



Tuesday 30th August, 2022

Spectral functions of the Holstein polaron: exact and approximate solutions

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*Scientific Computing Laboratory
Center for the Study of Complex Systems
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Republic of Serbia*

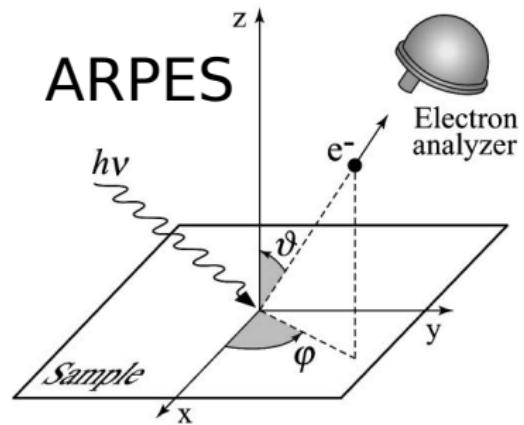
Holstein model

Hamiltonian:

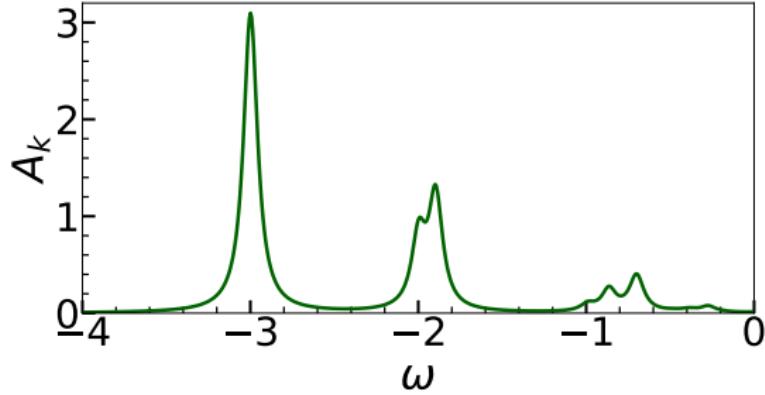
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We calculate:

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Damascelli et al., Rev. Mod. Phys. 75, 473 (2003)



