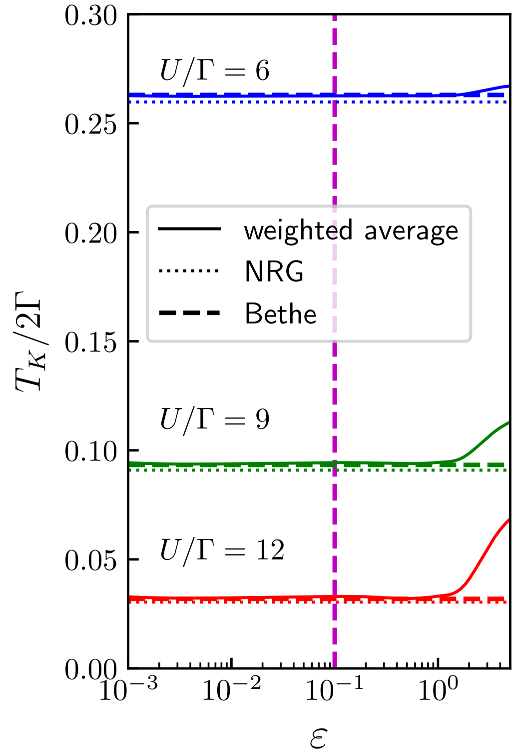


3) ADD BAYESIAN INFERENCE



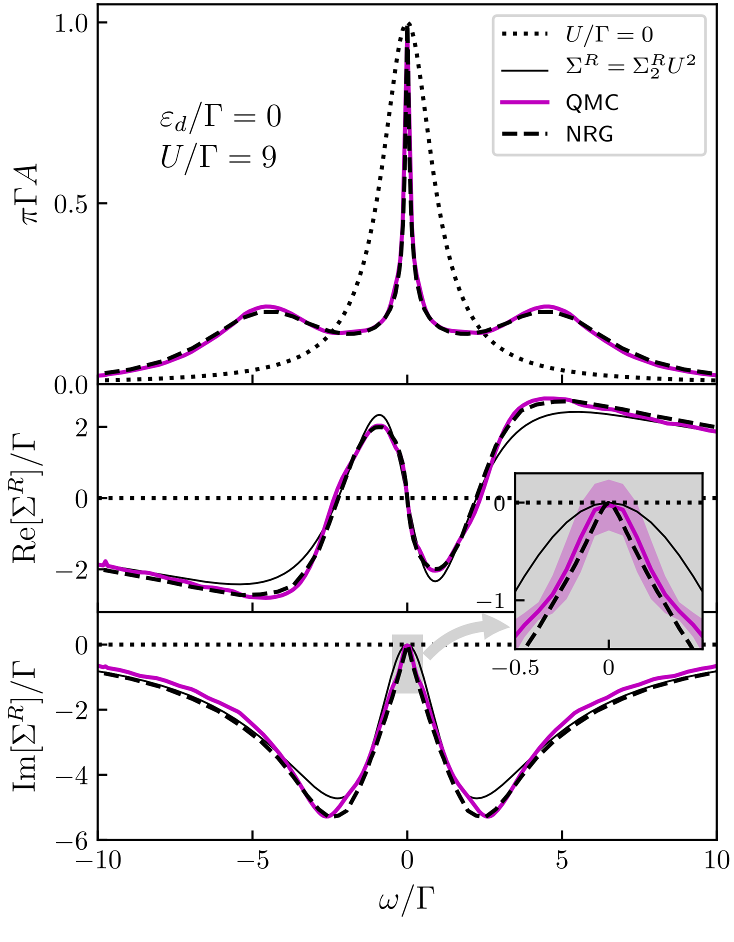
