Exploring the Kondo physics of the single impurity Anderson model by means of the variational cluster approach

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Introduction

Motivation

- **Benchmark** the variational cluster approach (VCA) and cluster perturbation theory (CPT)
- **Renewed interest** in quantum impurity models by:
  - ▶ non-equilibrium situations in nano devices
  - ▶ solver for DMFT

Single Impurity Anderson Model [1]

$$\hat{\mathcal{H}}_{\text{SIAM}} = \hat{\mathcal{H}}_{\text{conduction}} + \hat{\mathcal{H}}_{\text{impurity}} + \hat{\mathcal{H}}_{\text{hybridization}}$$

$$\hat{\mathcal{H}}^{L}_{\text{conduction}} = \epsilon_s \sum_{i}^{L} \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} - t \sum_{\langle i,j \rangle\, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma}$$

$$\hat{\mathcal{H}}_{\text{impurity}} = \epsilon_f \sum_{\sigma} f^{\dagger}_{\sigma} f_{\sigma} + U\, \hat{n}^{f}_{\uparrow} \hat{n}^{f}_{\downarrow}$$

$$\hat{\mathcal{H}}_{\text{hybridization}} = -V \sum_{\sigma} c^{\dagger}_{I\sigma} f_{\sigma} + f^{\dagger}_{\sigma} c_{I\sigma}\,.$$

- t ... hopping integral, U ... on-site repulsion
- ϵ_i ... on-site energy, V ... hybridization matrix element

Variational cluster approach [2]

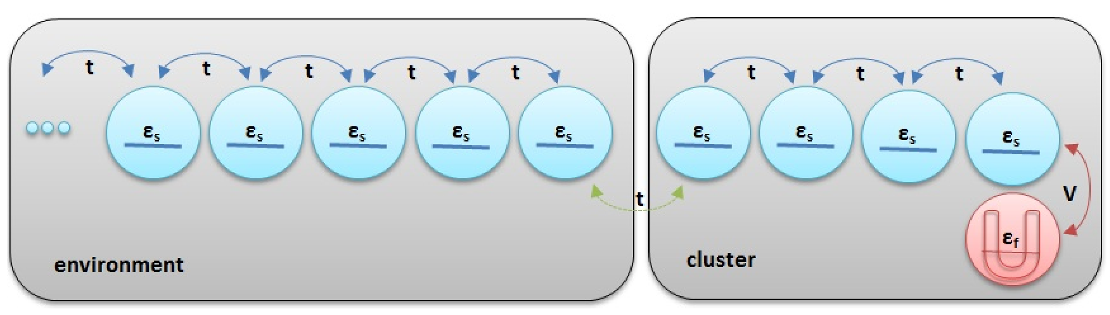
- The variational cluster approach (VCA$_\Omega$) is based on the self-energy functional approach (SFA) [3,4] and provides the single-particle Green's function.
- Grand potential Ω as functional of the Green's function G:

$$\Omega[\mathrm{G}] = \Phi[\mathrm{G}] - \mathrm{Tr}\left(\left(\mathrm{G}_0^{-1} - \mathrm{G}^{-1} \right) \mathrm{G} \right) + \mathrm{Tr}\ln\left(-\mathrm{G}\right)$$

- The Luttinger-Ward functional $\Phi[\mathrm{G}]$ [5] may be eliminated by constructing a reference system g:

$$\Omega[\Sigma] = \Omega'[\Sigma] + \mathrm{Tr}\ln\left(-\left(\mathrm{g}_0^{-1} - \Sigma\right)\right) - \mathrm{Tr}\ln\left(-\left(\mathrm{G}_0^{-1} - \Sigma\right)\right)$$

  - ▶ G ... total Green's function, $_0$ ... free Green's function
  - ▶ g ... Green's function of the reference system
- We choose a reference system consisting of two subsystems:
  - ▶ a cluster of length L including the impurity site
  - ▶ a semi-infinite non-interacting chain



- The self-energy is parameterized by the single-particle parameters x of the model. The physical Green's function makes the grand potential functional stationary.

