DMRG methods for dynamical properties of electron-phonon systems at finite temperatures

David Jansen[1], Janez Bonča[2,3], and Fabian Heidrich-Meisner[1]

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[3]University of Ljubljana

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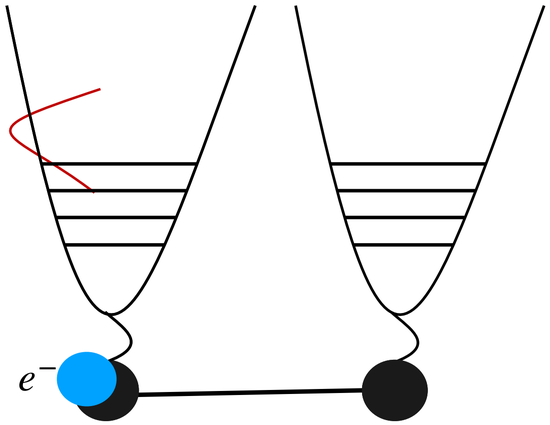
Recent Progress in Many-Body Theories XXI

SFB 1073

GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN IN PUBLICA COMMODA SEIT 1737

$[q,p]=i\hbar$

Outline



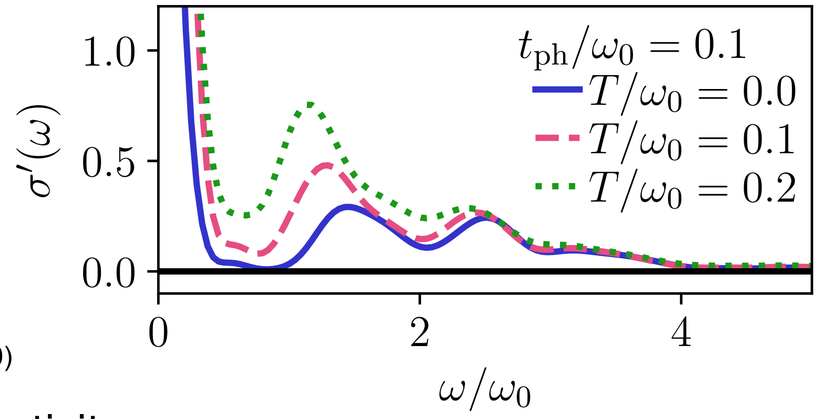
Motivation: Electron-phonon coupling

Holstein model

Numerical methods: DMRG with LBO

Finite temperature

DJ, Bonča and Heidrich-Meisner, Phys. Rev. B **102**, 165155 (2020)



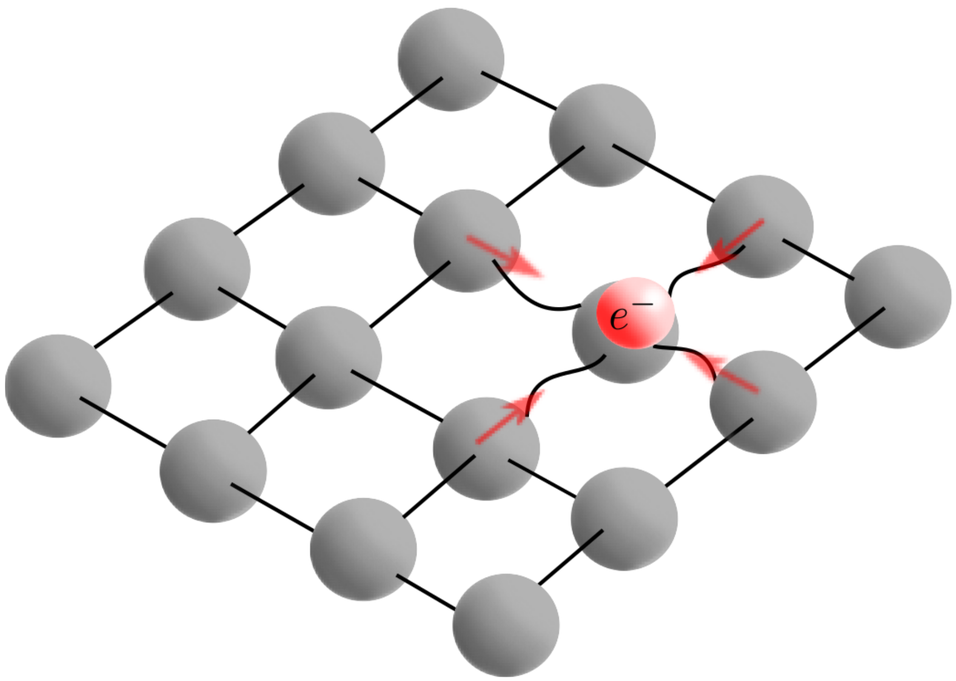
Results: Spectral functions and optical conductivity

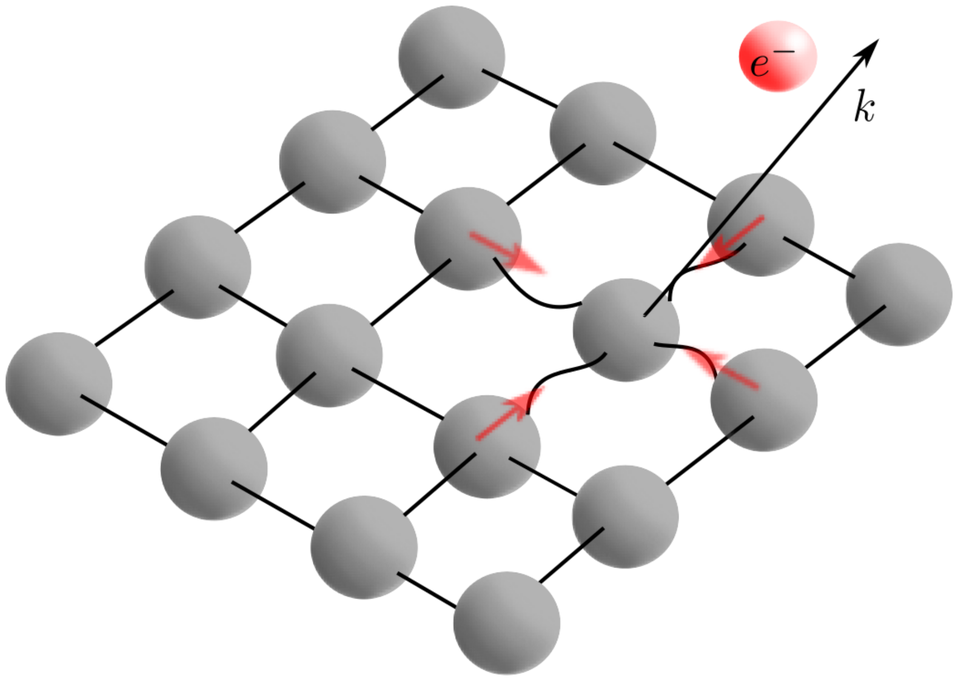
DJ, Bonča and Heidrich-Meisner, arXiv:2206.00985 (2022) (accepted in PRB)

Summary and outlook

Motivation: Electron-phonon interaction

Electon causes lattice vibrations
→ polaron



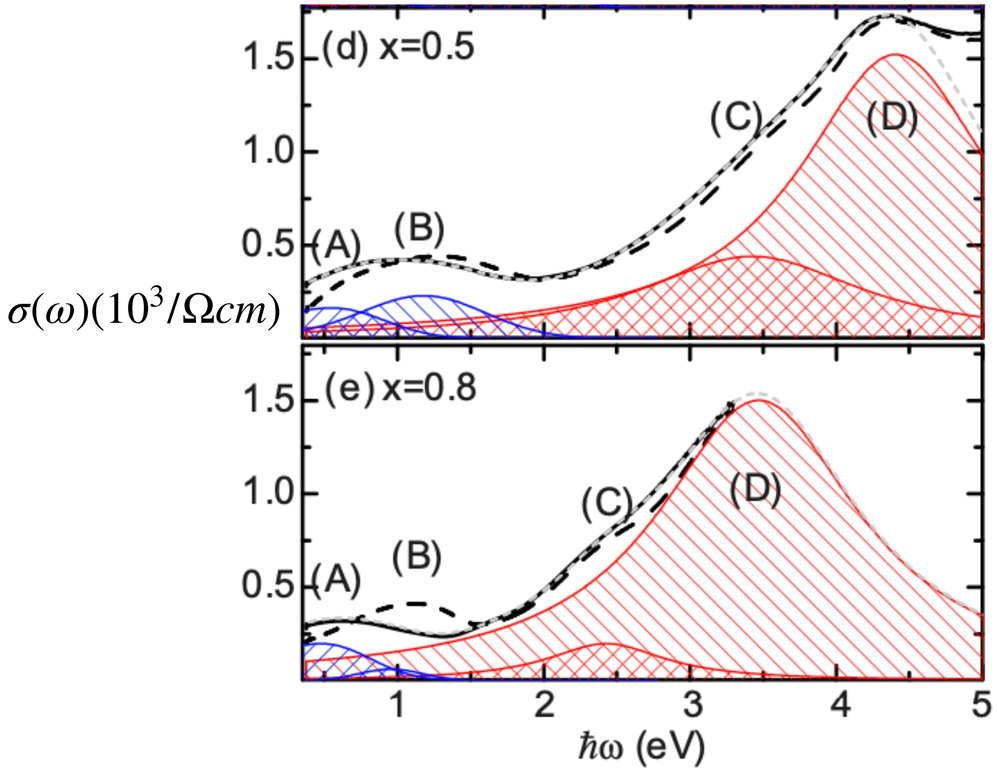


Motivation: Electron-phonon interaction

Experimentally accessible

Narrow bandwidth manganite $Pr_{1-x}Ca_xMnO_3$

Many results can be understood by small polaron theory



Mildner et al., Phys. Rev. B **92**, 035145 (2015)

Holstein model

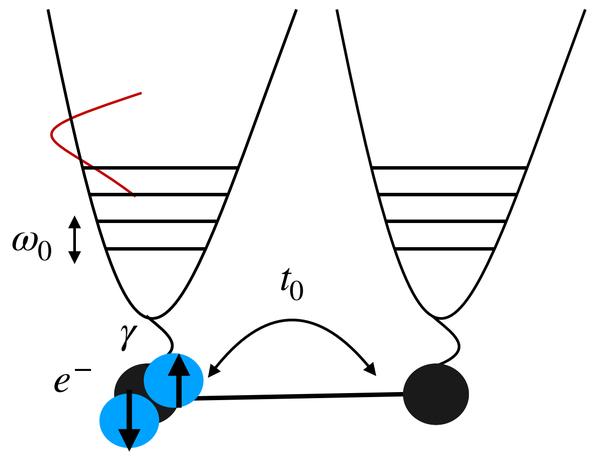
Electrons and local harmonic oscillators