3) ADD BAYESIAN INFERENCE

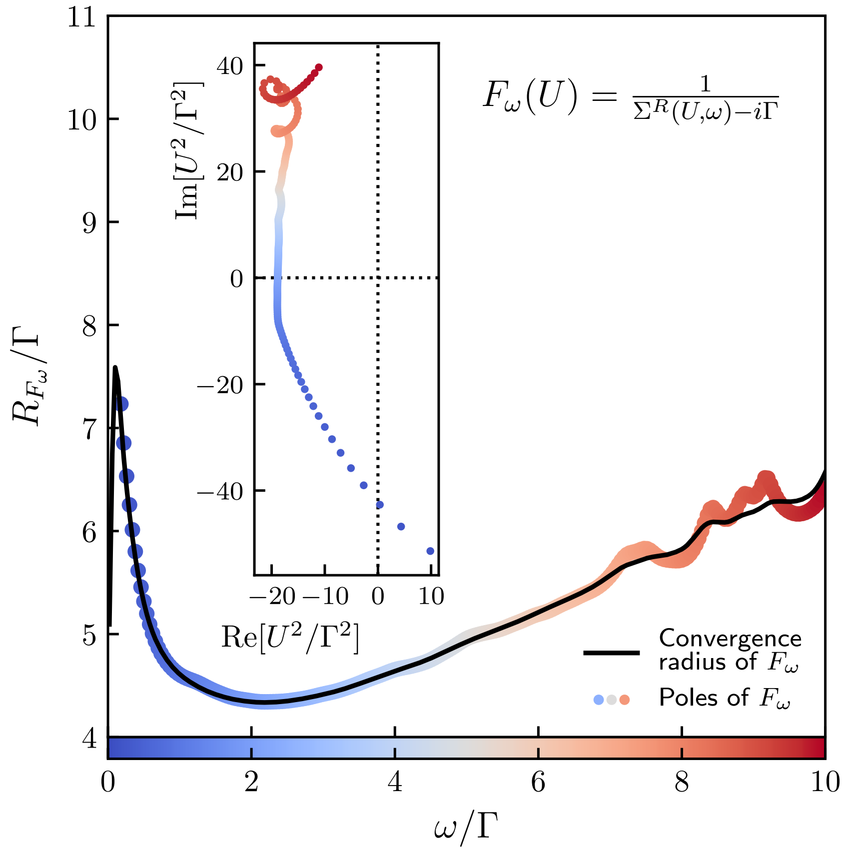




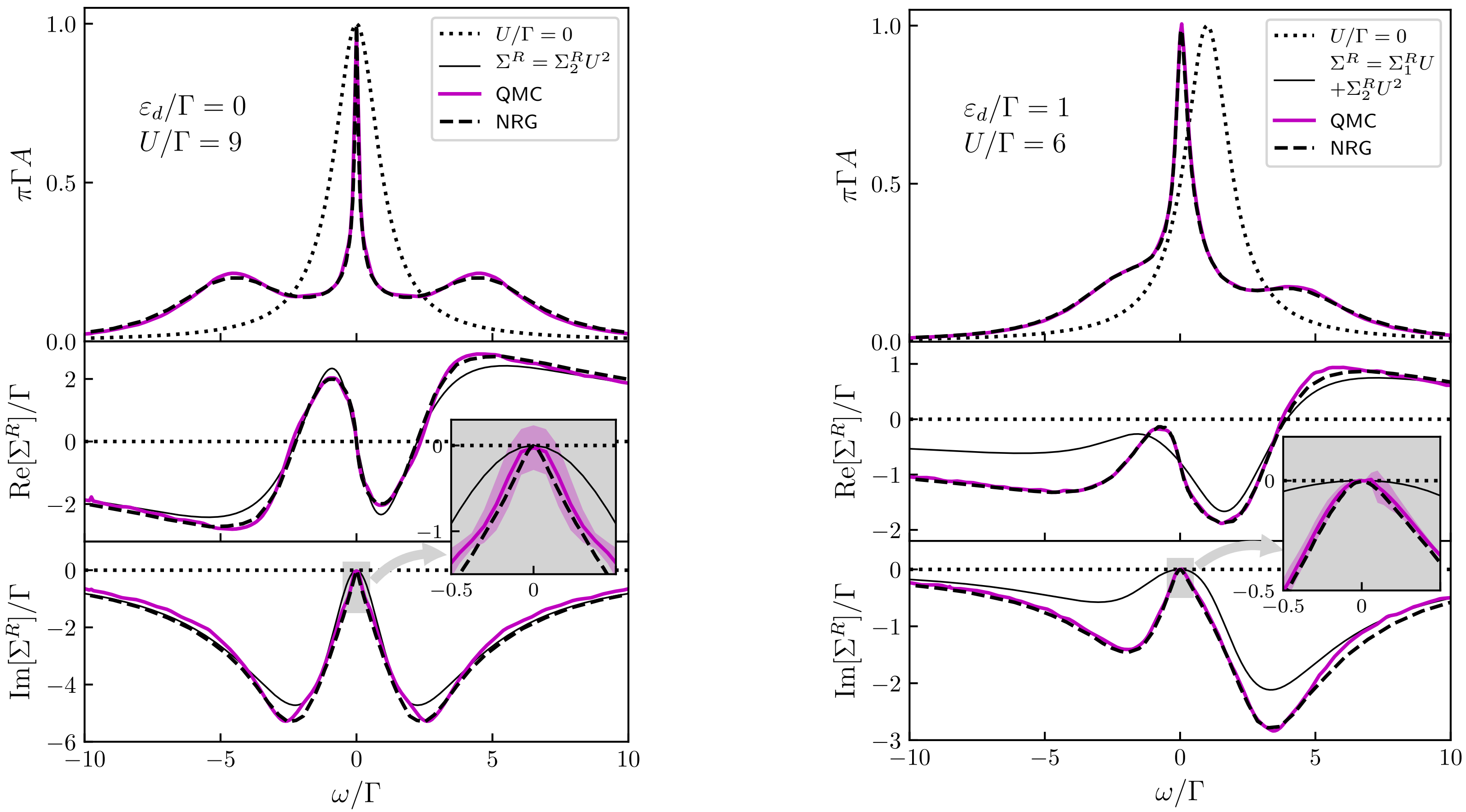
(Rq: NRG changed not QMC)

