A finite-frequency functional RG approach to the single impurity Anderson model

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Outline

- The single impurity Anderson model
- The energy-independent fRG approximation
- A frequency-dependent fRG scheme
  - discretization of the Matsubara frequency axis
  - numerical efficiency
- Spectral functions for the SIAM
- Does the fRG capture the Kondo scale?

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

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

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

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

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

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

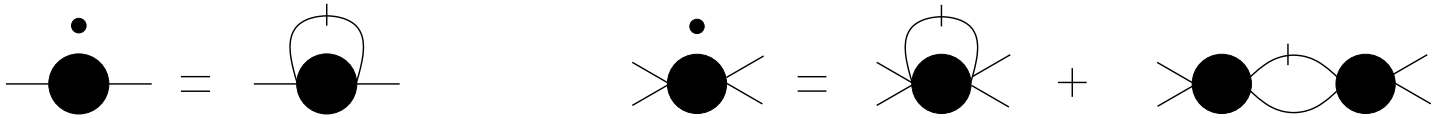
Hybridisation energy: $\Gamma = \Gamma_L + \Gamma_R$, where $\Gamma_s = \pi t_s^2 \rho_s = \text{const.}$ (wide-band limit)

Energy-independent fRG

- Introduce infrared cutoff in Matsubara frequency space:

$$\mathcal{G}^0(i\omega) \to \mathcal{G}^{0,\Lambda}(i\omega) = \mathcal{G}^0(i\omega)\Theta_\Lambda(|\omega| - \Lambda)$$

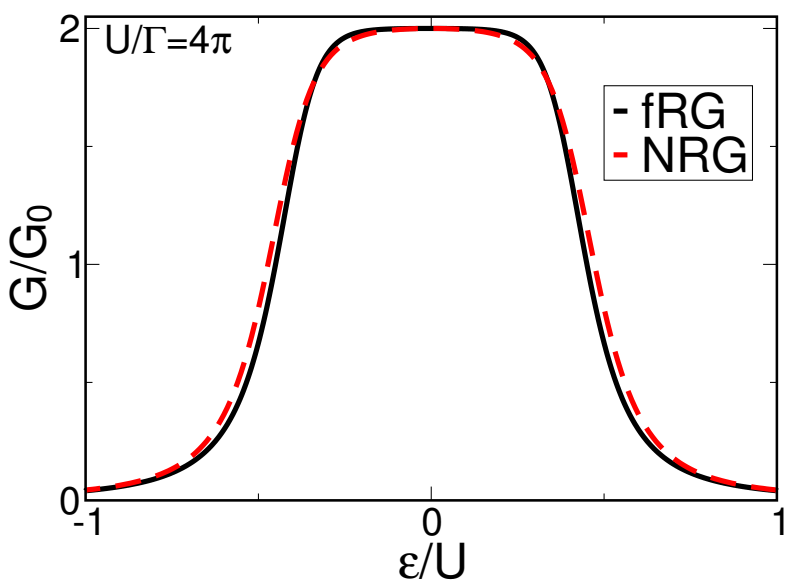
- Differentiating the single-particle irreducible vertex functions γ w.r.t. the cutoff parameter Λ yields an infinite hierachy of flow equations:

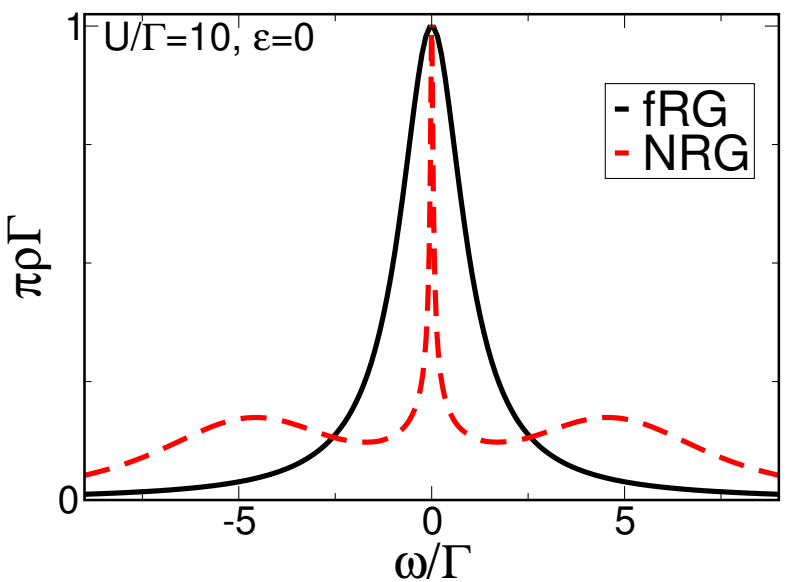


- Truncation procedure employed for SIAM-like models:

  (a) neglect the contribution of γ_3 to the flow of γ_2
  (b) neglect the frequency dependence of γ_2

- **Zero-frequency** (**finite-frequency**) properties are described **well** (**badly**):





Finite-frequency fRG

Next logical step: **account for the frequency-dependence** of γ_2. This is physically interesting since

- more 'complex' systems can practically not be tackled by **NRG** due to the limitation of **numerical resources**.
- an extended fRG scheme may provide a reliable tool to compute **non-equilibrium properties** of the SIAM.

Straight-forward way of implementing frequency-dependence:

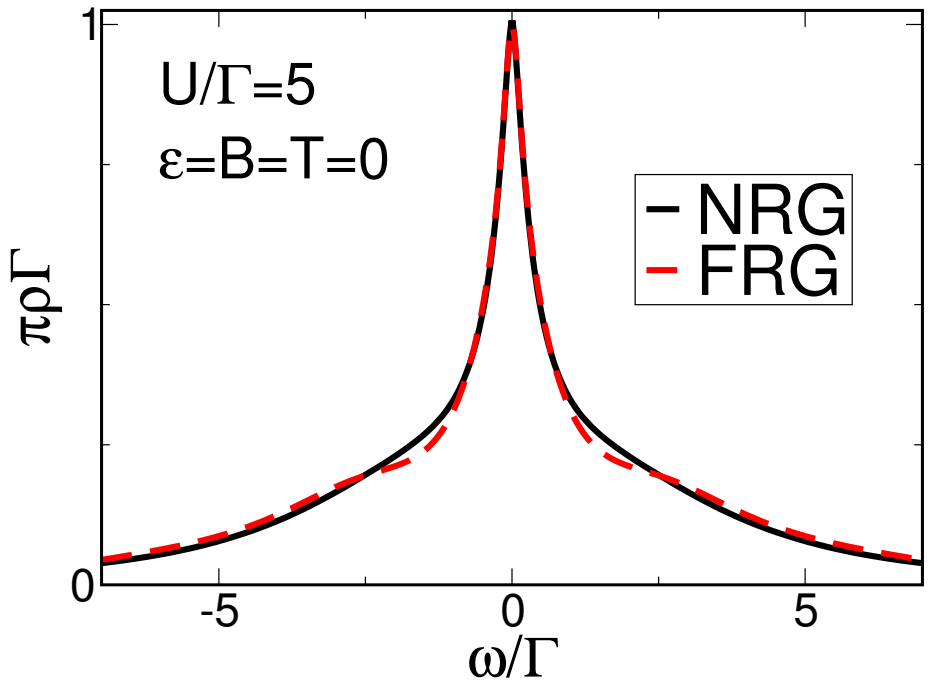
Parametrize the self-energy $\Sigma^\Lambda(i\omega)$ and the two-particle vertex $\gamma_2^\Lambda(i\omega_1', i\omega_2'; i\omega_1, i\omega_2)$ using a **discrete mesh of N Matsubara frequencies**:

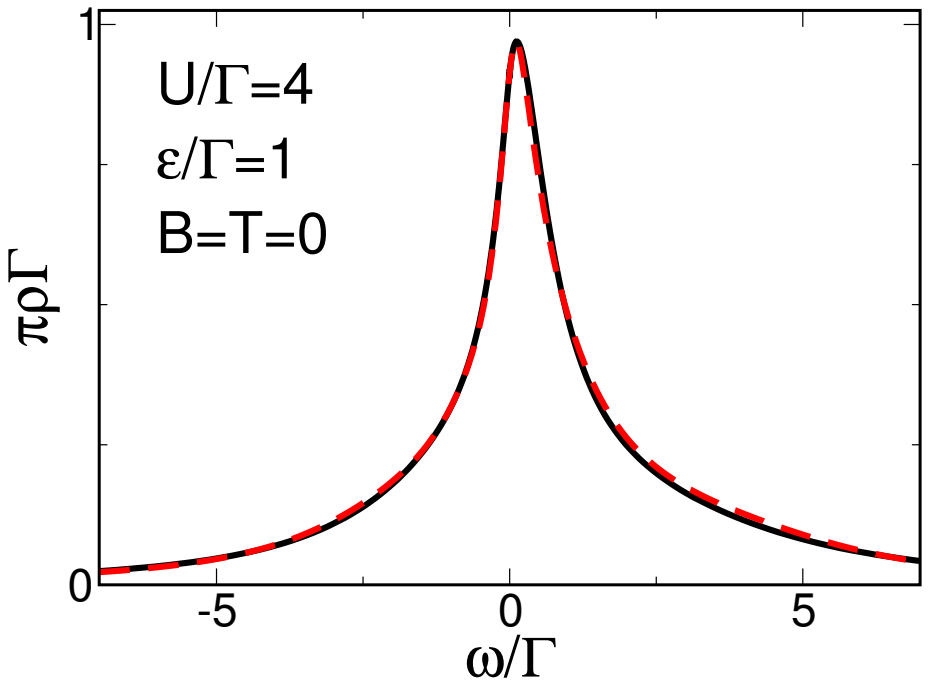
$$\omega_n = \omega_0 \frac{a^n - 1}{a - 1} \qquad \text{or} \qquad \omega_n = \omega_0 a^n$$

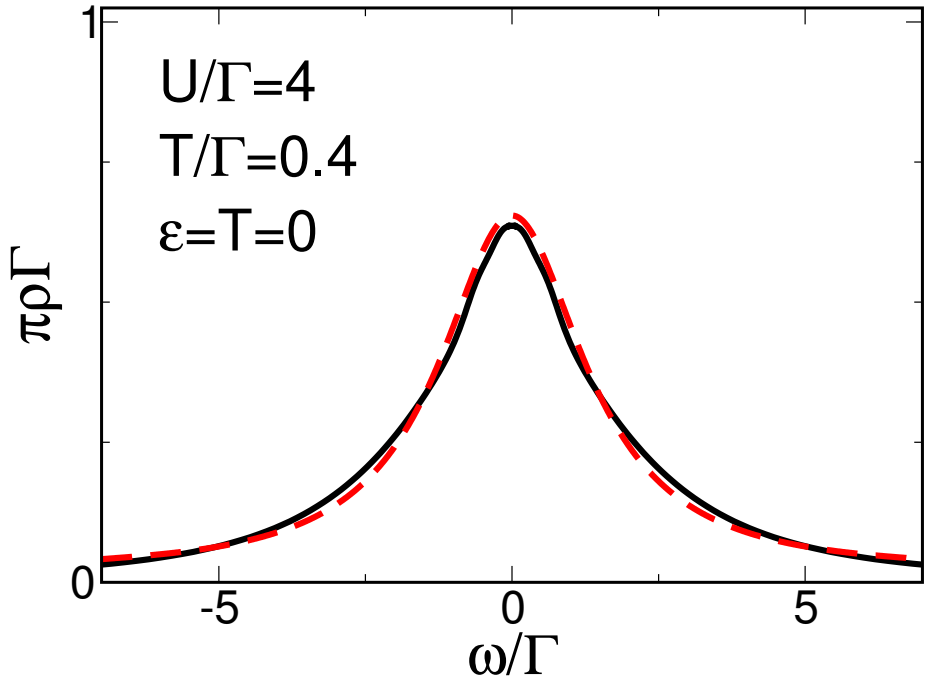
and **verify that physical properties are independent of the actual choice of the discretization**.

