

RECENT PROGRESS IN REAL TIME DIAGRAMMATIC MONTE-CARLO

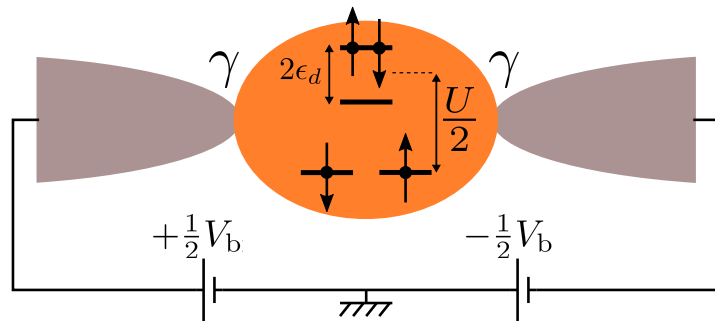
Xavier WAIN TAL,

CEA Grenoble, Pheligs IRIG

With CORENTIN BERTRAND, Olivier Parcollet, and Serge Florens

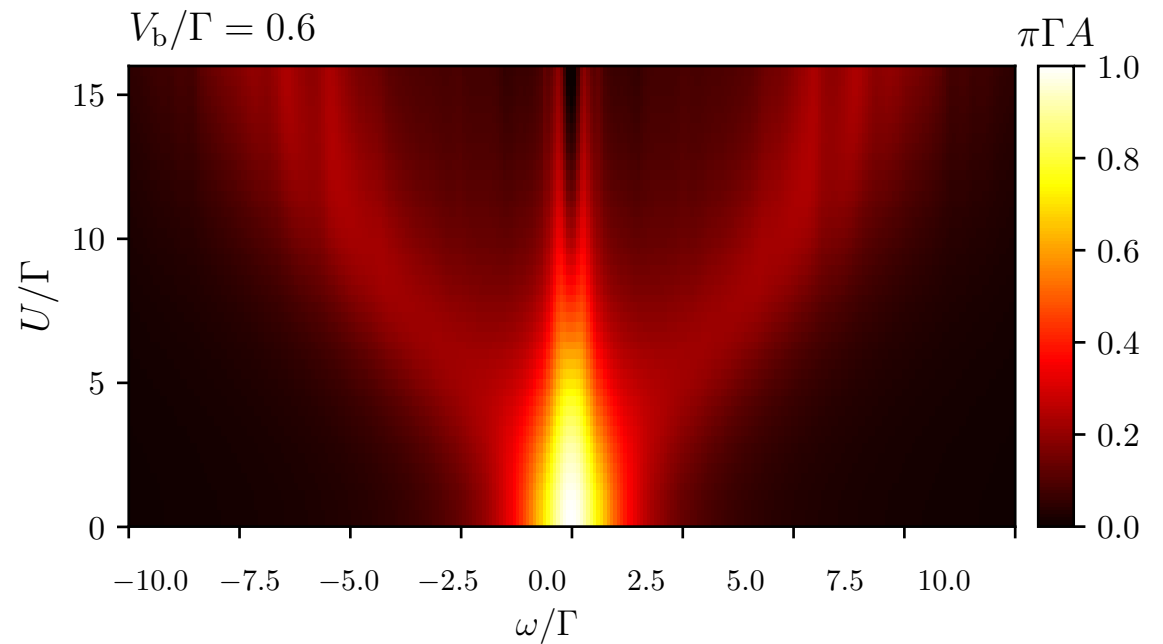
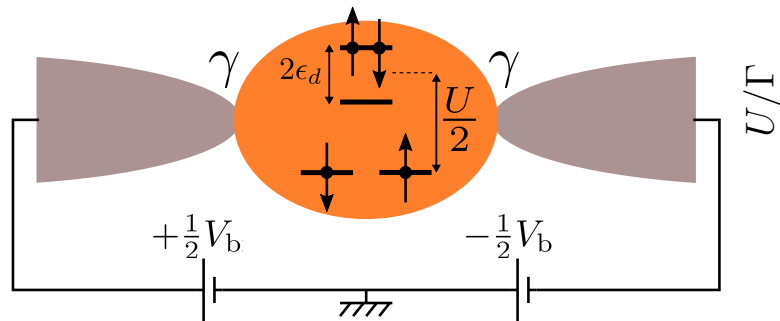
ARXIV: 1903.11646

THE OUT-OF-EQUILIBRIUM ANDERSON IMPURITY



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

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OUTLINE

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

- HOW TO CALCULATE THE F_n ?

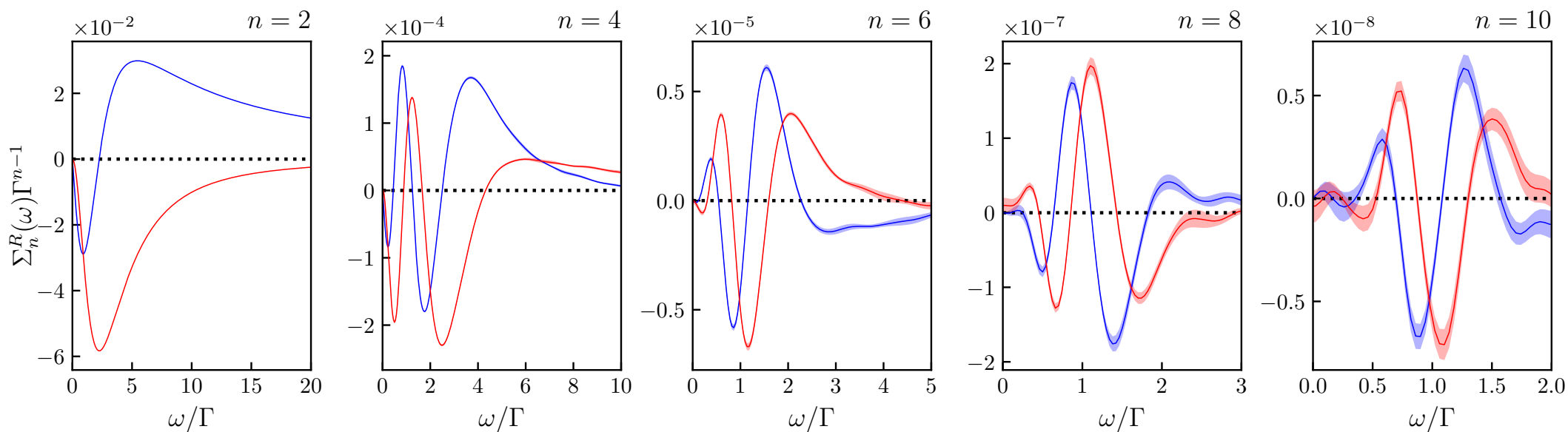
(Alternative: expansion in power of hybridization, see Gull & Cohen)

- HOW TO RECONSTRUCT $F(U)$ FROM THE F_n ?

TAKE THE ANALYTICAL STRUCTURE OF $F(U)$ SERIOUSLY

- BACK TO THE ANDERSON IMPURITY

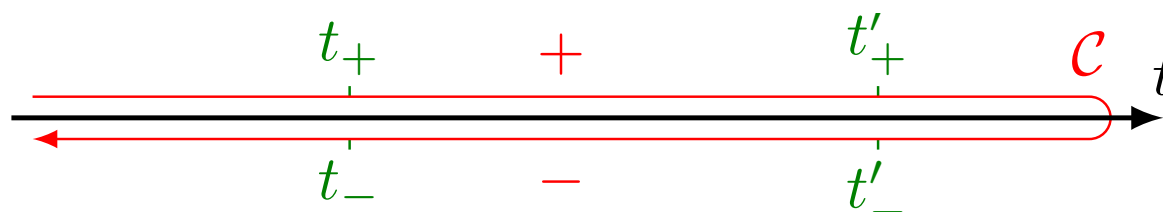
HOW TO CALCULATE THE F_N ?



KELDYSH FORMALISM IN A NUTSHELL

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

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



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

1) BARE EXPANSION

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

2ⁿ sum cancels
disconnected
diagrams

$$\mathbf{M}_n = \begin{pmatrix} g_{k_1 i_1}^<(\bar{u}_1, \bar{u}_1) & g_{k_1 j_1}^<(\bar{u}_1, \bar{u}_1) & g_{k_1 i_2}^c(\bar{u}_1, \bar{u}_2) & \dots & g_{k_1 j}^c(\bar{u}_1, \bar{t}') \\ g_{l_1 i_1}^<(\bar{u}_1, \bar{u}_1) & g_{l_1 j_1}^<(\bar{u}_1, \bar{u}_1) & g_{l_1 i_2}^c(\bar{u}_1, \bar{u}_2) & \dots & g_{l_1 j}^c(\bar{u}_1, \bar{t}') \\ g_{k_2 i_1}^c(\bar{u}_2, \bar{u}_1) & g_{k_2 j_1}^c(\bar{u}_2, \bar{u}_1) & g_{k_2 i_2}^<(\bar{u}_2, \bar{u}_2) & \dots & g_{k_2 j}^c(\bar{u}_2, \bar{t}') \\ \dots & \dots & \dots & \dots & \dots \\ g_{k_n i_1}^c(\bar{u}_n, \bar{u}_1) & g_{k_n j_1}^c(\bar{u}_n, \bar{u}_1) & g_{k_n i_2}^c(\bar{u}_n, \bar{u}_2) & \dots & g_{k_n j}^c(\bar{u}_n, \bar{t}') \\ g_{l_n i_1}^c(\bar{u}_n, \bar{u}_1) & g_{l_n j_1}^c(\bar{u}_n, \bar{u}_1) & g_{l_n i_2}^c(\bar{u}_n, \bar{u}_2) & \dots & g_{l_n j}^c(\bar{u}_n, \bar{t}') \\ g_{ii_1}^c(\bar{t}, \bar{u}_1) & g_{ij_1}^c(\bar{t}, \bar{u}_1) & g_{ii_2}^c(\bar{t}, \bar{u}_2) & \dots & g_{ij}^c(\bar{t}, \bar{t}') \end{pmatrix}$$



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

Known non-interacting functions.

