Finite-frequency Matsubara FRG for the SIAM

– Final status report –

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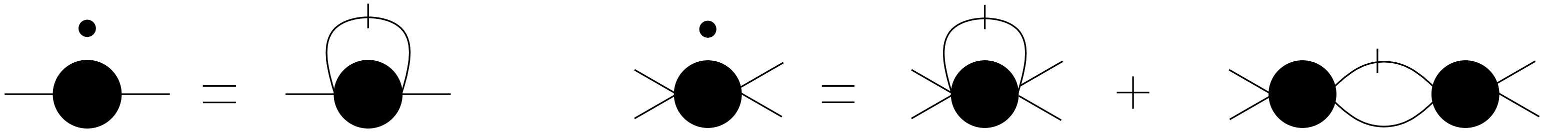
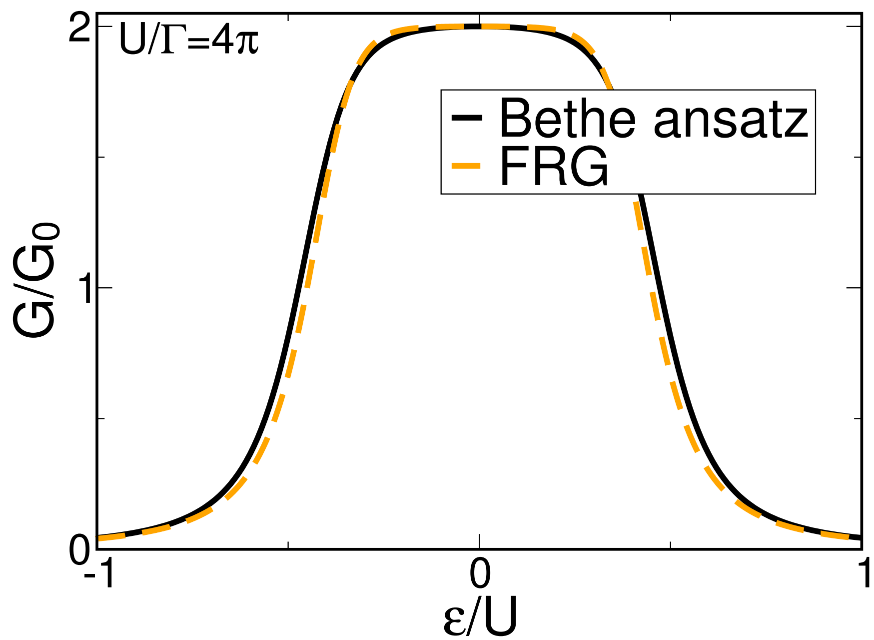
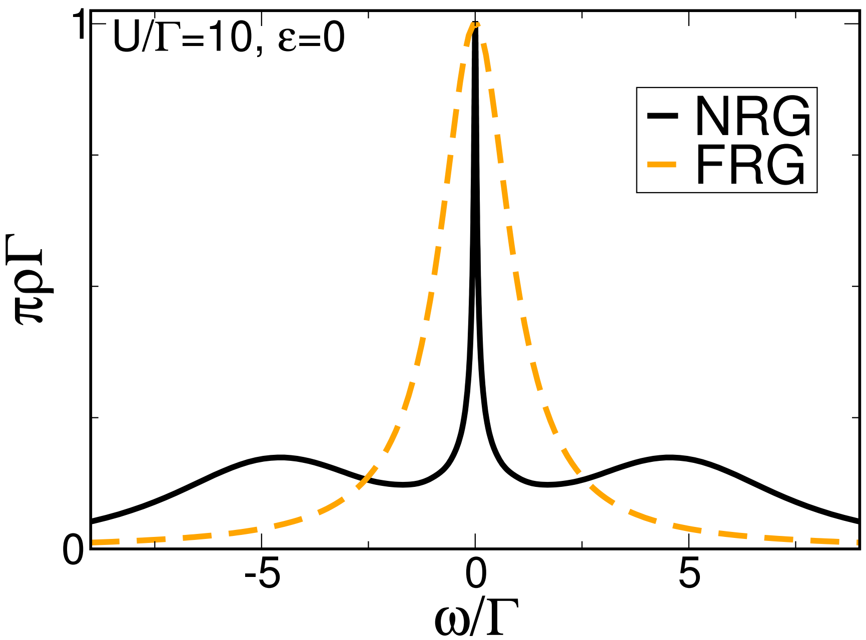
The Stage

