Tuesday 30th August, 2022

Spectral functions of the Holstein polaron: exact and approximate solutions

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Republic of Serbia

Holstein model

Hamiltonian:

$$H = -t_0 \sum_i \left(c_i^\dagger c_{i+1} + H.c. \right) - g \sum_i n_i \left(a_i^\dagger + a_i \right) + \omega_0 \sum_i a_i^\dagger a_i$$

We calculate:

- QP prop: m^*, E_p
- **Spec. fun.** $A_k(\omega)$
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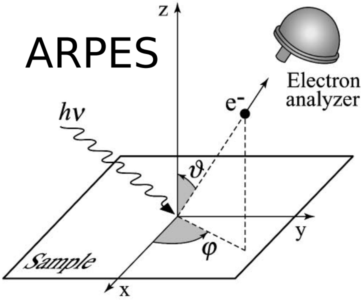

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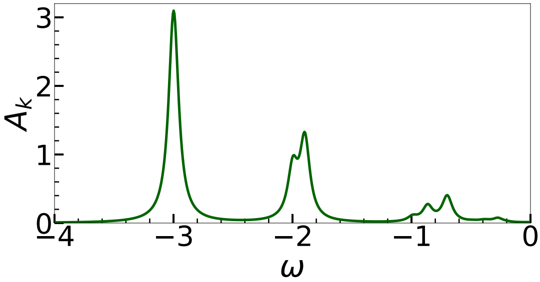

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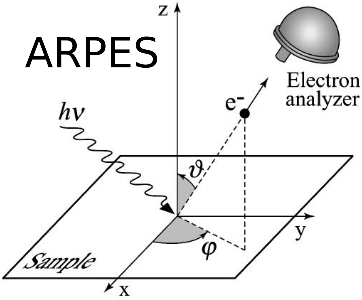

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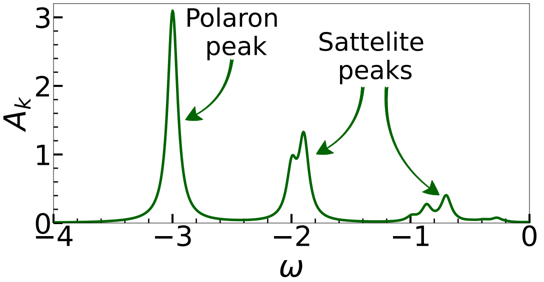

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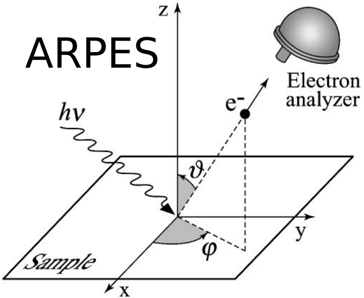

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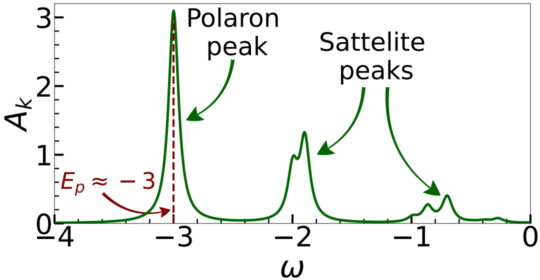

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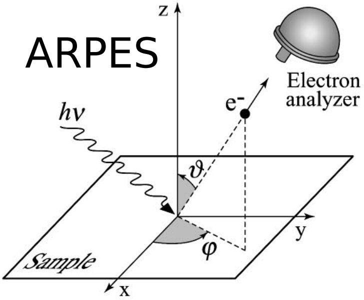

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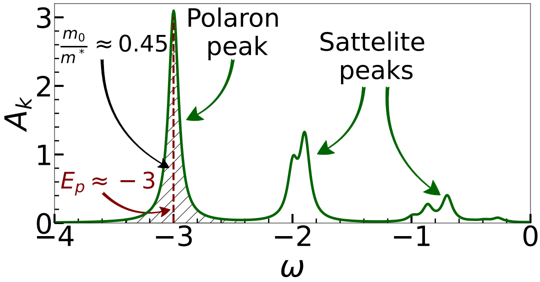

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$$C_k(\tau) = \int_{-\infty}^{\infty} A_k(\omega) e^{-\omega\tau} d\omega$$