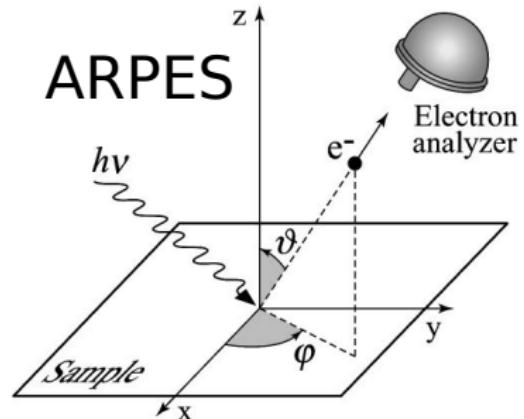
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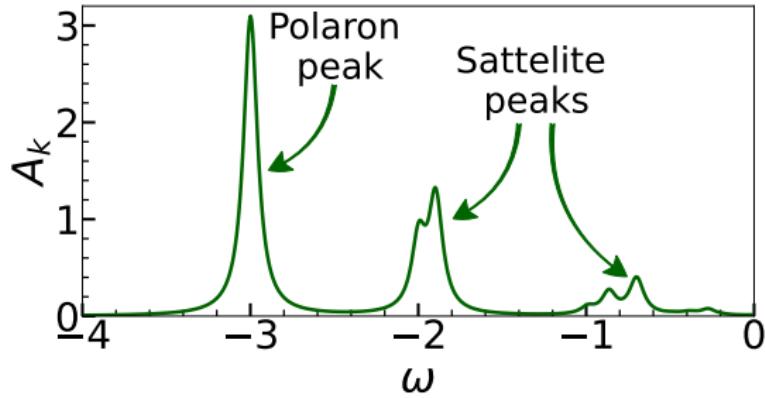
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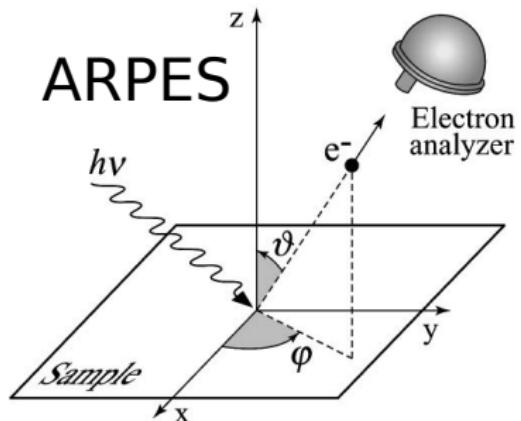
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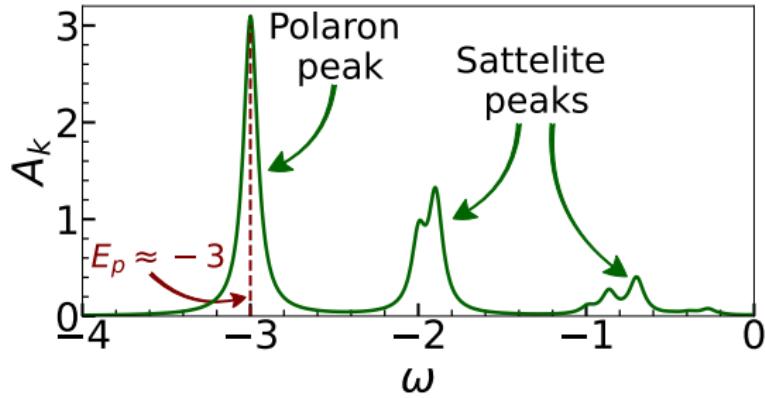
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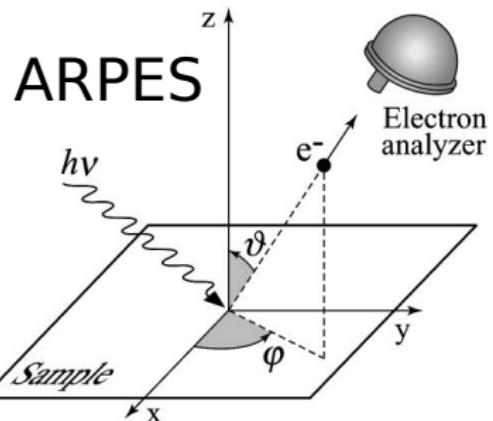
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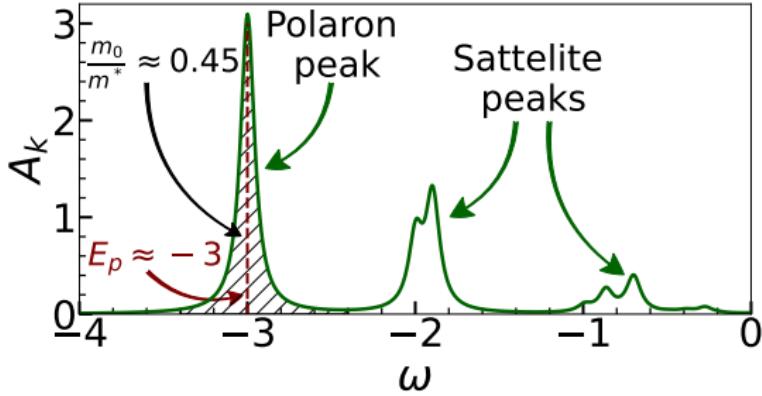
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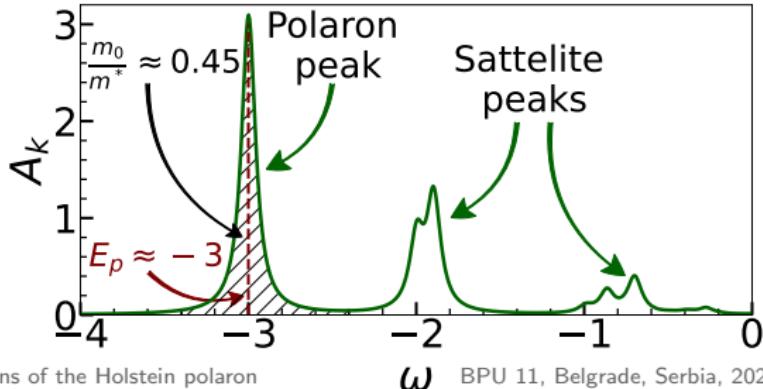
$$C_k(\tau) = \int_{-\infty}^{\infty} A_k(\omega) e^{-\omega\tau} d\omega$$

