Strongly correlated quantum impurity problems

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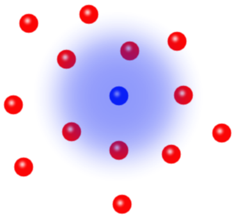
Quantum Matter: Computation Meets Experiments

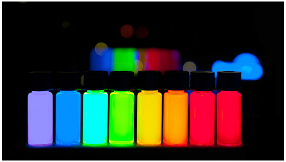
Quantum impurities



Impurity models are **simple** $\left\{ \begin{array}{l} \rightarrow \text{easy} \\ \rightarrow \text{fundamental} \end{array} \right.$

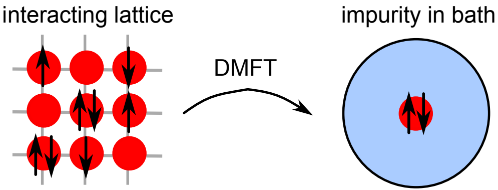
Examples:

- Fröhlich polaron
- Kondo impurity
- Transport through quantum dots



[quantum dots for sale on `www.plasmachem.com`]

Dynamical Mean Field Theory



- Approximation: local lattice self-energy
- Exact in the limit of infinite dimensions
- Mapping to one or several impurities

$\Rightarrow$ good **impurity solvers** are crucial

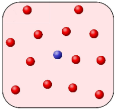
Reviews e.g. [Georges *et. al.*, Rev. Mod. Phys. 68, 13 (1996); Kotliar *et. al.*, Rev. Mod. Phys. 78, 865 (2006); Aoki *et. al.*, Rev. Mod. Phys. 86, 779 (2014)]

Outline

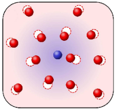
- Introduction
- **The Fermi polaron**
- The spin-boson model
- Conclusions

The Fermi polaron

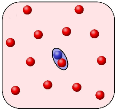
A single **mobile** impurity interacting with a **sea of fermions**



weak attraction: mean-field of the medium



stronger attraction: polaron "dressed" with a cloud of atoms



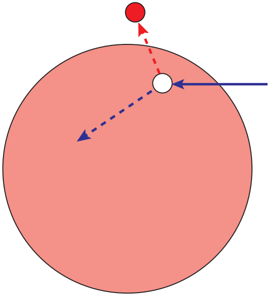
strong attraction: molecular bound state

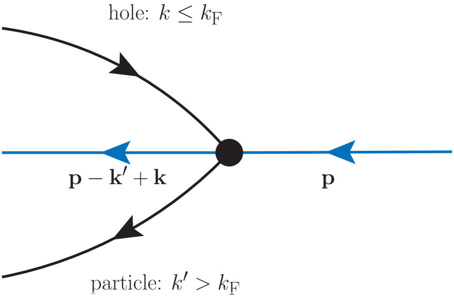
[image: Schirotzek, Wu, Sommer, Zwierlein, PRL **102**, 230402 (2009)]

The Fermi polaron

Hamiltonian

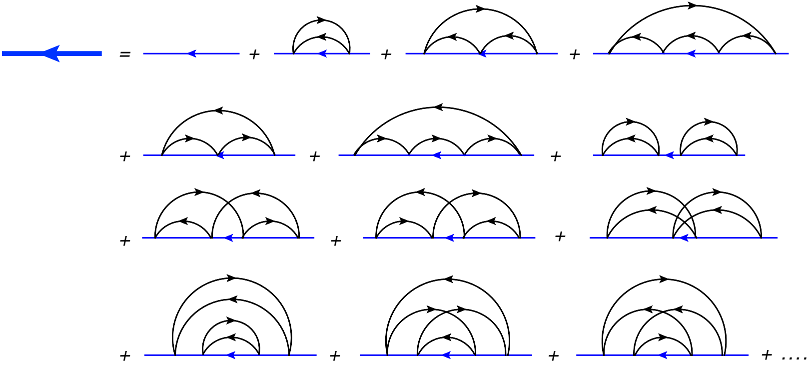
$$H = \sum_{\mathbf{k}} \left(\epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \epsilon'_{\mathbf{k}} b^\dagger_{\mathbf{k}} b_{\mathbf{k}} \right) + g_0 \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} b^\dagger_{\mathbf{p}-\mathbf{k}'+\mathbf{k}} c^\dagger_{\mathbf{k}'} c_{\mathbf{k}} b_{\mathbf{p}}$$