2) KERNEL EXPANSION

$$\mathbf{M}_n = \begin{pmatrix} g_{k_1 i_1}^<(\bar{u}_1, \bar{u}_1) & g_{k_1 j_1}^<(\bar{u}_1, \bar{u}_1) & g_{k_1 i_2}^c(\bar{u}_1, \bar{u}_2) & \dots & g_{k_1 j}^c(\bar{u}_1, \bar{t}') \\ g_{l_1 i_1}^<(\bar{u}_1, \bar{u}_1) & g_{l_1 j_1}^<(\bar{u}_1, \bar{u}_1) & g_{l_1 i_2}^c(\bar{u}_1, \bar{u}_2) & \dots & g_{l_1 j}^c(\bar{u}_1, \bar{t}') \\ g_{k_2 i_1}^c(\bar{u}_2, \bar{u}_1) & g_{k_2 j_1}^c(\bar{u}_2, \bar{u}_1) & g_{k_2 i_2}^<(\bar{u}_2, \bar{u}_2) & \dots & g_{k_2 j}^c(\bar{u}_2, \bar{t}') \\ \dots & \dots & \dots & \dots & \dots \\ g_{k_n i_1}^c(\bar{u}_n, \bar{u}_1) & g_{k_n j_1}^c(\bar{u}_n, \bar{u}_1) & g_{k_n i_2}^c(\bar{u}_n, \bar{u}_2) & \dots & g_{k_n j}^c(\bar{u}_n, \bar{t}') \\ g_{l_n i_1}^c(\bar{u}_n, \bar{u}_1) & g_{l_n j_1}^c(\bar{u}_n, \bar{u}_1) & g_{l_n i_2}^c(\bar{u}_n, \bar{u}_2) & \dots & g_{l_n j}^c(\bar{u}_n, \bar{t}') \\ \hline g_{ii_1}^c(t, \bar{u}_1) & g_{ij_1}^c(t, \bar{u}_1) & g_{ii_2}^c(t, \bar{u}_2) & \dots & g_{ij}^c(t, \bar{t}') \end{pmatrix}$$

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

$$G_{xx'}^{aa'}(t, t') = g_{xx'}^{aa'}(t, t') + \int du \sum_{b,y} (-1)^b g_{xy}^{ab}(t, u) K_{yx'}^{ba'}(u, t')$$

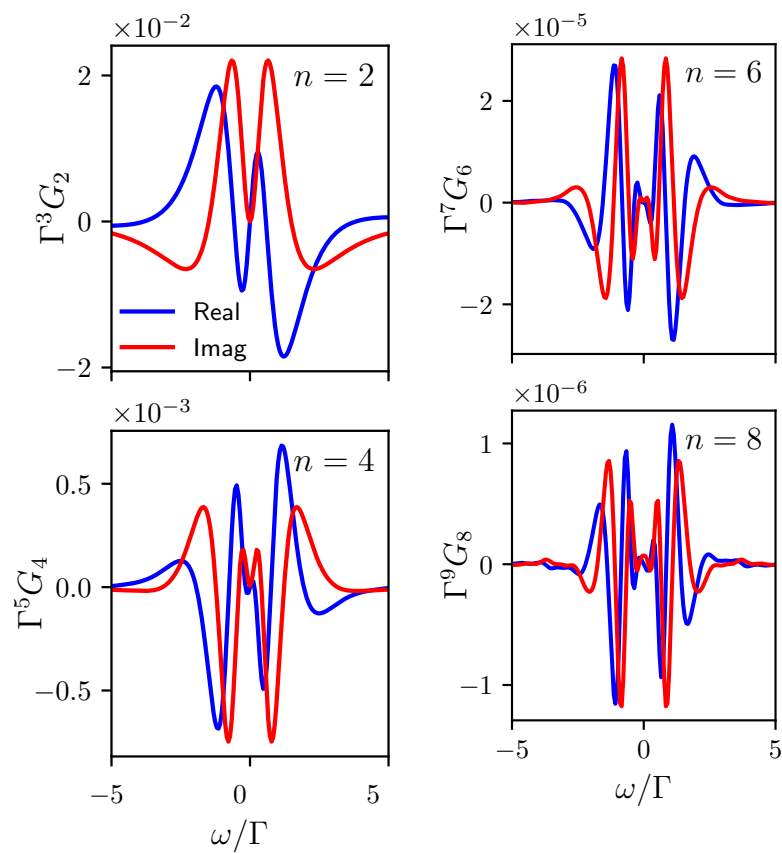
3) HIGHER ORDER KERNEL

$$\bar{K}_{xy}^{ab}(t, u) = -2iU \sum_z V_{yz}(u) F_{xyz}^{ab}(t, u)$$

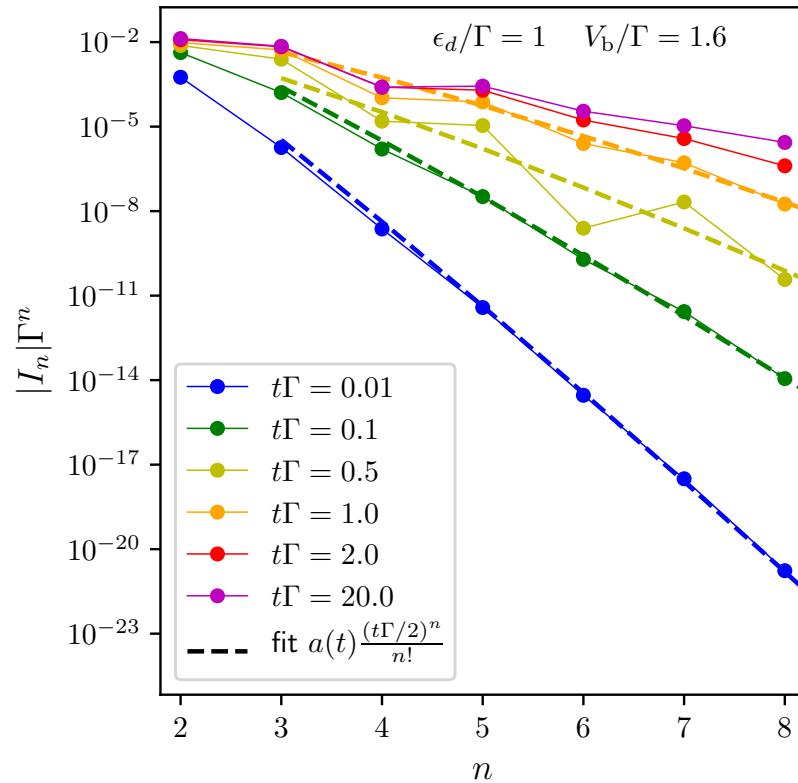
$$F_{xx'z}^{aa'}(t, t') \equiv (-i)^2 \left\langle T_c \hat{\mathbf{c}}(x, t, a) \hat{\mathbf{c}}^\dagger(x', t', a') \left[\hat{\mathbf{c}}^\dagger(z, t', a') \hat{\mathbf{c}}(z, t', a') - \alpha_z \right] \right\rangle$$

→ Re-expand a second time over one raw.
(lower the noise)