$$A_k(\omega) = -\frac{1}{\pi} \text{Im} G_k(\omega)$$

$$G_k(\omega) = \frac{1}{\omega + 2t_0 \cos k - \Sigma_k(\omega)}$$

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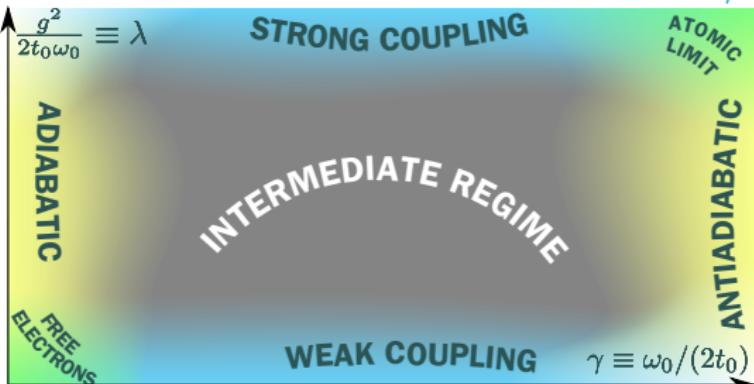
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Mitrić et al., Phys. Rev. Lett. 129, 096401 (2022)

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- Self-consistent Migdal approximation (SCMA)
- Hierarchical equations of motion (HEOM)
- Quantum Monte Carlo (QMC)
- Exact diagonalization (ED)

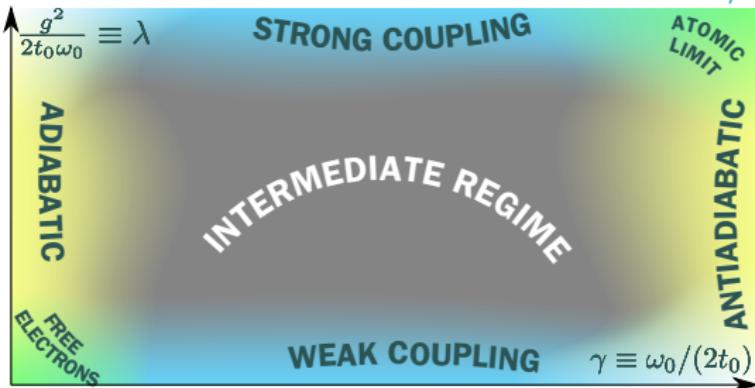
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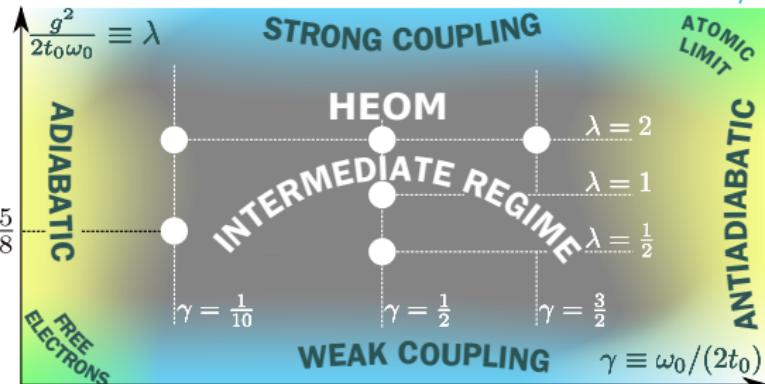
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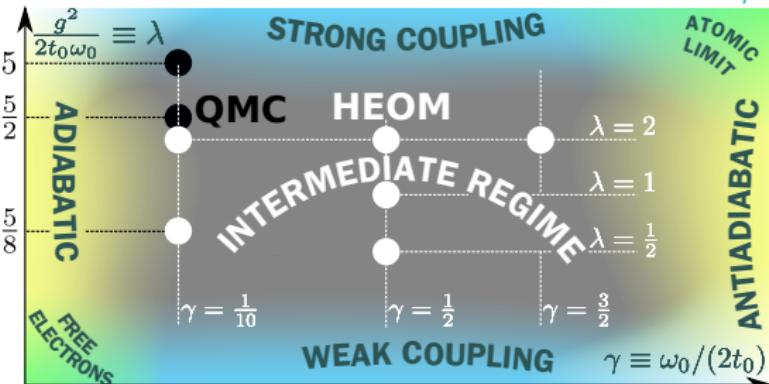
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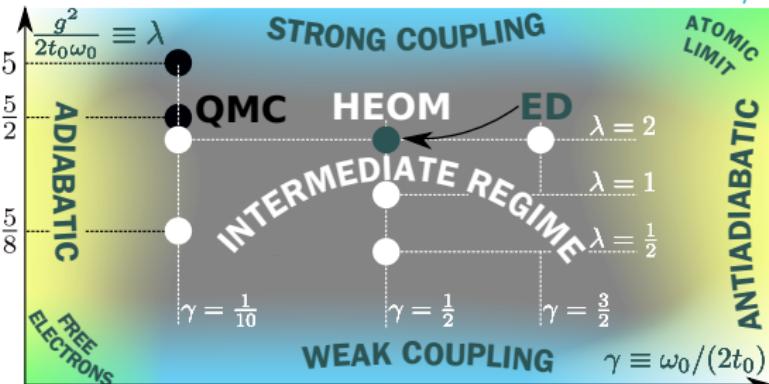
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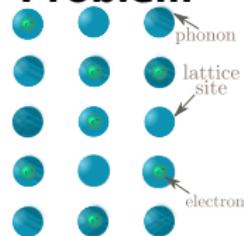
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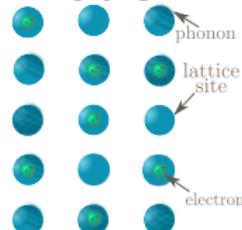
Dynamical mean-field theory(DMFT)