SOME EQUILIBRIUM BENCHMARKS

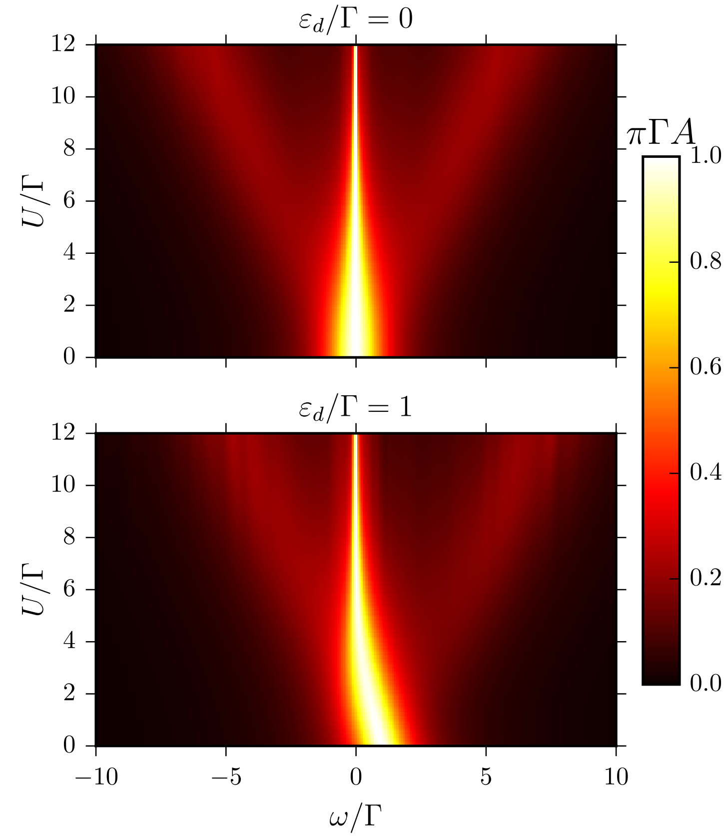




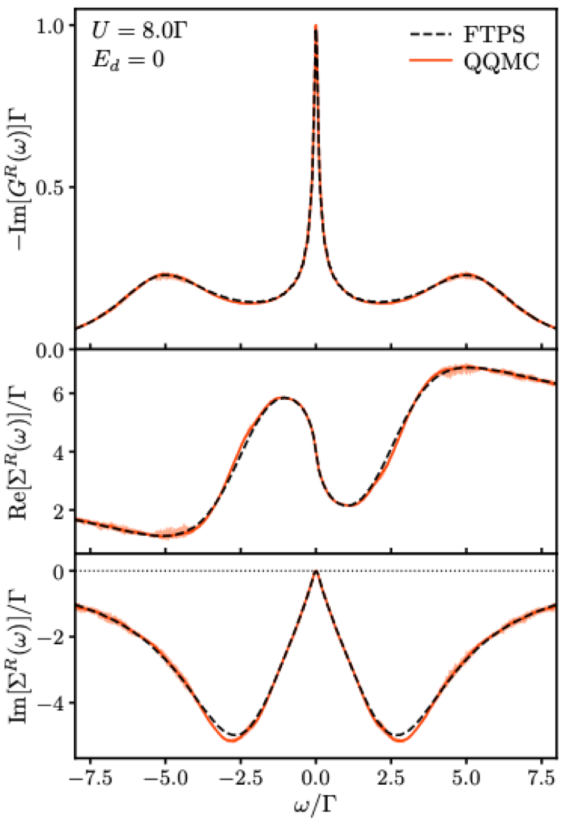
SOME EQUILIBRIUM BENCHMARKS

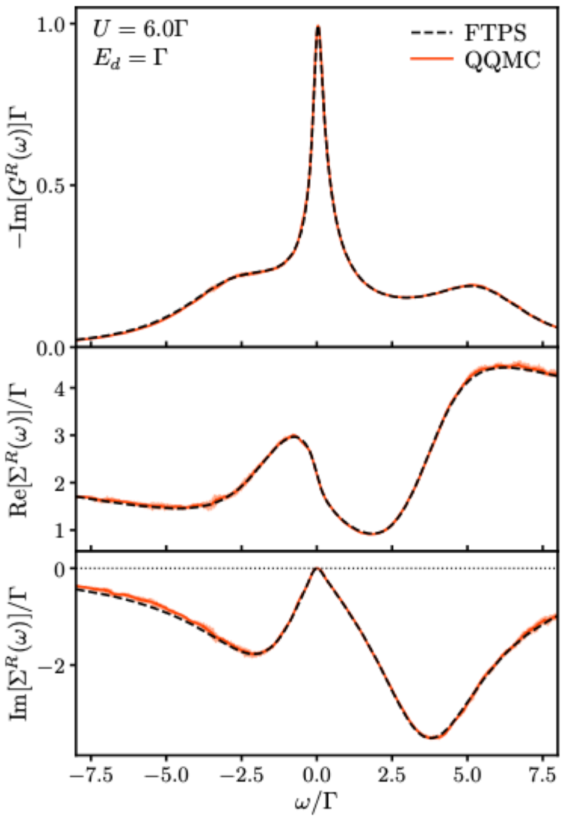