- Single Impurity Anderson Model ($\rightarrow$ Severin)
- 1P-irreducible Matsubara FRG with sharp multiplicative Θ-cutoff
- usual flow equation hierachy:



- truncation procedure usually employed for SIAM-like models:
  (a) neglect the contribution of γ_3 to the flow of γ_2
  (b) neglect the frequency dependence of γ_2
- **zero**/**finite**-frequency properties are described **well**/**badly**:





Finite-frequency FRG

Straight-forward way of implementing frequency-dependence:

- regard γ_2 as a function of three indep. bosonic frequencies ν_i

  $\rightarrow$ preserves symmetries automatically

- parametrize the self-energy $\Sigma^\Lambda(i\omega)$ and the two-particle vertex $\gamma_2^\Lambda(i\nu_1, i\nu_2, i\nu_3)$ using a discrete mesh of N Matsubara frequencies:

$$\omega_n = \omega_0 a^n, \qquad n = 0 \ldots N-1$$

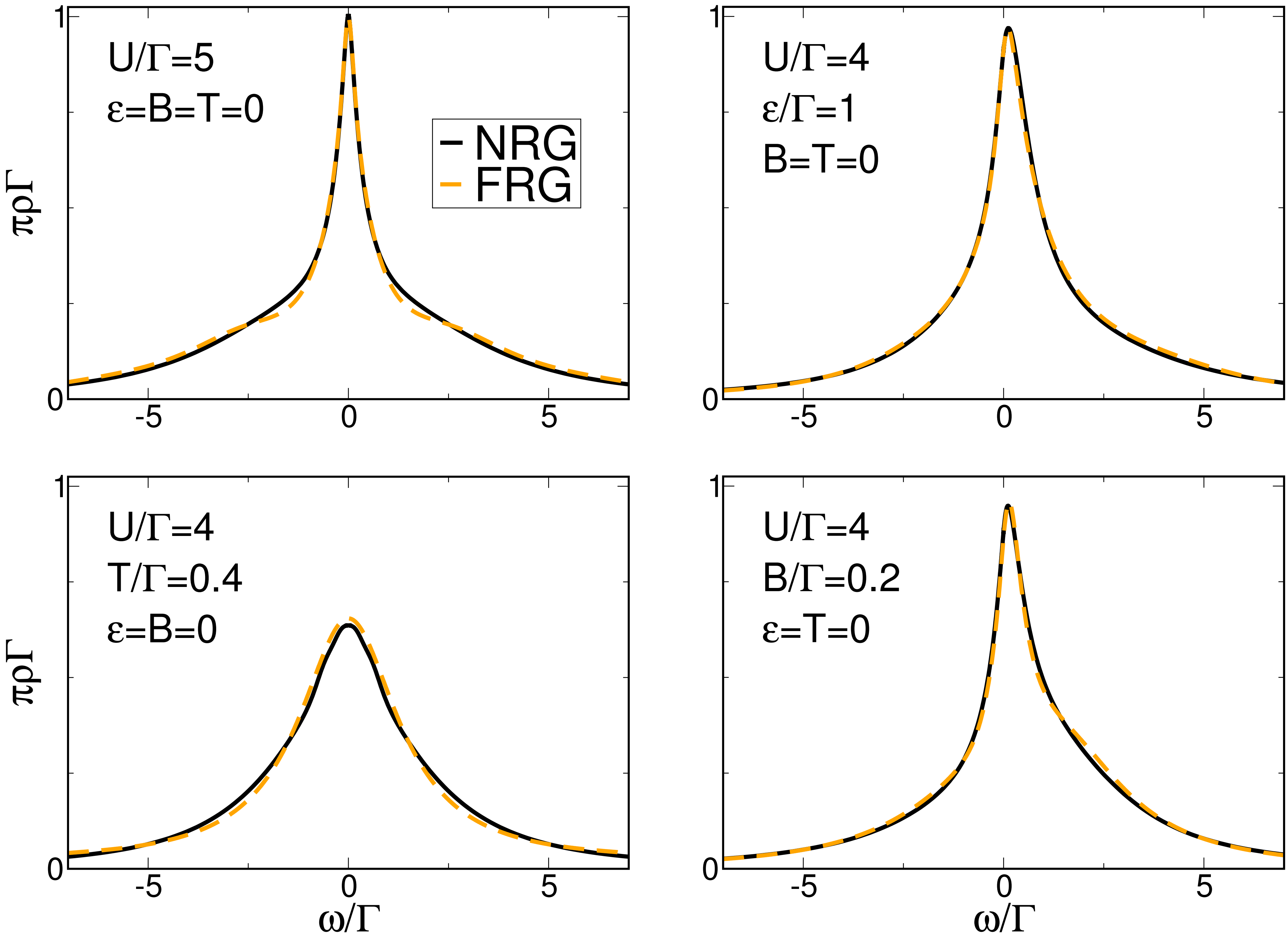
Important numerical aspect:

verify that physical properties are independent of the actual choice of the discretization!

Technical issues:

- compute spectral function from (ill-controlled) Padé approximation
- replace $S^\Lambda \mathcal{G}^\Lambda \rightarrow -\dot{\mathcal{G}}^\Lambda \mathcal{G}^\Lambda$ (Katanin 2004)

Results: small to intermediate U



Numerical efficiency

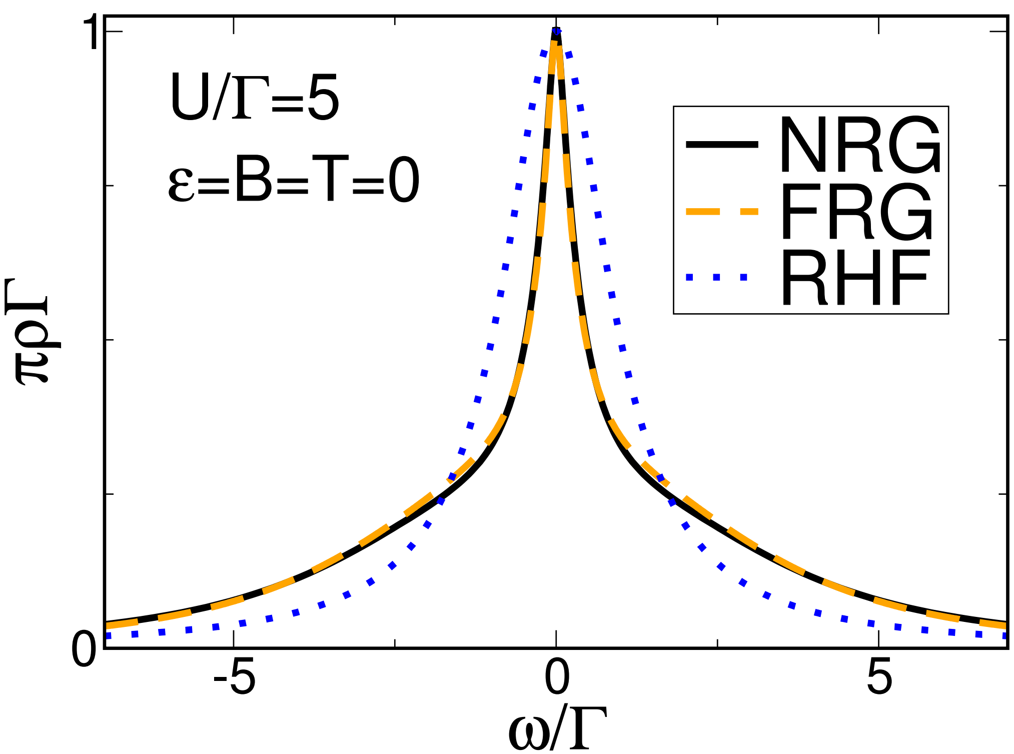
The FRG works well for arbitrary parameters and intermediate U.

It is, however, numerically demanding.