$$\Omega(\mathrm{x}') = \Omega'(\mathrm{x}') + \mathrm{Tr}\ln\left(-\mathrm{G}(\mathrm{x}')\right) - \mathrm{Tr}\ln\left(-\mathrm{g}(\mathrm{x}')\right)$$

- The stationarity condition becomes:

$$\nabla_{\mathrm{x}'} \Omega(\mathrm{x}') \overset{!}{=} 0$$

- The total Green's function may be obtained by a Dyson-like equation: $\mathrm{G}^{-1} = \mathrm{g}^{-1} - \mathrm{T}$
  - ▶ T holds the cluster-environment hopping as well as all variations made to single-particle parameters

References

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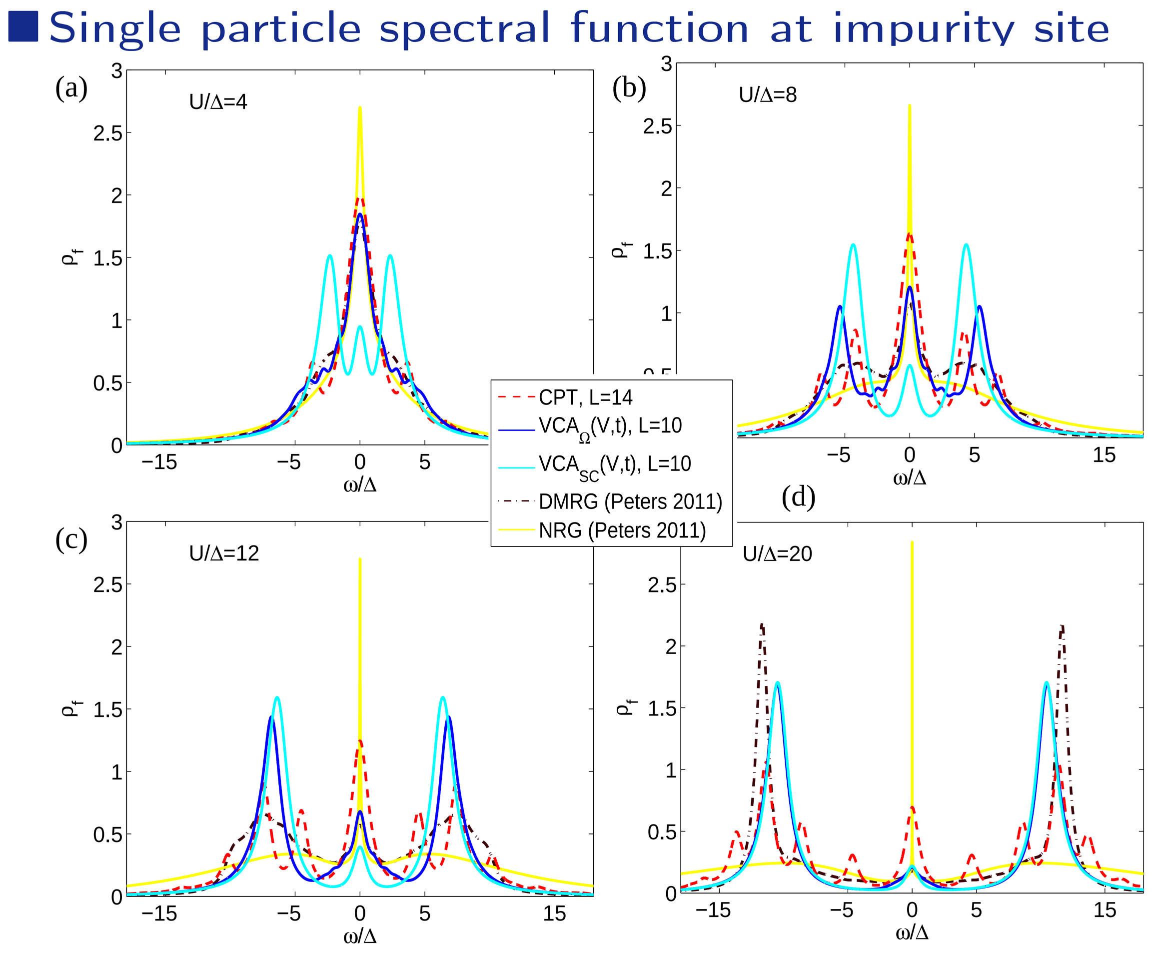
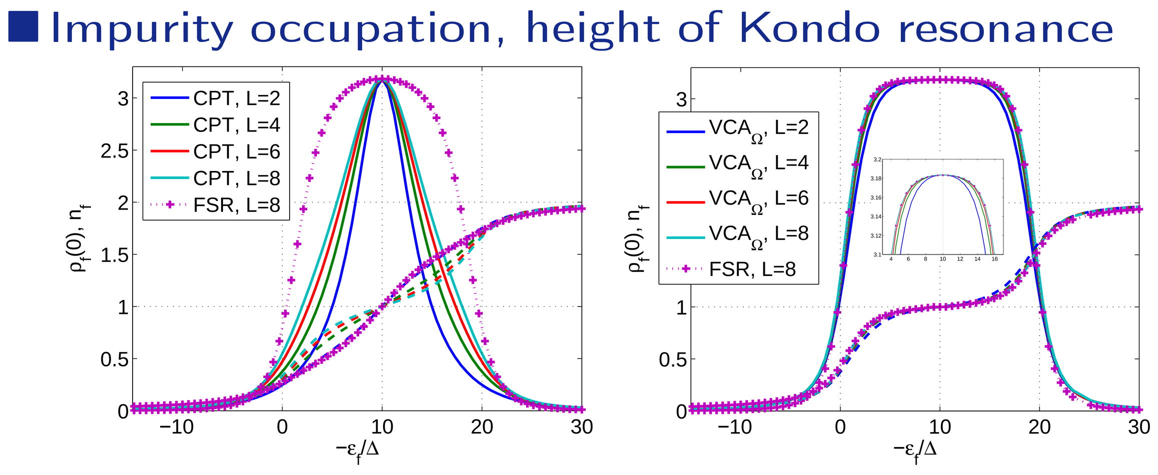
Results I