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

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

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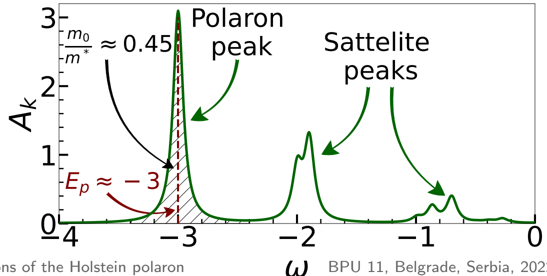

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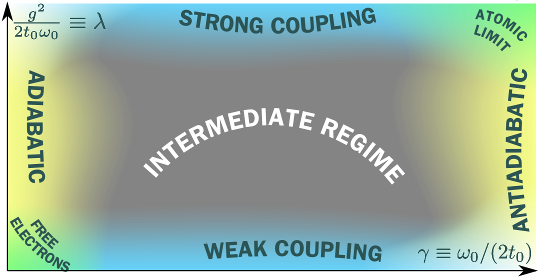

Mitrić et al., Phys. Rev. Lett. **129**, 096401 (2022)

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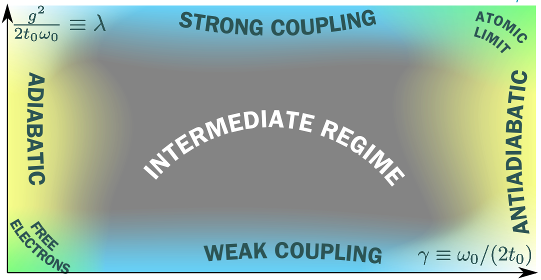

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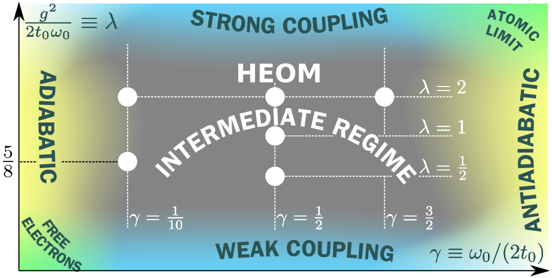

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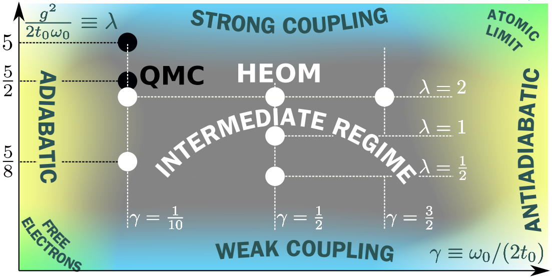

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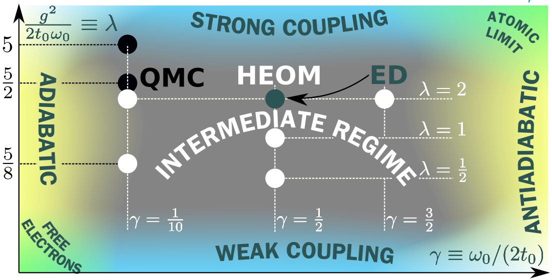

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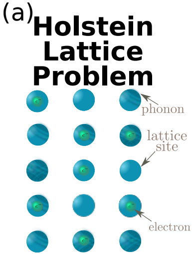

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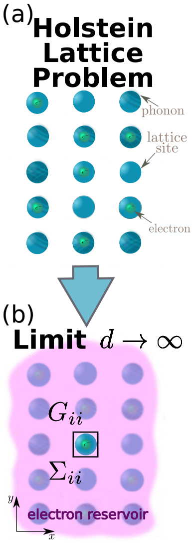

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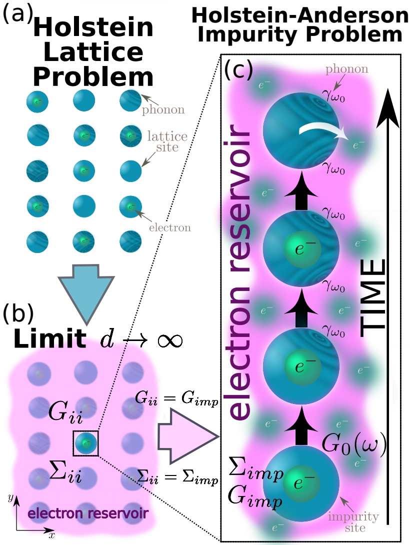