Approximation to increase efficiency:

$$\begin{aligned}\dot{\gamma}_2 = &- \text{PP-term}\ (\boldsymbol{\nu_1}, \nu_2 = 0, \nu_3 = 0) \\ &- \text{PH-term}\ (\nu_1 = 0, \boldsymbol{\nu_2}, \nu_3 = 0) \\ &+ \text{HP-term}\ (\nu_1 = 0, \nu_2 = 0, \boldsymbol{\nu_3})\end{aligned} \Rightarrow$$

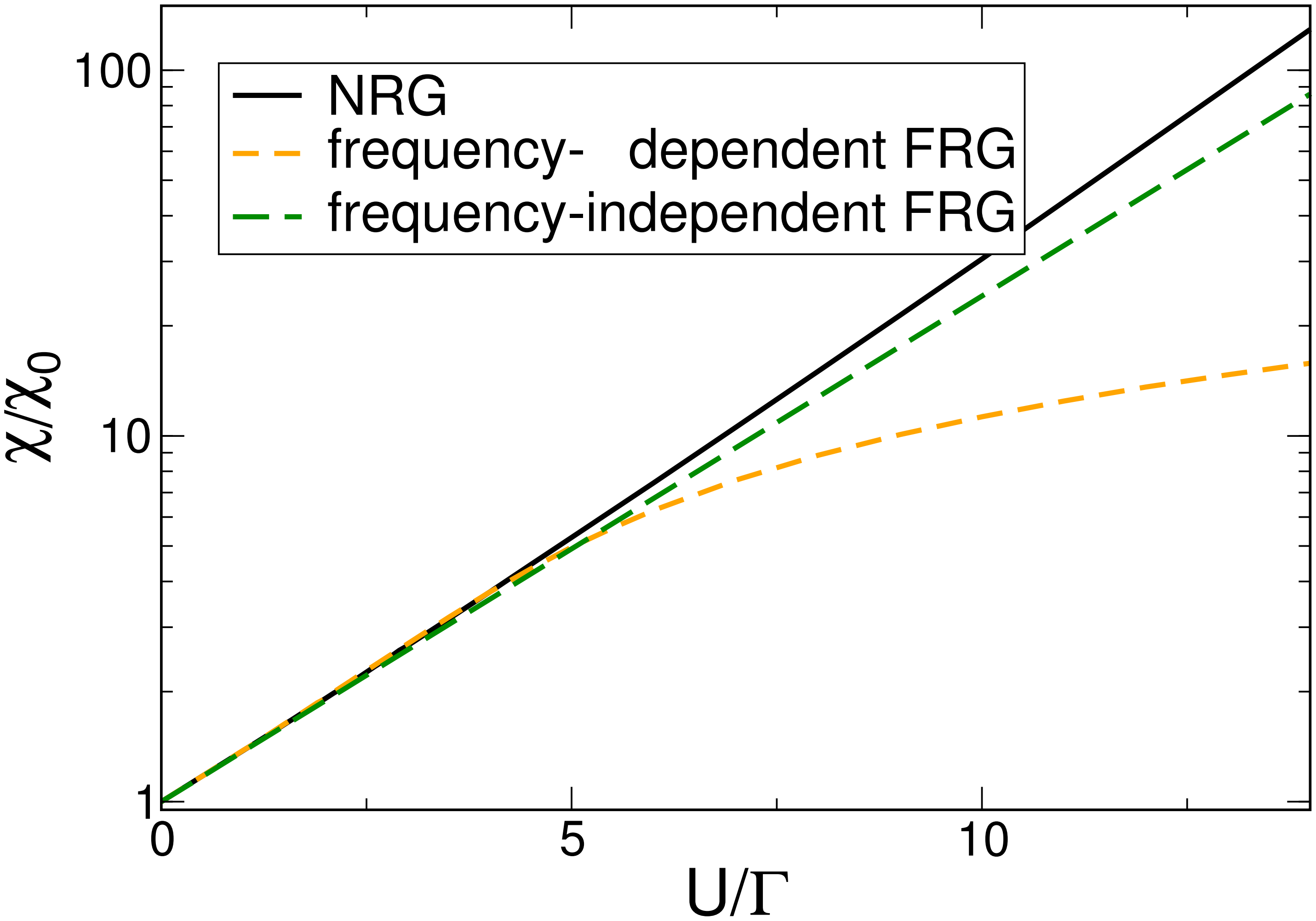
one-dimensional frequency meshes only



At intermediate U, reliable results can be obtained with minor numerical effort!

Large U: the Kondo scale

quantities governed by T_K: spin susceptibility, effective mass, width of the Kondo resonance, ...



Frequency-independent FRG shows exponential behavior.

