Light bipolarons stabilized by strong Peierls electron-vibration coupling: A new hope for high-T_c superconductivity

John Sous

UBC $\rightarrow$ Columbia (MRSEC)

JS, Chakraborty, Krems and Berciu, PRL 121, 247001 (2018)
JS, Nocera, Feiguin and Berciu, in preparation

Funding: NSERC & NSF DMR-1420634

March 4th, 2020

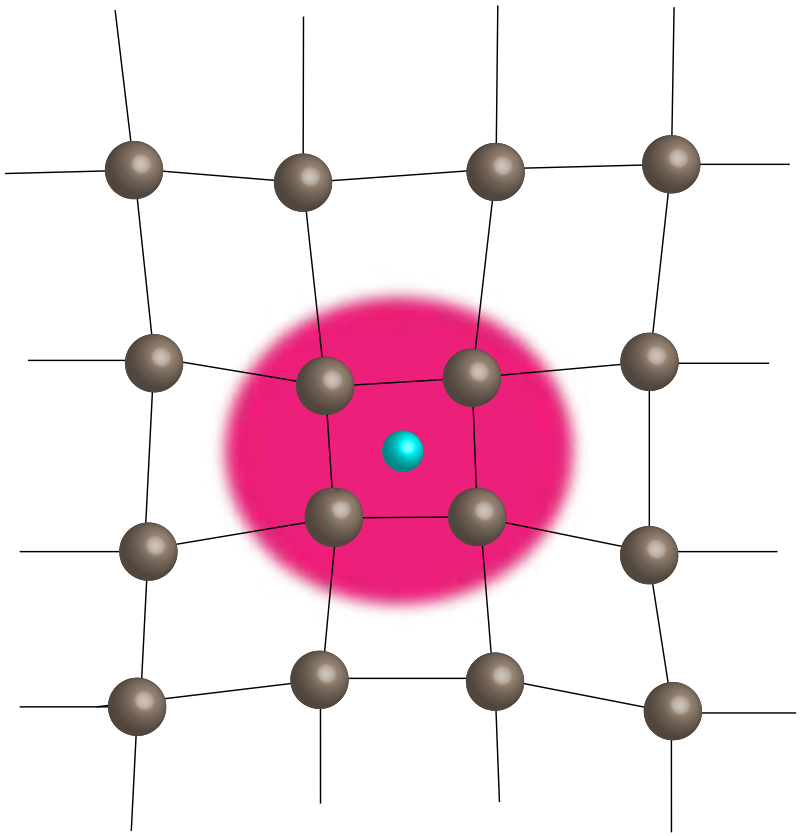
Talk plan:

- Overview of research:
  Coupling to environmental modes &/or disorder (in & out of equilibrium)

- Focus talk on ***Peierls bipolarons***

Coupling to environmental modes &/ disorder (in & out of equilibrium):
Routes to new states of matter

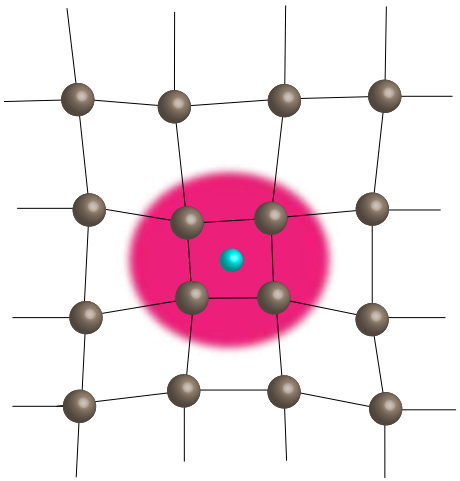
Lattice polarons: Peierls coupling



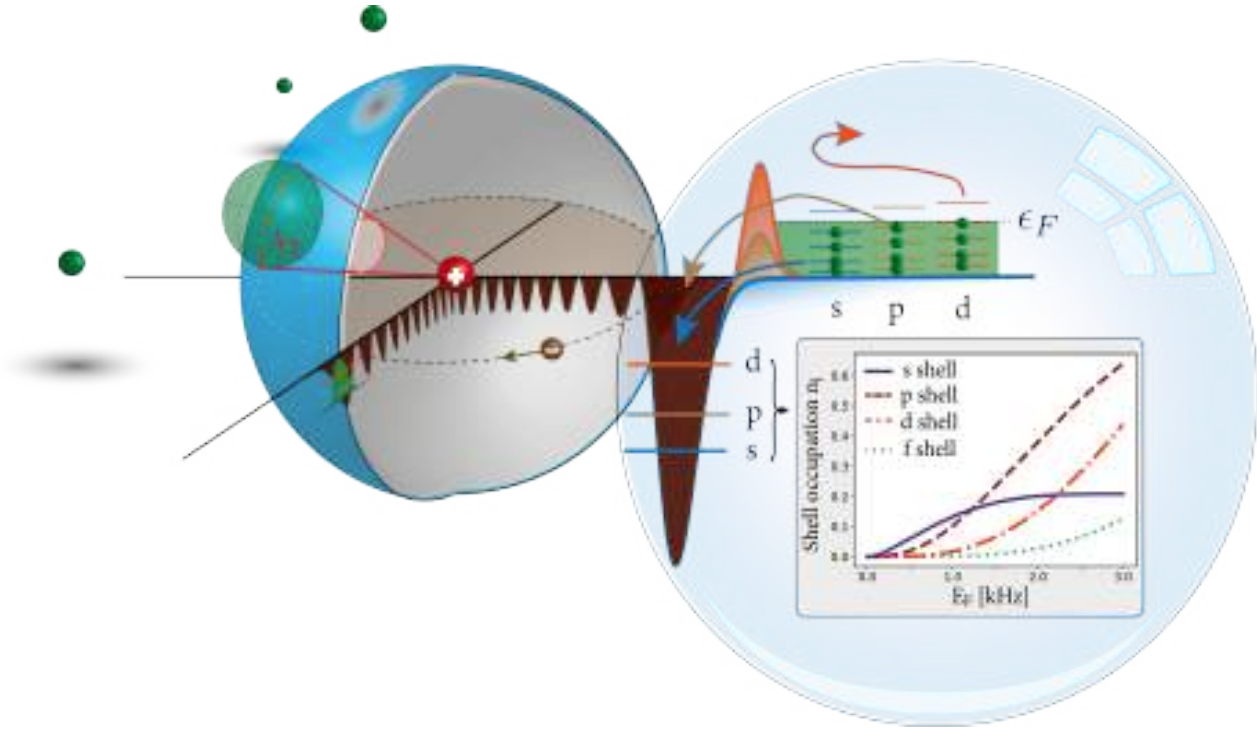
JS, Chakraborty, Krems, Berciu, Sc. Rep. 2017; PRA 2017; PRL 2018, ...