(a) **Holstein
Lattice
Problem**

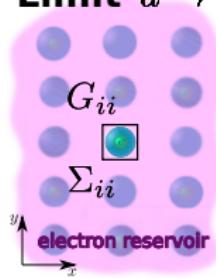


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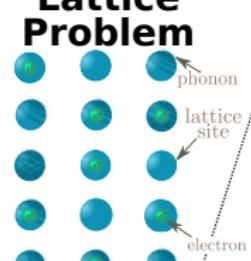


(b) **Limit $d \rightarrow \infty$**

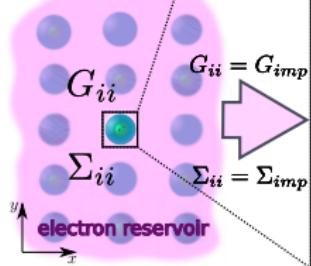


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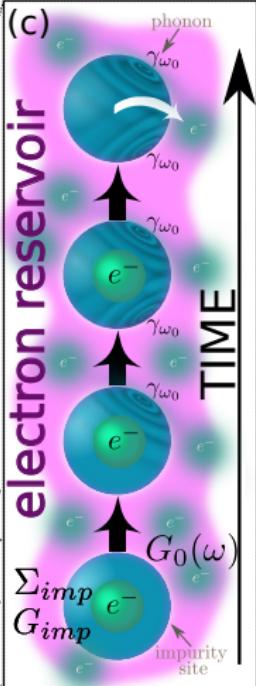
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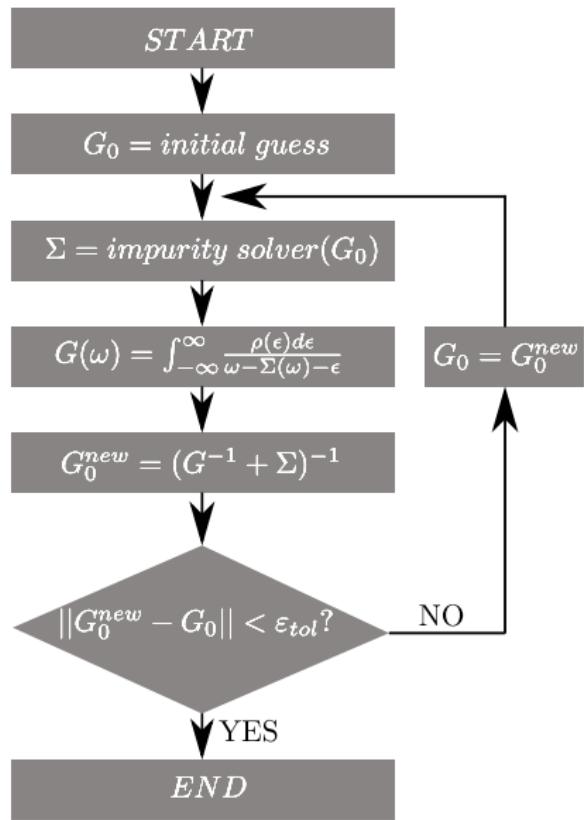