Frequency- dependent FRG shows no exponential behavior.

Discussion

Frequency-dependent FRG:

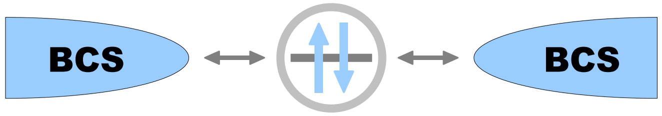
- gives better results at small to intermediate U
- there is no exponential energy scale

BUT: there are numerical (discretization) issues!

- choose N large enough so that results are converged $\surd$
- different ways to parametrize γ_2 do not give coinciding results in the strong coupling regime (limitation of num. resources ?!)
- why does the non-Katanin scheme break down for large U?
  - ⋆ frequency discretization?
  - ⋆ fundamental reasons (neglection of γ_3)?

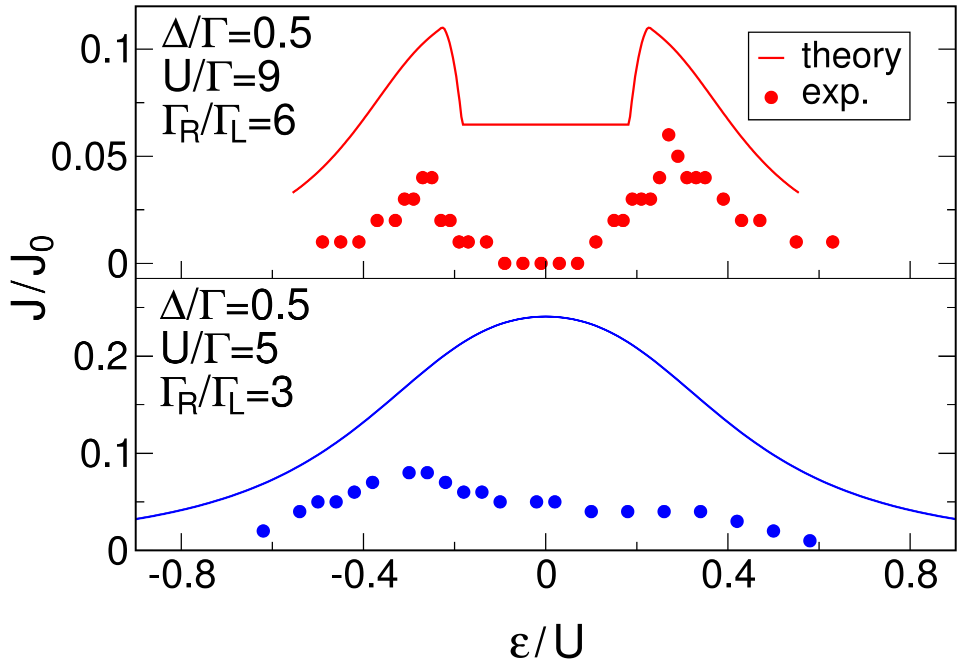
So what?

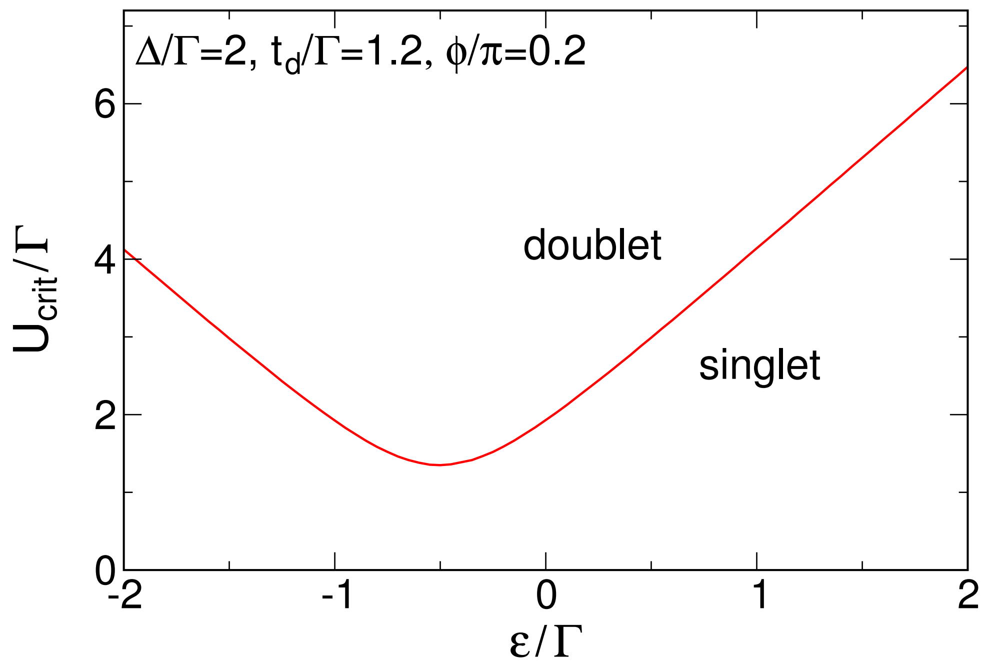
Consider SIAM with BCS leads:



- low-energy physics: governed by an interplay of the Kondo effect and induced superconductivity (ratio T_K/Δ)
- interesting quantity: supercurrent as a function of the gate voltage
- advantage: interesting physics at intermediate U

Zero-frequency FRG works fine for **zero temperature**!





Finite-frequency FRG needed to treat **finite temperatures**!

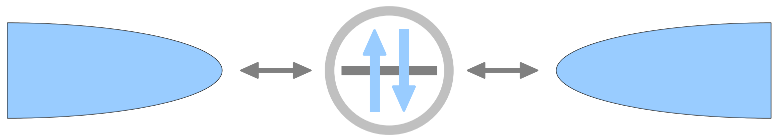
Frequency-dependent FRG can be used to fast compute finite-energy properties of the SIAM at small to intermediate U.

There is no exponential energy scale.

Thank you for your attention!

Single Impurity Anderson Model

The SIAM describes an impurity of **interacting** spin up and down **electrons coupled to** a bath of **Fermi-liquid leads**.



The low-energy physics of this model is dominated by the **Kondo effect.** The Hamiltonian consists of three parts, $H = H_{\text{dot}} + H_{\text{leads}} + H_{\text{coup}}$, where

$$H_{\text{dot}} = \sum_{\sigma} \epsilon_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow}$$

$$H_{\text{leads}} = \sum_{s=L,R} \sum_{k\sigma} \epsilon_{sk} c_{sk\sigma}^{\dagger} c_{sk\sigma}$$

$$H_{\text{coup}} = \sum_{s=L,R} t_s \left(c_{s\sigma}^{\dagger} d_{\sigma} + d_{\sigma}^{\dagger} c_{s\sigma} \right)$$

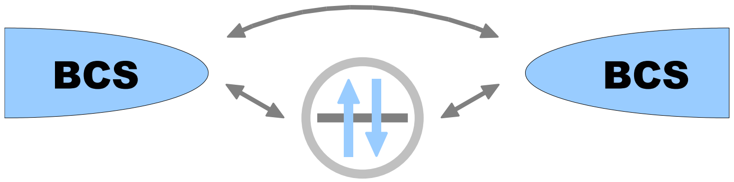
Single-particle energy: $\epsilon_{\sigma} = \epsilon - U/2 \pm B/2$

Local electron operators at the impurity site: $c_{s\sigma} = \sum_k c_{sk\sigma}/\sqrt{N}$

Hybridisation energy: $\Gamma = \Gamma_L + \Gamma_R$, where $\Gamma_s = \pi t_s^2 \rho_s =$ const. (wide-band limit)

The QD Josephson junction

Model Hamiltonian:



$$H^{\text{dot}} = (\epsilon - U/2) \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow}$$ **quantum dot**