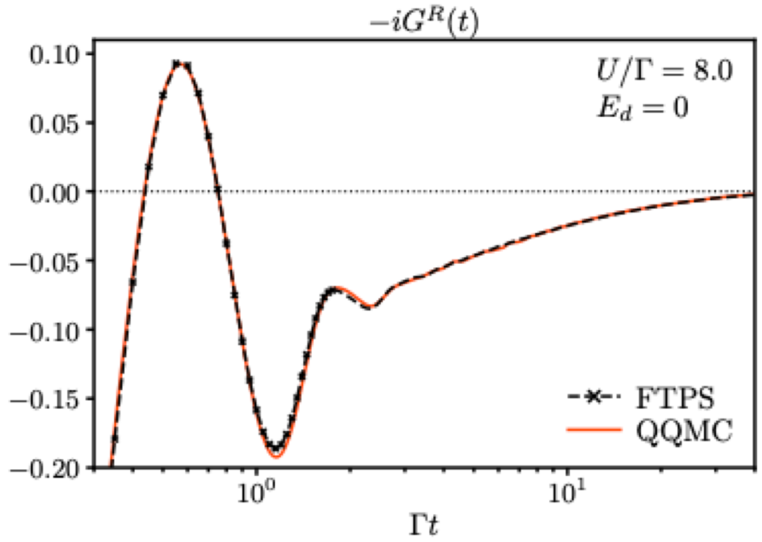
SOME EQUILIBRIUM BENCHMARKS



SOME EQUILIBRIUM BENCHMARKS



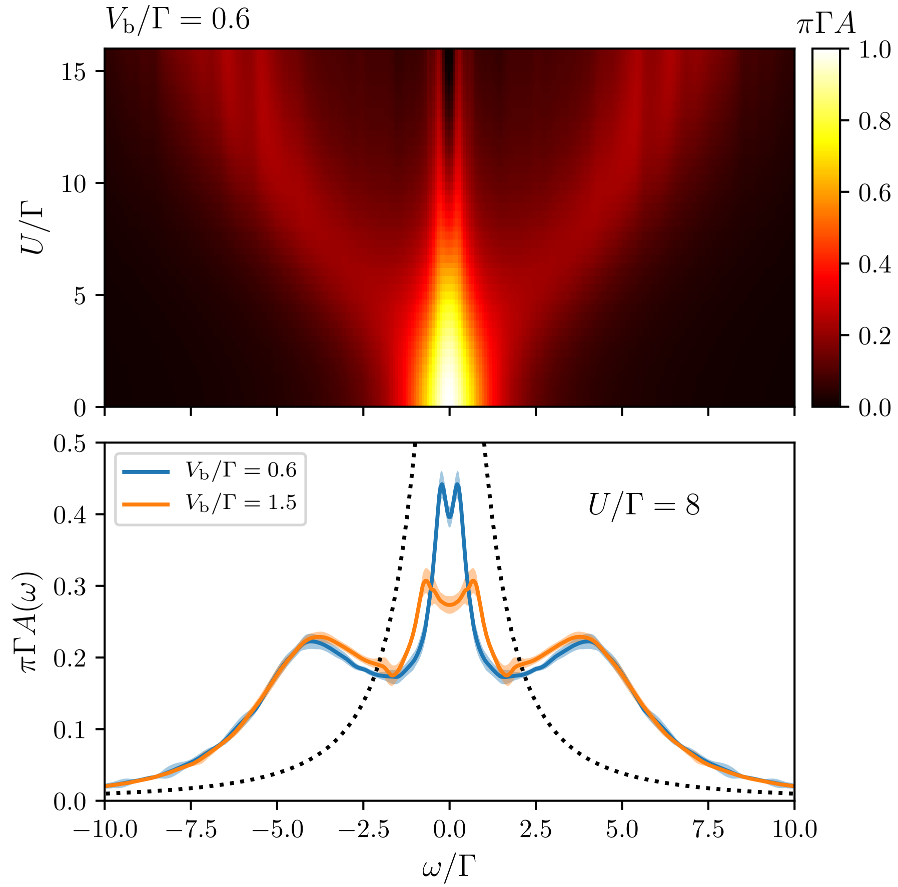


