Spectral function of the Anderson impurity model at finite temperatures

Functional and Numerical Renormalization Group approaches

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Motivation

Theoretical interest in the Anderson Impurity Model

- *non-equilibrium* description of quantum dots (see talks of S. Andergassen, M. Pletyukhov, S. Jakobs)
- at *equilibrium*, impurity solvers for Dynamical Mean-Field Theory (multi-orbital generalizations)

Comparison of two complementary *non-perturbative* approaches to the Anderson Impurity Model:

1. Numerical Renormalization Group (NRG) at finite temperatures
2. Functional Renormalization Group (FRG) with partial bosonization in the spin-fluctuation channel (Hubbard-Stratonovich decoupling)

- A. Isidori, D. Roosen, L. Bartosch, W. Hofstetter, P. Kopietz, Phys. Rev. B **81**, 235120 (2010)

Previous FRG studies of the Anderson Model

1. frequency-independent approaches

only low-energy properties ($\omega = 0$) are accessible, e.g.,

- quasiparticle weight $Z(U)$
- static spin-susceptibility $\chi_s(U)$
- ...

- C. Karrasch, T. Enss, and V. Meden, Phys. Rev. B **73**, 235337 (2006)
- L. Bartosch *et al.*, J. Phys.: Condens. Matter **21**, 305602 (2009)

2. finite-frequency approaches without bosonization

not satisfactory in the strong-coupling limit

- R. Hedden *et al.*, J. Phys.: Condens. Matter **16**, 5279 (2004)
- C. Karrasch *et al.*, J. Phys.: Condens. Matter **20**, 345205 (2008)
- S. G. Jakobs *et al.*, Phys. Rev. B. **81**, 195109 (2010)

Functional integral representation

Particle-hole symmetric Anderson Model

- half-filling, $\langle \hat{n} \rangle = 1$
- no magnetic field, $h = 0$
- wide band limit, $\Delta(i\omega) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{i\omega - \epsilon_{\mathbf{k}}} \rightarrow -i\Delta \, \mathrm{sign}\, \omega$

Partial *bosonization* in the transverse spin-fluctuation channel: dominant channel at strong-coupling

- $\mathcal{Z} = \int \mathcal{D}[\bar{d}, d, \bar{\chi}, \chi] \, e^{-S_0[\bar{d},d,\bar{\chi},\chi] - S_{\text{int}}[\bar{d},d,\bar{\chi},\chi]}$
- $S_0[\bar{d}, d, \bar{\chi}, \chi] = -\int_\omega \sum_\sigma \Big[i\omega - \Delta(i\omega) \Big] \bar{d}_{\omega\sigma} d_{\omega\sigma} + \int_{\bar{\omega}} U^{-1} \bar{\chi}_{\bar{\omega}} \chi_{\bar{\omega}}$
- $S_{\text{int}}[\bar{d}, d, \bar{\chi}, \chi] = \int_{\bar{\omega}} \int_\omega \Big[\bar{d}_{\omega+\bar{\omega}\uparrow} d_{\omega\downarrow} \chi_{\bar{\omega}} + \bar{d}_{\omega\downarrow} d_{\omega+\bar{\omega}\uparrow} \bar{\chi}_{\bar{\omega}} \Big]$

Our FRG method

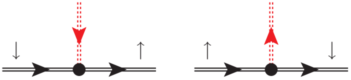
Cutoff scheme

- infrared cutoff only in the *bosonic* propagator

Truncation scheme

- neglect RG flow of vertices

- fermion-boson vertices: $\Gamma_\Lambda\{\omega\} \approx \Gamma_0 \equiv 1$



- fermionic propagator: $G_\Lambda(i\omega) = \dfrac{1}{i\omega + i\Delta\,\mathrm{sign}\,\omega - \Sigma_\Lambda(i\omega)}$

- bosonic propagator: $F_\Lambda(i\bar{\omega}) = \dfrac{1}{U^{-1} - \Pi_\Lambda(i\bar{\omega}) + R_\Lambda(i\bar{\omega})}$

Energy scales

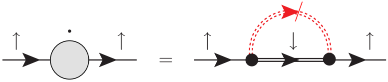
- U on-site Coulomb repulsion
- $\Delta = \pi\rho|V|^2$ hybridization energy

- $\Sigma_\Lambda(i\omega)$ fermionic self-energy
- $\Pi_\Lambda(i\bar{\omega})$ spin-flip susceptibility
- $R_\Lambda(i\bar{\omega})$ cutoff function