Single particle spectral function at impurity site



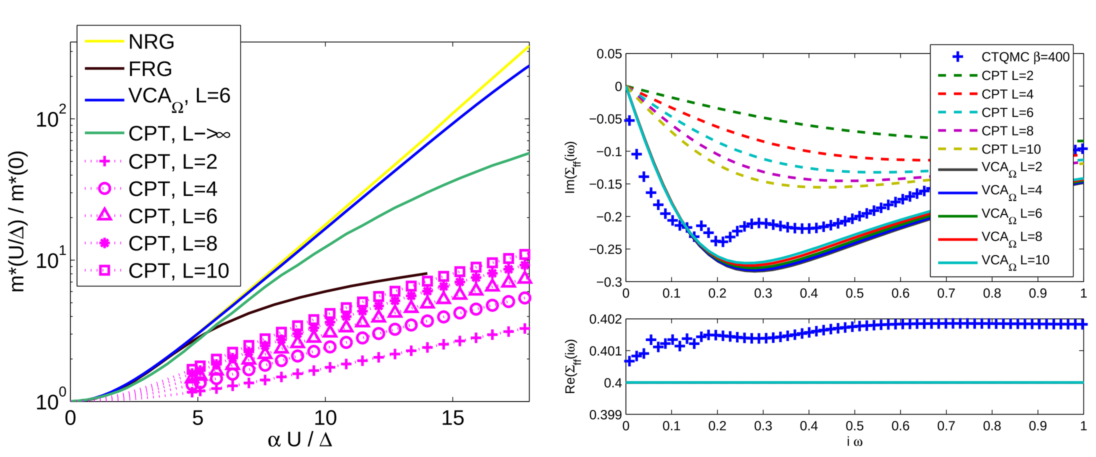
Impurity occupation, height of Kondo resonance



- ▶ CPT results slowly converge with increasing cluster size.
- ▶ VCA shows **rapid convergence** within very small sizes of the cluster part of the reference system.
- ▶ VCA reproduces the pinning of the Kondo peak remarkably well.
- ▶ The **Friedel sum rule** [8] is "naturally" fulfilled within VCA$_\Omega$ using variational parameters $\{\epsilon_s, \epsilon_f\}$:

$$\rho_{f,\sigma}(0) = \frac{\sin^2\left(\pi < n^f_\sigma >\right)}{\pi\Delta}\,.$$