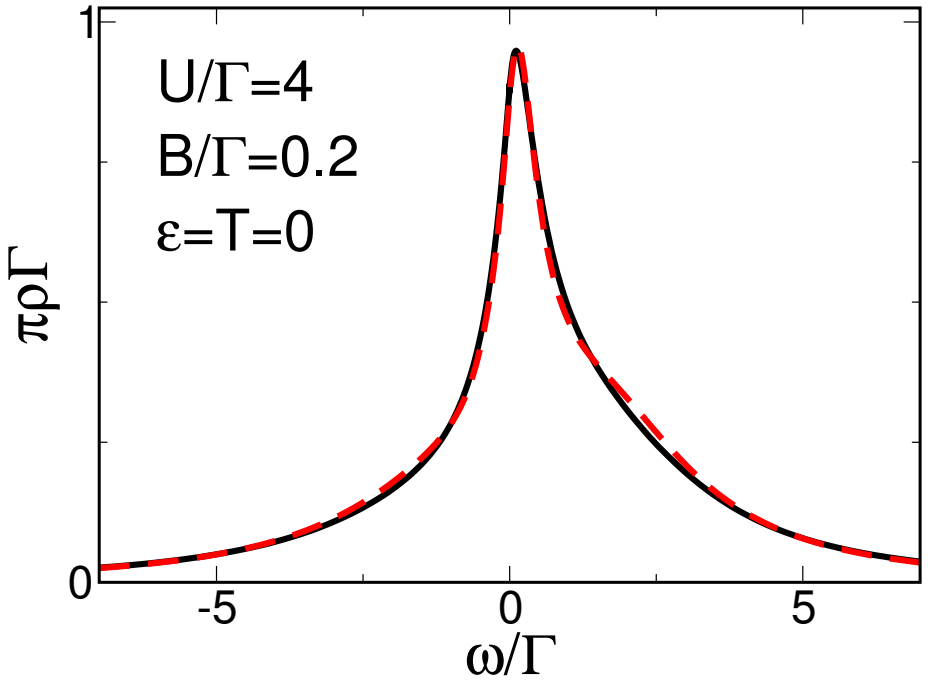
In addition: replace $S^\Lambda \mathcal{G}^\Lambda \to -\dot{\mathcal{G}}^\Lambda \mathcal{G}^\Lambda$ (Katanin 2004)

Small to intermediate U









Numerical efficiency

- FRG works well at intermediate U, but is numerically demanding.
- Idea to **increase numerical efficiency**: introduce new (bosonic) frequencies

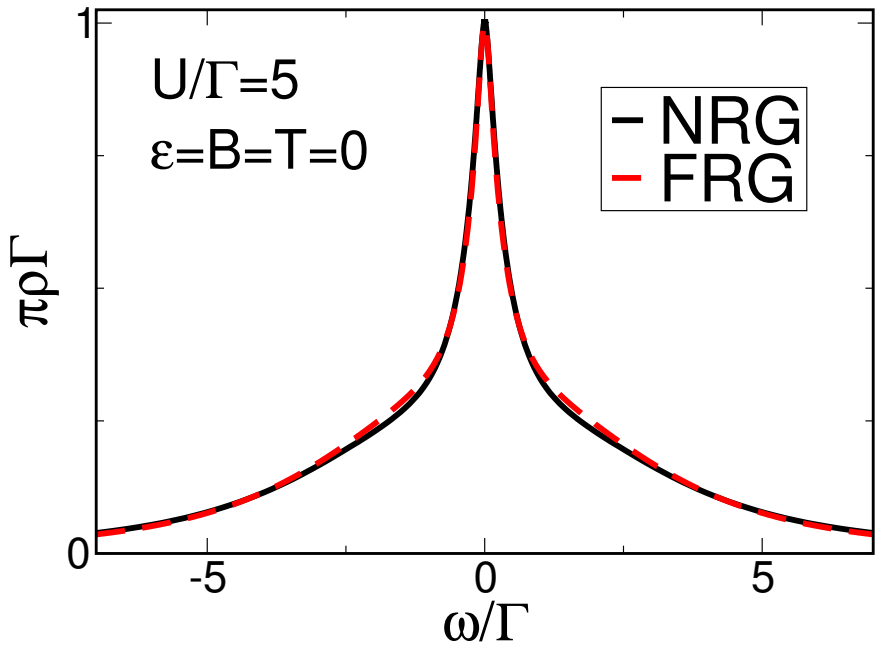
$$\nu_1 = \omega_1' + \omega_2' \qquad \nu_2 = \omega_1' - \omega_1 \qquad \nu_3 = \omega_2' - \omega_1$$