Coupling to environmental modes &/ disorder (in & out of equilibrium):
Routes to new states of matter

Lattice polarons



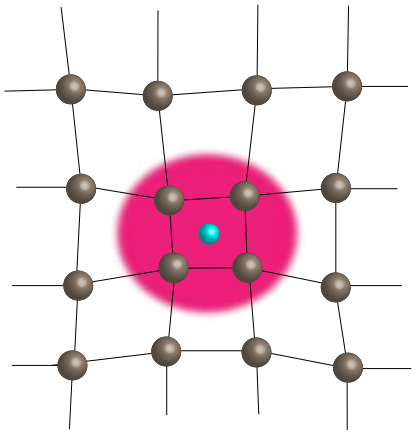
Rydberg polarons



JS, Sadeghpour, Killian, Demler, Schmidt, PRRes. 2020 (in press)

Coupling to environmental modes &/ disorder (in & out of equilibrium):
Routes to new states of matter

Lattice polarons



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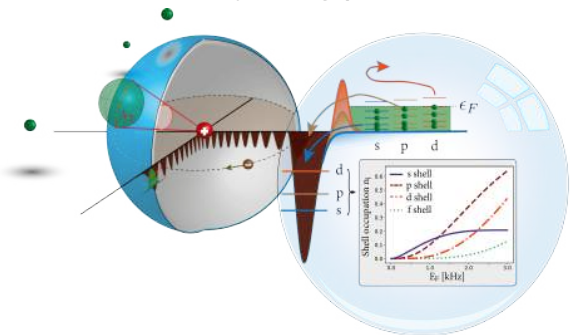
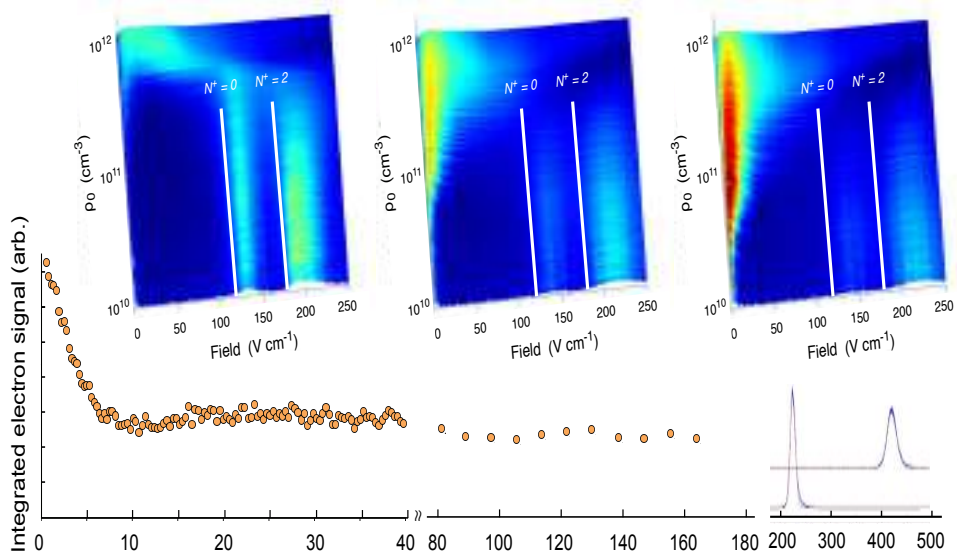
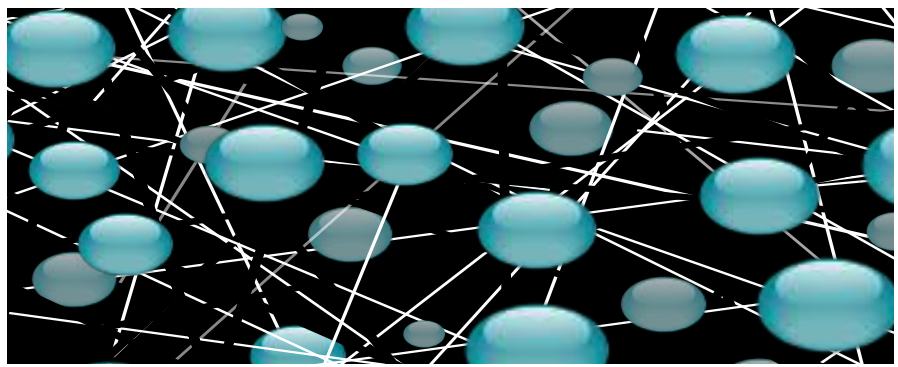