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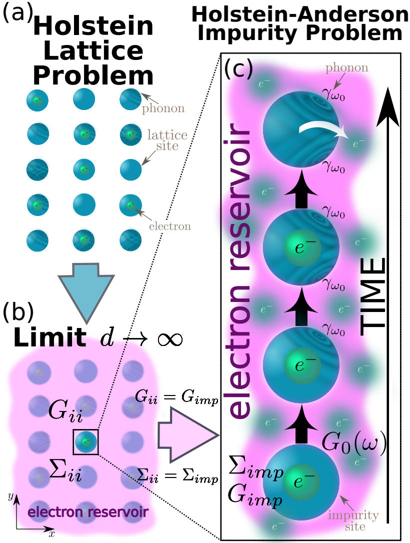

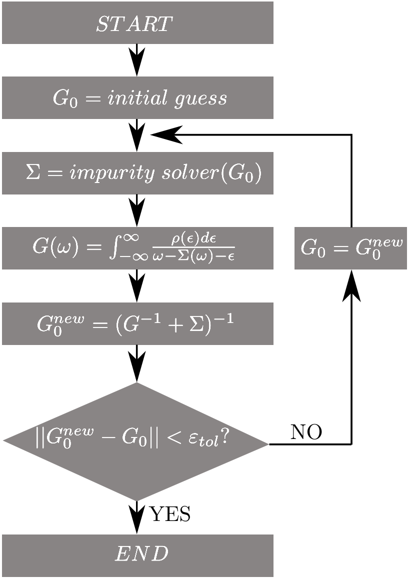

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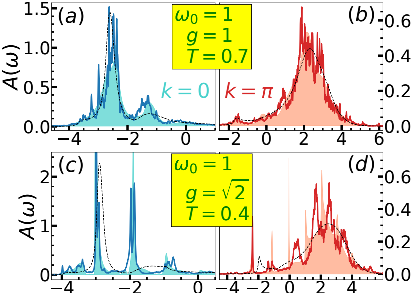
Results: Spectral functions



Parameter regime:
Left Fig:

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

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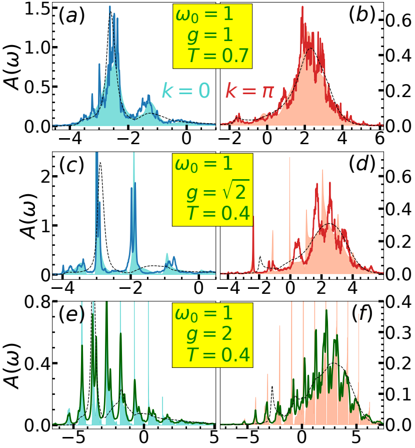

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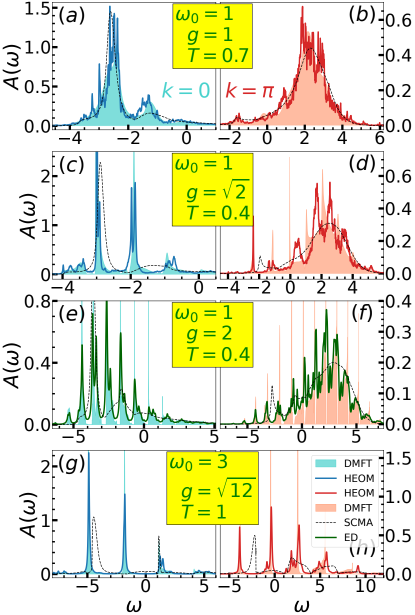

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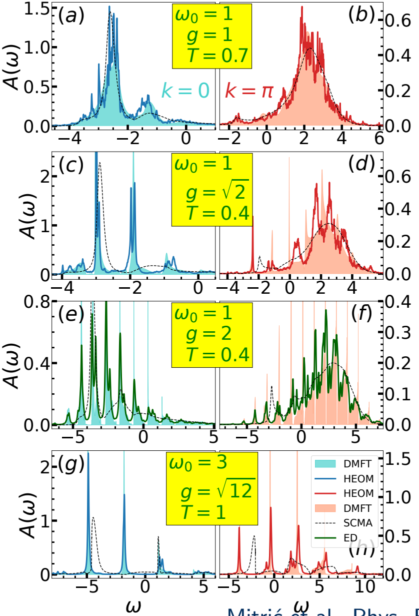