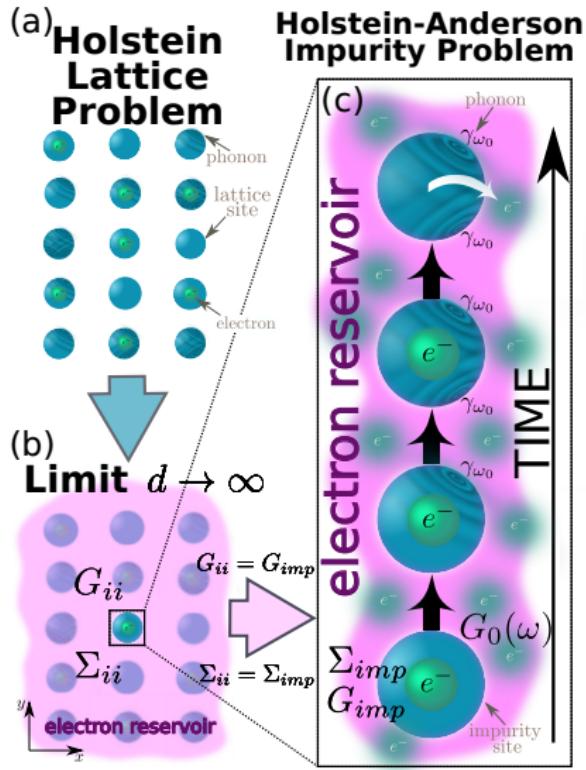
(b) Limit $d \rightarrow \infty$



Holstein-Anderson Impurity Problem



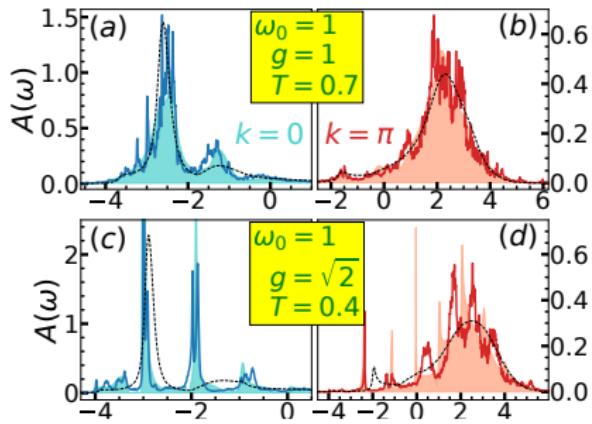
Dynamical mean-field theory(DMFT)



Mitrić et al., Phys. Rev. Lett. 129, 096401 (2022)

Spectral functions of the Holstein polaron

Results: Spectral functions

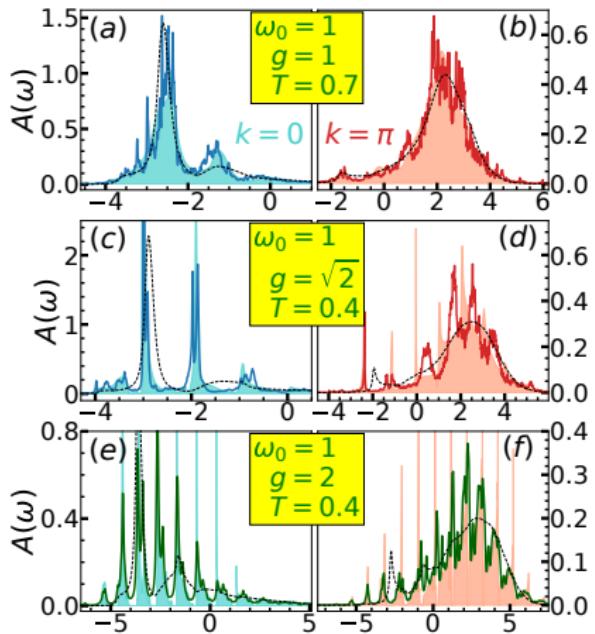


Parameter regime:
Left Fig:

- (a)–(d) Intermediate
- (e)–(f) Strong
- (g)–(h) Atomic

- Weak

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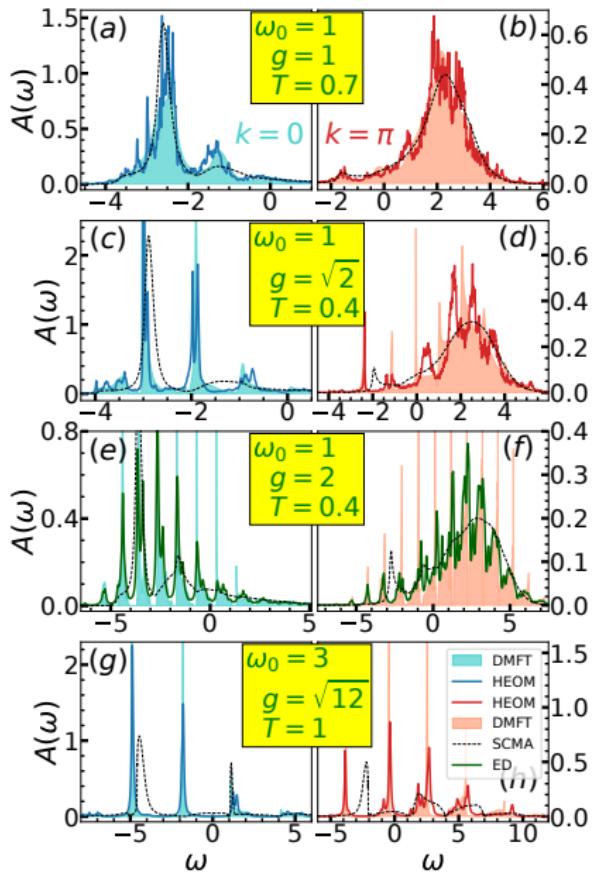


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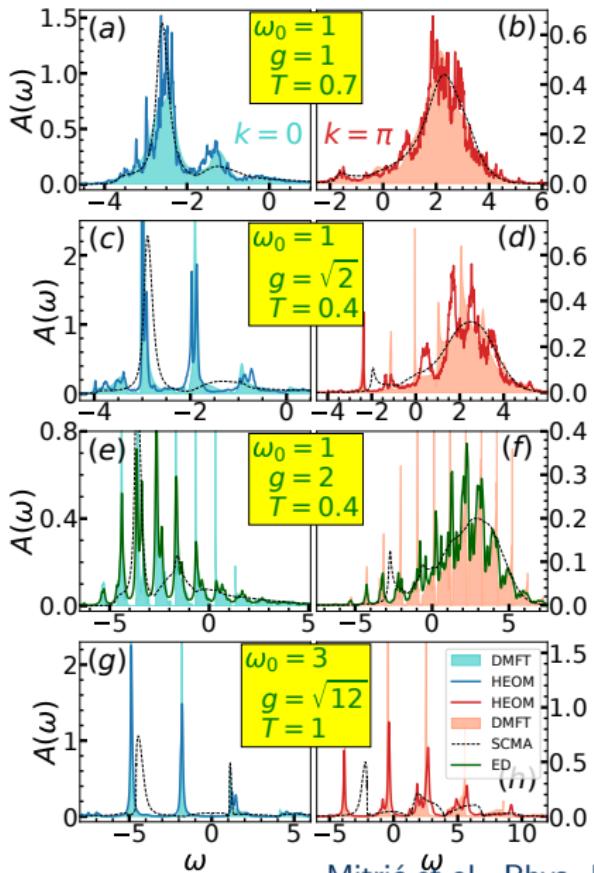
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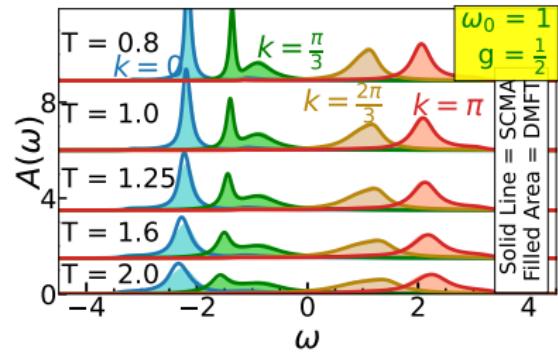
Parameter regime:

Left Fig:

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Bottom Fig:

- Weak



Results: 1D Quasiparticle properties

- Effective mass: DMFT vs DMRG

E. Jeckelmann and S. R. White, Phys. Rev. B 57, 6376 (1998)

- Ground state energy: DMFT vs Global-local variational approach A. H. Romero, D. W. Brown, and K. Lindenberg, J. Chem. Phys. 109, 6540 (1998)

The figure consists of two side-by-side plots. The left plot shows the logarithm of the effective mass ratio, $\log_{10}(m^*/m_0)$, on the y-axis (ranging from 0 to 3), versus the coupling strength g/ω_0 on the x-axis (ranging from 0 to 3). It contains six data series: $\omega_0 = 0.2$ (DMRG squares, blue dashed line), $\omega_0 = 0.2$ (DMFT circles, blue solid line), $\omega_0 = 1$ (DMRG diamonds, orange dashed line), $\omega_0 = 1$ (DMFT triangles, orange solid line), $\omega_0 = 4$ (DMRG circles, green dashed line), and $\omega_0 = 4$ (DMFT line, green solid line). The right plot shows the ground state energy E_p/ω_0 on the y-axis (ranging from -12 to 0) versus $(g/\omega_0)^2$ on the x-axis (ranging from 0 to 12). It contains eight data series for different values of γ^{-1} : 1 (blue circles), 2 (green squares), 4 (red diamonds), 6 (brown inverted triangles), 8 (purple circles), and 10 (grey asterisks). The legend indicates that markers represent DMFT and solid lines represent the Global-local (G-L) approach. A text box in the right plot states "Markers = DMFT" and "Solid Line = G-L".

Mitrić et al., Phys. Rev. Lett. 129, 096401 (2022)

Petar Mitrić [IPB]

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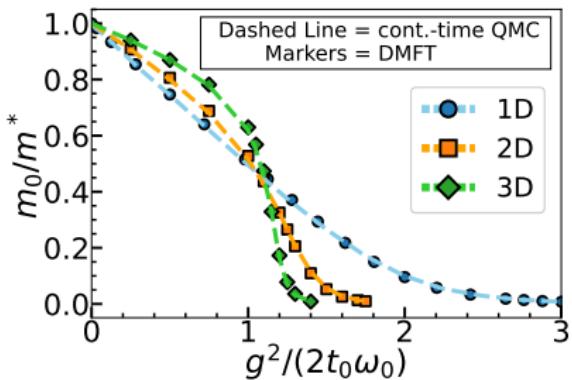
BPU 11, Belgrade, Serbia, 2022

Higher dim. QP prop. and im. time corr. func.

- Effective mass: DMFT vs Continuous-time QMC

Kornilovitch, Phys. Rev. Lett. 81, 5382 (1998)

- Imaginary time correlation functions ($\omega_0 = 1$, $g = \sqrt{2}$)