FRG flow equations

- flow equation for the fermionic self-energy $\Sigma_\Lambda(i\omega)$

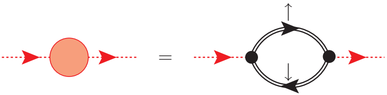
$$\partial_\Lambda \Sigma_\Lambda(i\omega) = \int_{\bar{\omega}} \dot{F}_\Lambda(i\bar{\omega}) G_\Lambda(i\omega - i\bar{\omega})$$



- single-scale propagator: $\dot{F}_\Lambda(i\bar{\omega}) = [-\partial_\Lambda R_\Lambda(i\bar{\omega})][F_\Lambda(i\bar{\omega})]^2$

- skeleton equation for the spin-flip susceptibility $\Pi_\Lambda(i\bar{\omega})$

$$\Pi_\Lambda(i\bar{\omega}) = -\int_{\omega} G_\Lambda(i\omega) G_\Lambda(i\omega - i\bar{\omega})$$



$$\int_\omega \equiv \begin{cases} \frac{1}{\beta} \sum_{\omega_n} & \text{if } T > 0 \\ \int \frac{d\omega}{2\pi} & \text{if } T = 0 \end{cases}$$

Litim cutoff:

$$R_\Lambda(i\bar{\omega}) = \frac{1}{\pi \Delta^2} (\Lambda - |\bar{\omega}|) \Theta(\Lambda - |\bar{\omega}|)$$

Numerical implementation of FRG

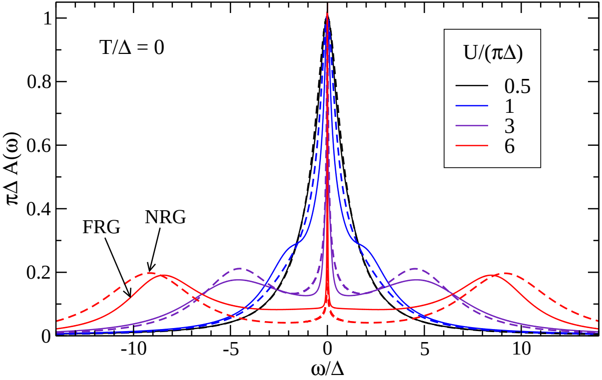
Discretization of the Matsubara axis

- $\boldsymbol{T = 0}$
  - numerical stability: $\begin{cases} \omega_{\min} & \ll & Z(U)\Delta \\ \omega_{\max} & \gg & \max(\Delta, U) \end{cases}$
  - $\omega_n = \omega_{\min} \dfrac{a^n - 1}{a - 1}, \qquad n = 1, \ldots, N$
  - $\omega_{\min} \sim 10^{-6}\Delta, \quad a \sim 1.06, \quad N \sim 400$
- $\boldsymbol{T > 0}$
  - numerical stability: $\omega_{\max} \gg \max(\Delta, U)$
  - $\omega_n = (2n+1)\pi/\beta, \qquad \bar{\omega}_n = 2n\pi/\beta$
  - $N \sim 500 \div 1000$

Analytic continuation to real frequencies

- Padé approximation of the Matsubara self-energy: $\Sigma(\omega) = \Sigma(i\omega_n \to \omega + i0^+)$

FRG and NRG spectral functions at $T/\Delta = 0$, for several Coulomb interactions



- correct *width* and *position* of the Hubbard bands at strong coupling
- at intermediate coupling $U/(\pi\Delta) \approx 1$ FRG overestimates the role of the interaction