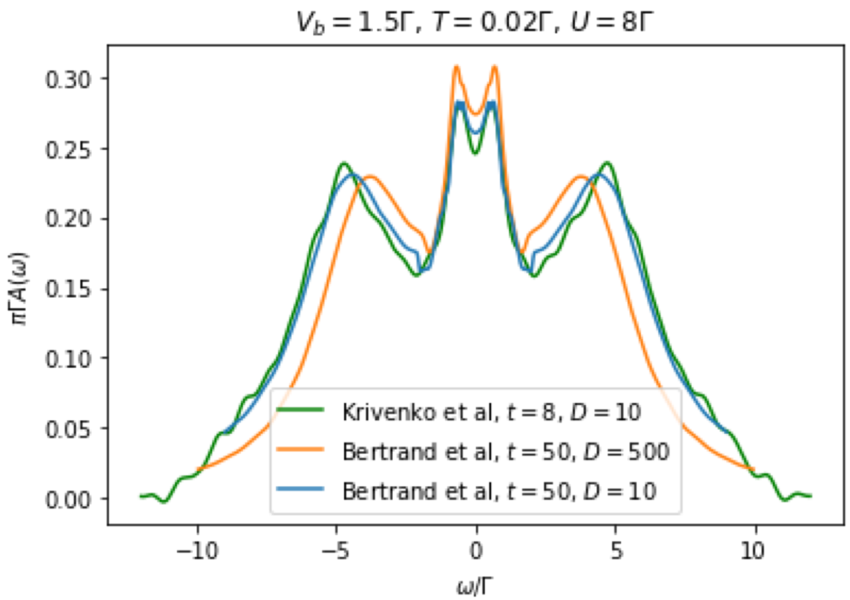


AND BACK TO NON-EQUILIBRIUM

Igor Krivenko,[1] Joseph Kleinhenz,[1] Guy Cohen,[2,*] and Emanuel Gull

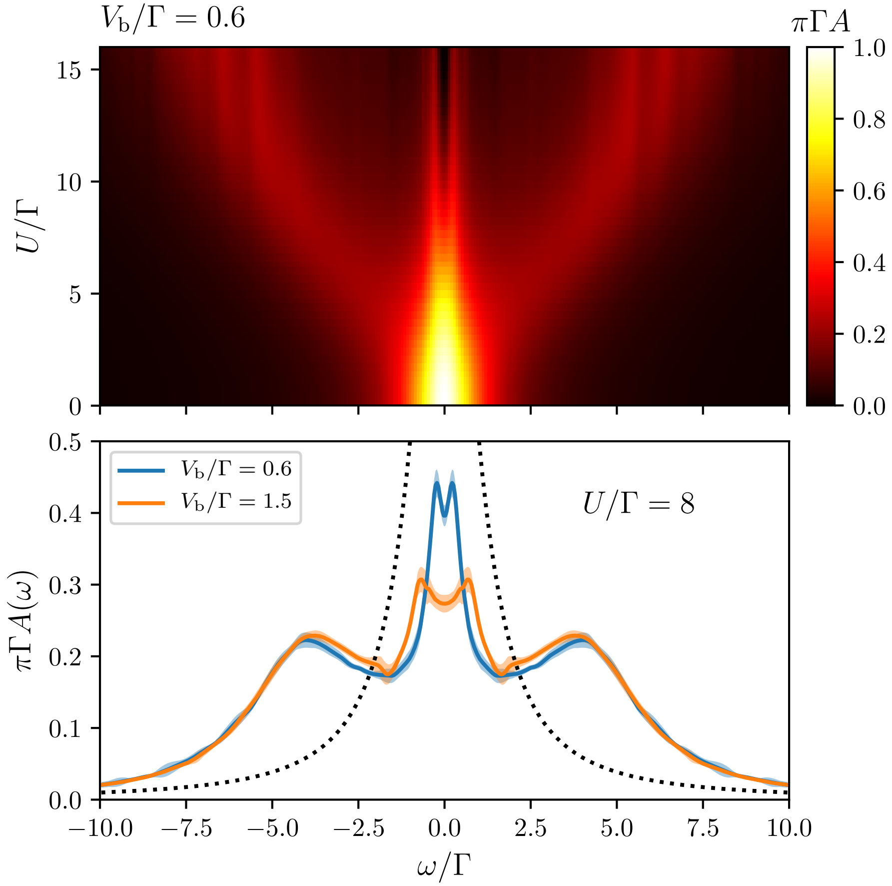