Low energy properties



- The **Kondo temperature** (symmetric SIAM) is given by **Bethe Ansatz** [8]

$$T_K = \sqrt{\frac{\Delta U}{2}}\, e^{-\gamma \frac{\pi}{8\Delta} U}\,, \quad \gamma = 1$$

- The **effective mass** (quasiparticle renormalization) is **inversely proportional** to the Kondo temperature [9]:

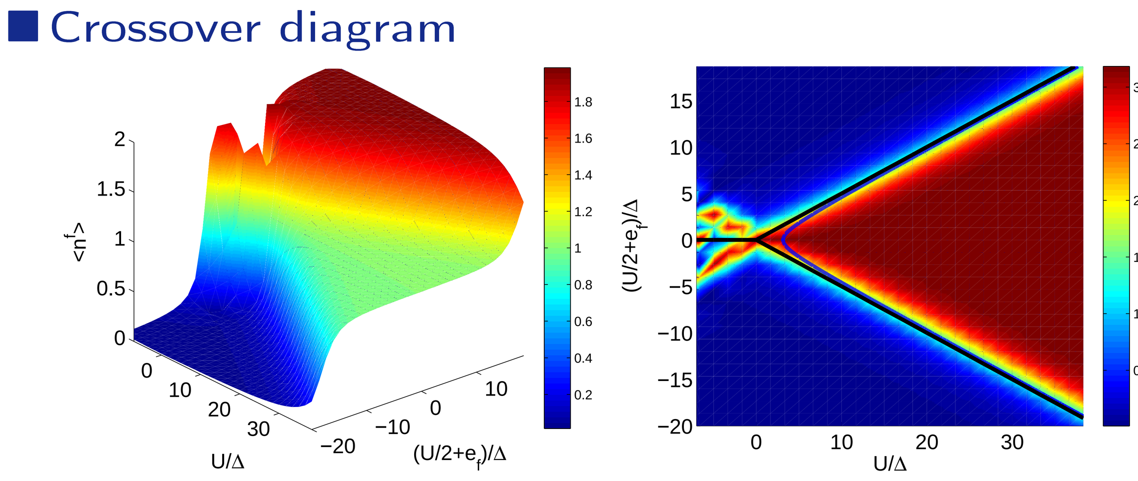
$$m^*(U) = 1 - \left.\frac{d[\mathrm{Im}\,\Sigma^{\sigma}_{ff}(i\omega, U)]}{d\,\omega}\right|_{\omega=0^+}$$

- Obtaining the Kondo scale by means of the **static spin-susceptibility**, the **full-width at half maximum** or the **spectral weight of the Kondo resonance** shows exactly the **same behavior**.
- **VCA$_\Omega$ yields an exponential scale in U** but does not give the correct pre-factor in the exponent. The pre-factor correction to the Bethe Ansatz result may be calculated analytically for a two-site reference system and is given by