Long-lived disordered molecular plasma

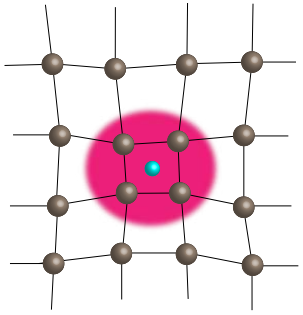




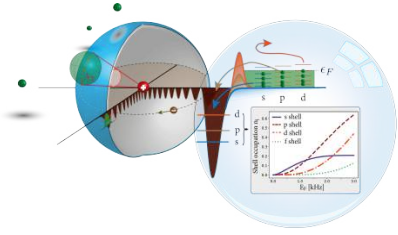
JS and Grant, PRL 2018; NJP 2019

Coupling to environmental modes &/ disorder (in & out of equilibrium):
Routes to new states of matter

Lattice polarons



Rydberg polarons



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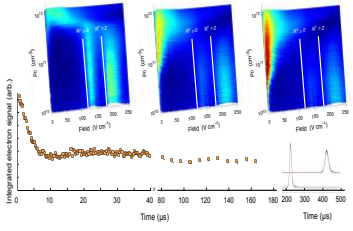
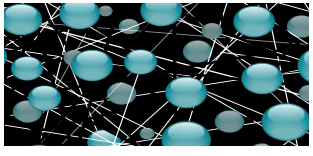
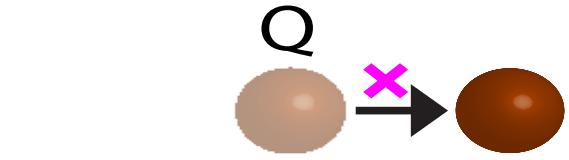
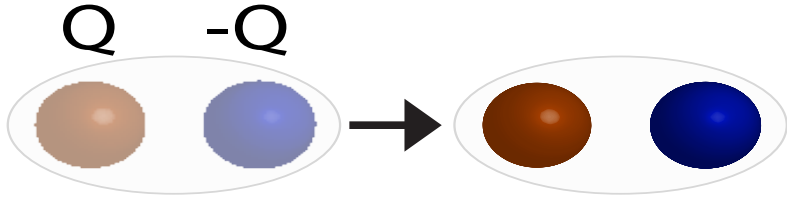
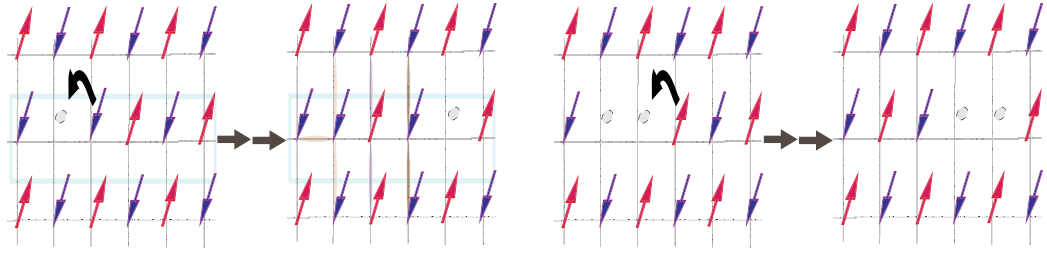




Fractons







JS and Pretko, under consideration (two articles)

Today's talk:

Light bipolarons in Peierls e-ph systems: A route to high-T_c superconductivity

Polaron = electron dressed by phonons
Bipolaron = two polarons bound through phonon exchange
Peierls coupling = coupling electron hopping to lattice distortion

JS, Chakraborty, Krems and Berciu, PRL 2018 & **JS**, Nocera, Feiguin and Berciu, in preparation

Light bipolarons in Peierls e-ph systems: A route to high-T_c superconductivity

Motivation

Methods

Peierls polarons

Peierls bipolarons

Peierls multi-polarons > bipolarons

Peierls bipolarons: The why?

Importance of electron-phonon interaction

$H = T_{\mathrm{el}} + H_{\mathrm{ph}} + V_{\mathrm{e-ph}}$

Modify electronic properties:

+ polaronic dressing

+ induce electron-electron interactions

Q: What electronic phases result from strong e-ph coupling?

+ Strong-coupling superconductivity?

Phonon-mediated superconductivity

BCS superconductivity

Weak e-ph coupling induces a retarded attractive interaction between e's

$\rightarrow$ binds e's, forming Cooper pairs

$\Rightarrow$ Cooper pairs condense

Q: Strong coupling superconductivity?

Strong e-ph coupling

$\rightarrow$ binds e's, forming tightly bound bosonic pairs = bipolarons

$\Rightarrow$ bosonic pairs condense

Strong e-ph coupling: A fast review of the Holstein mode

Understanding of strong e-ph coupling based on a simplified models of charge density coupled to phonons:

Holstein model:

$$V_{\mathrm{e-ph}}^{\mathrm{Holstein}} = g_{\mathrm{Holstein}} \sum_i c_i^\dagger c_i X_i$$

Summary of Holstein polaron physics:

+ Heavy polarons: local dressing of e's potential energy
+ Attractive phonon-mediated interactions: mostly local
+ Very heavy bipolarons: onsite pairs

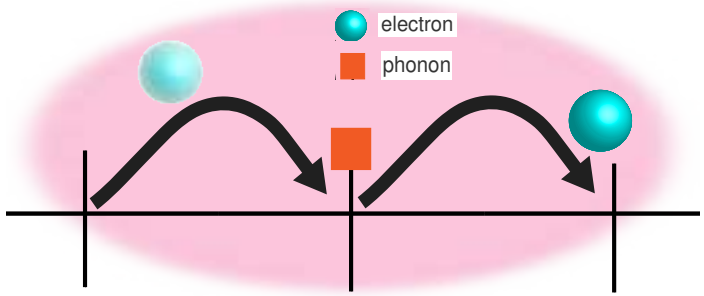
Bonča, Katrašnik, Trugman, PRL 2000; Bonča & Trugman, PRB 2001; Goodvin, Berciu, Sawatzky PRB 2006; many others

Strong-coupling superconductivity based on Holstein model?