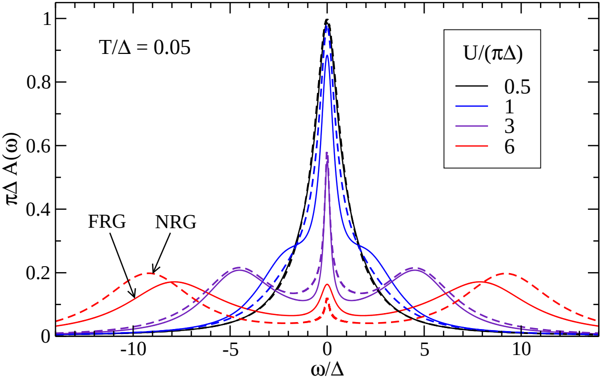
- Friedel sum rule

$$\left|\pi\Delta A(0) - 1\right| < 0.01$$

- integrated spectral weight

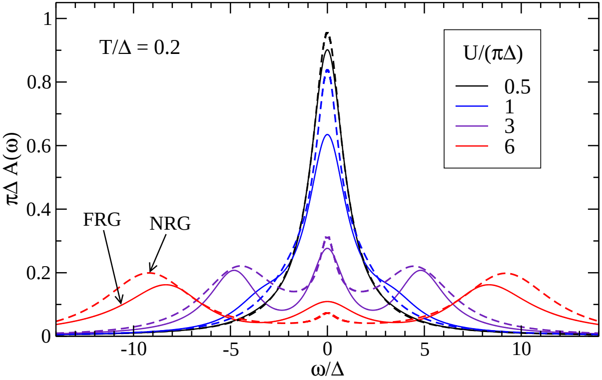
$$\left|\int_{-\infty}^{\infty} d\omega\, A(\omega) - 1\right| < 0.03$$

FRG and NRG spectral functions at $T/\Delta = 0.05$, for several Coulomb interactions



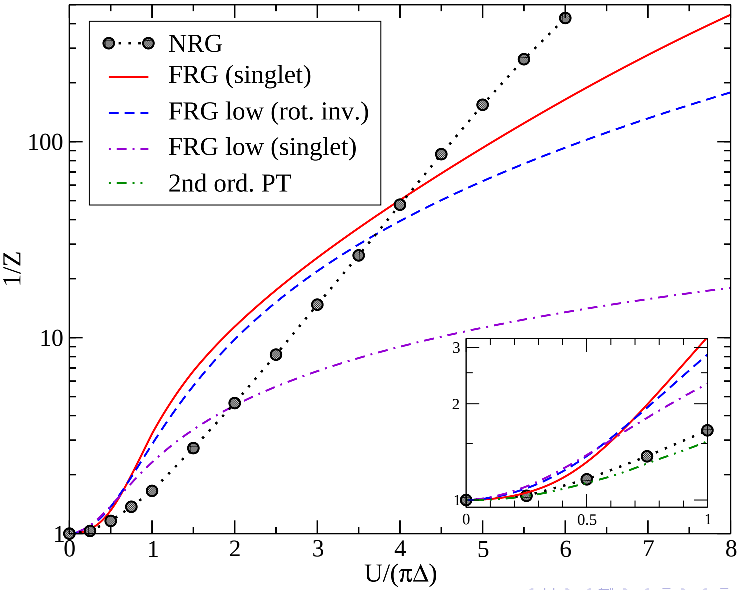
- correct *width* and *position* of the Hubbard bands at strong coupling
- at intermediate coupling $U/(\pi\Delta) \approx 1$ FRG overestimates the role of the interaction

FRG and NRG spectral functions at $T/\Delta = 0.2$, for several Coulomb interactions



- correct *width* and *position* of the Hubbard bands at strong coupling
- at intermediate coupling $U/(\pi\Delta) \approx 1$ FRG overestimates the role of the interaction

Inverse quasi-particle weight $1/Z$ at $T = 0$



Improvements

1. **Magnetic field cutoff**

   - $\Lambda \equiv h$: magnetic field as a cutoff for the fermionic bare propagator,
     $G_{0\sigma}^{-1}(i\omega) = i\omega - \Delta(i\omega) + \sigma\Lambda$
   - $\Lambda \neq 0 \;\Rightarrow\; G_{\Lambda\uparrow} \neq G_{\Lambda\downarrow}$: finite magnetization $\Sigma_{\Lambda\sigma}(i0) = -\sigma\frac{U}{2}m_\Lambda \neq 0$
   - choose the initial magnetization m_{Λ_0} such that $\lim_{\Lambda\to 0} m_\Lambda = 0$

   Results

   - improves $Z(U)$ in the weak-coupling regime $U/(\pi\Delta) \leq 1$
   - fails in describing the strong-coupling limit

2. **Flowing bosonization** [S. Flörchinger and C. Wetterich, Phys. Lett. B **680**, 371 (2009)]

   - work in progress ...

Conclusions

The present FRG scheme: partial bosonization, with IR-cutoff in the bosonic sector, keeping the full frequency structure of the fermionic self-energy and spin-flip susceptibility

- quantitatively good agreement between NRG's and FRG's spectral functions, especially at strong coupling
- the solution is stable at all energy scales and captures both the strong narrowing of the Kondo peak and the high-energy features (unfortunately, no exponential Kondo scale at large U)
- more flexible than the NRG, a simple FRG truncation can be used to solve more complex impurity problems (e.g., as DMFT impurity solver)