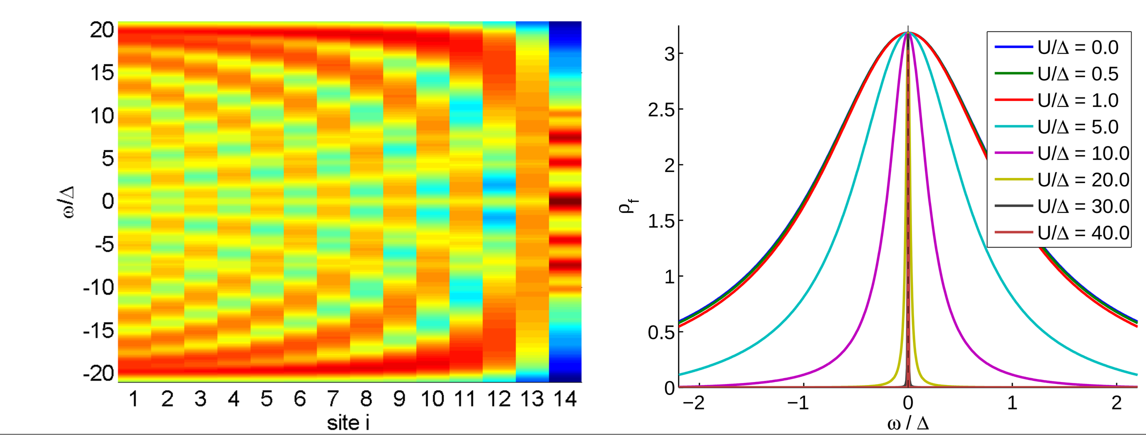
$$\gamma = \frac{1}{\alpha} = 0.6511$$

Results II

Crossover diagram



Spatially resolved spectrum / Kondo peak



Nonequilibrium situation

- Initial state: **three decoupled systems in equilibrium**

  left lead - cluster - right lead

  - ▶ At some time t_0 the **coupling is switched on**.
  - ▶ We are interested in the long time **steady-state properties**.
- **Keldysh - formalism** to obtain steady-state properties
- **VCA$_{SC}$ reformulated** in terms of self-consistently determined variational parameters where the self-consistency conditions are static expectation values [10] (for example the particle number if the variational parameter is the on-site energy):

$$\left\langle \hat{n}^f_\sigma \right\rangle_{\text{cluster},\epsilon'_f,\epsilon'_s} \overset{!}{=} \left\langle \hat{n}^f_\sigma \right\rangle_{\text{CPT},\epsilon_f,\epsilon_s,\epsilon'_f,\epsilon'_s}$$

- Green's functions calculated in **Keldysh space on the real energy axis**:

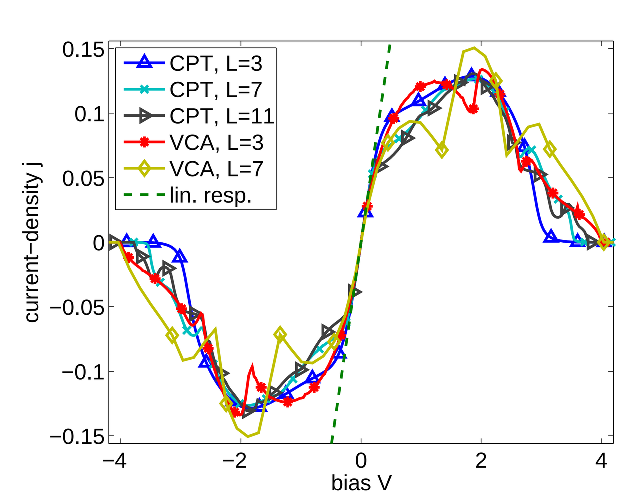
$$\tilde{\mathrm{G}}(\omega) = \begin{pmatrix} \mathrm{G}^{\text{ret}}(\omega) & \mathrm{G}^{\text{keld}}(\omega,\mu) \\ 0 & \mathrm{G}^{\text{adv}}(\omega) \end{pmatrix}$$

- The initial $\mathrm{G}^{\text{keld}}(\omega,\mu)$ of the decoupled system is given by

$$\mathrm{G}^{\text{keld}}(\omega,\mu) = \left(\mathrm{G}^{\text{ret}}(\omega) - \mathrm{G}^{\text{adv}}(\omega)\right)\left(1 - 2p_{\text{FD}}(\omega,\mu,\beta)\right)$$

  - ▶ $p_{\text{FD}}(\omega,\mu,\beta)$ ... Fermi-Dirac distribution
- The **current-density** is given by:

$$I_{ij} = t\,\mathrm{Re}\left(\mathrm{G}^{\text{keld}}_{ij}(t=0)\right) = \frac{t}{2}\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \mathrm{Re}\left(\mathrm{G}^{\text{keld}}_{ij}(w) - \mathrm{G}^{\text{keld}}_{ji}(w)\right)$$



Conclusions

- VCA$_\Omega$ captures all qualitative features of the spectral features of the SIAM including
  - ▶ Kondo resonance and exponential scaling in U
  - ▶ formation of Hubbard bands (width and position)
  - ▶ fulfills Friedel sum rule in all parameter regions

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