BARE DATA



A WARNING ON CONVERGENCE RADIUS



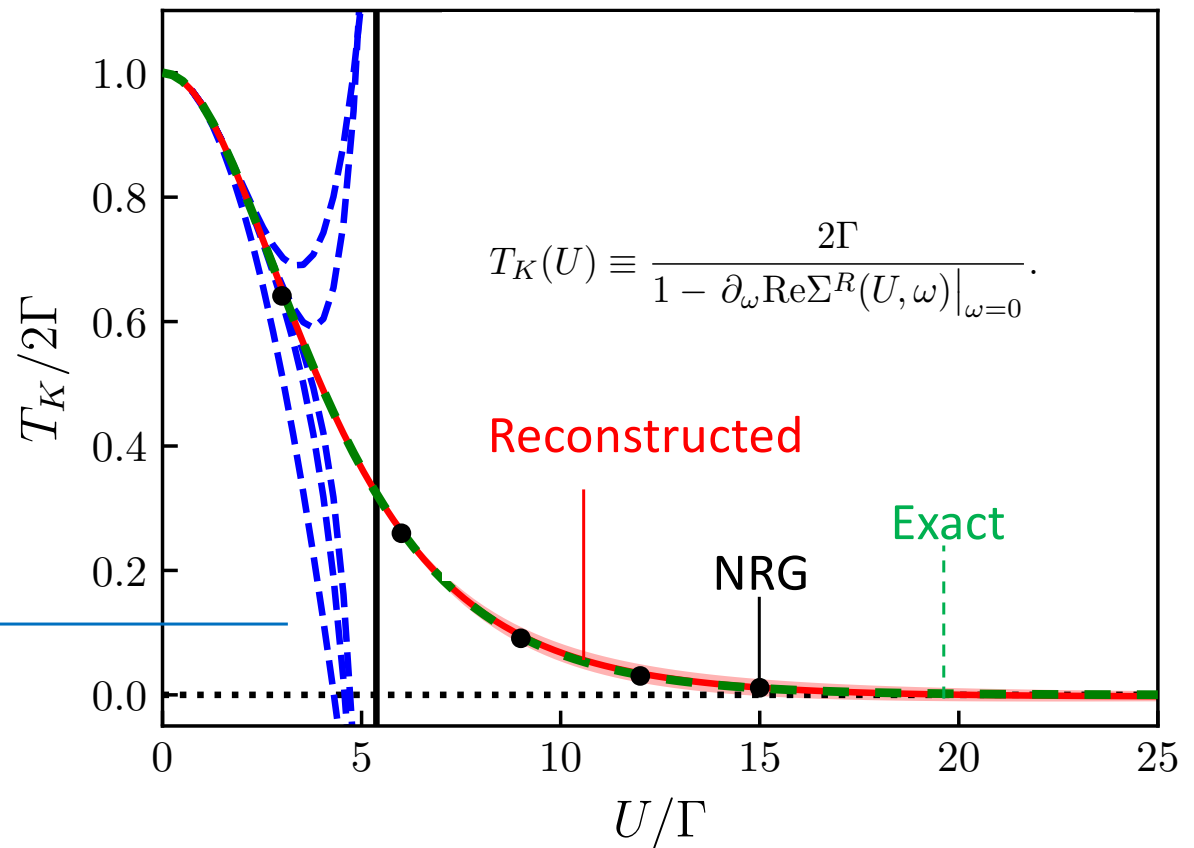
We work directly in the stationary limit

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

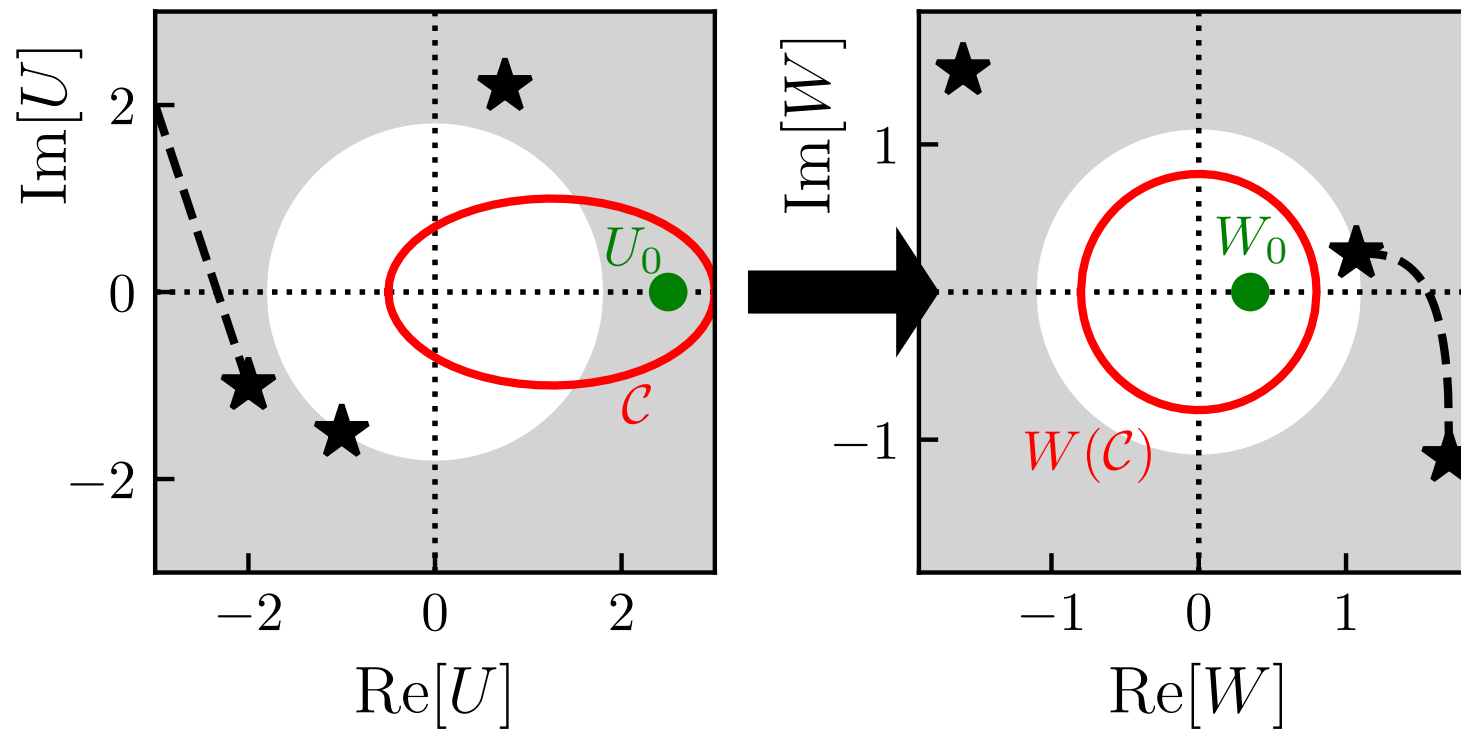
HOW TO RECONSTRUCT $F(U)$ FROM F_N ?

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

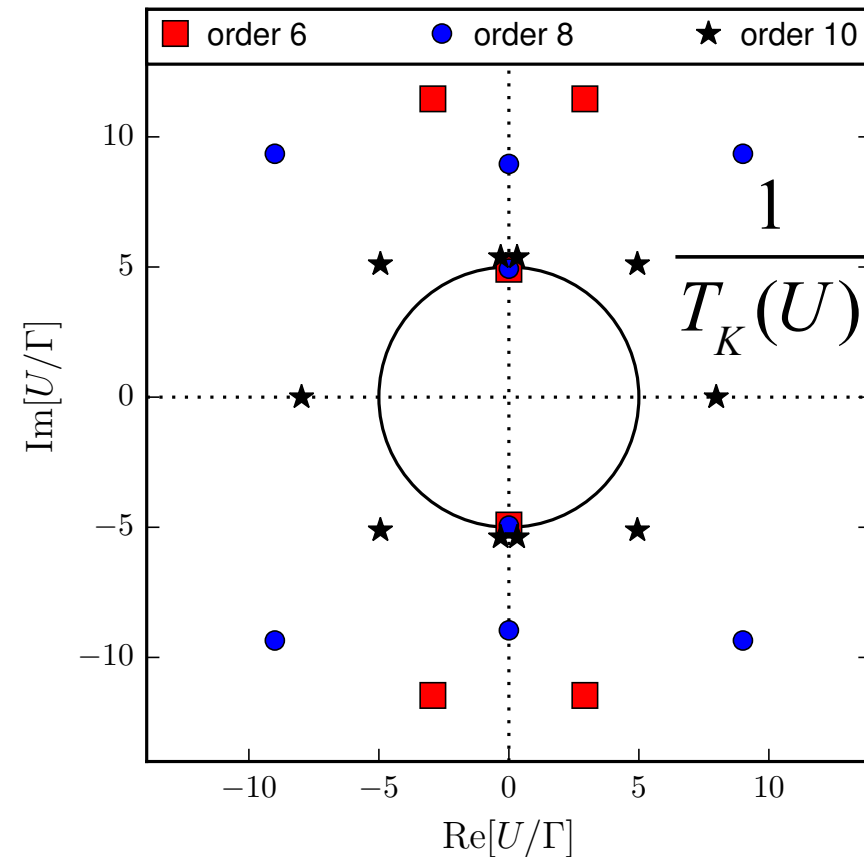
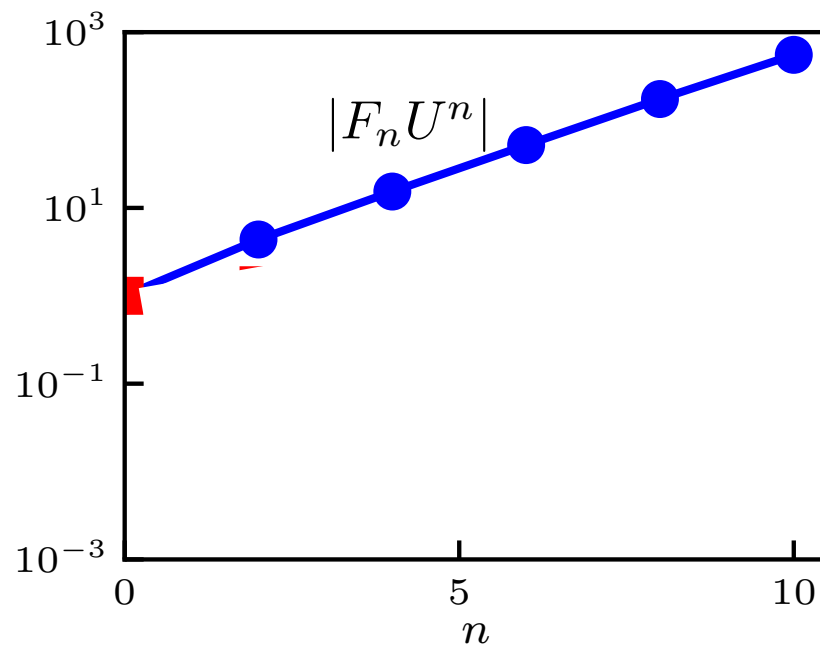
Truncated sum