arXiv:1904.11527v1

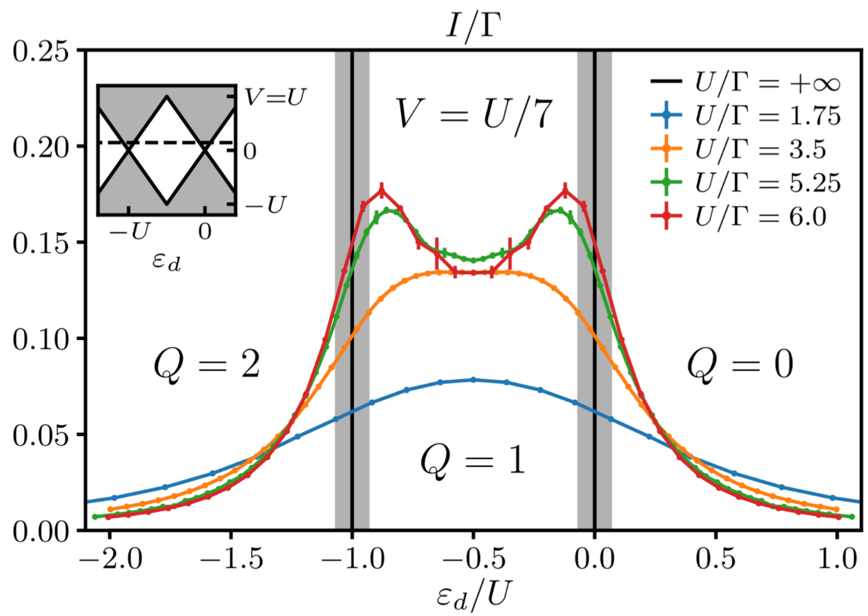




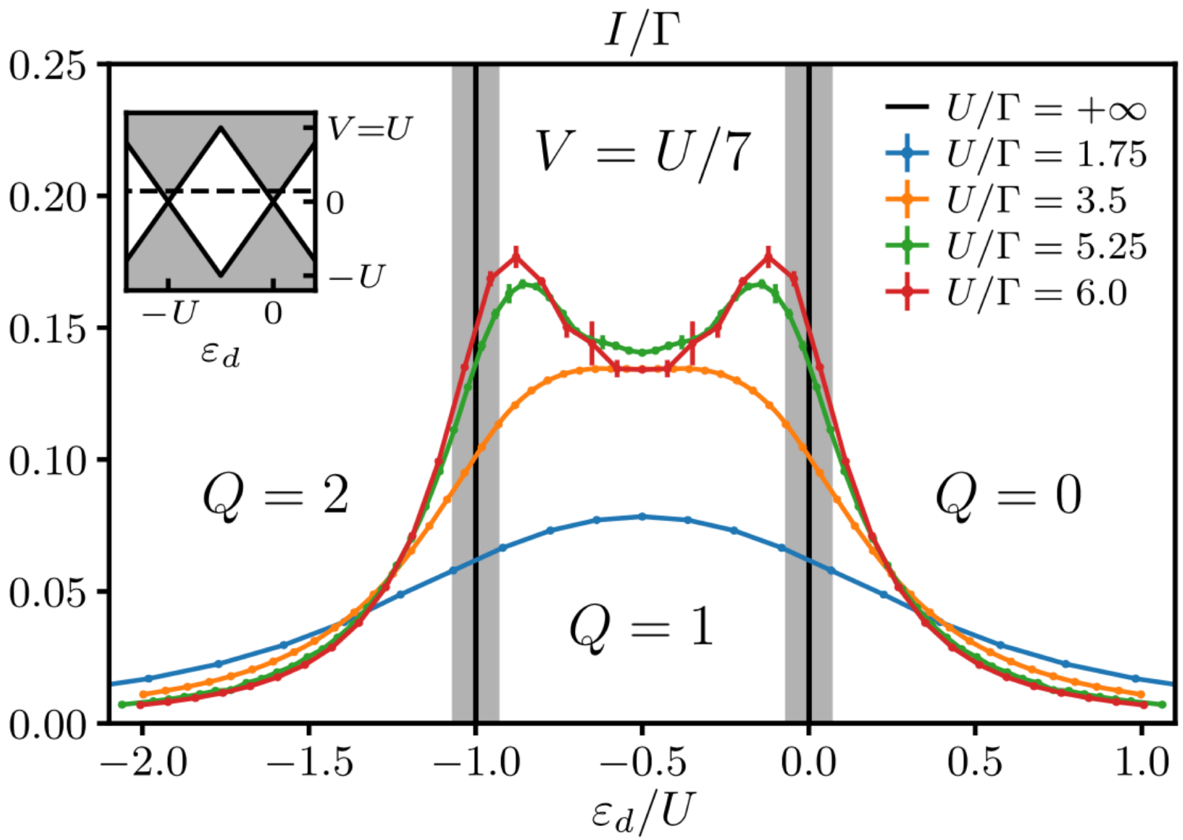
(PRELIMINARY COMPARAISON DIFFERENT BATH AND TIMES)