Electron hopping

Phonon energy

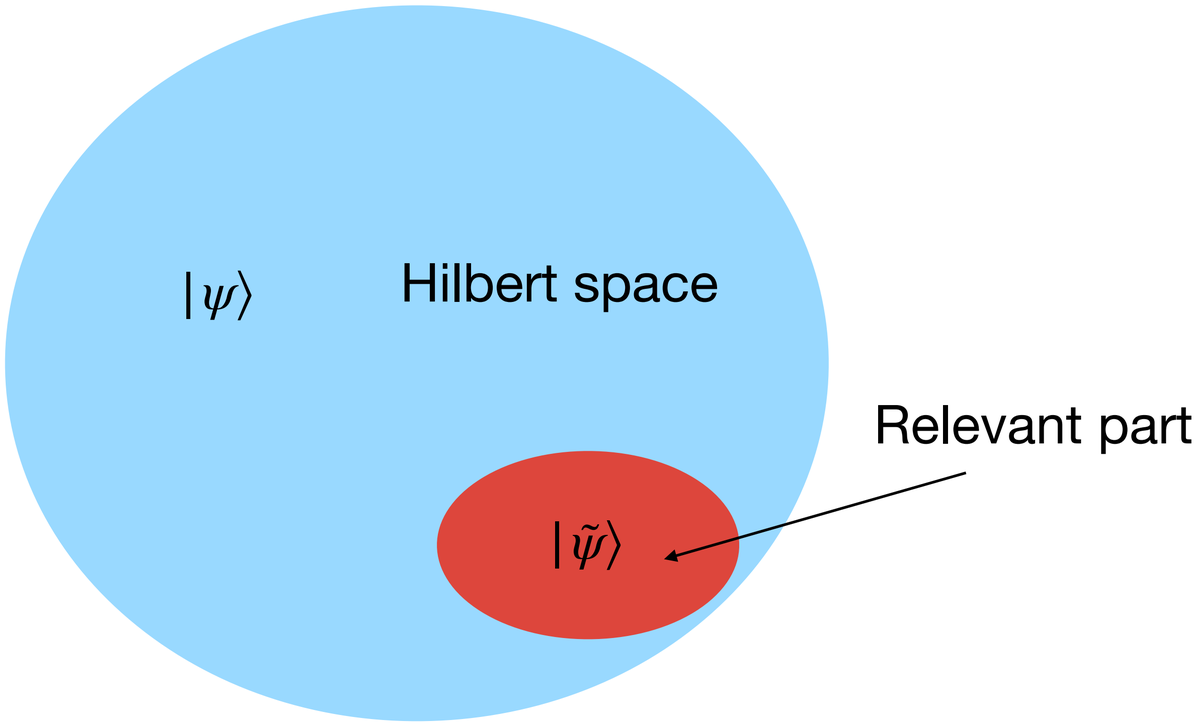
Electron-phonon coupling

Total Hilbert space $\sim M^L$



$$H = -t_0 \sum_{i,\sigma} (c^\dagger_{i,\sigma} c_{i+1,\sigma} + h.c.) + \omega_0 \sum_i b_i^\dagger b_i + \gamma \sum_{i,\sigma} n_{i,\sigma}(b_i + b_i^\dagger)$$

Summary of DMRG



White, Phys. Rev. Lett. **69,** 2863 (1992)
Schollwöck, Rev. Mod. Phys. **77**, 259 (2005)
Orús, Ann. Phys. **349**, 117 (2014)

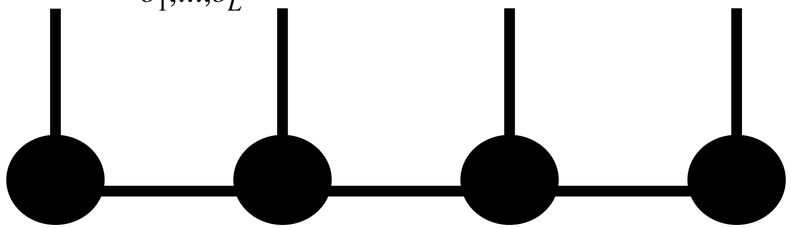
Here: 1 dimension!

Describe state in Hilbert space

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c^{\sigma_1\ldots\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle$$

Truncate $|\psi\rangle$
by selecting the most important states

$$|\tilde{\psi}\rangle = \sum_{\sigma_1,\ldots,\sigma_L} M^{\sigma_1} M^{\sigma_2} \ldots M^{\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle =$$



Flexible!
Ground-state search
Non-equilibrium dynamics
Finite-temperature

Verstraete et al., Phys. Rev. Lett. **93**, 207204 (2004)
White, Phys. Rev. Lett. **102**, 190601 (2009)
Paeckel et al., Ann. Phys., **411**, 167998 (2019)

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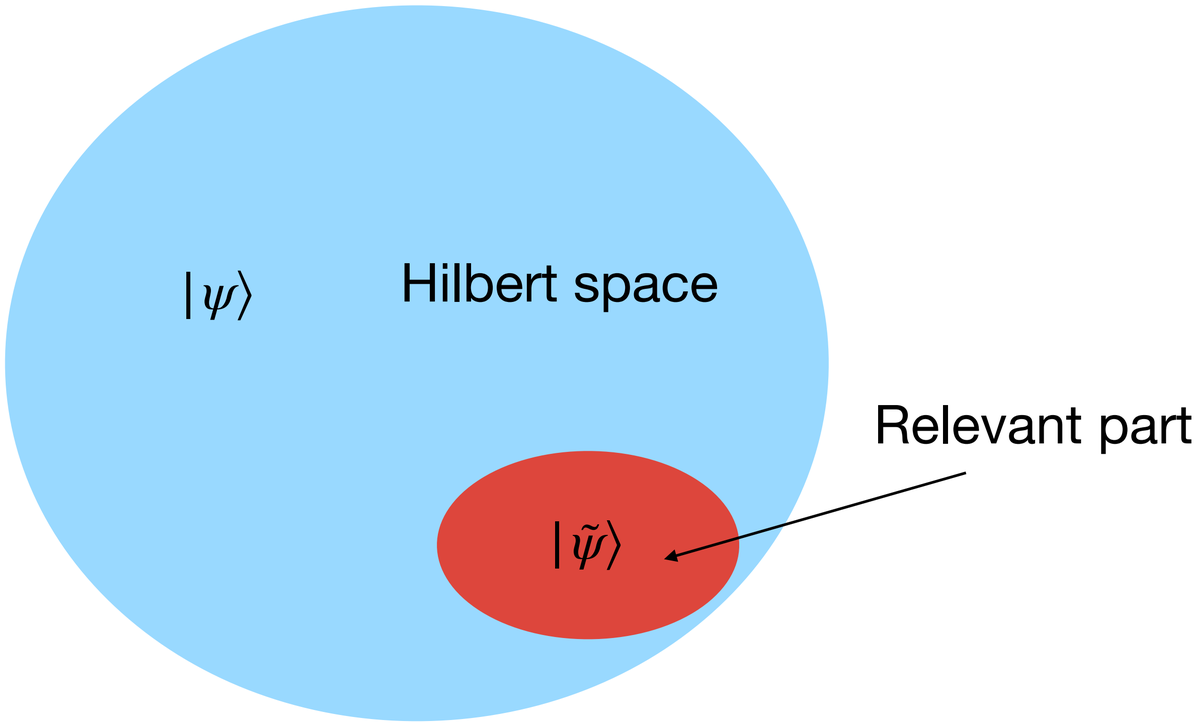

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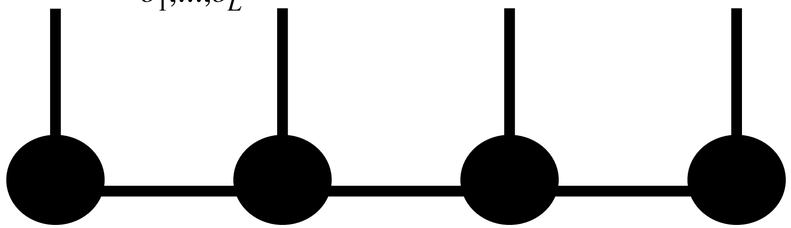
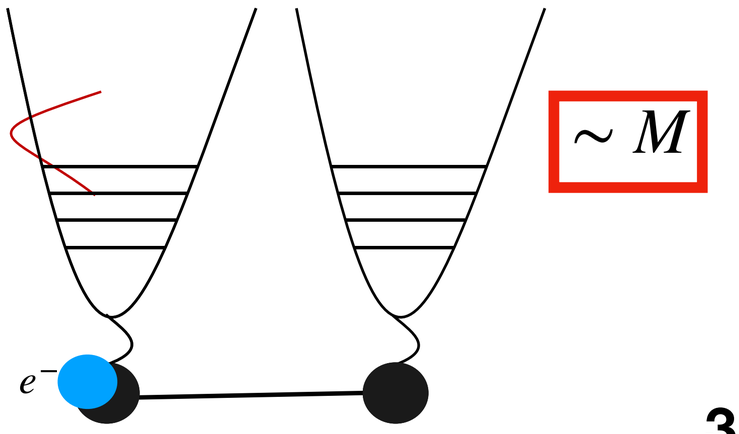


Flexible!
Ground-state search
Non-equilibrium dynamics
Finite-temperature
IT IS FUN!

Verstraete et al., Phys. Rev. Lett. **93**, 207204 (2004)
White, Phys. Rev. Lett. **102**, 190601 (2009)
Paeckel et al., Ann. Phys., **411**, 167998 (2019)

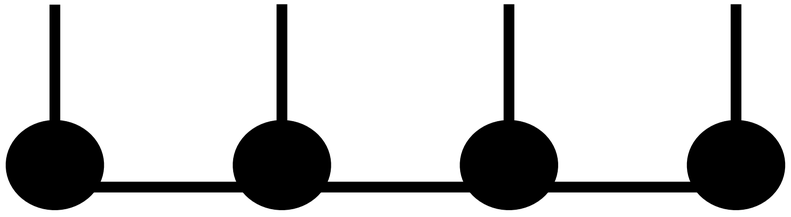
Challenges:

1: Large local Hilbert spaces: LBO



2: Finite temperature: Purification

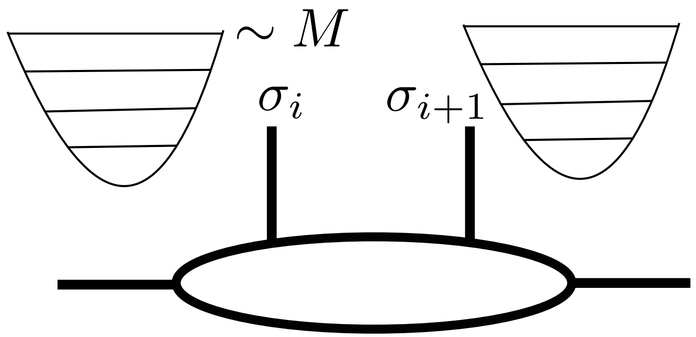
Only pure states



3: Restrictions in time-evolution: pTDVP

Challenge 1: LBO

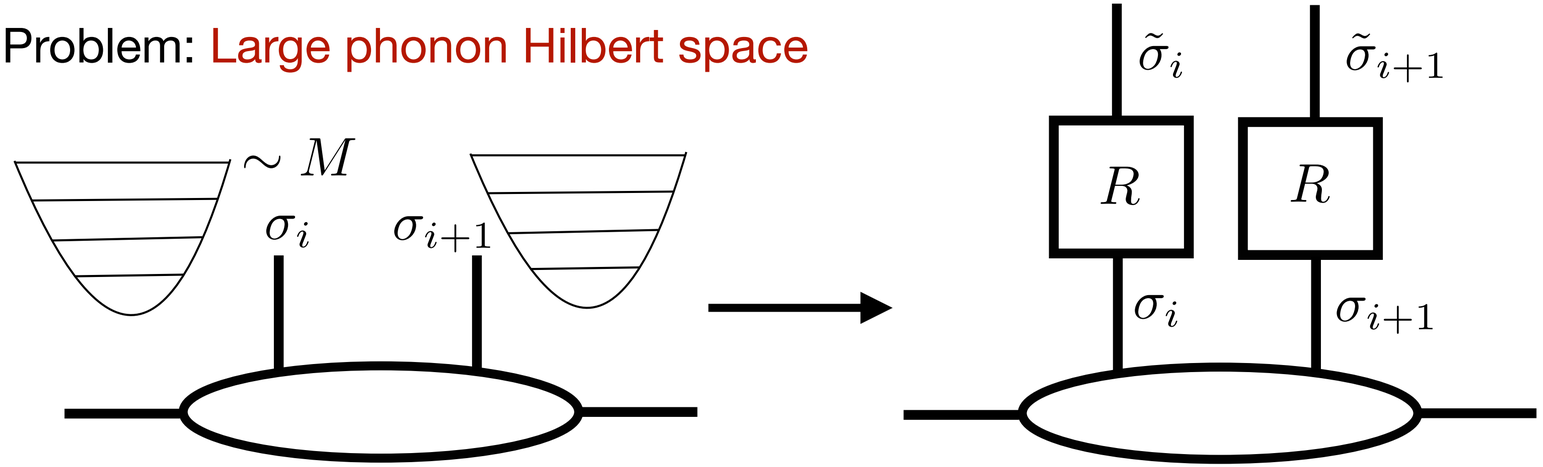
Problem: Large phonon Hilbert space



Computational effort $\sim d^3$

Challenge 1: LBO

Problem: Large phonon Hilbert space



$$\rho^i |\phi^i_\alpha\rangle = w^i_\alpha |\phi^i_\alpha\rangle$$

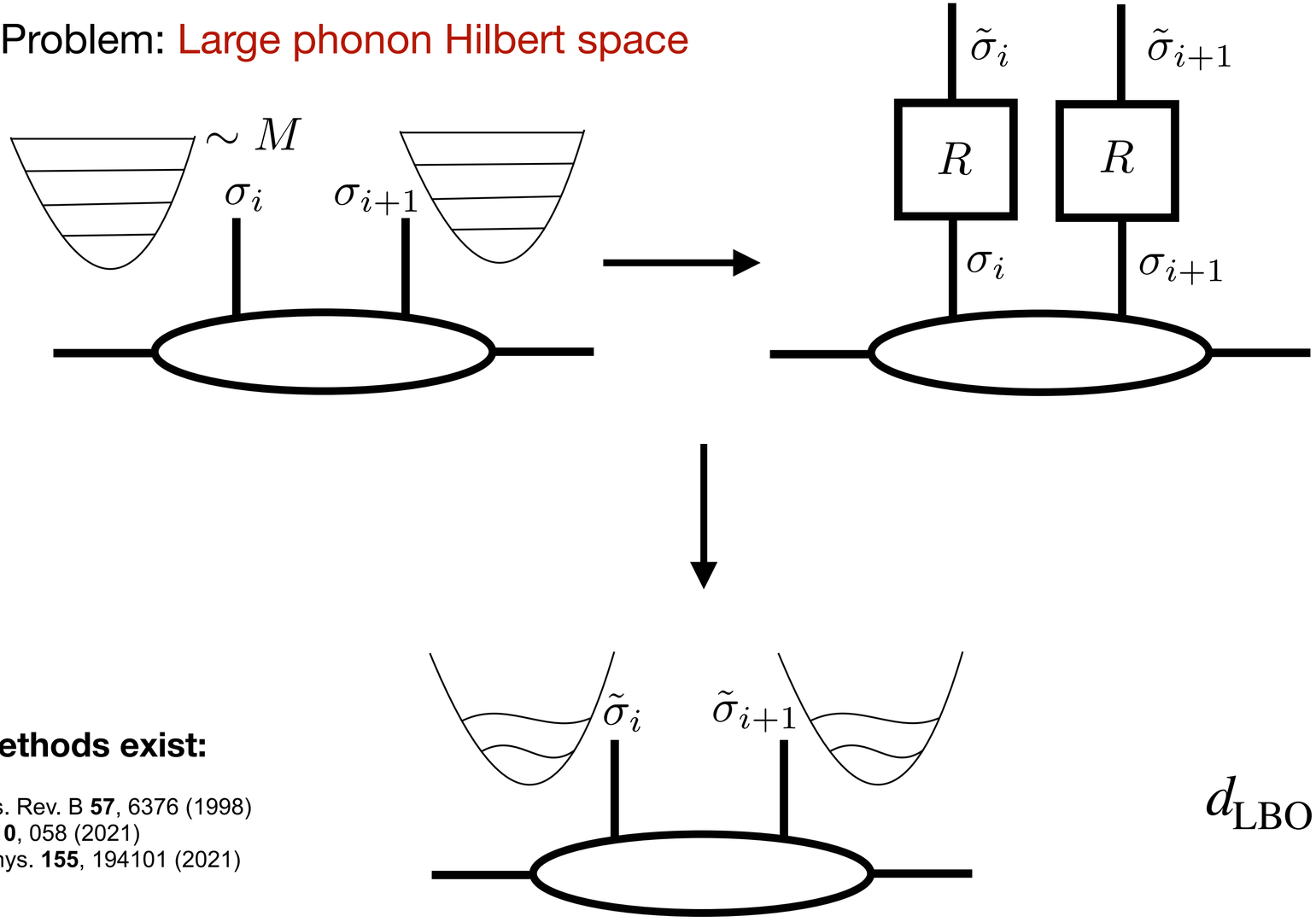
Computational effort $\sim d^3$

Diagonalize reduced single-site density matrix: Truncate!

Zhang, Jeckelmann and White, Phys. Rev. Lett. **80**, 2661 (1998)

Challenge 1: LBO

Problem: Large phonon Hilbert space



$$d_{\mathrm{LBO}} \ll d$$

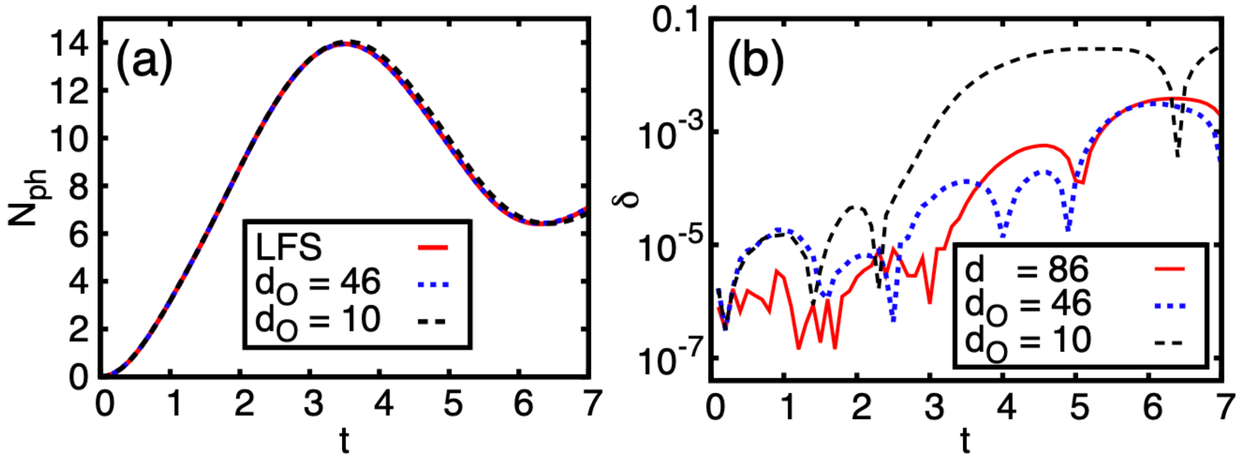
Other clever methods exist:

Jeckelmann and White, Phys. Rev. B **57**, 6376 (1998)
Köhler at el., SciPost Phys. **10**, 058 (2021)
Mardazad et al., J. Chem. Phys. **155**, 194101 (2021)

Challenge 1: LBO

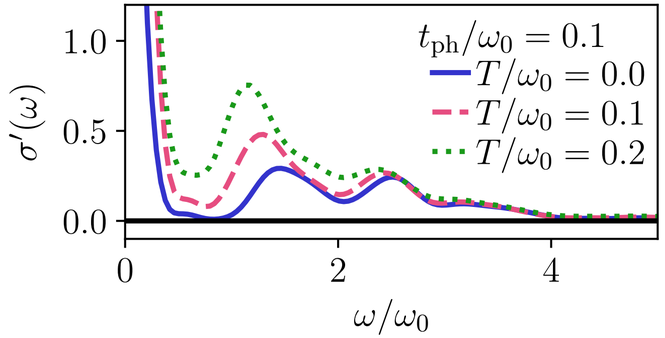
Time evolution:

Brockt, Dorfner, Vidmar, Heidrich-Meisner, Jeckelmann, Phys. Rev. B **92**, 241106 (2015)
Herbrych, Dorfner, Dagotto, Heidrich-Meisner, Phys. Rev. B **101**, 035134 (2020)
DJ, Jooss and Heidrich-Meisner, Phys. Rev. B **104**, 195116 (2021)



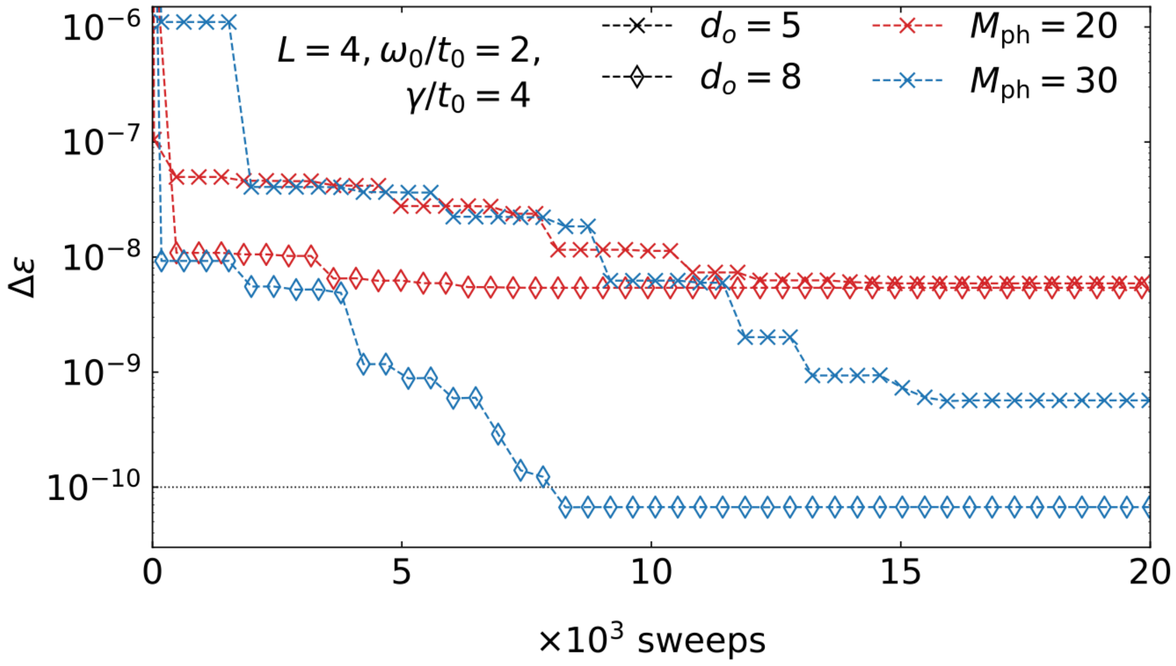
Finite tempertaure:

DJ, Bonča, Heidrich-Meisner, Phys. Rev. B **102**, 165155 (2020)
DJ, Bonča, Heidrich-Meisner, arXiv:2206.00985 (2022) (accepted in PRB)



Ground state:

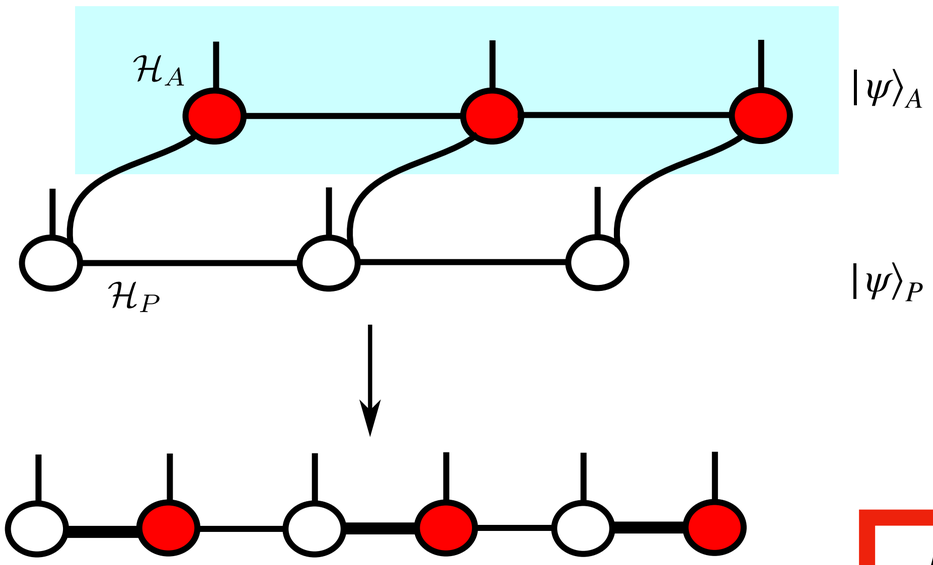
Stolpp, Herbrych, Dorfner, Dagotto, Heidrich-Meisner, Phys. Rev. B **101**, 035134 (2020)
Guo, Weichselbaum, von Delft, Vojta, Phys. Rev. Lett. **108**, 160401 (2012)



Challenge 2: Finite temperature

$$\langle \hat{O} \rangle_\beta = \frac{1}{Z} \sum_n e^{-E_n \beta} \langle n | \hat{O} | n \rangle$$