Diagrammatic expansion

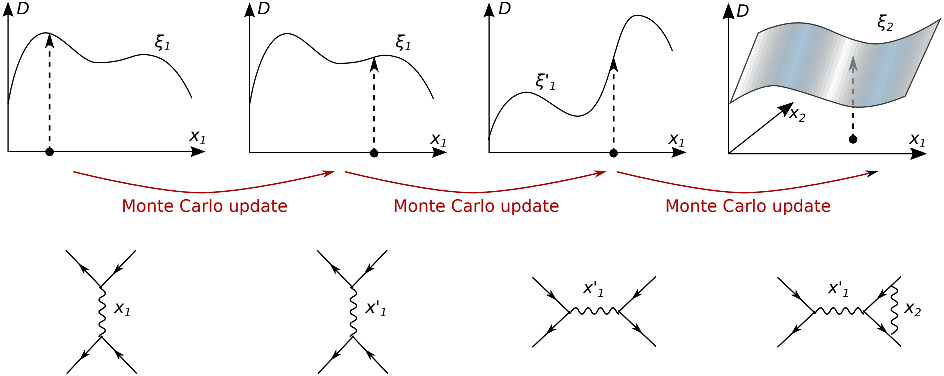
Full impurity Green's function $G(\mathbf{k},\tau) = -\theta(\tau)\langle b_{\mathbf{k}}(\tau) b^{\dagger}_{\mathbf{k}}(0)\rangle$
Expansion in the free Green's function and coupling constant:



- Excitation of multiple particle-hole pairs
- Impurity exchanges momentum with particles and holes

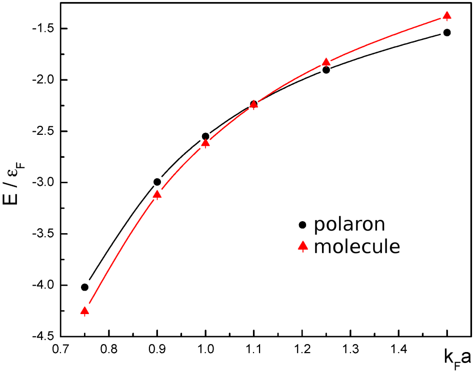
Sampling of diagrams

$$Q(\mathbf{y}) = \sum_{n=0}^{\infty} \sum_{\xi_n} \int d\mathbf{x}_1 \dots d\mathbf{x}_n D(\xi_n, \mathbf{y}, \mathbf{x}_1, \dots, \mathbf{x}_n)$$



The Fermi polaron

Exact nature of the phase transition to the molecule state

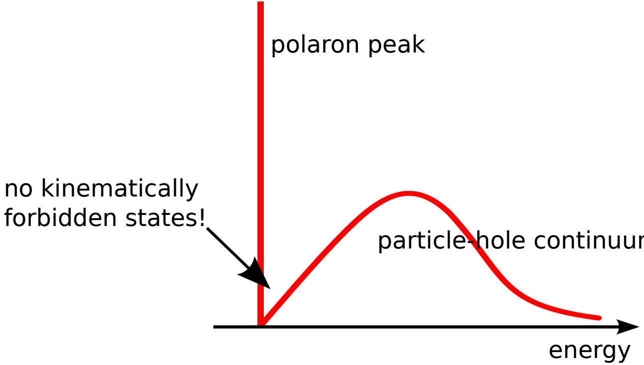


[Prokof'ev & Svistunov, PRB **77**, 125101 and 020408 (2008)]