Bipolarons could undergo Bose-Einstein condensation at dilute electron concentrations

$$k_B T_c \propto \hbar^2 n_{BP}^{2/3} / m_{BP}$$

n_{BP}: concentration of bipolarons
m_{BP}: mass of bipolarons



But, as the e-ph coupling increases, m_B grows $\rightarrow$ $\mathrm{small}\, T_c$

High-T_c bipolaronic superconductivity is impossible

Chakraverty, Ranninger, Feinberg, PRL 1998

Peierls challenges Holstein

Phonons also modulate the distance between sites:

$\Rightarrow$ electron hopping couples to the lattice:

$$g_{\text{Peierls}} \sum_{i,j} c_i^\dagger c_j (X_i - X_j)$$

Peierls physics

+ Inter-site/bond coupling

+ dimerization in polyacetylene

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Peierls polarons

Peierls bipolarons

Peierls multi-polarons > bipolarons

Methods

Methods

- Momentum Average (MA) Green fn. method Berciu, PRL 2006

  Method development: First extension to large bipolarons

  JS et al. (Sc. Rep. 2017 & PRL 2018)

- Variational exact diagonalization (VED) Bonča, Katrašnik, Trugman, PRL 2000; Bonča & Trugman, PRB 2001; Chakraborty, Tezuka, Min PRB 2014

- Density-Matrix Renormalization Group (DMRG) White PRL (1992); Nocera

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Peierls bipolarons

Peierls multi-polarons > bipolarons

Peierls polarons

Single electron coupled to phonons:
$H = T_{\mathrm{el}} + H_{\mathrm{ph}} + V_{\mathrm{e-ph}}$

$$V_{\mathrm{e-ph}}^{\mathrm{Peierls}} = g_{\mathrm{Peierls}} \sum_{i,j} c_i^\dagger c_j (X_i - X_j)$$

Dimensionless coupling $\lambda_{\mathrm{p}} = \frac{2 g_{\mathrm{Peierls}}^2}{\Omega_{\mathrm{ph}} t}$

Phonon frequency $\Omega_{\mathrm{ph}} = \sqrt{\frac{K}{M}} \sim$ electron hopping t

Peierls polarons:

+ Sharp polaronic transition: at λ_{p}^c (m_P^* diverges)
+ $\lambda_{\mathrm{P}} < \lambda_{\mathrm{P}}^c$: the polaron becomes heavier as λ_{p} increases
+ $\lambda_{\mathrm{P}} > \lambda_{\mathrm{P}}^c$: the polaron becomes lighter as λ_{p} increases

Marchand et al., PRL 2010

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Peierls bipolarons

Peierls multi-polarons > bipolarons

Peierls bipolarons

JS, Chakraborty, Krems and Berciu, PRL 2018

The bipolaron problem in 1D Peierls e-ph system

Methods:

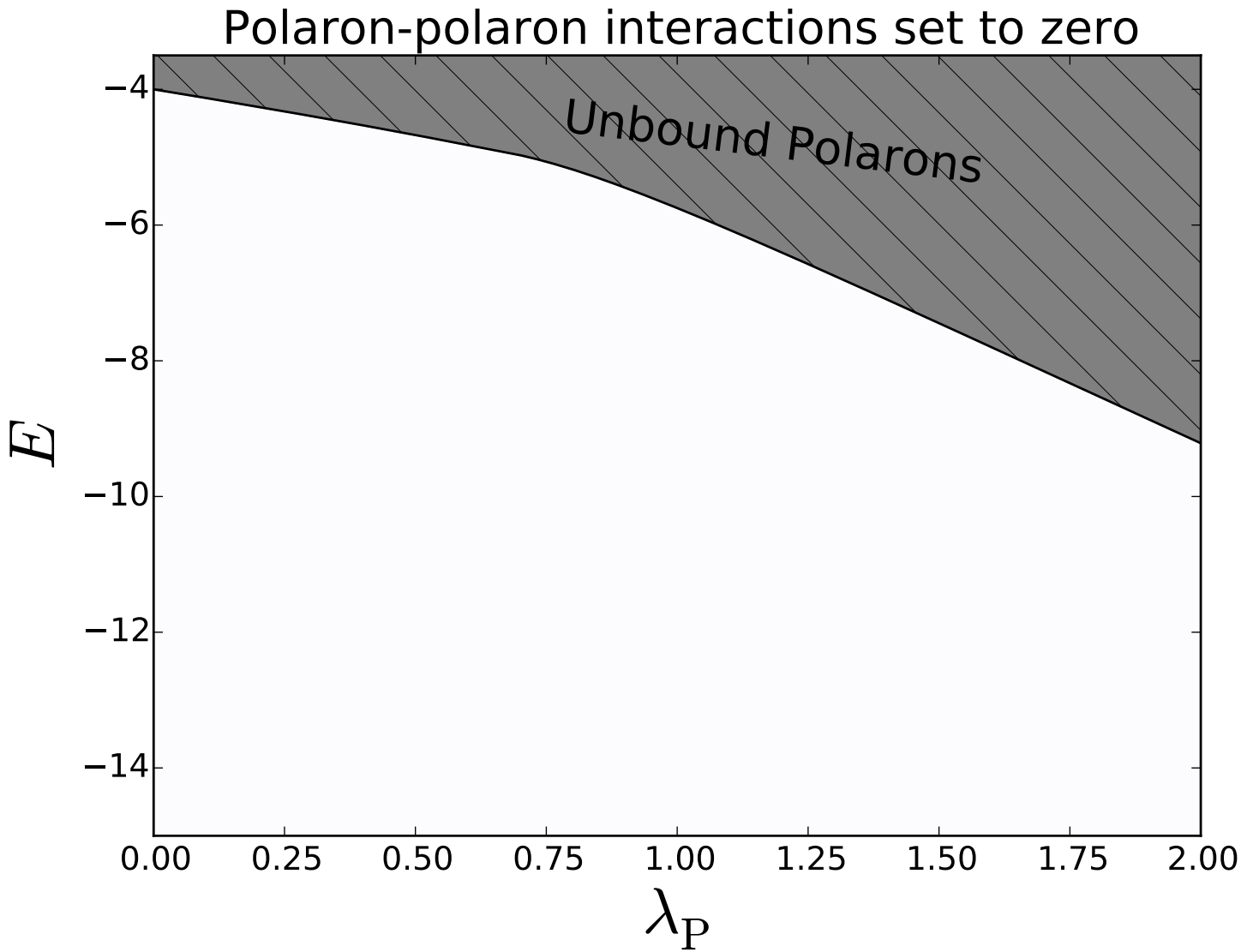
Numerics from MA & VED

Analytics from perturbative diagrams

Peierls bipolarons

JS, Chakraborty, Krems and Berciu, PRL 2018

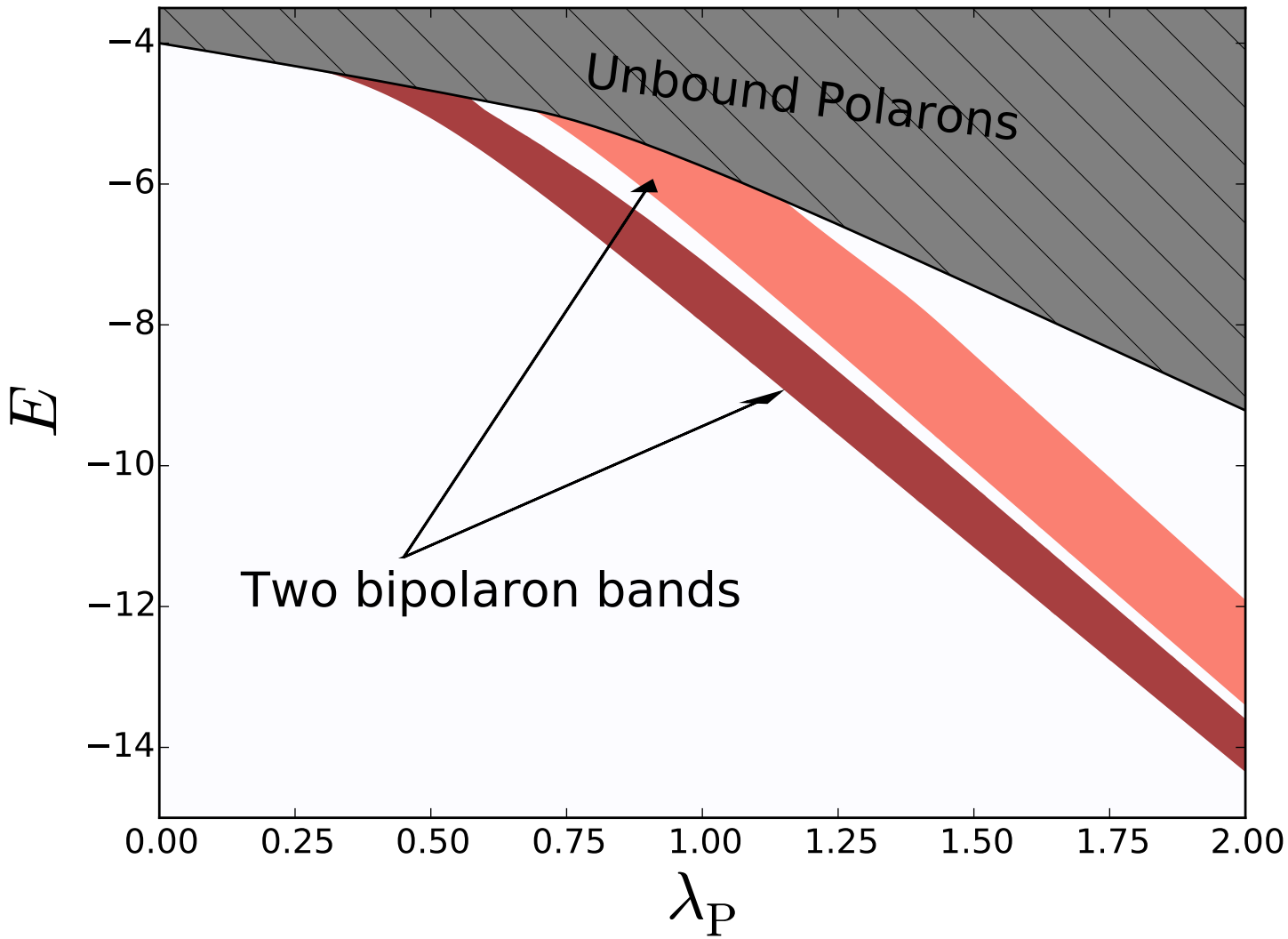
Energy spectrum



Peierls bipolarons

JS, Chakraborty, Krems and Berciu, PRL 2018

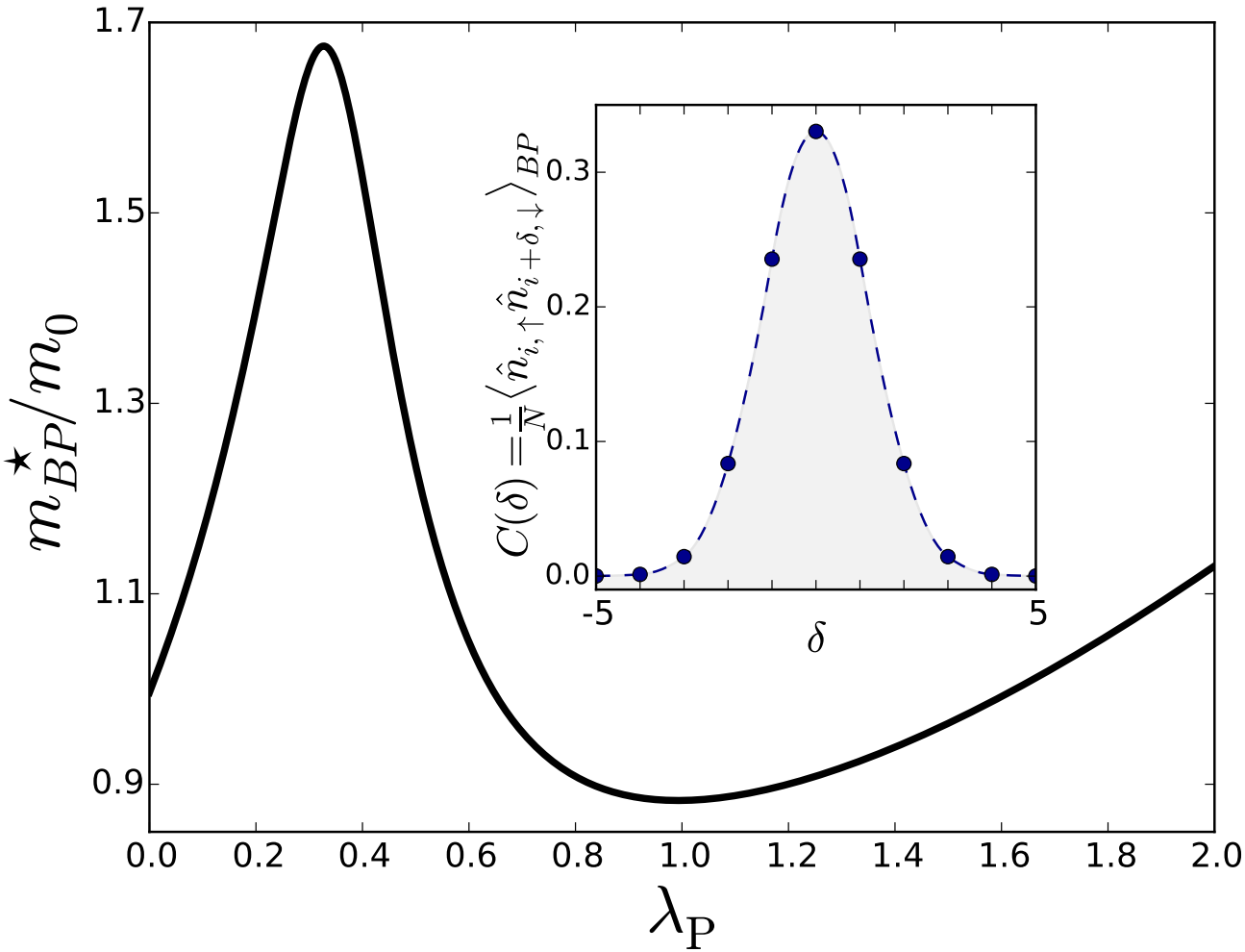
Energy spectrum: Two bipolaron states



Peierls bipolarons

***JS**, Chakraborty, Krems and Berciu, PRL 2018*

Light bipolaron



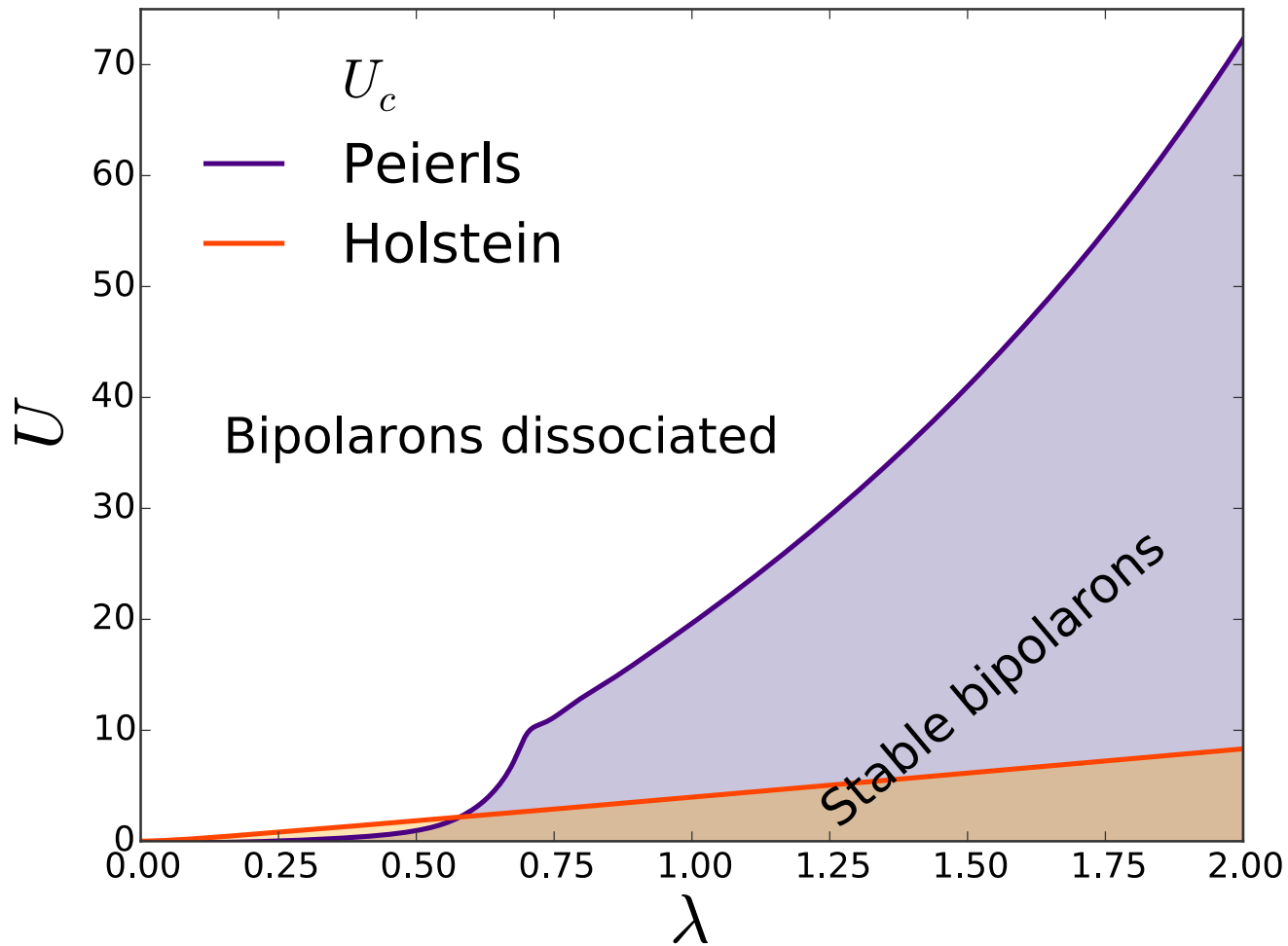
m_0: mass of two free electrons

Peierls bipolarons

JS, Chakraborty, Krems and Berciu, PRL 2018