Purification

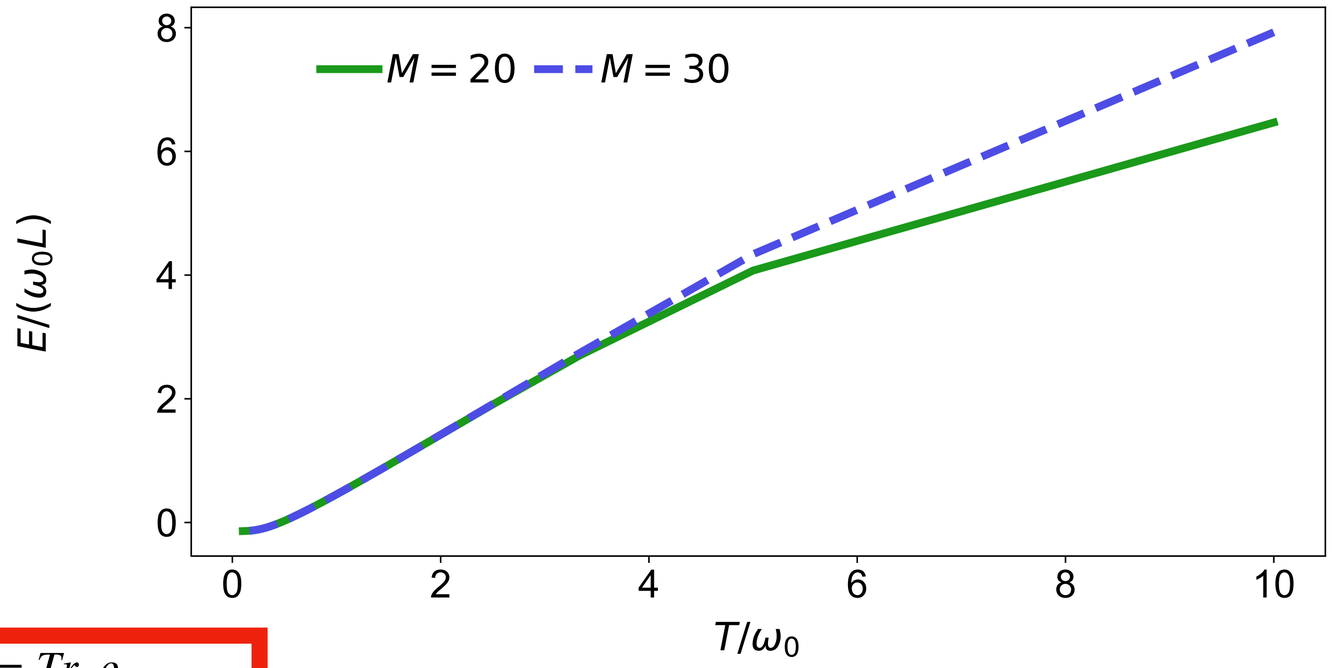


Verstraete et al., Phys. Rev. Lett. **93**, 207204 (2004)

$$\rho_P = Tr_A \rho$$

$$|\psi_\beta\rangle = e^{-\beta \hat{H}/2} |\psi_0\rangle$$

$$L = 21, \gamma/\omega_0 = \sqrt{2}, t_0/\omega_0 = 1$$



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Purification gives correct physics in low temperature regime!

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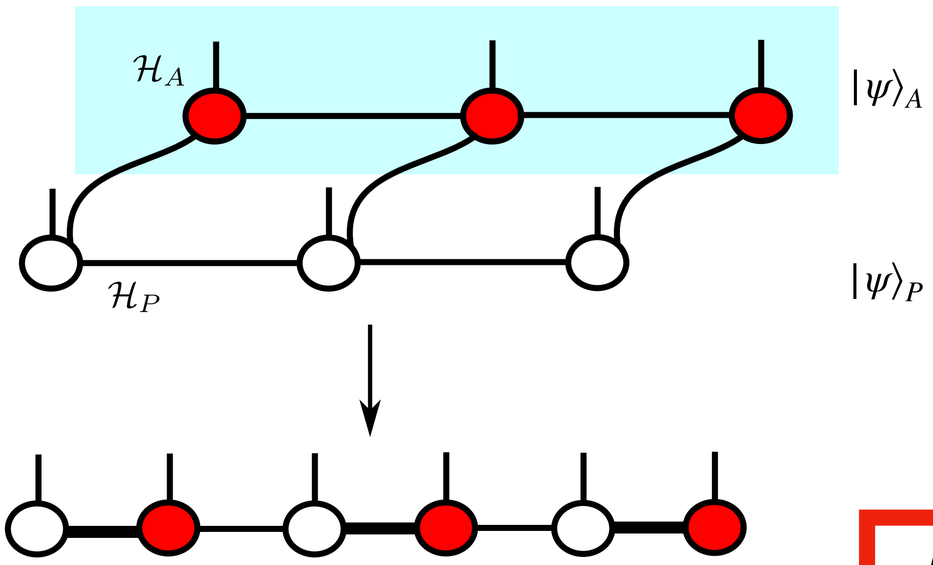

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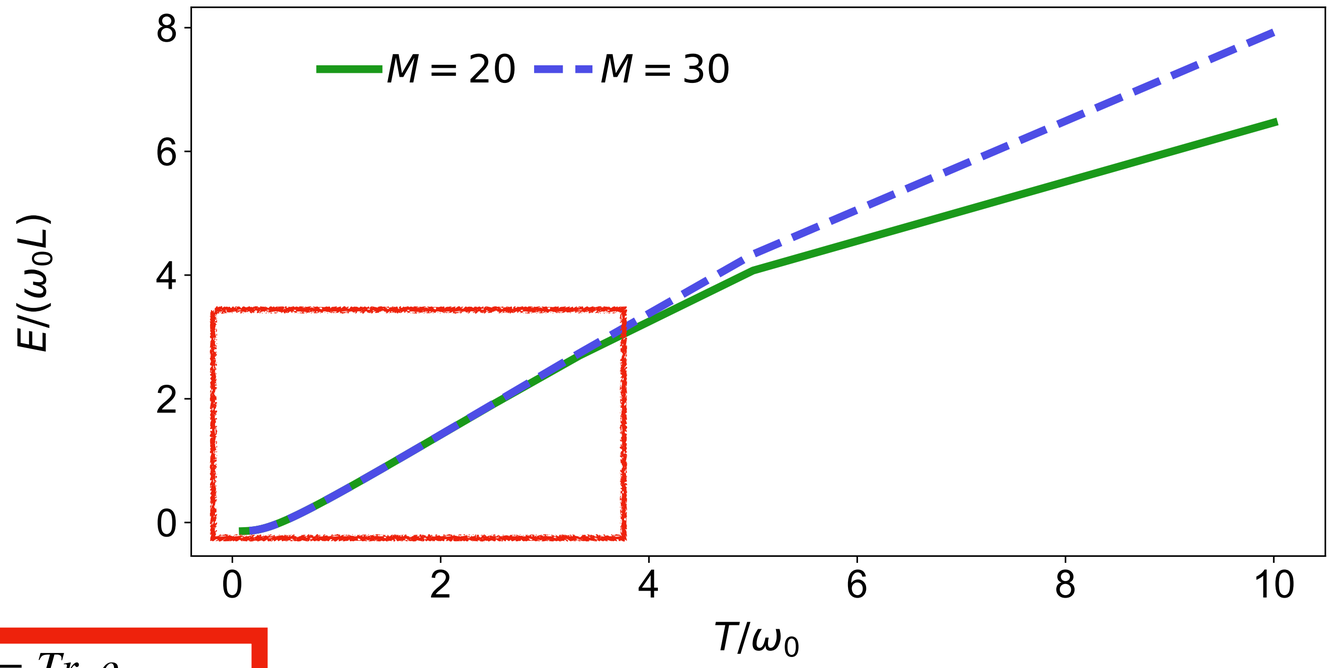

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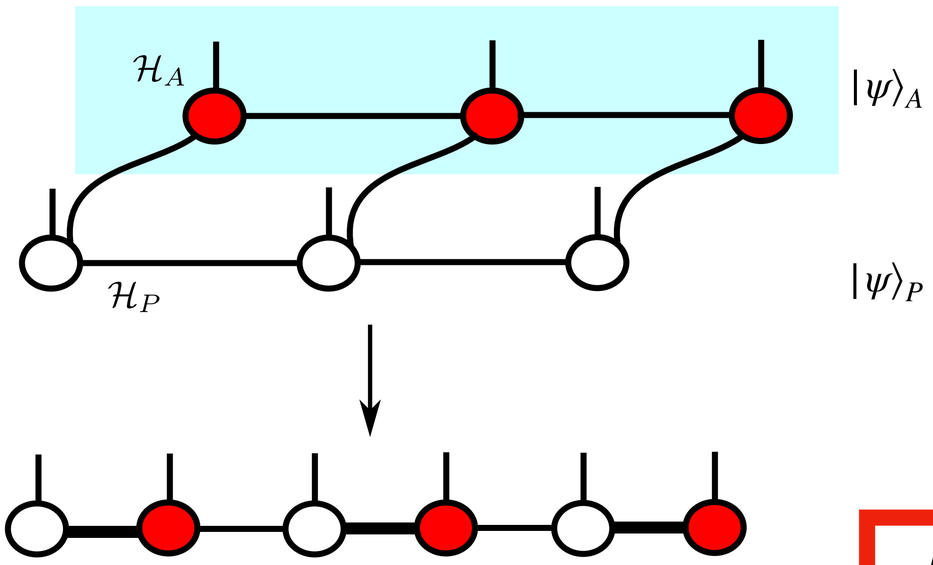

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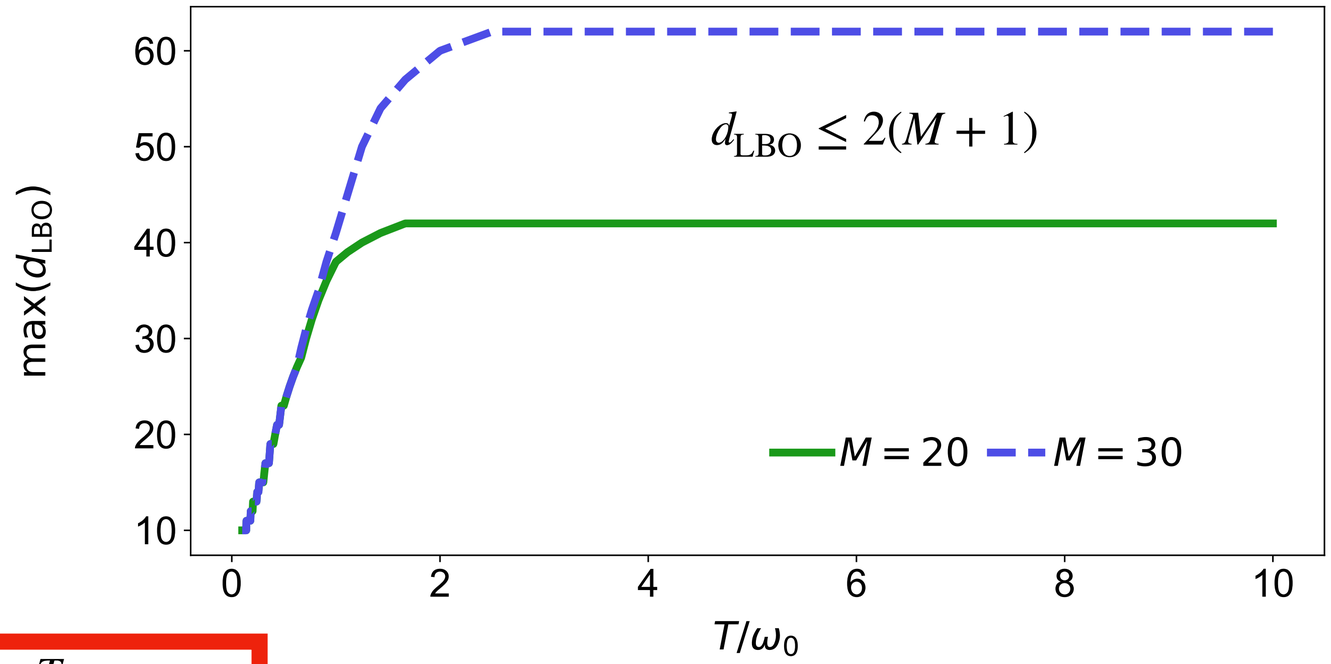
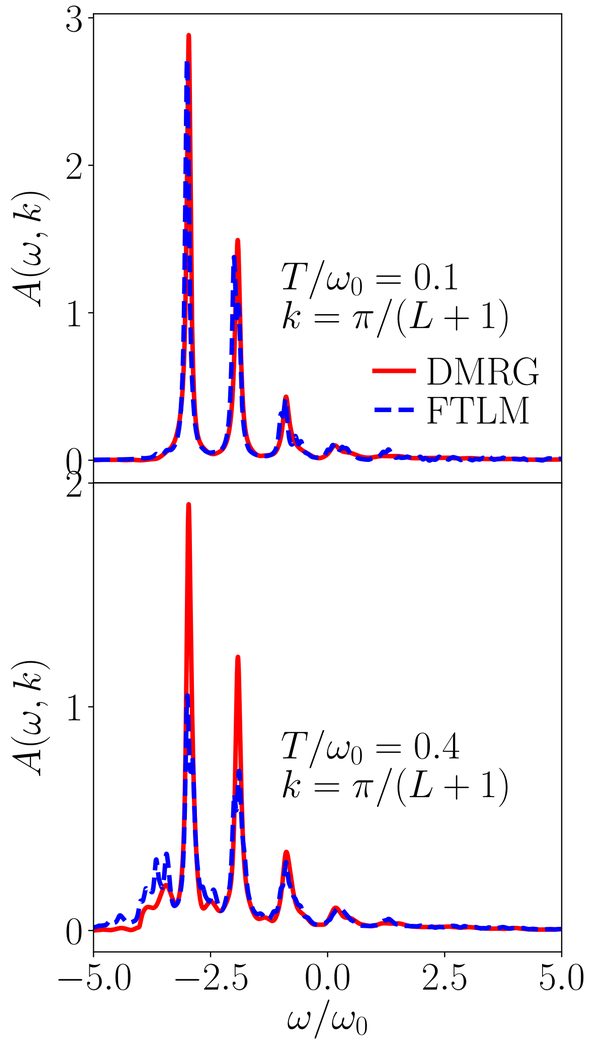