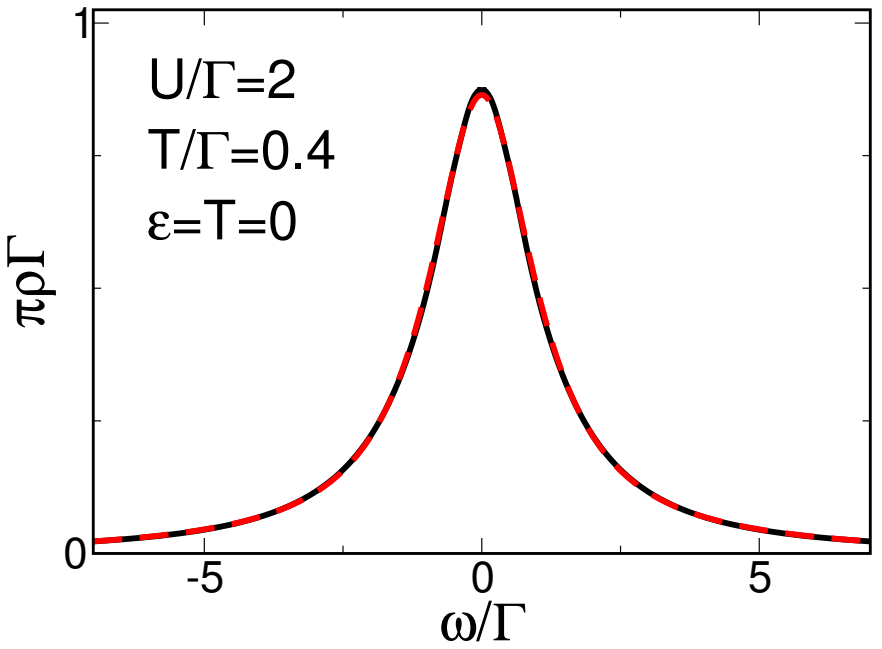
and approximate the flow equation for the two-particle vertex as

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

$\Rightarrow$ three **one-dimensional frequency meshes** instead of a three-dimensional one