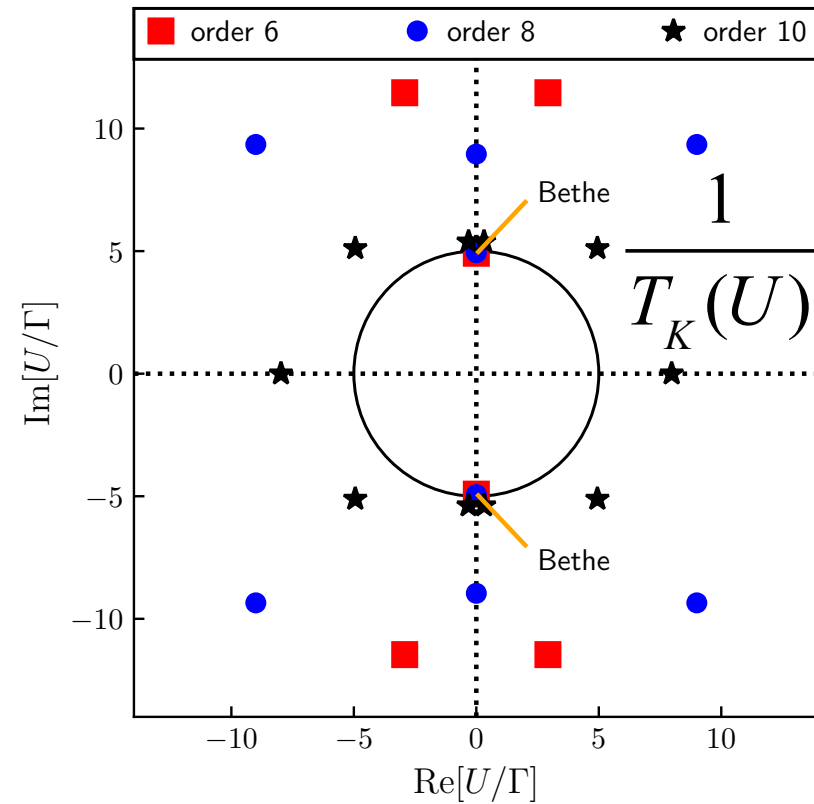
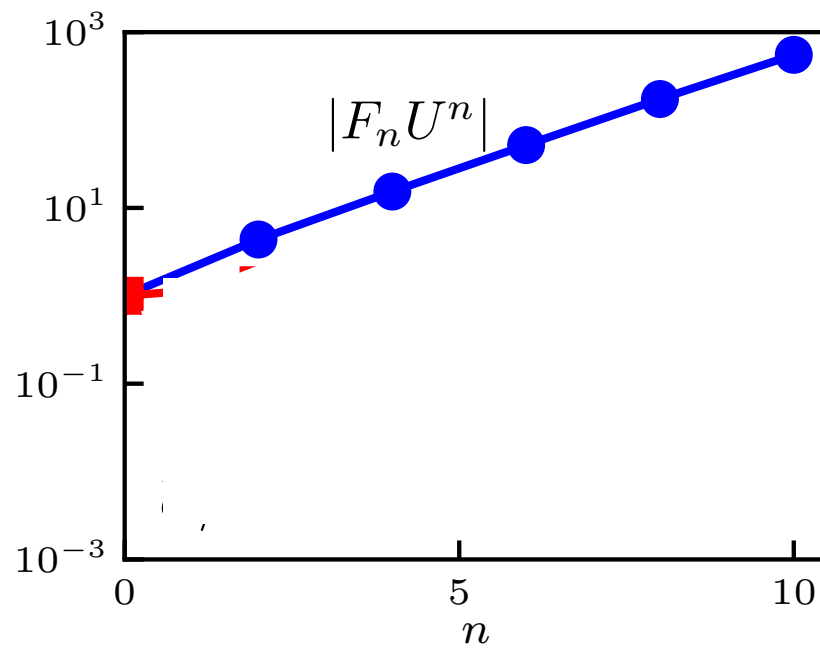
SEPARATION PROPERTY HYPOTHESIS



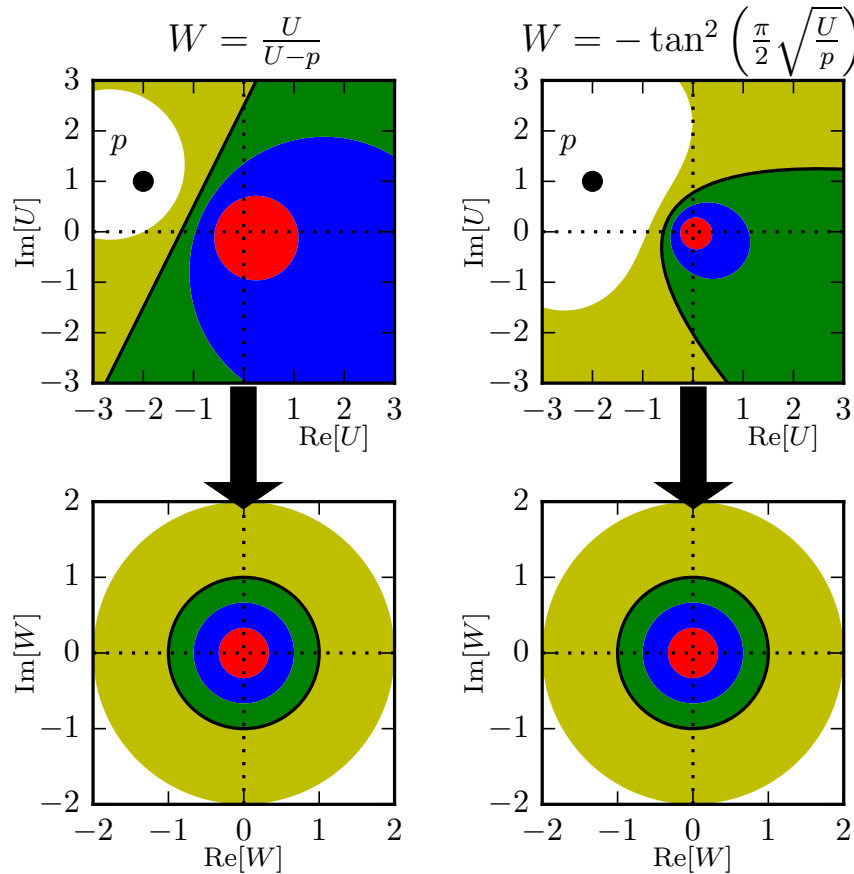
1) FIND THE POLES / ZEROS OF THE INVERSE



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2) DESIGN THE CONFORMAL TRANSFORM