Against Coulomb: $H + U \sum_i n_{i,\uparrow} n_{i,\downarrow} + \cdots$

Peierls defeats Holstein



Peierls bipolarons

JS, Chakraborty, Krems and Berciu, PRL 2018

Unconventional properties:

+ Light bipolarons even at large λ_{P}

+ Peierls bipolarons more stable against Coulomb repulsion than Holstein bipolarons

Pairing mechanism:

Phonons mediate pair-hopping interactions

$$\sim \alpha \sum_{i,j,\sigma} f(i,j) c^{\dagger}_{j,\sigma} c^{\dagger}_{j+\delta,-\sigma} c_{i+\delta,-\sigma} c_{i,\sigma}$$

Peierls bipolarons

***JS**, Chakraborty, Krems and Berciu, PRL 2018*

Strongly bound yet light bipolarons at strong coupling $\rightarrow$
possible high-T_c BEC superconductivity

Stability of bipolarons against bipolaron-bipolaron interactions?

Light bipolarons in Peierls e-ph systems: A route to high-T_c superconductivity

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Peierls bipolarons

Peierls multi-polarons > bipolarons

Peierls multi-polarons > bipolarons

***JS**, Nocera, Feiguin and Berciu, in preparation*

Up to six electrons in 1D Peierls e-ph system

$\Downarrow$

zero/dilute-density limit

Methods:

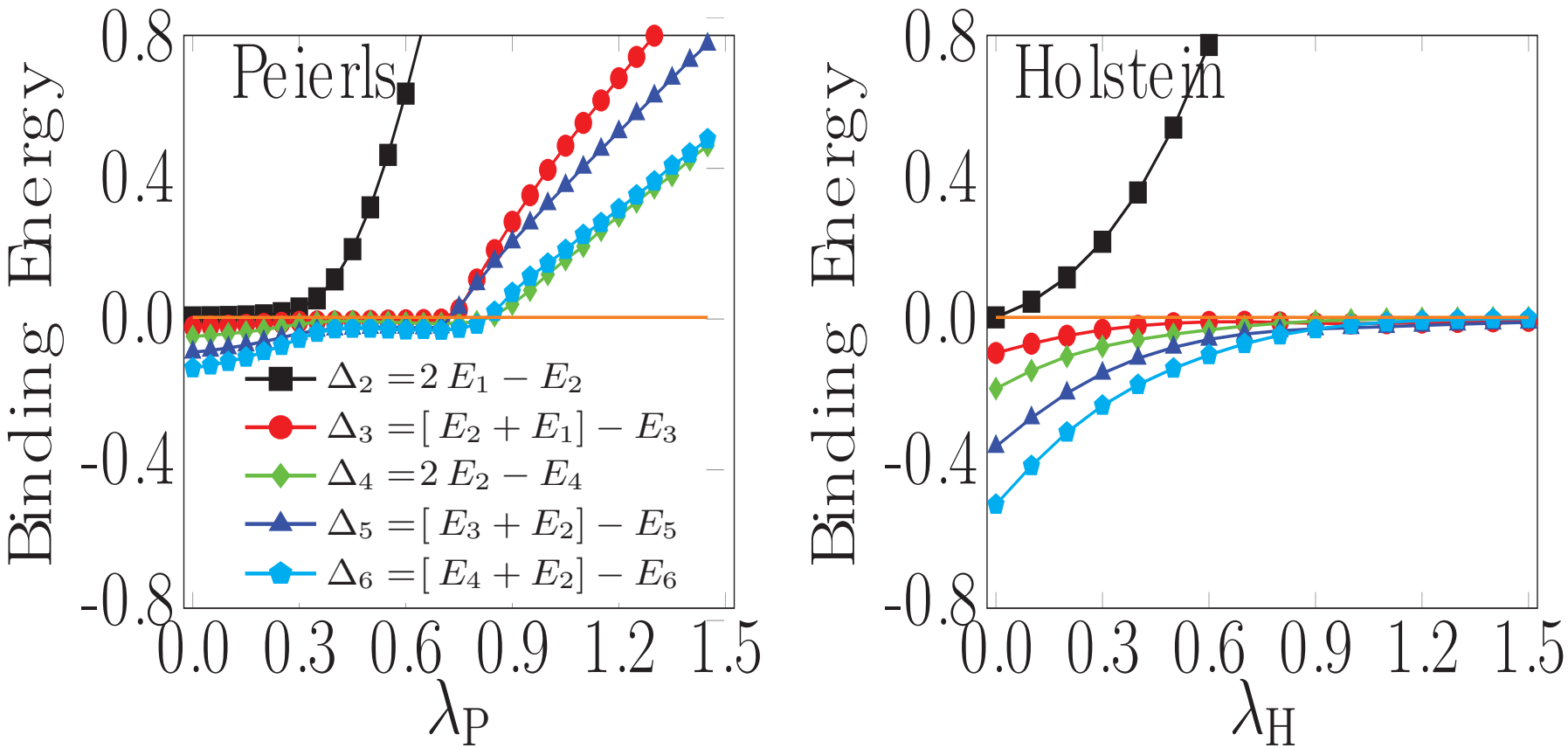
Numerics from DMRG

Analytics under development

Peierls multi-polarons > bipolarons

JS, Nocera, Feiguin and Berciu, in preparation

Bipolarons, tripolarons, tetrapolarons, pentapolarons & sextapolarons

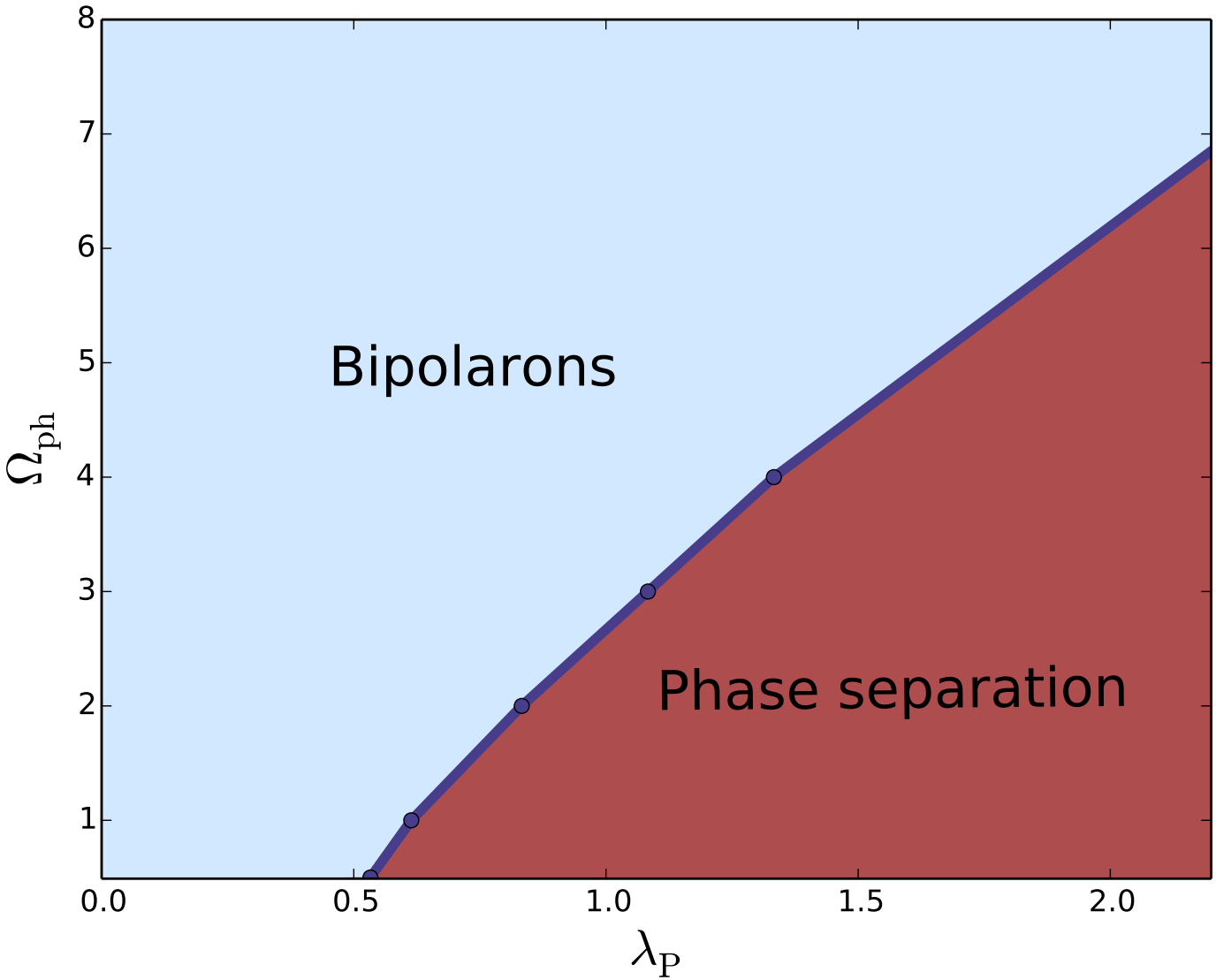


Bipolarons stable till $\lambda_P^c \sim 0.7$

Peierls phase diagram

JS, Nocera, Feiguin and Berciu, in preparation

Bipolaron condensate vs phase separation



Peierls bipolarons: Towards high-T_c BEC superconductivity

- Dilute electron concentration
  $\lambda_{\mathrm{P}} < \lambda_{\mathrm{P}}^{c}$: bipolaron phase
- Light bipolarons

Bipolaronic high-T_c superconductivity

Future directions:

- **?** Materials:
  - Chevrel phase compounds Chen, Millis, Reichman, PRM 2018
  - Alkali-doped organics Qin, Fabrizio, Naghavi, Tosatti, PRB 2014
  - Bismuth oxides Naamneh, · · · , Plumb, arXiv:1808.06135 2018; Li, Johnston, arXiv:1901.07612 2019
- **?** Theoretical studies in 2D & 3D