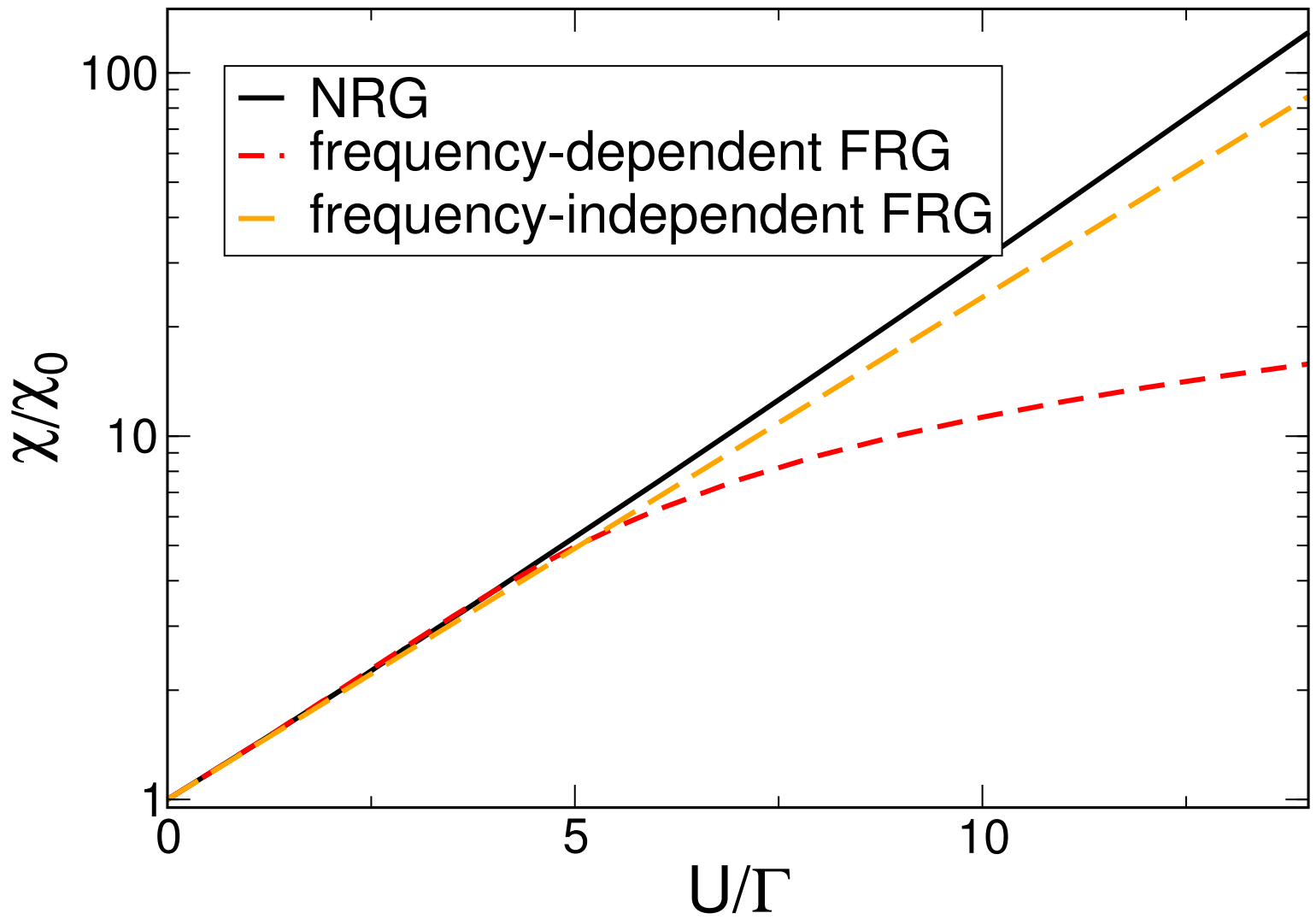
- The resulting approximation works well for intermediate U:





Large U: the Kondo scale

Spin susceptibility: $\chi(U) = \frac{\partial}{\partial B}\big(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle\big)\big|_{B=0} \sim 1/T_K$



Frequency-independent fRG shows **exponential behaviour**.

Frequency-dependent fRG shows **no exponential behaviour**.

Discussion

At **small to intermediate U**, one gets **better results** if the frequency-dependence of γ_2 is accounted for; however, the frequency-dependent scheme does **not contain an exponential energy scale** (in χ, m^*, ...)!

BUT: there are **numerical** (discretization) **issues**!