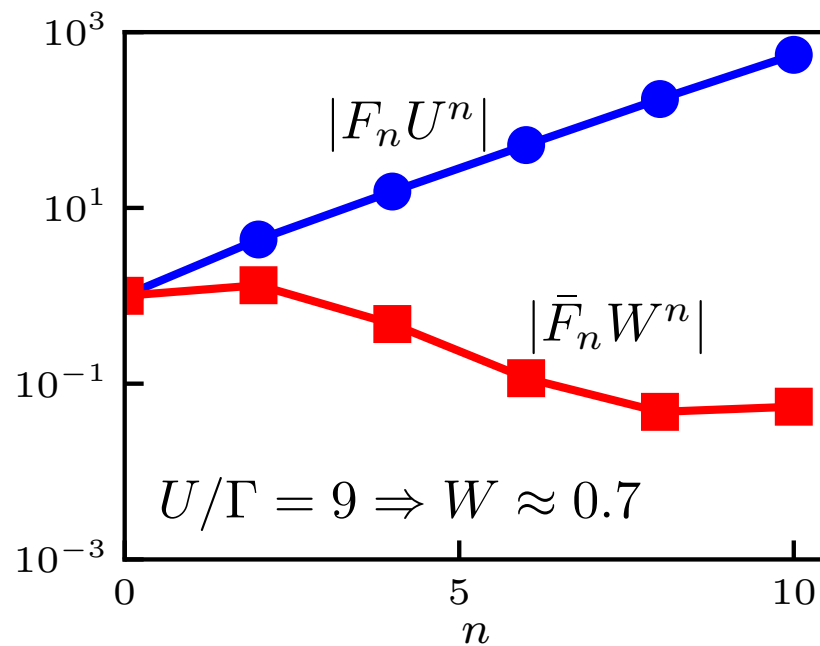
$$F(U(W)) = \sum_n \bar{F}_n W^n$$

$W(U)$: exact

$U(W)$: truncated

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

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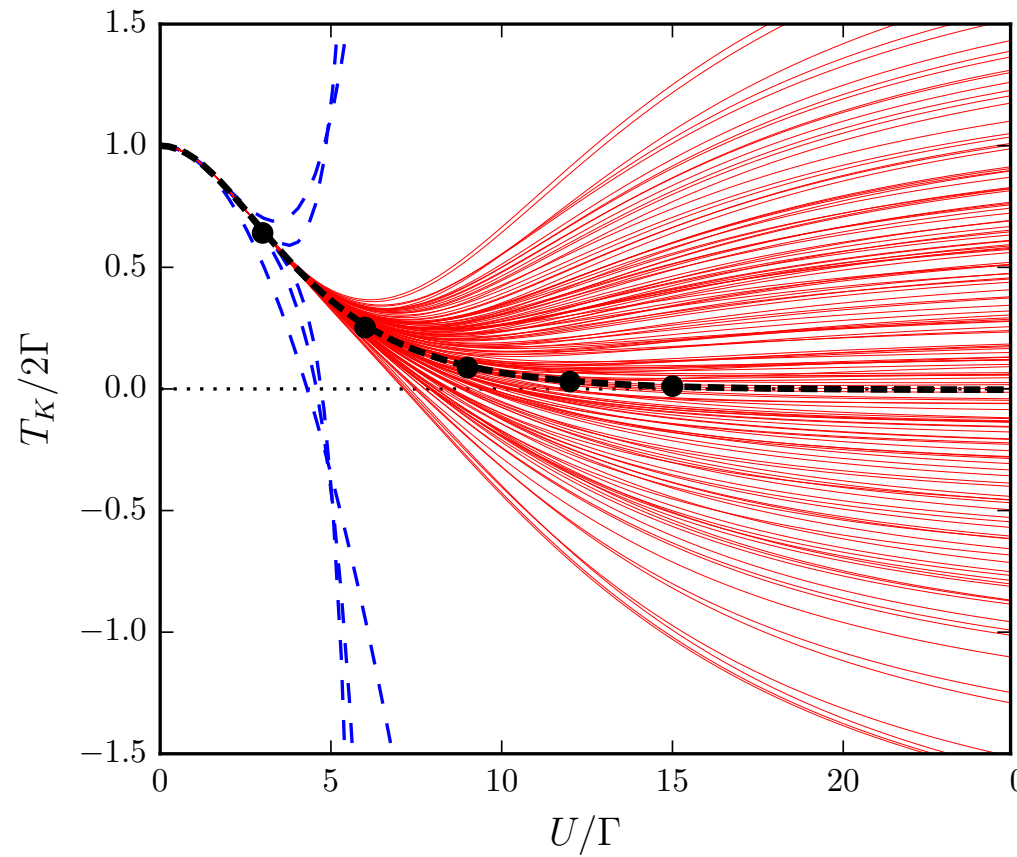
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$W(U)$: exact

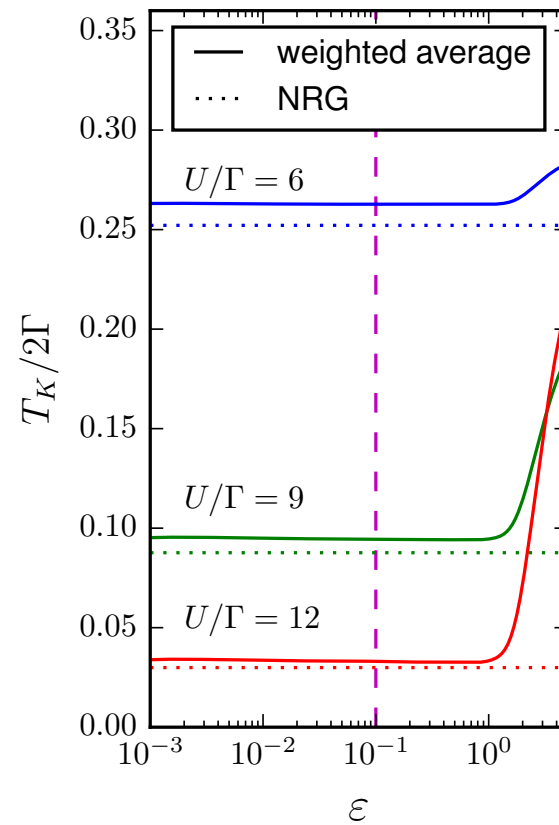
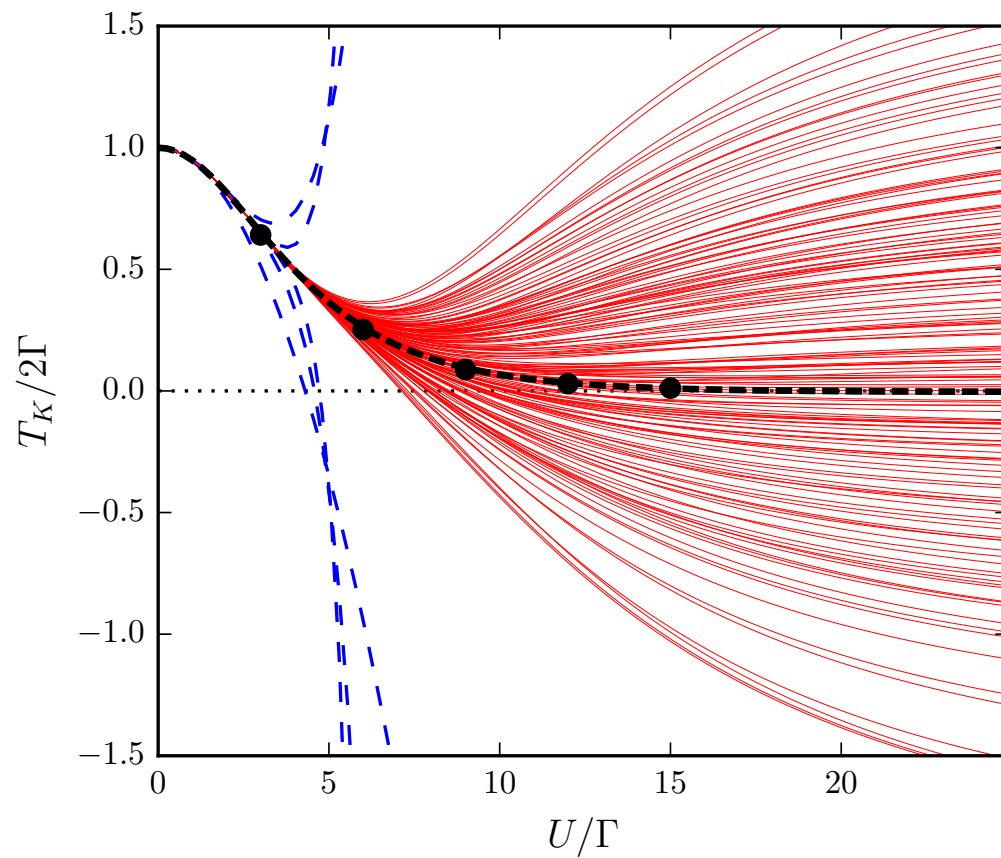
$U(W)$: truncated

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

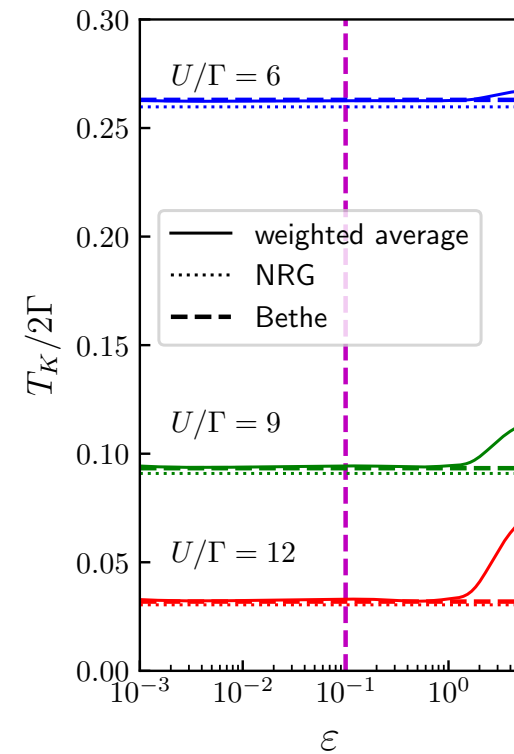
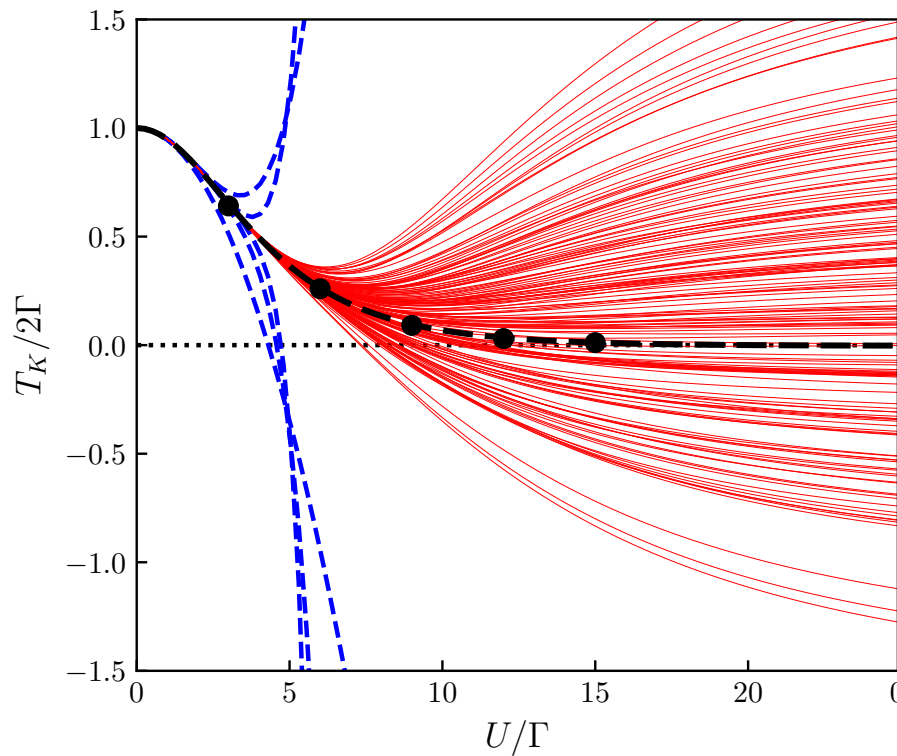
3) ADD BAYESIAN INFERENCE