AND BACK TO NON-EQUILIBRIUM

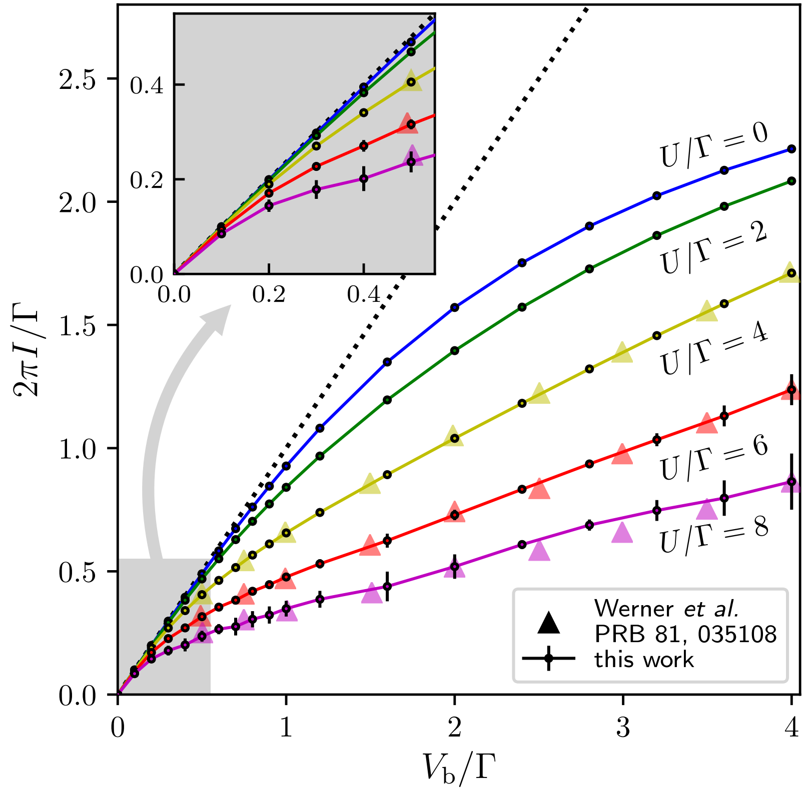


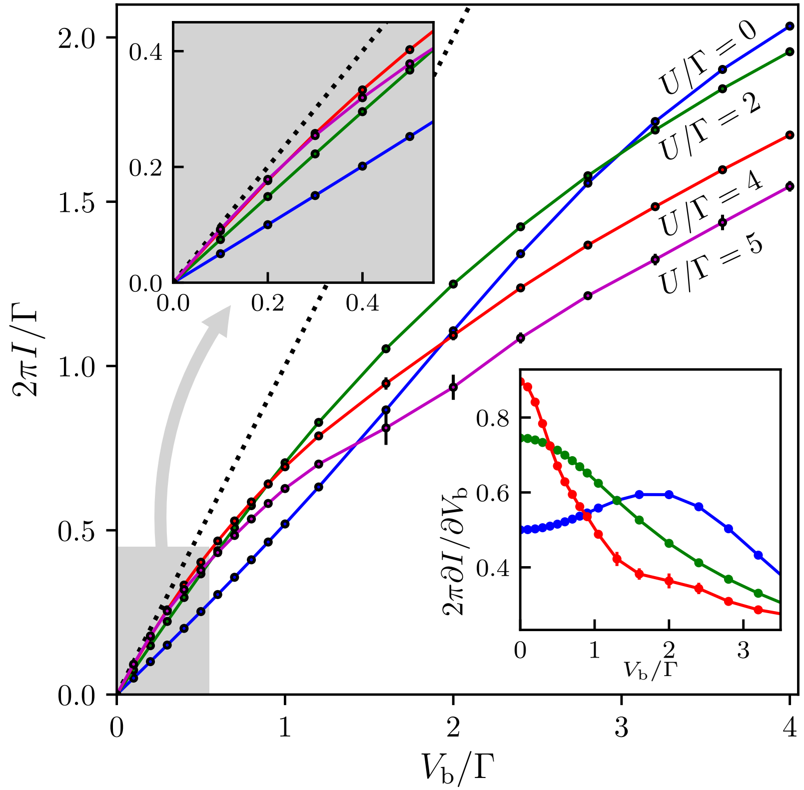


AND BACK TO NON-EQUILIBRIUM



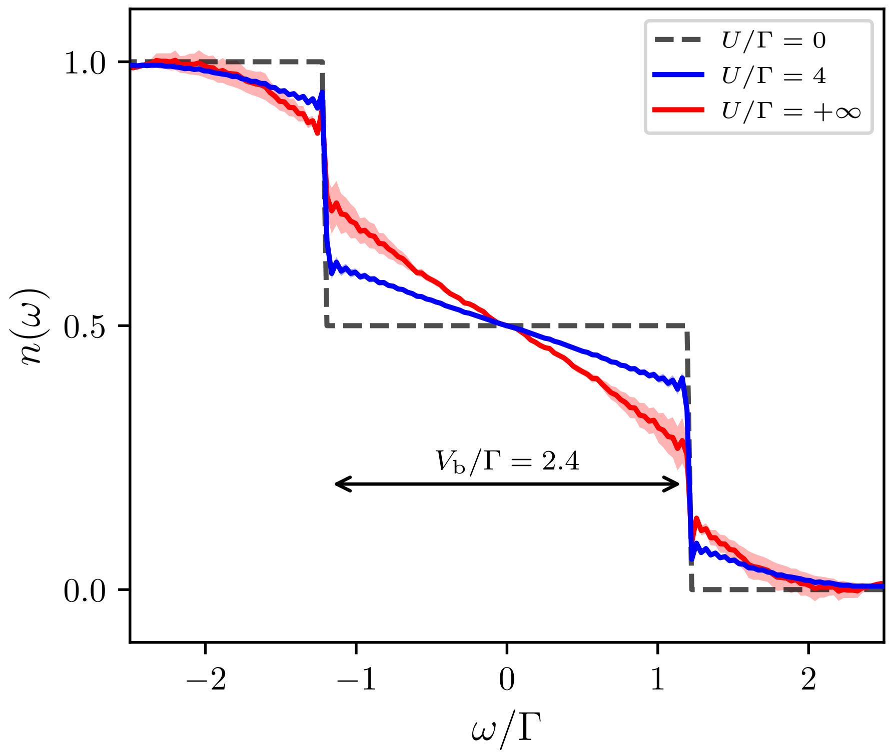
AND BACK TO NON-EQUILIBRIUM





NON-EQUILIBRIUM DISTRIBUTION FUNCTION

$$n(\omega) = \frac{iG^{<}(\omega)}{2\,\mathrm{Im}[G^R(\omega)]}$$



CONCLUSION

MORE TECHNICAL PROGRESS NEEDED

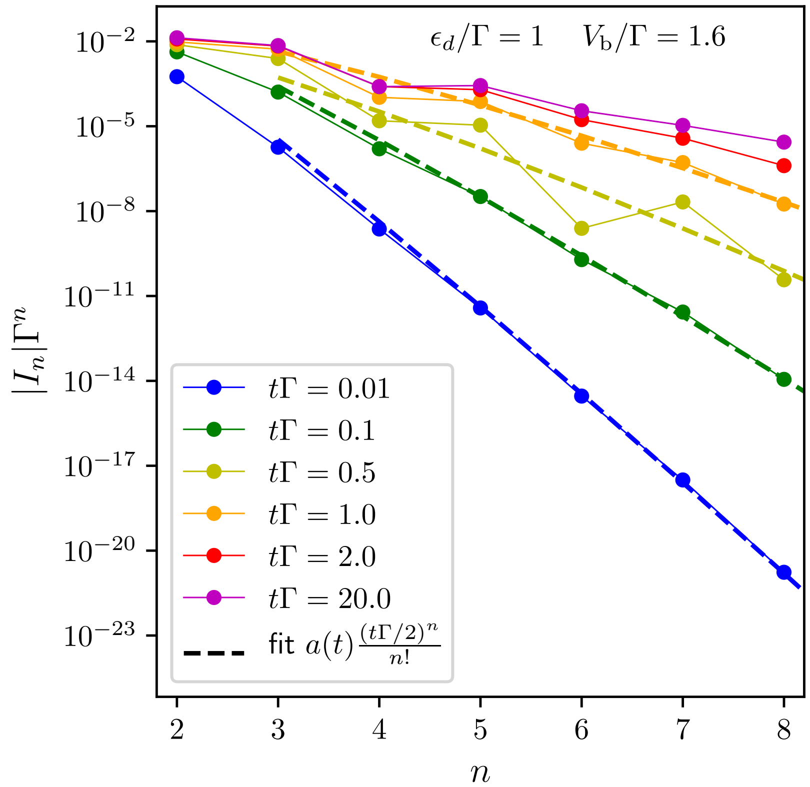
- Improved sampling & implementation (coming up soon)
- Terms and Counter-terms

MORE APPLICATIONS

- Lattice (in progress)
- DMFT (also in progress)
- Nanoelectronics (0.7 anomaly)
- Few qubits & their baths
- Eventually an open source software

PHYSICAL REVIEW LETTERS **125,** 047702 (2020)
PHYSICAL REVIEW X **9,** 041008 (2019)
PHYSICAL REVIEW B **100**, 125129 (2019)
PHYSICAL REVIEW B **91**, 245154 (2015)

A WARNING ON CONVERGENCE RADIUS



We work directly in the stationary limit

$$\lim_{n\to\infty}\lim_{t\to\infty} O_n(t) \neq \lim_{t\to\infty}\lim_{n\to\infty} O_n(t)$$