- **choose N large enough** so that results are converged $\surd$
- **different ways to parametrize γ_2** can be shown to give **coinciding results for intermediate U, but not in the strong coupling regime** (limitation of numerical resources ?!)
- it is unclear, whether the **non-Katanin scheme breaks down completely** for large U because of the **frequency discretization** or for **fundamental reasons** (neglection of γ_3)

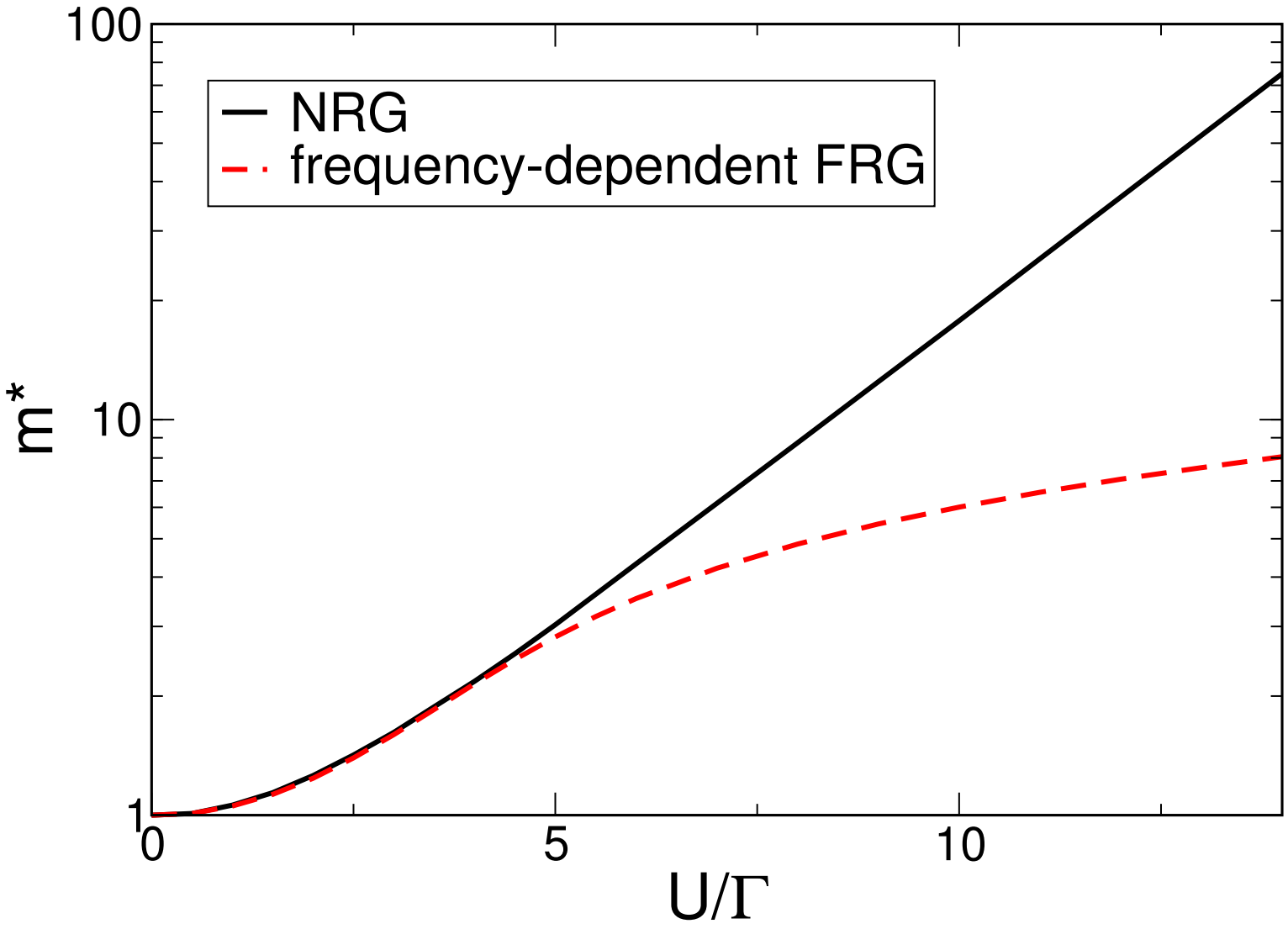
Frequency-dependent fRG can be used to fast compute finite-energy properties of the SIAM at small to intermediate U.

There is no exponential energy scale (in χ, m^*, ...).

Thank you for your attention!

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