DJ, Bonča and Heidrich-Meisner, Phys. Rev. B **102**, 165155 (2020)

Purification gives correct physics in low temperature regime!

Spectral functions

$L = 21, \gamma/\omega_0 = \sqrt{2}, t_0/\omega_0 = 1$



Polaron spectral function

$$G^{>}_{T,0}(m,n,t) = -i\langle \hat{c}_m(t)\hat{c}^{\dagger}_n(0)\rangle_{T,0}$$

$$\rightarrow A(\omega,k) = -\frac{1}{2\pi} Im[G^{>}_{T,0}(k,\omega)]$$

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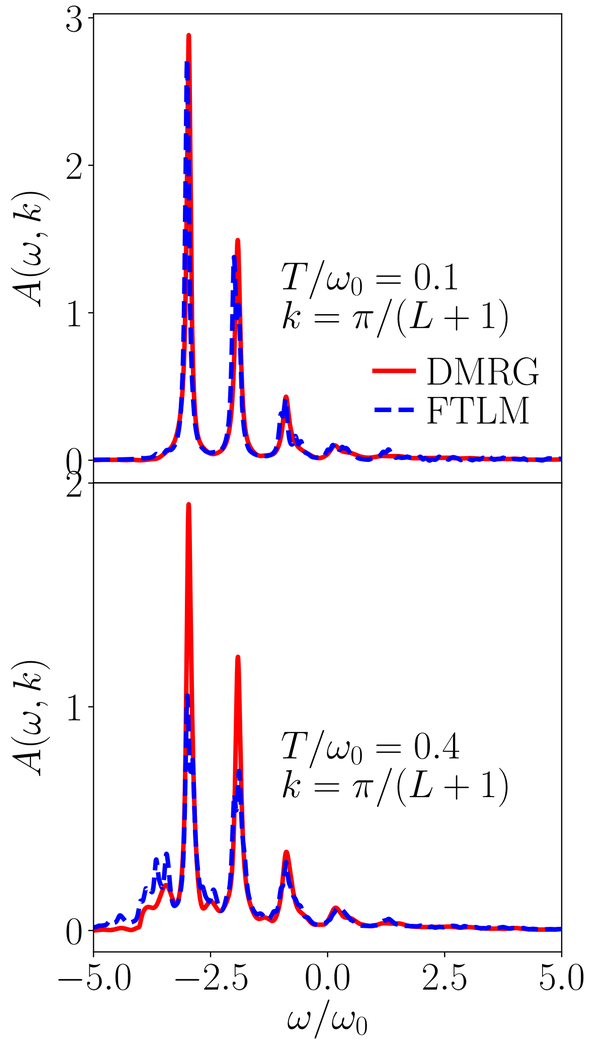

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$$G^{>}_{T,0}(m,n,t) = -\,i\langle \hat{c}_m(t)\hat{c}^{\dagger}_n(0)\rangle_{T,0}$$

$$\longrightarrow A(\omega,k) = -\frac{1}{2\pi} Im[G^{>}_{T,0}(k,\omega)]$$

Electron emission function

$$G^{<}_{T,1}(m,n,t) = i\langle \hat{c}^{\dagger}_m(0)\hat{c}_n(t)\rangle_{T,1}$$

$$\longrightarrow A^{+}(\omega,k) = -\frac{1}{2\pi} Im[-G^{<}_{T,1}(k,\omega)]$$

Large systems

Temperature dependence

Full momentum resolution

Phonon spectral function

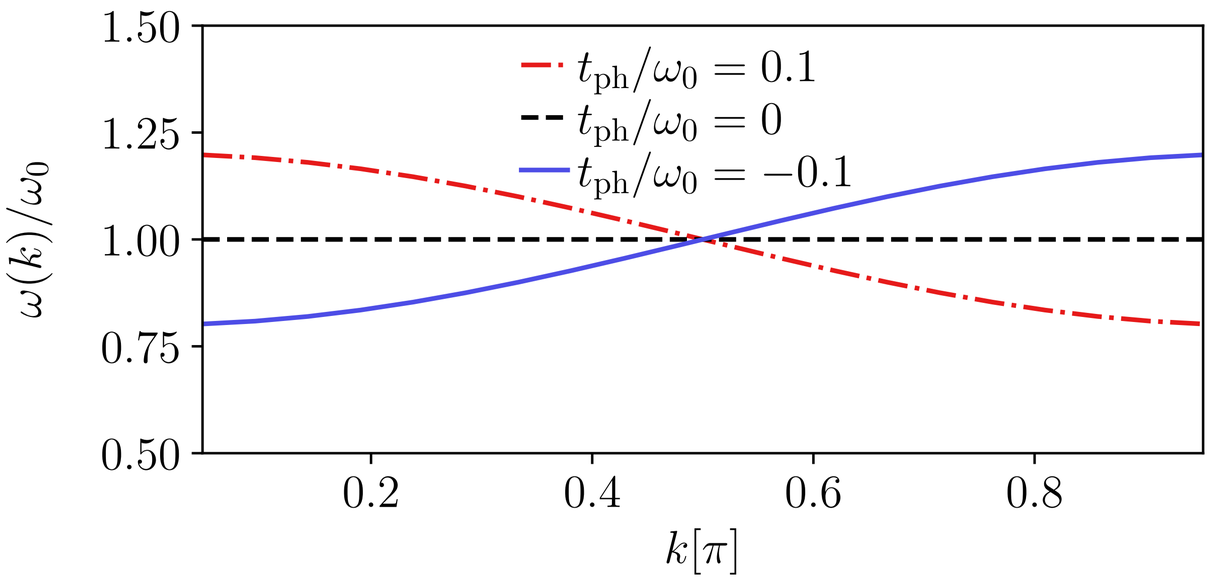
$$D^{>}_{T,1}(m,n,t) = -\,i\langle \hat{X}^{\dagger}_m(t)\hat{X}_n(0)\rangle_{T,1}$$

$$\longrightarrow B(\omega,k) = -\frac{1}{2\pi} Im[D^{>}_{T,1}(k,\omega)]$$

DJ, Bonča and Heidrich-Meisner, Phys. Rev. B **102**, 165155 (2020)

Adding dispersion

$$+t_{\mathrm{ph}} \sum_i (b_i^\dagger b_{i+1} + h.c.)$$



Influence on CDW formation in 2D with QMC — Costa et al., Phys. Rev. Lett. **120**, 187003 (2018)

Polaron effective mass — Dominic et al., Phys. Rev. B **88**, 060301(R) (2013)

Optical conductivity and spectral functions in the ground state — Bonča and Trugman, Phys. Rev. B **103**, 054304 (2021)

How to get $\sigma(\omega)$

Linear response theory $J(\omega) = \sigma(\omega)E(\omega)$, $\sigma'(\omega) = Re[\sigma(\omega)]$

With $\sigma'(\omega) = \dfrac{1 - e^{-\omega/T}}{\omega} \displaystyle\int_0^\infty dt\, Re[e^{i\omega t}\langle J(t)J(0)\rangle_T]$

And $J = i \displaystyle\sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} - h.c.)$

Need $\langle J(t)J(0)\rangle_T$

Finite temperature: Purification

Verstraete et al., Phys. Rev. Lett. **93**, 207204 (2004)
Karrasch et al., New J. Phys. **15**, 083031 (2013)
Kennes and Karrasch, Comput. Phys. Commun. **200**, 37 (2016)

Time evolution real and imaginary

→ (p)2TDVP with LBO and 1TDVP!

Zhang, Jeckelmann and White, Phys. Rev. Lett. **80**, 2661 (1998)
Haegeman et al., Phys. Rev. Lett. 1**07**, 070601 (2011)
Secular et al., Phys. Rev. B 1**01**, 235123 (2020)

Lots of research

Goodvin et al., Phys. Rev. Lett. **107**, 076403 (2011)
Schubert et al., Phys. Rev. B **72**, 104304 (2005)
Zhang et al., Phys. Rev. B **60**, 14092 (1999)
Fratini and Ciuchi, Phys. Rev. B **74**, 075101 (2006)
Bonča and Trugman, Phys. Rev. B **103**, 054304 (2021)
+more

We:

Study polaron and bipolaron
Dispersive phonons
Different parameter regimes
Finite temperature
Relatively large systems

Challenge 3: Time evolution

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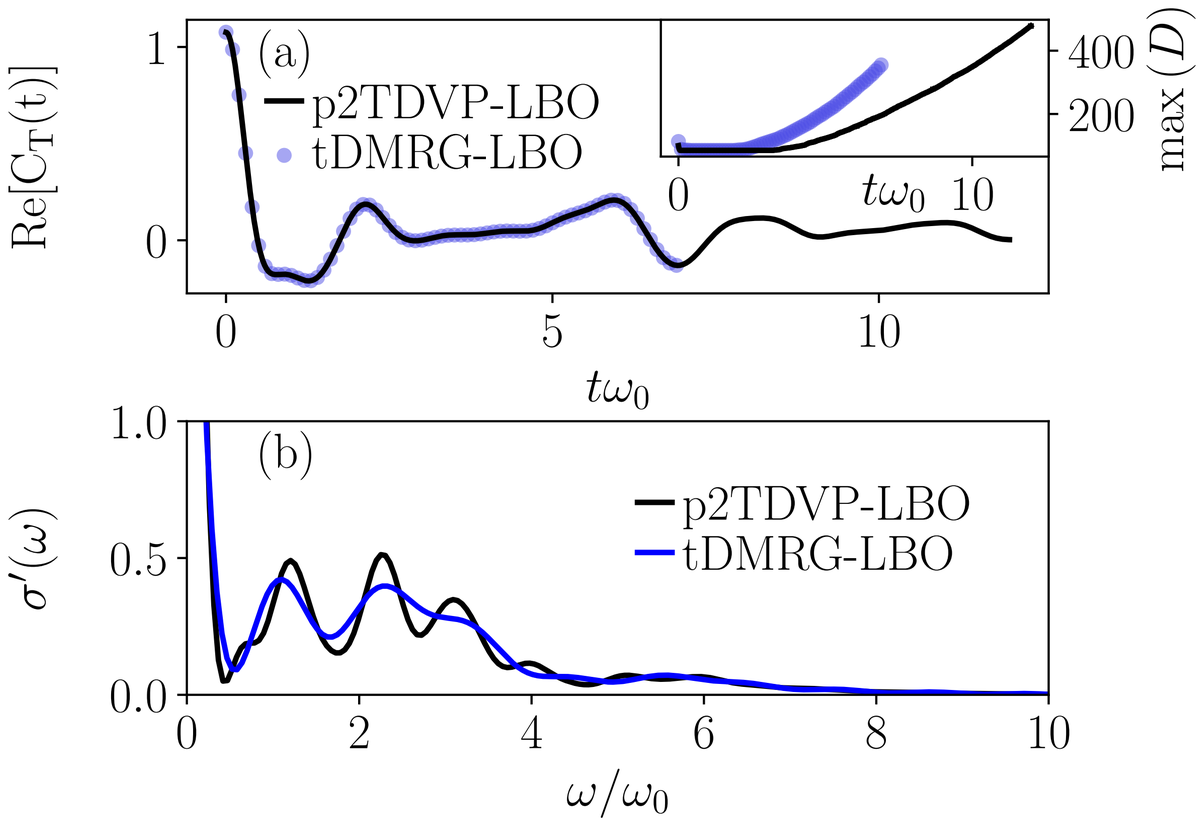