The Fermi polaron

First controlled calculation of the Fermi polaron **spectral function**

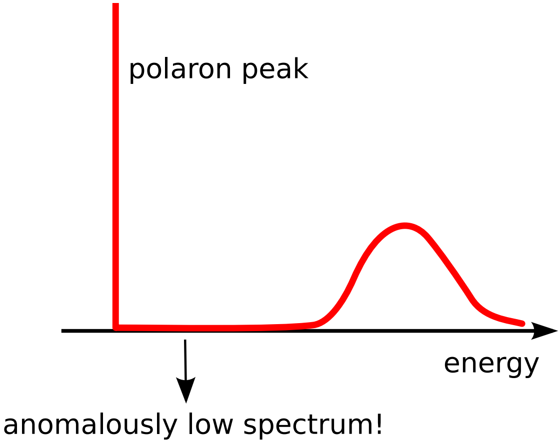
Expectation:



[Goulko, Mishchenko, Prokof'ev, Svistunov, PRA **94**, 051605(R) (2016)]
[Goulko, Mishchenko, Pollet, Prokof'ev, Svistunov, PRB **95**, 014102 (2017)]

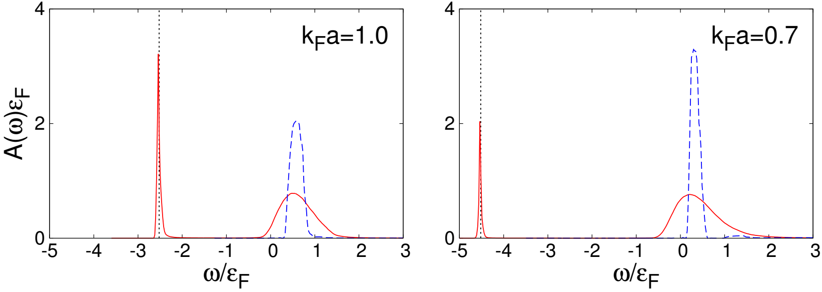
The Fermi polaron

Instead for $k_{\mathrm{F}} a \lesssim 1$ we find:



Spectral function from Green's function (analytic continuation)

$$-G(\tau) = \int_0^\infty e^{-\omega\tau} A(\omega) d\omega$$



[Goulko, Mishchenko, Prokof'ev, Svistunov, PRA **94**, 051605(R) (2016)]
[Goulko, Mishchenko, Pollet, Prokof'ev, Svistunov, PRB **95**, 014102 (2017)]

Outline

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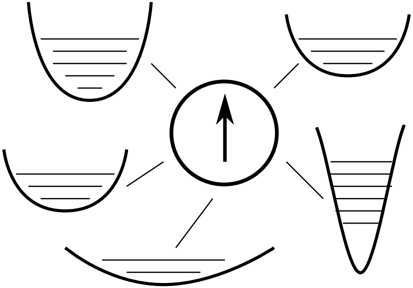
- **The spin-boson model**
- Conclusions

Spin-Boson Model

A **spin** (two-state system)
coupled to
a bath of **non-interacting harmonic modes**

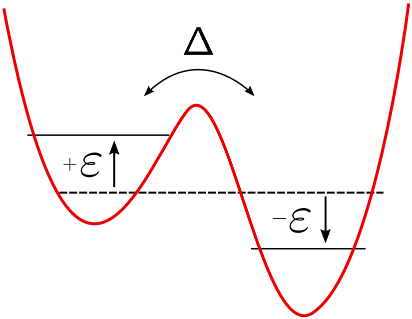


- Model for quantum dissipation
- Interactions with photons or phonons
- Fermi systems via bosonization

Spin-Boson Model

Hamiltonian two-state system:

$$H_s = \varepsilon\sigma_z + \Delta\sigma_x$$



Hamiltonian boson bath (harmonic oscillators):

$$H_b = \sum_k \hbar\omega_k \left(b_k^\dagger b_k + \frac{1}{2} \right)$$

Spin-Boson Model

Linear spin-bath coupling:

$$H_{\mathrm{int}} = \sigma_z \sum_k c_k x_k = \sigma_z \sum_k \frac{c_k}{\sqrt{2\omega_k}} \left(b_k^\dagger + b_k \right)$$

Spectral density:

$$\begin{aligned} J(\omega) &= \frac{\pi}{2} \sum_k \frac{c_k^2}{\omega_k} \delta(\omega - \omega_k) \\ &\propto \omega^{s} \omega_c^{1-s} f_{\mathrm{cutoff}}(\omega/\omega_c) \end{aligned}$$