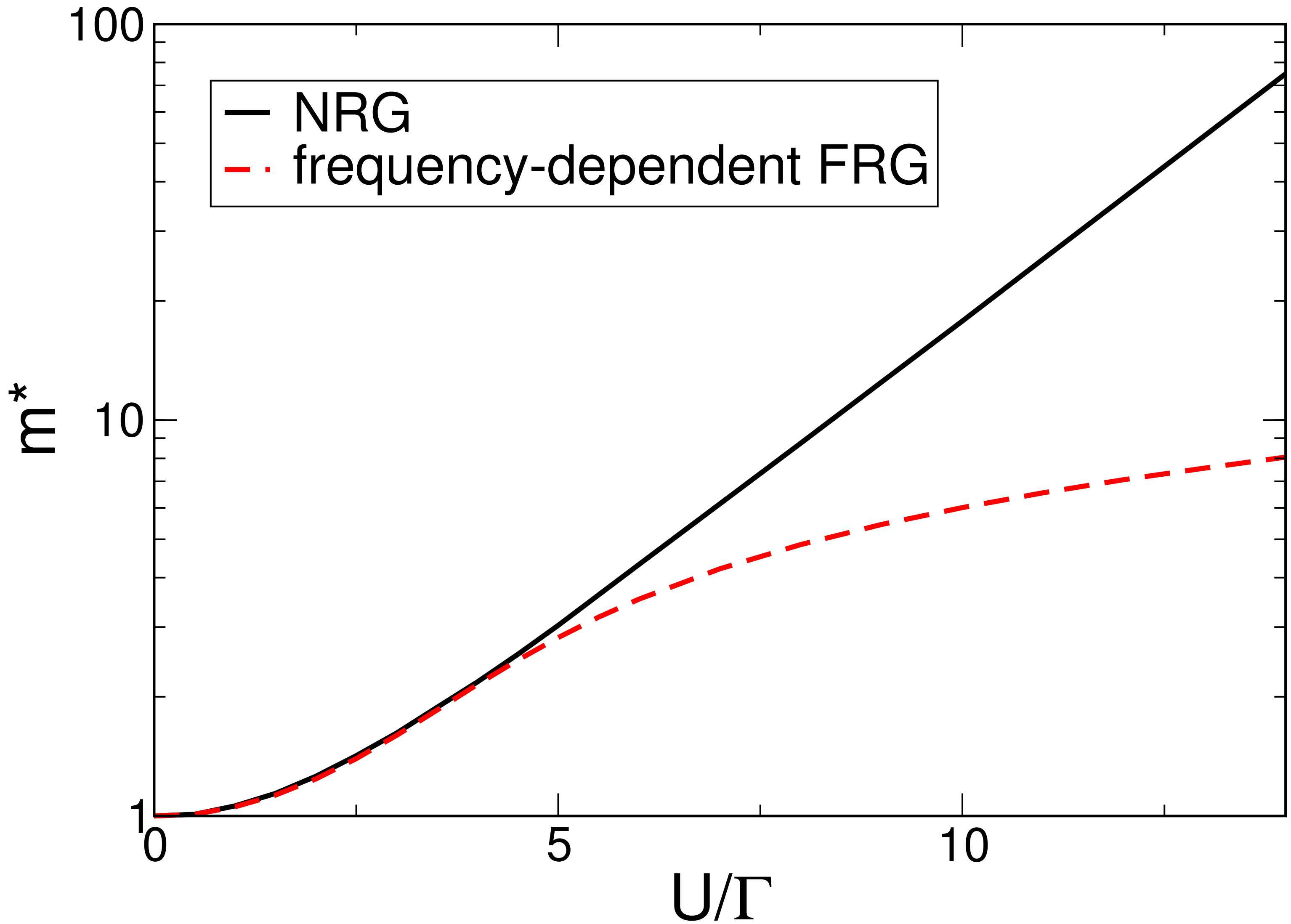
$$H^{\text{lead}}_{s=L,R} = \sum_{k\sigma} \epsilon_{sk} c^{\dagger}_{sk\sigma} c_{sk\sigma} - \Delta \sum_{k} \left[e^{i\phi_s} c^{\dagger}_{sk\uparrow} c^{\dagger}_{s-k\downarrow} + \text{H.c.} \right]$$ **BCS leads**

$$H^{\text{coup}}_{s=L,R} = -\, t_s \sum_{\sigma} c^{\dagger}_{s\sigma} d_{\sigma} + \text{H.c.}$$ **coupling QD-leads**

$$H^{\text{direct}} = -\, t_d \sum_{\sigma} c^{\dagger}_{L\sigma} c_{R\sigma} + \text{H.c.}$$ **direct coupling**

Kondo scale: the effective mass

Effective mass: $1/T_K \sim m^* = 1 - \mathrm{Im}\,\Sigma(i\omega_0)/\omega_0$



FRG does not show exponential behaviour!

Spin susceptibility