Brockt, Dorfner, Vidmar, Heidrich-Meisner, Jeckelmann, Phys. Rev. B **92**, 241106 (2015)
DJ, Bonča and Heidrich-Meisner, Phys. Rev. B **102**, 165155 (2020)
DJ, Bonča and Heidrich-Meisner, arXiv:2206.00985 (2022) (accepted in PRB)

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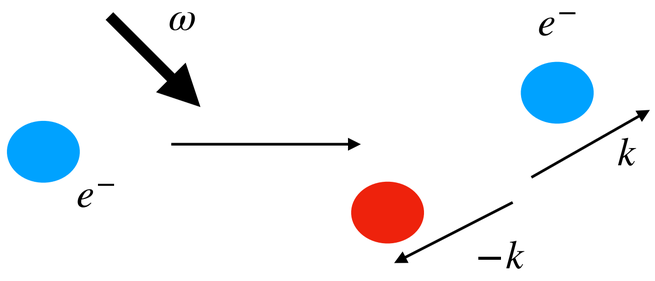
Haegeman et al., Phys. Rev. Lett. **107**, 070601 (2011)
Secular et al., Phys. Rev. B **101**, 235123 (2020)

Known that TDVP pefoms very well!

Paeckel et al., Ann. Phys., **411**, 167998 (2019)

Optical conductivity: Polaron

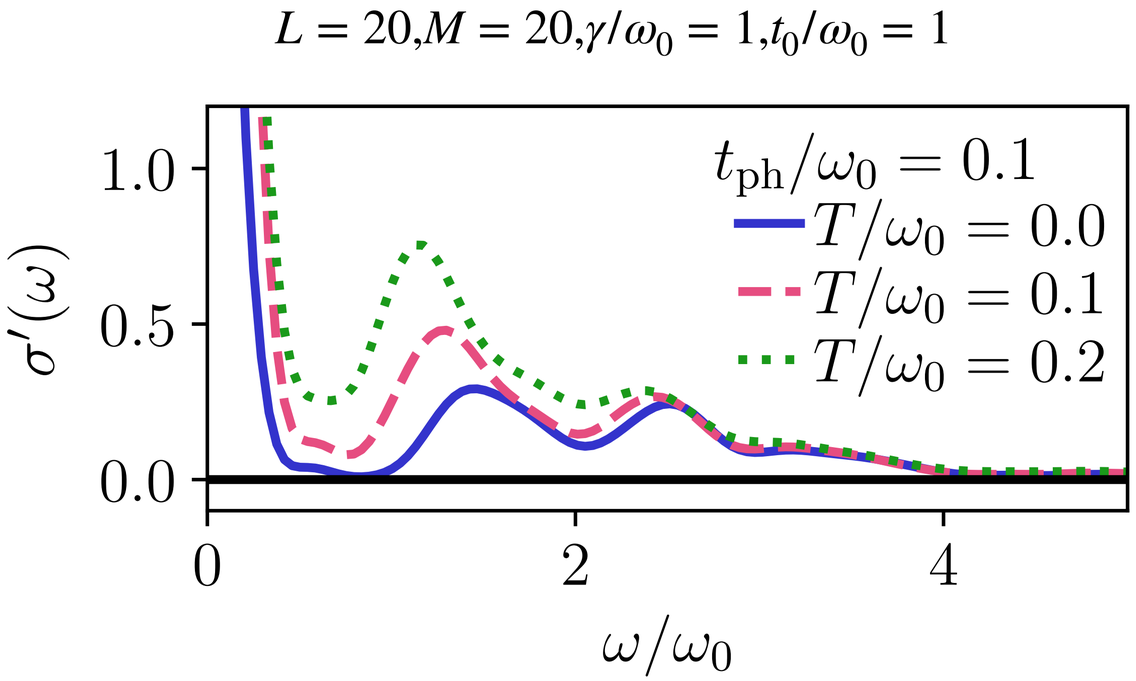
Electron emits a phonon



Spectrum goes from discrete to continuous

Peak shifts to lower frequencies

Enhanced spectral weight at low frequencies



DJ, Bonča and Heidrich-Meisner, arXiv:2206.00985 (2022) (accepted in PRB)

Born-Oppenheimer surfaces

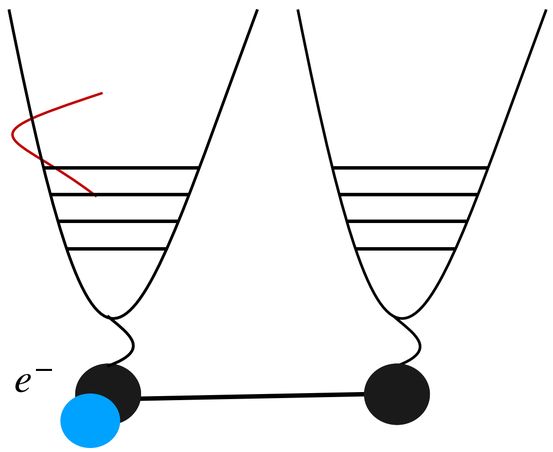
Look at the Holstein dimer, define $\tilde{\omega} = \omega_0 - t_{\text{ph}}$

Rewrite our Hamiltonian in terms of q, Q

with $Q = (x_1 + x_2))/\sqrt{2}, q = (x_1 - x_2)/\sqrt{2}$

Look at fixed phonon configurations

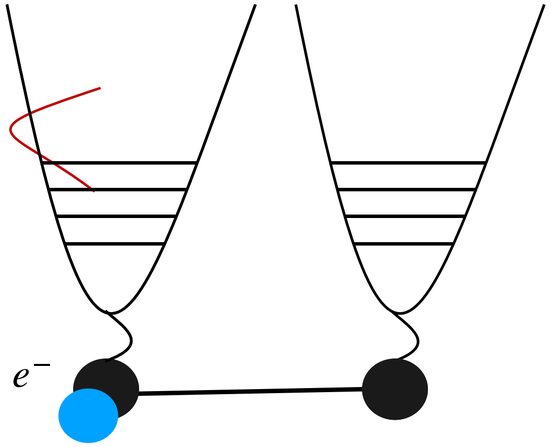
$H = H_{ekin} + \gamma[\bar{q}(n_1 - n_2)] + \frac{1}{2}\bar{q}^2(\omega_0 - t_{\text{ph}})$ and $\bar{q} = q\sqrt{m\omega_0/\hbar}$



Born-Oppenheimer surfaces

Diagonalize and get the eigenvalues

$$\begin{pmatrix} \frac{\bar{q}^2}{2}\tilde{\omega}_0 + \gamma\bar{q} & -t_0 \\ -t_0 & \frac{\bar{q}^2}{2}\tilde{\omega}_0 - \gamma\bar{q} \end{pmatrix}$$

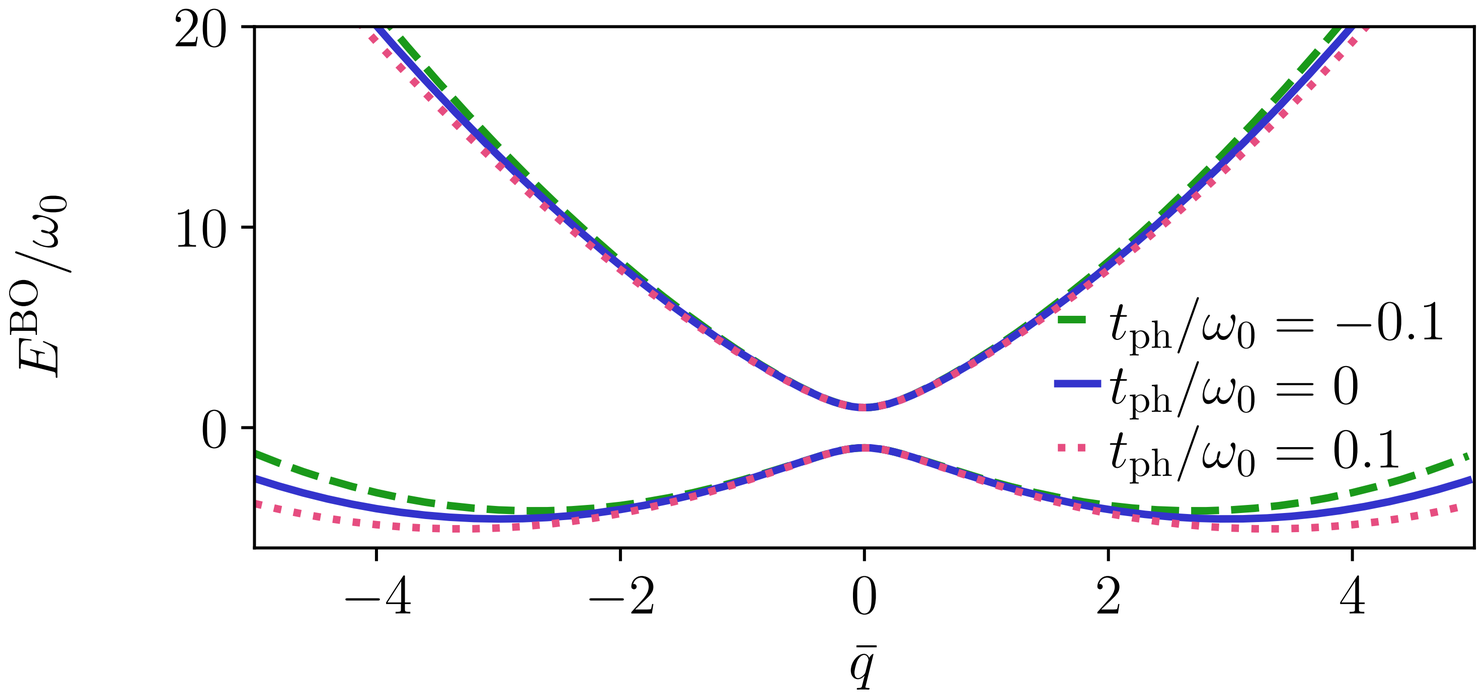


$$\longrightarrow \quad \boxed{E_{\pm}^{BO} = \frac{1}{2}(\bar{q}^2\tilde{\omega}_0 \pm 2\sqrt{(\gamma\bar{q})^2 + t_0^2})}$$

Born-Oppenheimer surfaces

Draw the surfaces

$$E_{\pm}^{BO} = \frac{1}{2}(\bar{q}^2\tilde{\omega}_0 \pm 2\sqrt{(\gamma\bar{q})^2 + t_0^2})$$