- $s = 1$: Ohmic
- $s > 1$: super-Ohmic
- $0 < s < 1$: sub-Ohmic

Diagrammatic expansion

Dynamical properties

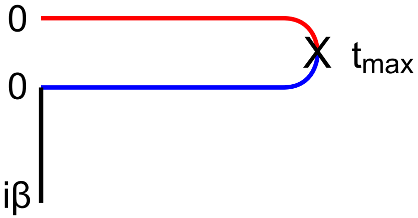
$\Downarrow$

Real-time evolution

$\Downarrow$

Keldysh contour expansion

$$\langle A(t)\rangle = \mathrm{Tr}\left[\rho_0 e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}\right] \quad \text{with} \quad \rho_0 = |0\rangle\langle 0|\frac{e^{-\beta H_b}}{Z}$$

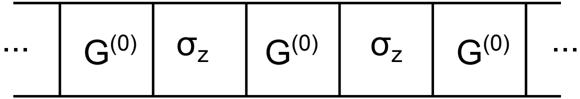


Diagrammatic expansion

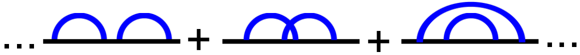
- Diabatic coupling expansion (in Δ)
- **System-bath coupling expansion** (in $H_{\rm int}$)

  $\Rightarrow$ factorizes into system and bath operators

  System part (matrix propagators):

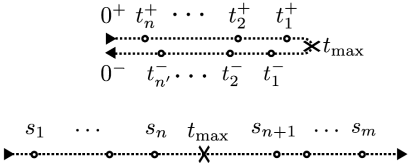


  Bath part (Wick's theorem):

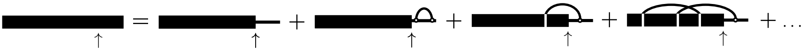


Inchworm algorithm

System observable at Keldysh fold



Efficient **real-time** Quantum Monte Carlo



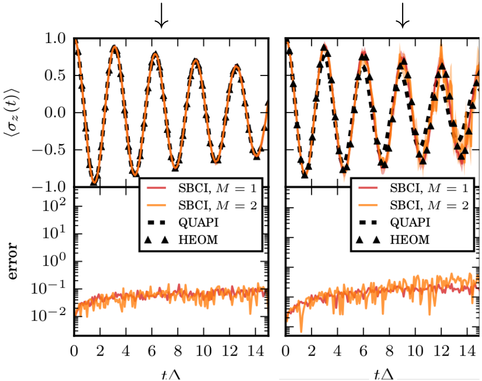
- Use cheap short term propagators to obtain long-term propagators
- Scaling reduces from exponential to polynomial

[Cohen, Gull, Reichman, Millis, PRL **115**, 266802 (2015)]

Spin-Boson Model: benchmarks

Non-equilibrium population difference $\langle \sigma_z(t) \rangle$

fast bath $\omega_c = 5\Delta$ slow bath $\omega_c = 0.25\Delta$

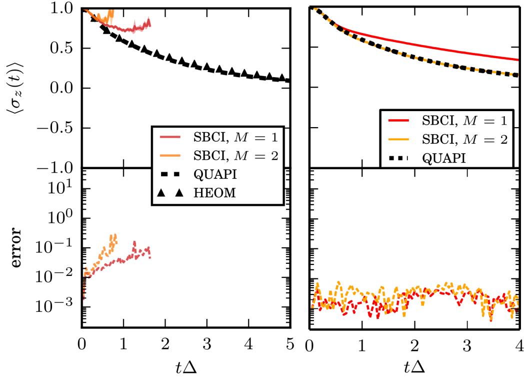


[Chen, Cohen, Reichman, JCP **146**, 054105 & 054106 (2017)]

- $\varepsilon = 0$
- weak coupling
- high temperature $\beta\Delta = 0.5$

Spin-Boson Model: benchmarks

Non-equilibrium population difference $\langle \sigma_z(t) \rangle$

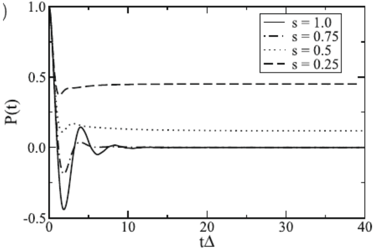


[Chen, Cohen, Reichman, JCP **146**, 054105 & 054106 (2017)]