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Bottom Fig:

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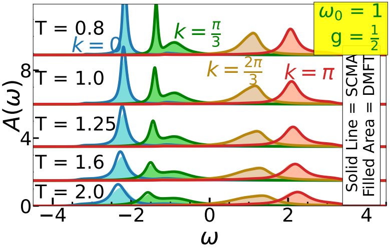


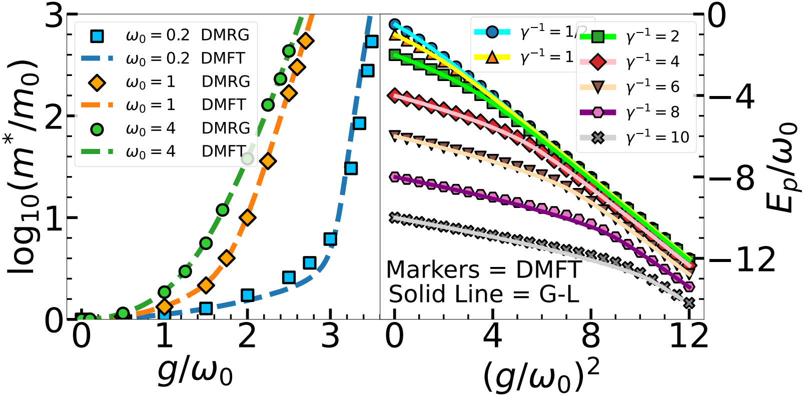
Mitrić et al., Phys. Rev. Lett. **129**, 096401 (2022)

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)



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

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

- Effective mass: DMFT vs Continuous-time QMC

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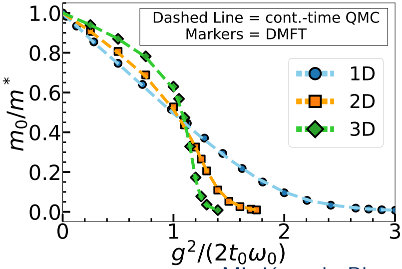
- Imaginary time correlation functions ($\omega_0 = 1$, $g = \sqrt{2}$)



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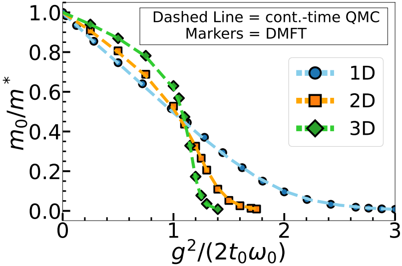

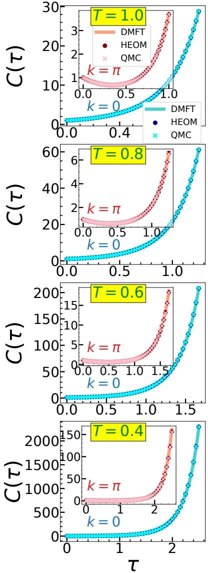

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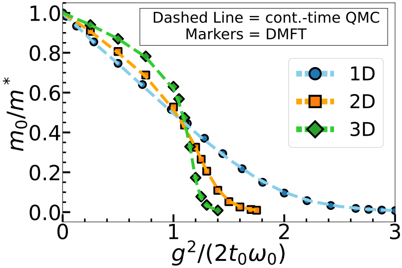

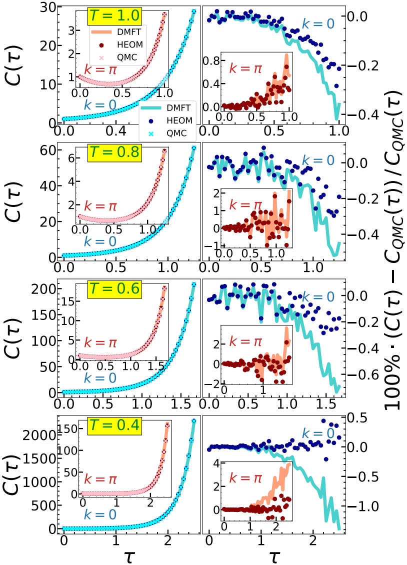

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Epilogue

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)