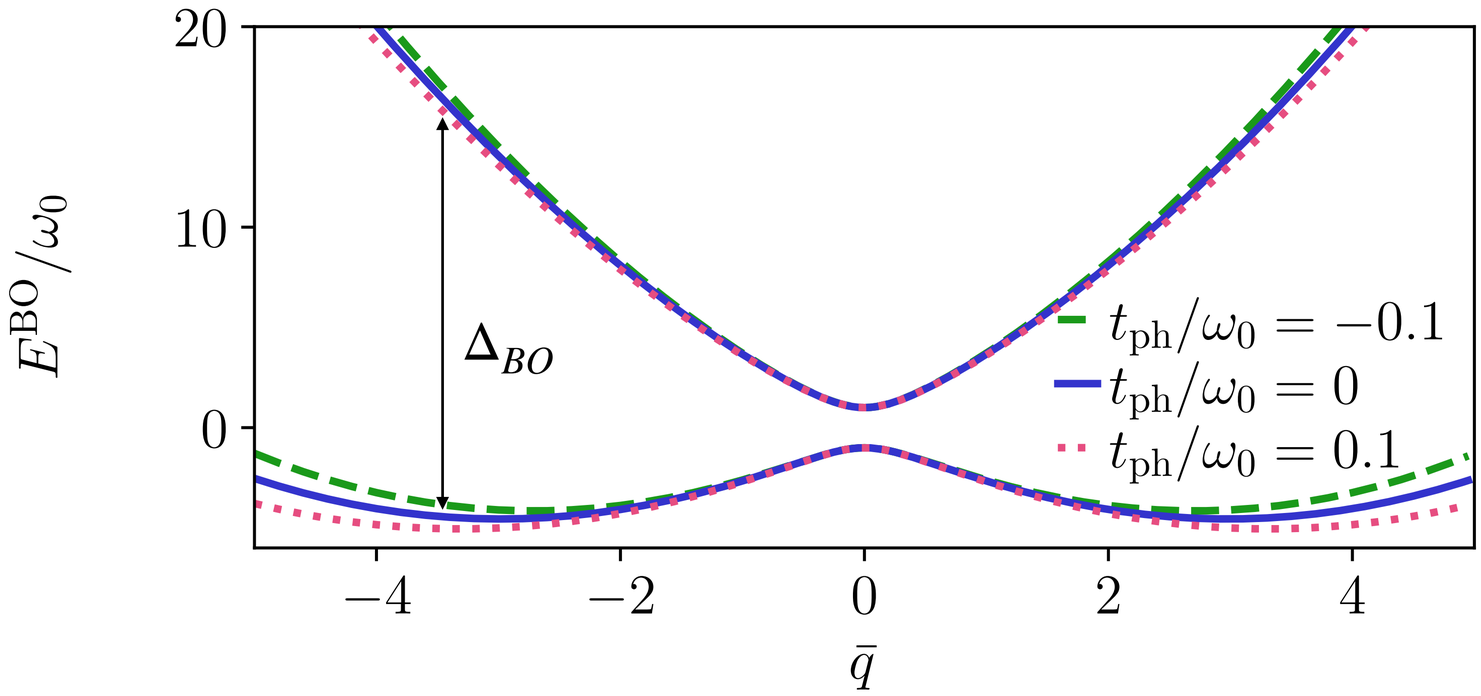


Born-Oppenheimer surfaces

Obtain formula $\sigma_{SC}(\omega) = \frac{1 - e^{-\beta\omega}}{\omega}\sqrt{\frac{2\pi}{\Delta_{BO}\alpha}}t_0^2 e^{-(\Delta_{BO}-\omega)^2/(2\Delta_{BO}\alpha)}$

$$\alpha = \tilde{\omega}_0 \coth(\beta\tilde{\omega}_0/2)$$

Without dispersion: Fratini and Ciuchi, Phys. Rev. B **74**, 075101 (2006)



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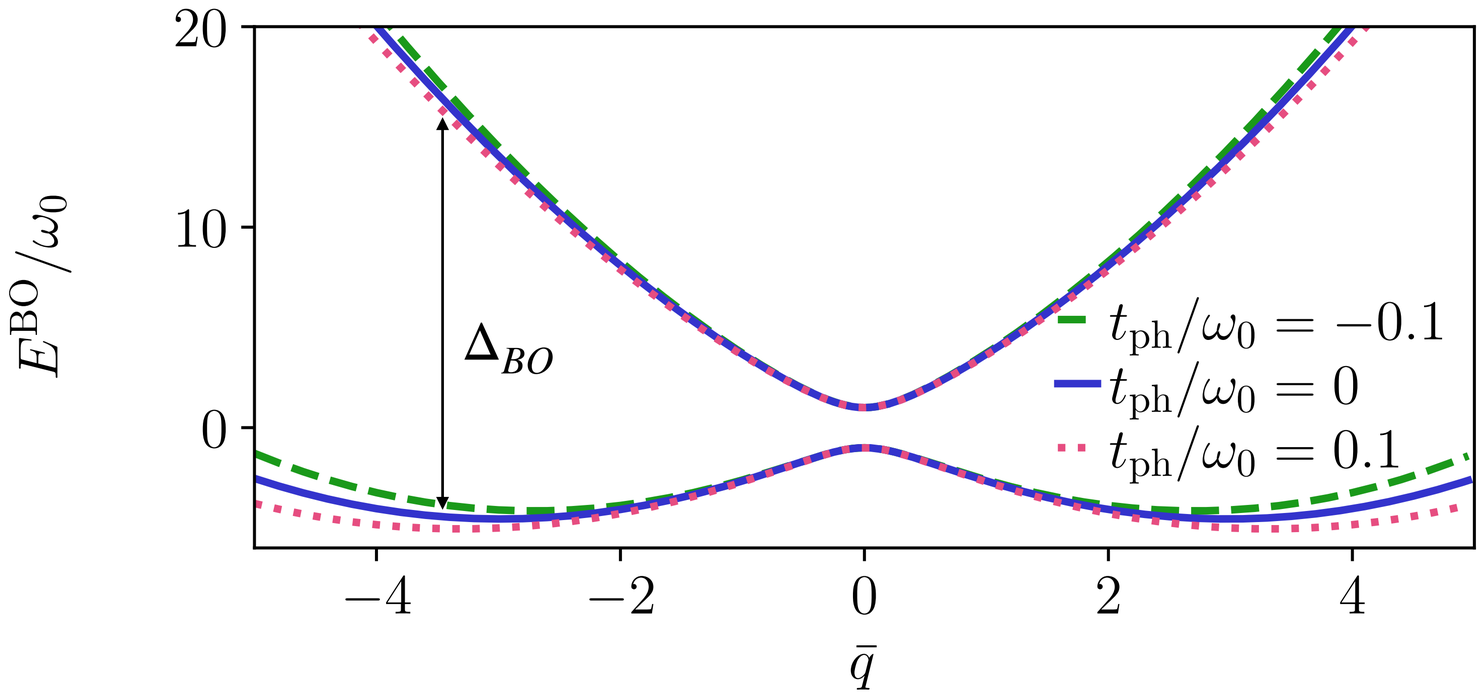

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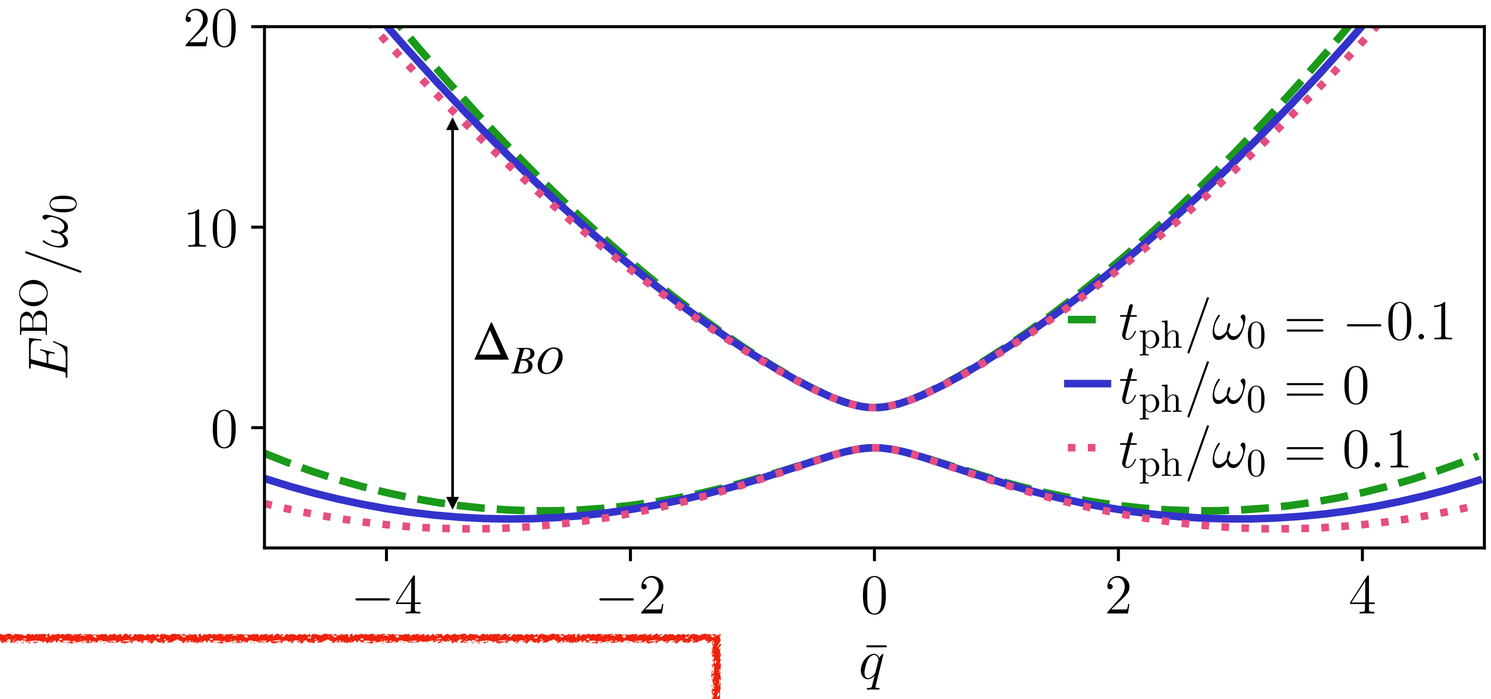


Valid for polarons and bipolarons!

Optical conductivity: Polaron

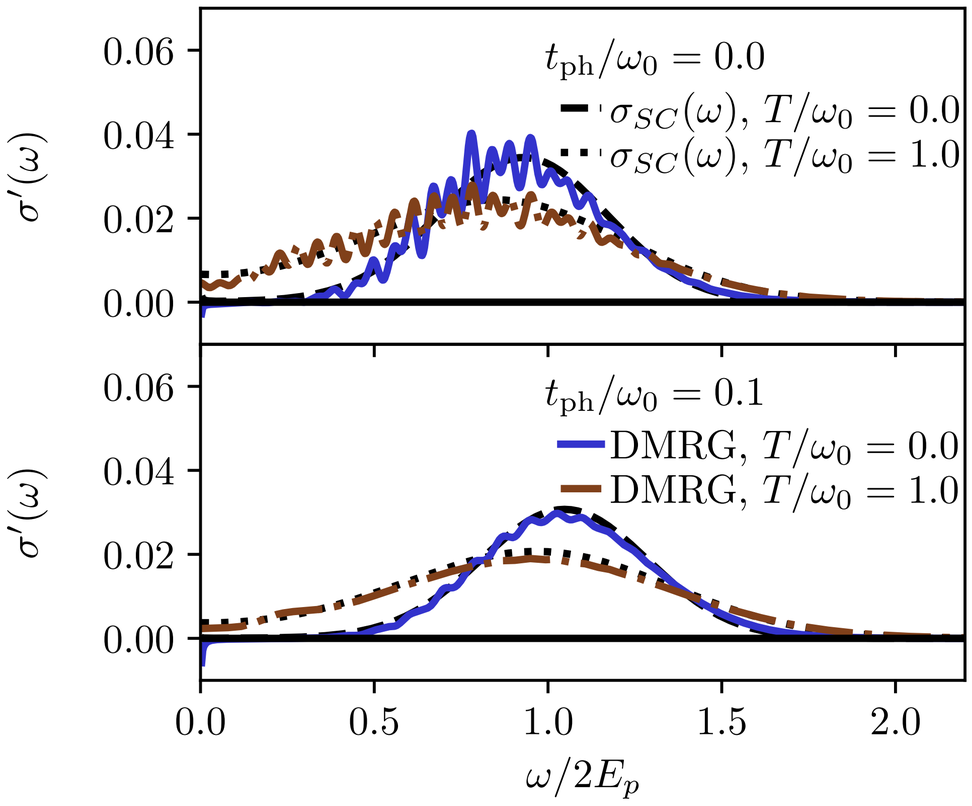
$$\sigma_{SC}(\omega) = \frac{1 - e^{-\beta\omega}}{\omega}\sqrt{\frac{2\pi}{\Delta_{BO}\alpha\tilde{\omega}_0}}t_0^2 e^{-(\Delta_{BO}-\omega)^2/(2\Delta_{BO}\tilde{\omega}_0\alpha)}$$

BO surfaces calculated for bipolaron

$\sigma_{SC}(\omega)$ fits well in all cases!