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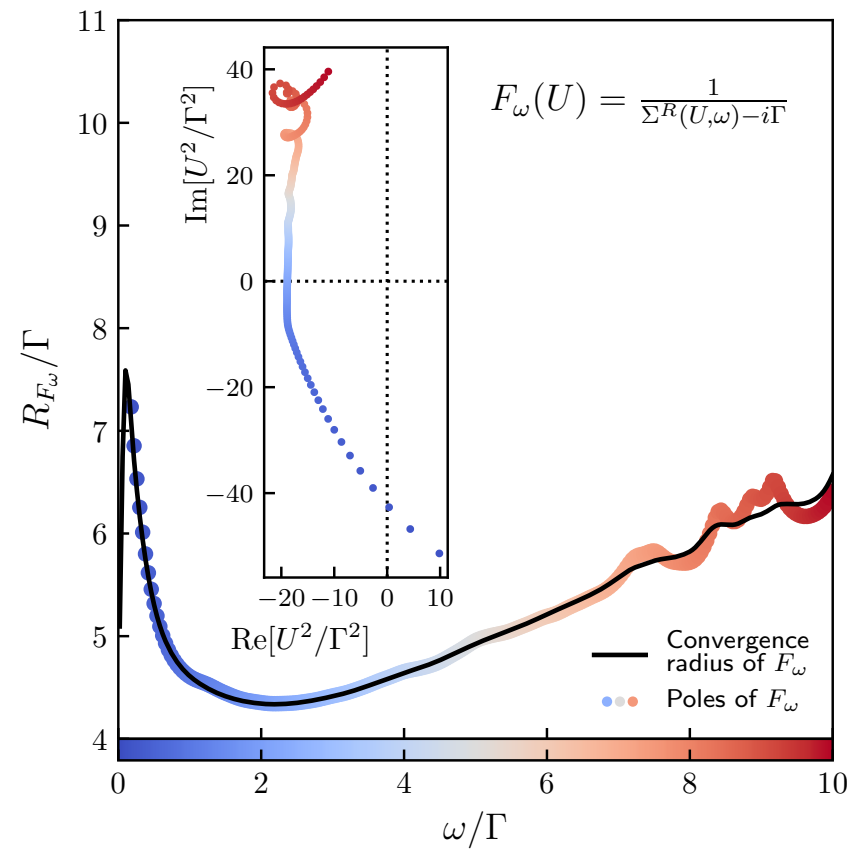
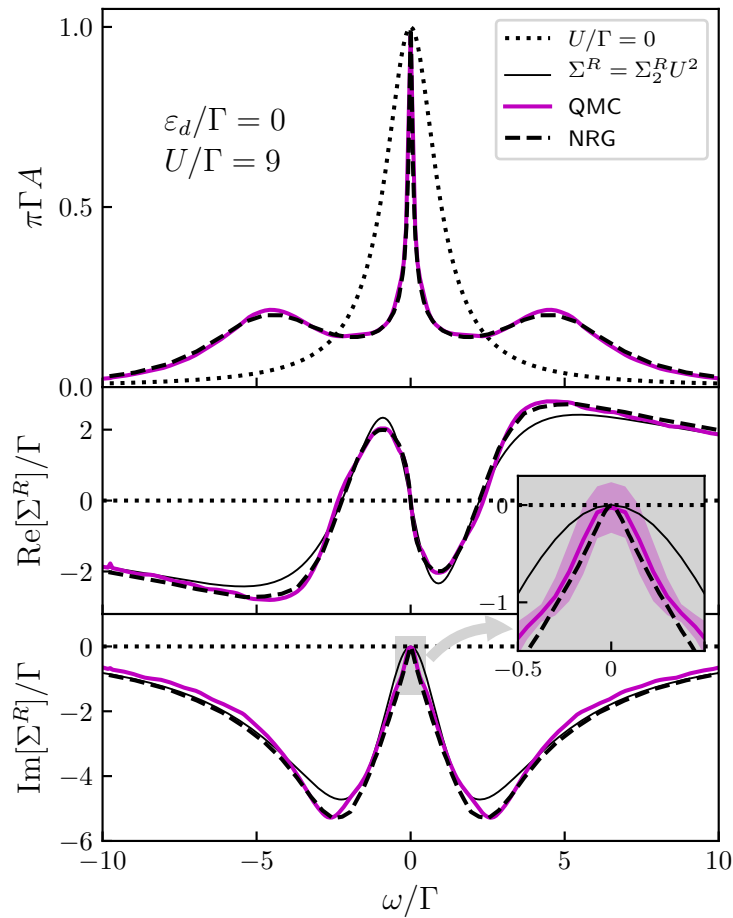


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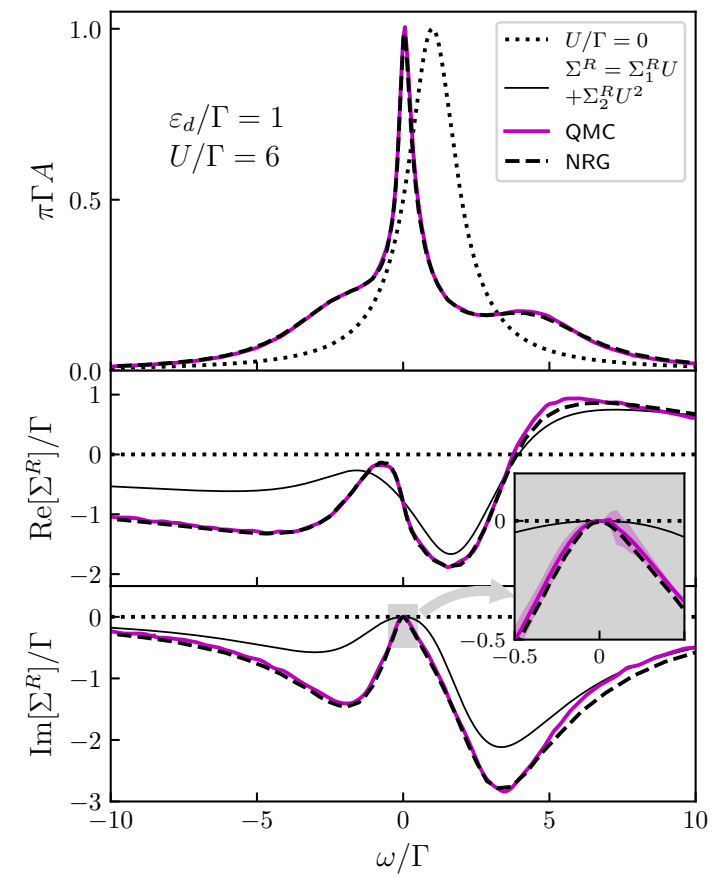
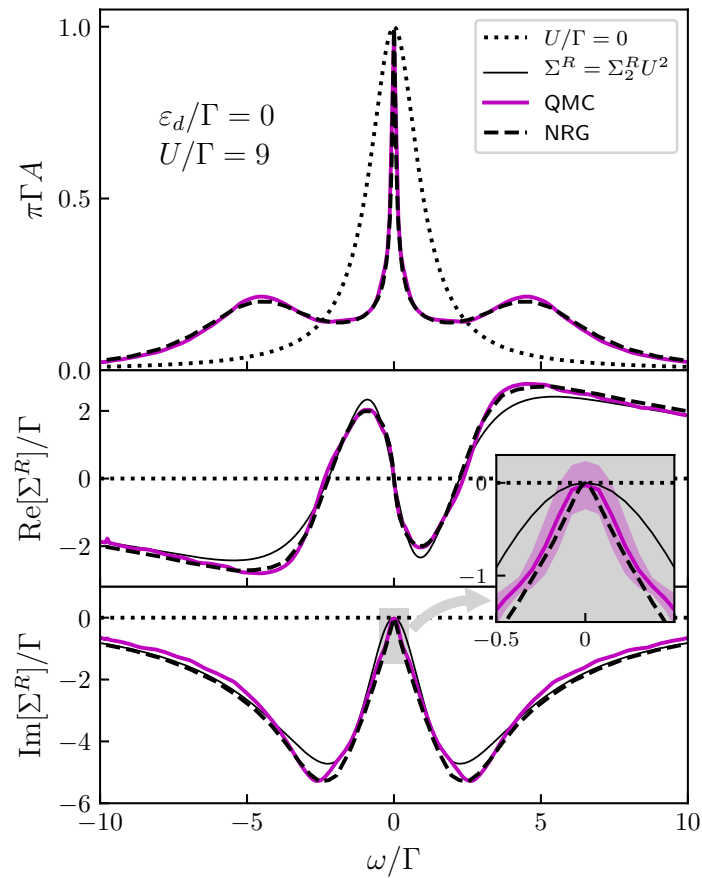