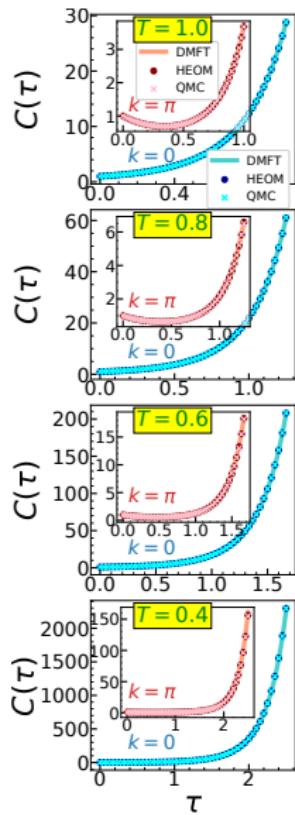
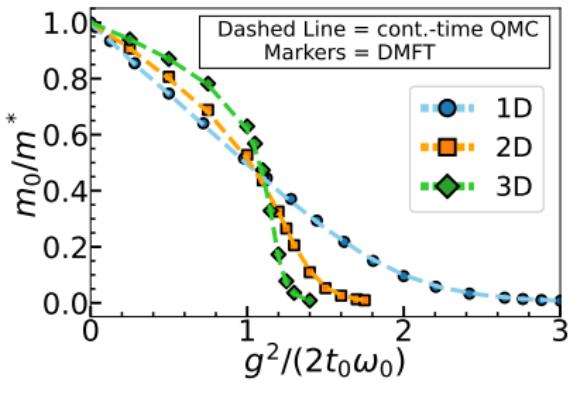
Mitrić et al., Phys. Rev. Lett. 129, 096401 (2022)

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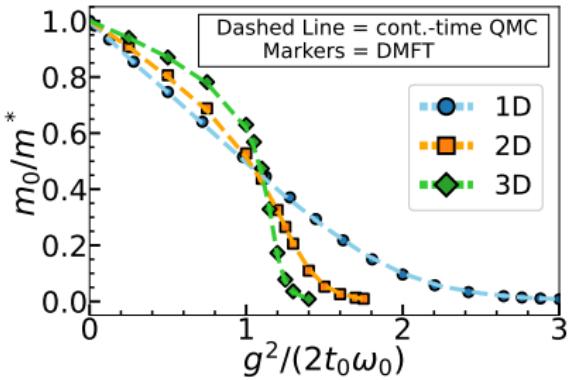
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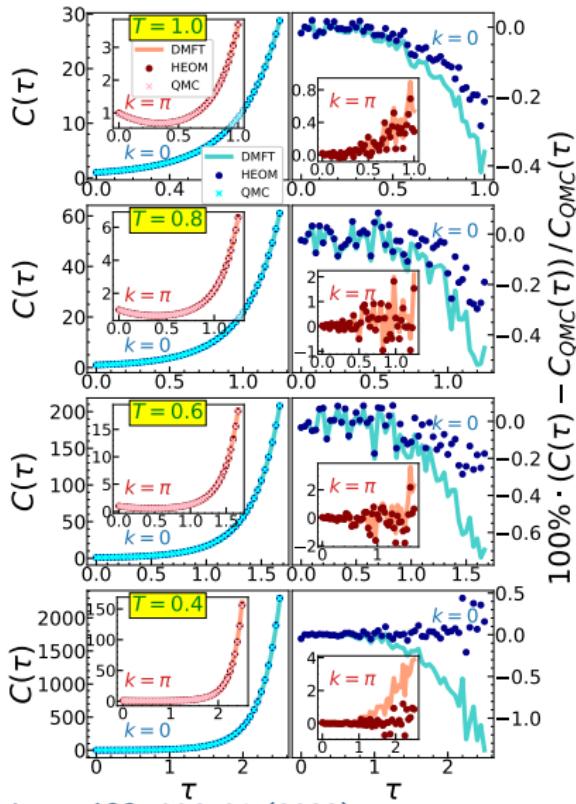
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Mitrić et al., Phys. Rev. Lett. 129, 096401 (2022)



Epilogue

Take-Home Message

DMFT gives highly accurate and numerically cheap approximate solutions of the Holstein model (nonlocal correlations in Holstein model are small)

- ❑ Covers the whole parameter regime which consists of ω_0, g, T, k and number of dimensions.
- ❑ Applicable both at the thermodynamic limit and on a chain with finite length.
- ❑ Drawback: Gives local $\Sigma_{\mathbf{k}}$.
- ❑ Possible applications to other systems:
 - ❑ Extended DMFT for the non-local electron-phonon interaction.
 - ❑ Statistical DMFT for the systems with disorder.
- ❑ all details in P. Mitrić, V.Janković, N. Vukmirović and D. Tanasković, Phys. Rev. Lett. **129**, 096401 (2022)