Main peak shifts to higher frequencies

$L = 20, M = 35, \gamma/\omega_0 = 3, t_0/\omega_0 = 1$



DJ, Bonča and Heidrich-Meisner, arXiv:2206.00985 (2022) (accepted in PRB)

Optical conductivity: Bipolaron

$$\sigma_{SC}(\omega) = \frac{1 - e^{-\beta\omega}}{\omega}\sqrt{\frac{2\pi}{\Delta_{BO}\alpha\tilde{\omega}_0}}t_0^2 e^{-(\Delta_{BO}-\omega)^2/(2\Delta_{BO}\tilde{\omega}_0\alpha)}$$

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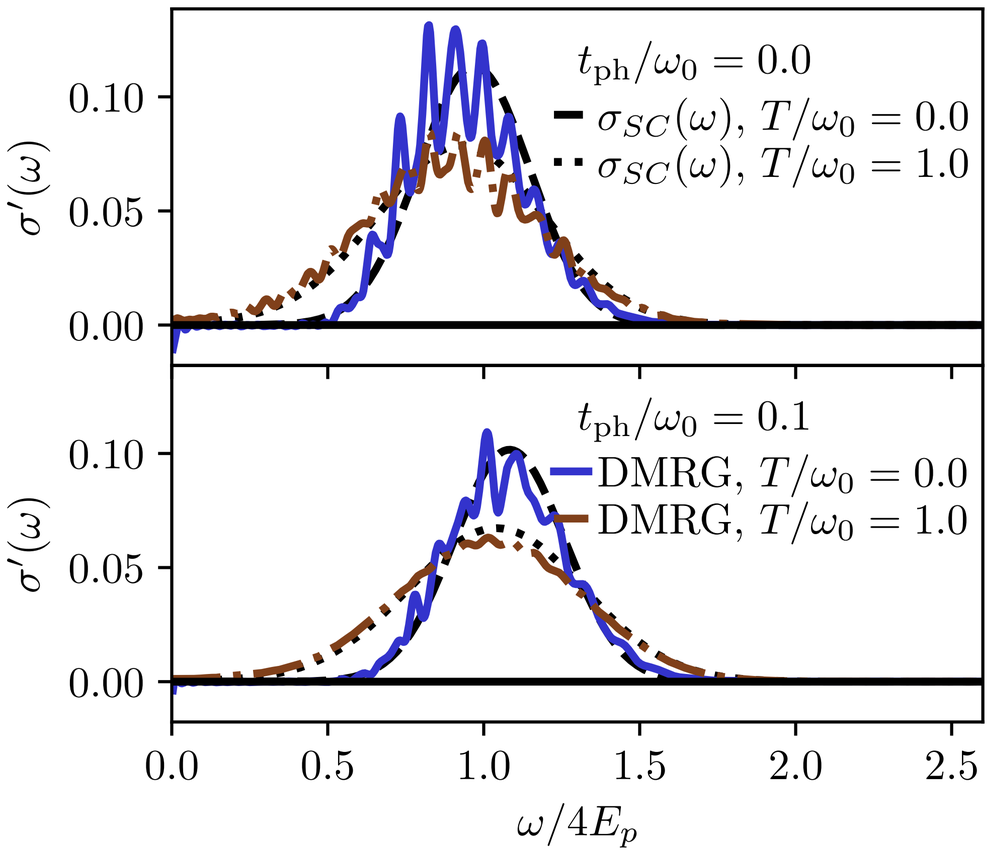


DJ, Bonča and Heidrich-Meisner, arXiv:2206.00985 (2022) (accepted in PRB)

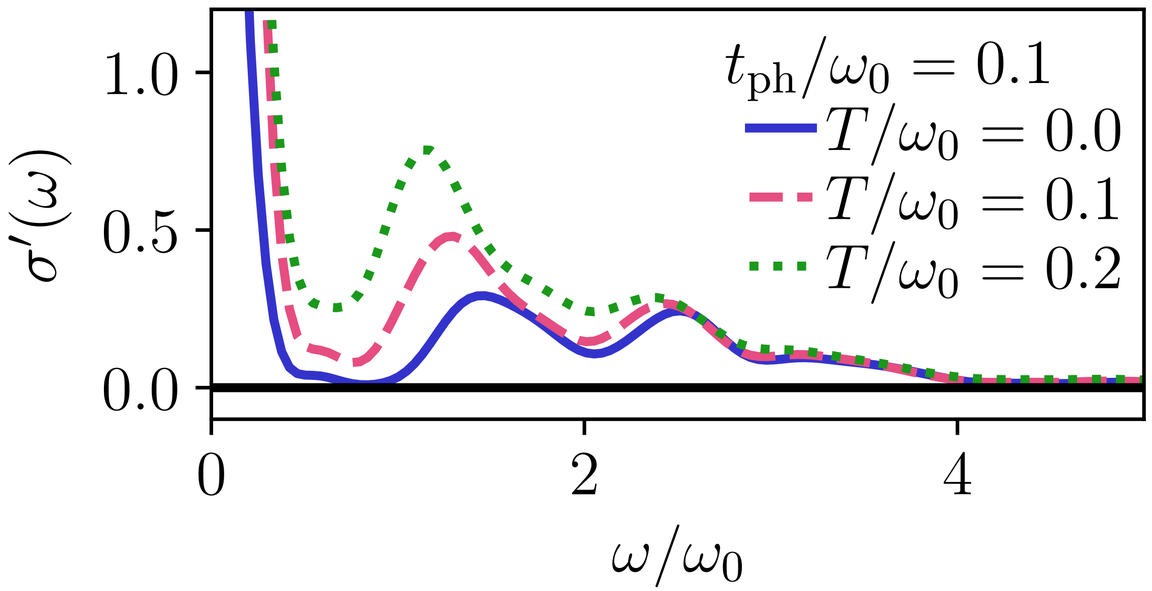
Summary and outlook

Electron-phonon systems

Finite temperature

DJ, Bonča and Heidrich-Meisner, Phys. Rev. B **102**, 165155 (2020)

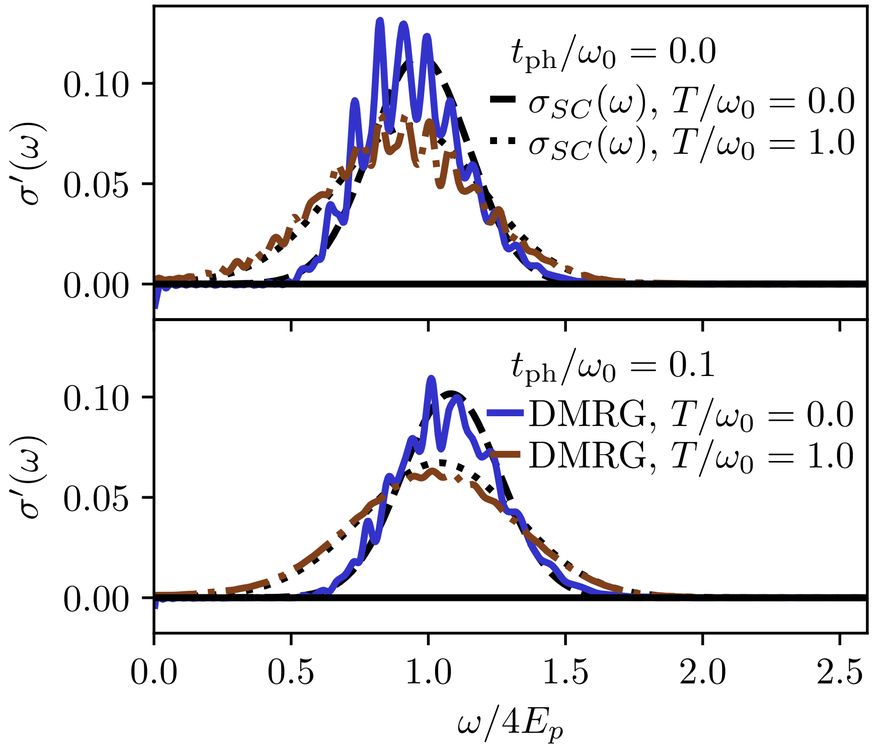
Using p2TDVP with LBO



Polarons and bipolarons

Weak and strong coupling

DJ, Bonča and Heidrich-Meisner, arXiv:2206.00985 (2022) (accepted in PRB)



Outlook

Thermal conductivity

DJ and Heidrich-Meisner, in preparation

Semi-classical treatment of phonons

ten Brink et al., J. Chem. Phys. **156,** 234109 (2022)

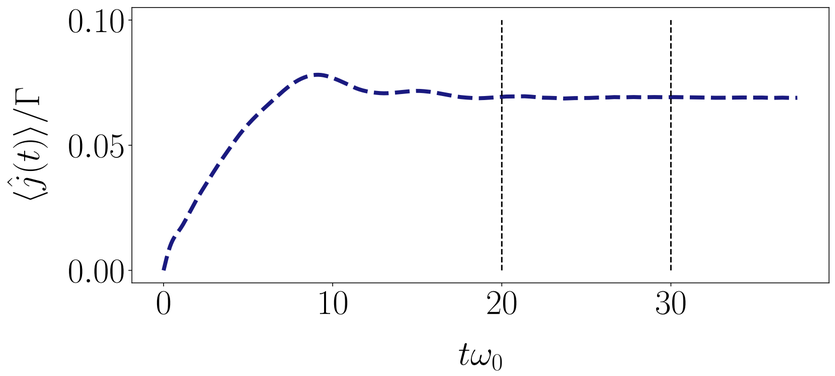
Transport and energy transfer in:

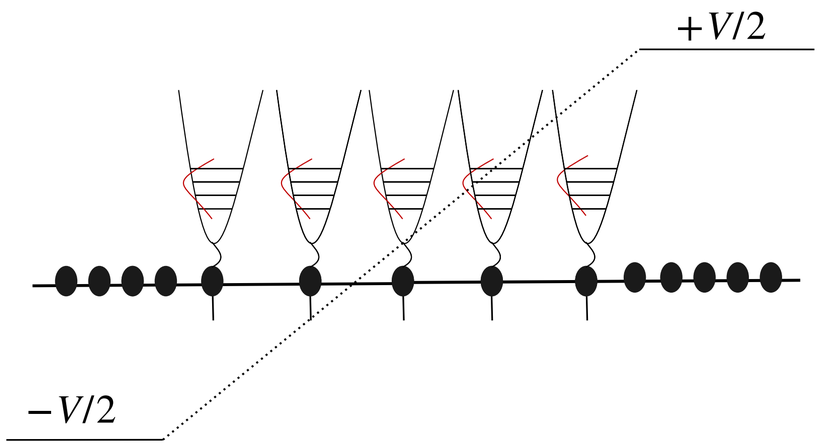
Hetero structures

DJ, Jooss and Heidrich-Meisner, Phys. Rev. B **104**, 195116 (2021)

Interfaces

$L = 236, \gamma/\omega_0 = 1, t_0/\omega_0 = 1, V/\omega_0 = 0.6$





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Interfaces

Thank you for your attention!

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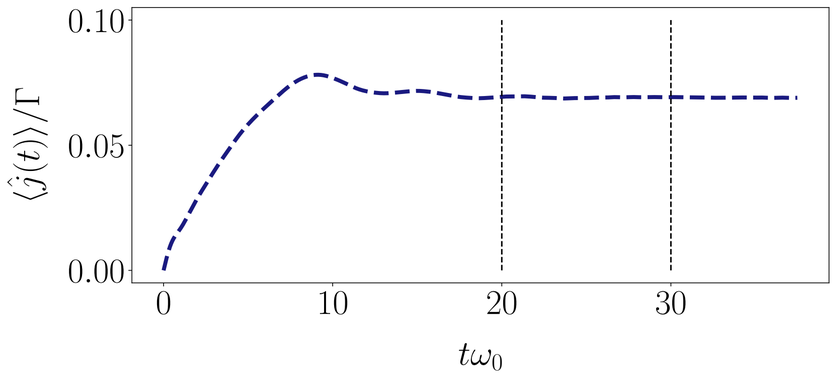

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