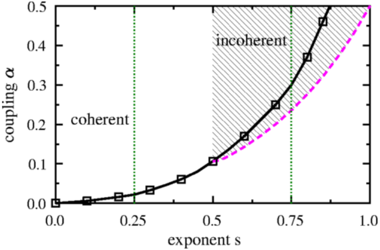
[current work with Chen, Cohen, Goldstein]

- $\varepsilon = 0$
- strong coupling
- high temperature $\beta\Delta = 0.5$
- fast bath $\omega_c = 5\Delta$

Spin-boson model: sub-Ohmic regimes



[Wang & Thoss, Chem.Phys. **370**, 78-86 (2010)]

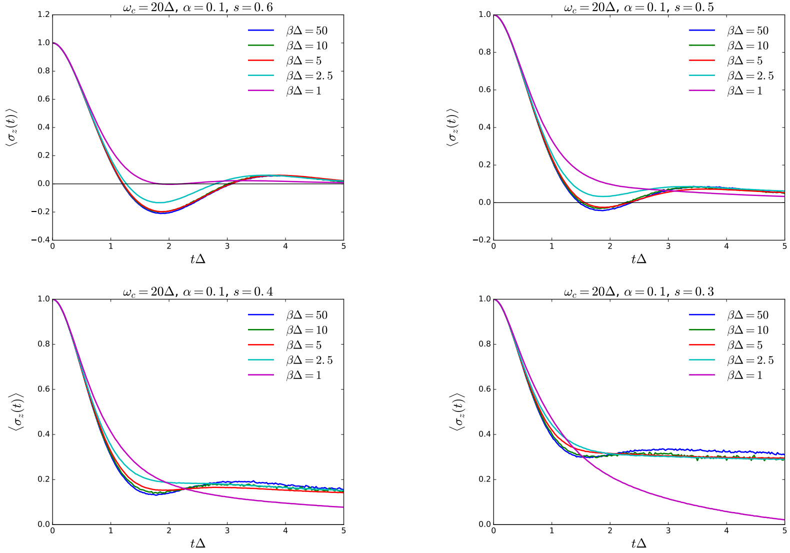


[Kast & Ankerhold, PRL **110**, 010402 (2013)]

- localization/delocalization phase transition
- critical exponents in the sub-Ohmic case
- coherence/decoherence crossover
- temperature-dependence not well understood yet

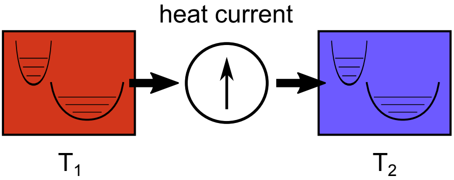
Spin-boson model: sub-Ohmic regimes

Preliminary data



Outlook: spin-boson model

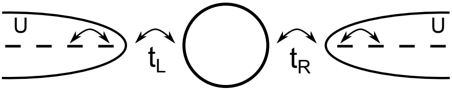
- Heat current through the two-level system coupled to two baths at different temperatures



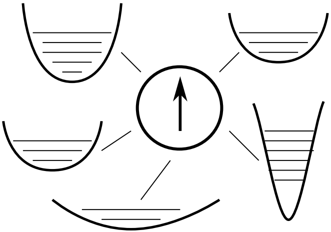
- Combining bosonic and fermionic baths (e.g. Anderson-Holstein model)

Outlook: bosonization

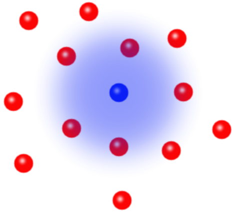
Single site coupled to (one or several) **interacting** electron leads



$\Downarrow$ bosonization



Summary



Impurity models are **simple** $\begin{cases} \rightarrow \text{easy} \\ \rightarrow \text{fundamental} \end{cases}$

Examples:

- Fermi polaron
- Spin-boson model
- Non-equilibrium

Controlled results:

- Precision calculations
- Discovery of new phenomena
- Fundamental understanding