(Rq: NRG changed not QMC)

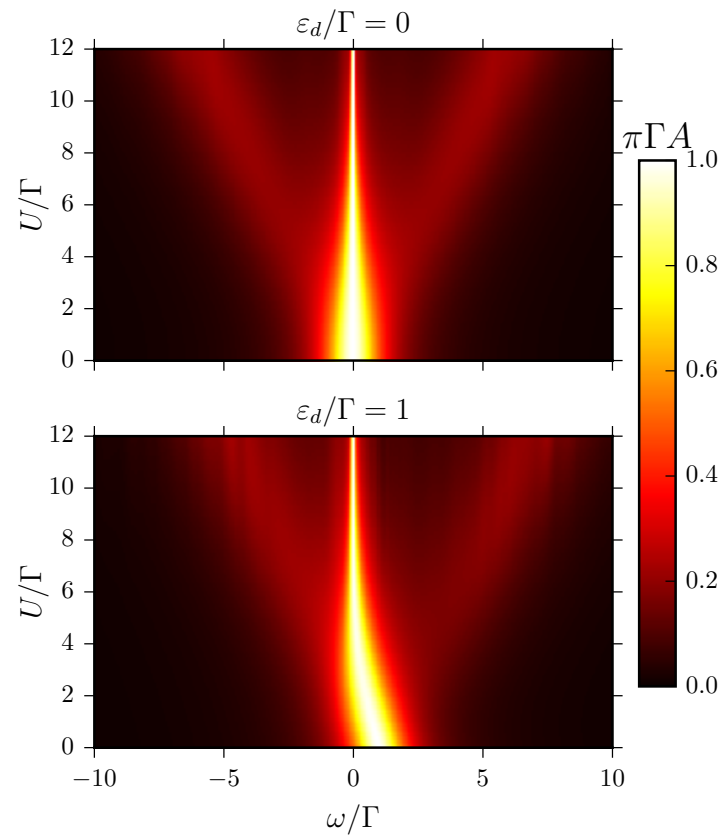
SOME EQUILIBRIUM BENCHMARKS



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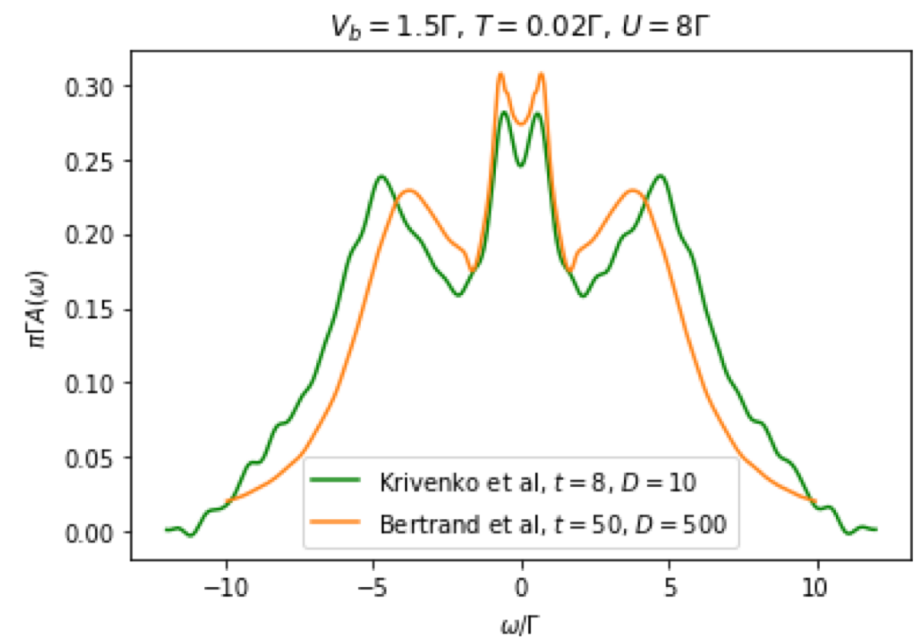
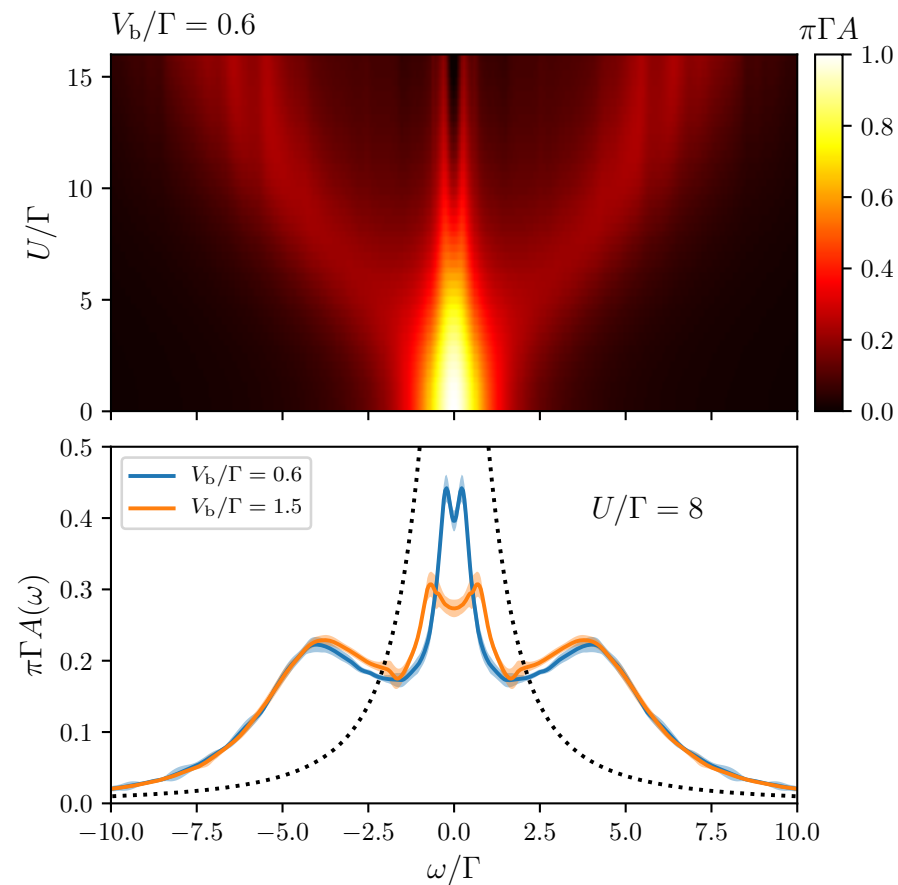


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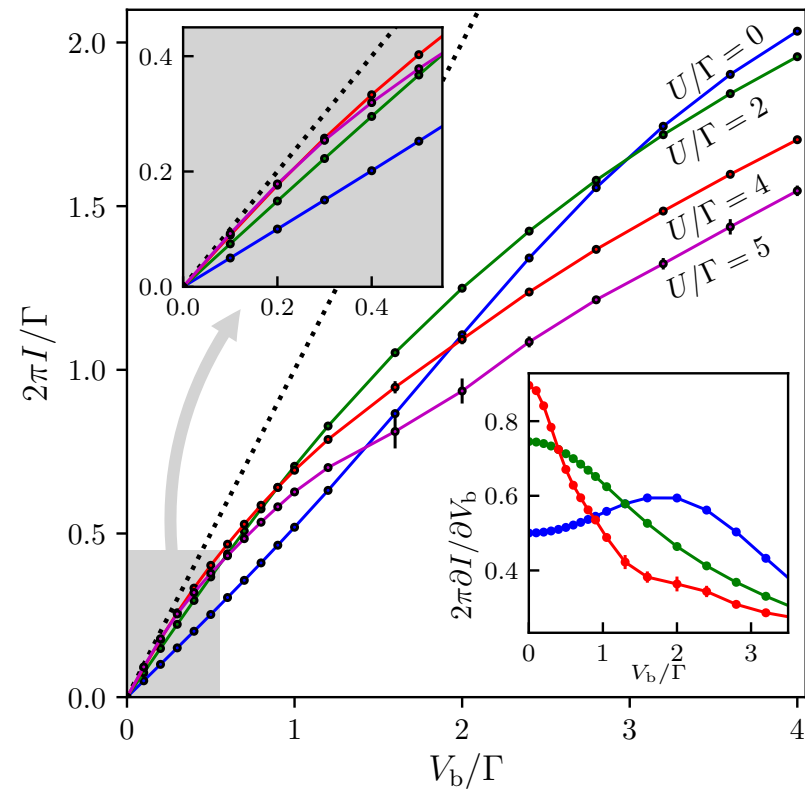
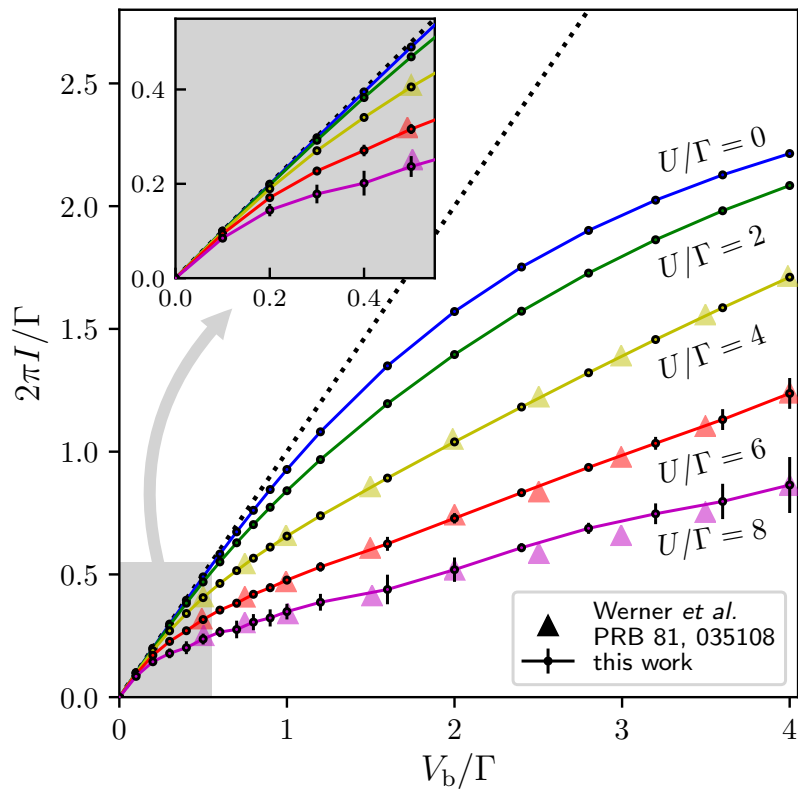
AND BACK TO NON-EQUILIBRIUM

Igor Krivenko,¹ Joseph Kleinhenz,¹ Guy Cohen,^{2,*} and Emanuel Gull
arXiv:1904.11527v1

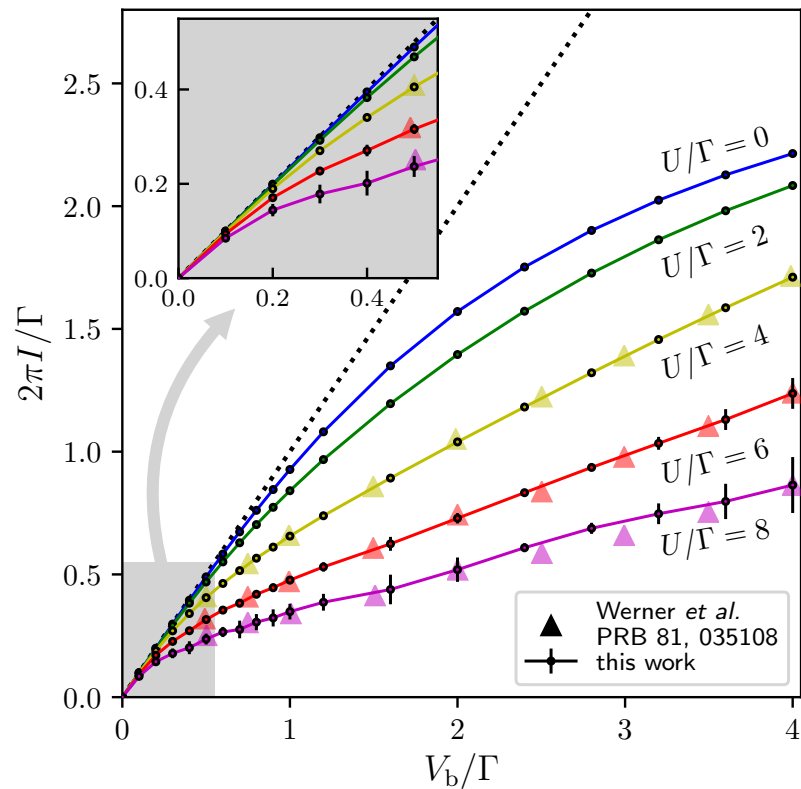


PRELIMINARY COMPARAISON
DIFFERENT BATH AND TIMES

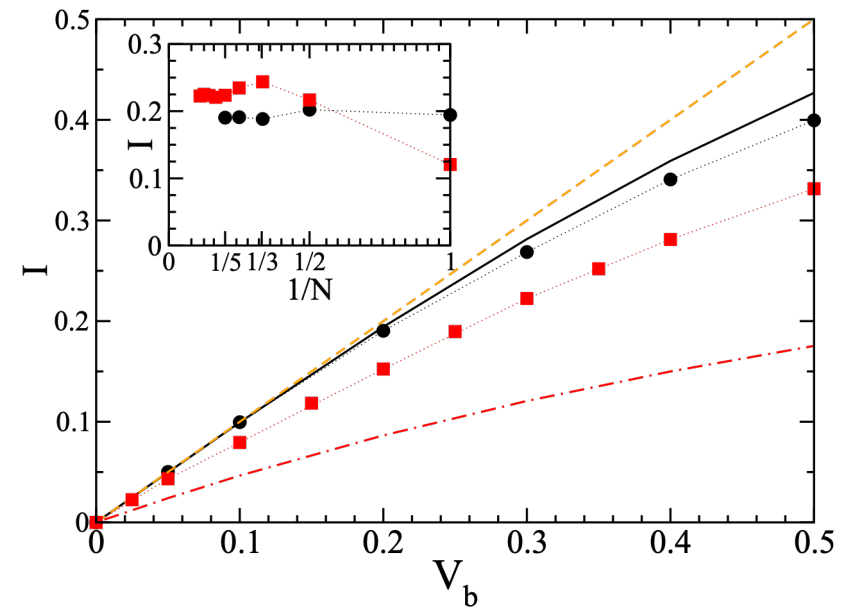
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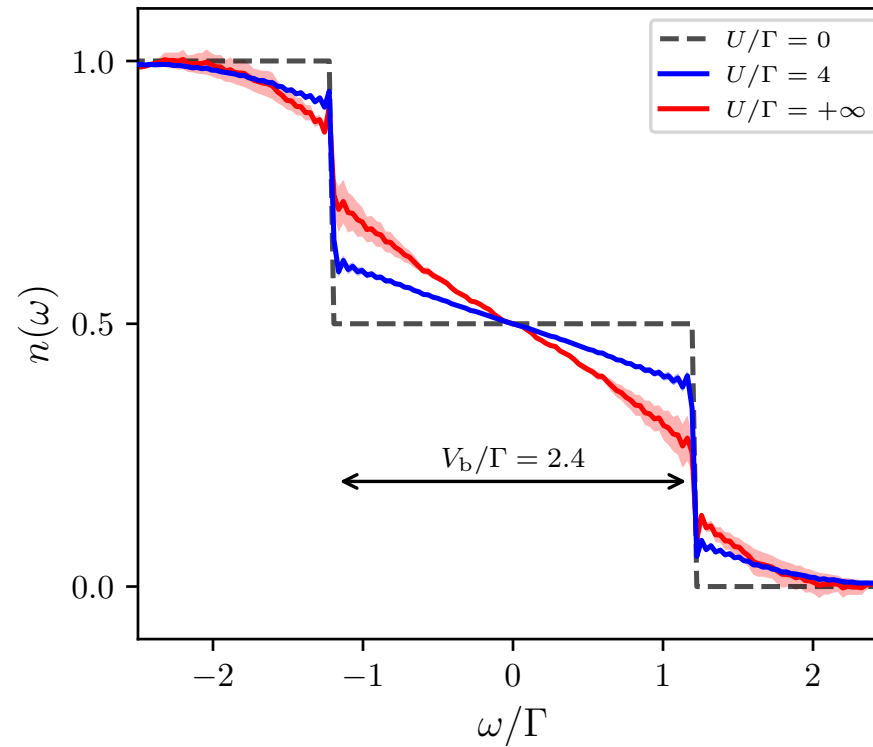


2 years ago: $U=2.4$



NON-EQUILIBRIUM DISTRIBUTION FUNCTION

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



CONCLUSION

MORE TECHNICAL PROGRESS NEEDED

- Improved sampling & implementation (coming up soon)
- Terms and Counter-terms
- Direct sampling in W variables / Self-energy

...

MORE APPLICATIONS

- Lattice (in progress)
- DMFT (also in progress)
- Nanoelectronics (0.7 anomaly)
- Few qubits & their baths