Numerical Study of Holstein Polarons

Part I. Self-Trapping Crossover
Part II. Disorder, Correlation, and Finite-Density Effects
Part III. Collective Phenomena – Quantum Phase Transitions

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Outline

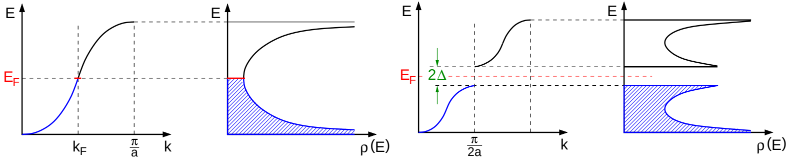
Lecture III: Collective Phenomena – Quantum Phase Transitions

- Introduction
  - Peierls instability
  - Peierls-Mott competition
- Metal insulator transition
  - Luttinger liquid characterisation
  - CDW characterisation
  - Phase diagram of the spinless fermion Holstein model
  - Phonon softening
- Peierls-insulator Mott-insulator transition
  - Ground-state properties
    Charge & spin structure factors
    Phonon distribution function
    Symmetry considerations
  - Excitations
    Photoemission
    Optical response
    Spin & charge excitation gaps
  - Intrinsic localised modes

related publications $\rightsquigarrow$ `http://theorie2.physik.uni-greifswald.de`

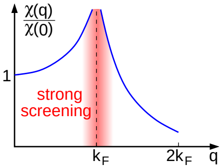
- Effect of electron-phonon coupling in low-D systems?

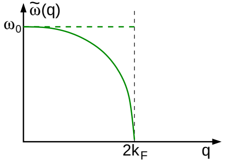
  $\rightsquigarrow$ structural distortions at commensurate band fillings n,
  famous example, Peierls instability:



EP driven metal insulator transition!

related: Kohn anomaly phonon softening



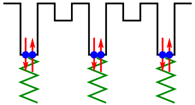


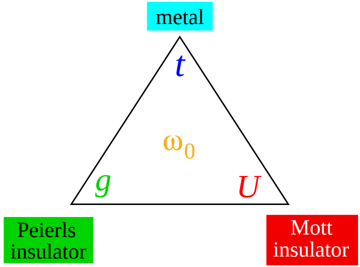
Lattice dynamics? Especially important in 1D!

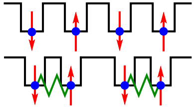
Peierls Mott transition

- Effect of Coulomb interaction?

ground state:







excitations?

electron-hole pairs
$\hookrightarrow$ QP behaviour!

quantum phase transitions
$\Leftarrow$??? $\Rightarrow$

massive • but gapless ↑
$\hookrightarrow$ spin-charge separation!

$\hookrightarrow$ quasi-1D materials: wide variety of broken-symmetry ground states & (partially) exotic excitations!

Part I: Metal-Insulator Transition

(Luttinger liquid vs charge-density-wave behaviour)

simplest model: 1D spinless fermion Holstein model at half-filling

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j - g\,\omega_0 \sum_i (b_i^\dagger + b_i) n_i + \omega_0 \sum_i b_i^\dagger b_i$$

N sites, N_e electrons with $n = N_e/N = 0.5$, dispersionless phonons, $T = 0$

parameters: $g^2 = \varepsilon_p/\omega_0$; $\lambda = \varepsilon_p/2t$, and $\alpha = \omega_0/t$

"known" results:

- $\lambda \nearrow$: quantum phase transition from a metallic (LL) to an insulating (Peierls distorted) phase; RG, QMC, GFMC, ED, DMRG, ... $\rightsquigarrow$ phase boundary, *but* significant discrepancies in the adiabatic intermediate coupling regime!
- $\omega_0 \to 0$: $\lambda_c \to 0$
- strong-coupling anti-adiabatic regime $\rightsquigarrow$ exactly solvable XXZ model: Kosterlitz -Thouless phase transition

Luttinger liquid parameters

- Characterisation of Luttinger liquids?

  Holstein model - gapless for small couplings $\rightsquigarrow$ Tomonaga-Luttinger universality class [Haldane LL conjecture (PRL 45, 1358 (1980))]:

  $$\boxed{n(k),\ \rho(\omega),\ G(x),\ \chi^{-1},\ \kappa^{-1},\ldots \leftrightharpoons K_\rho,\ u_\rho}$$

  interaction (stiffness) constant and charge velocity

- $\exists$ scaling relations!

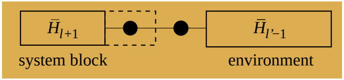
  (conformal field theory - Affleck, Cardy, Nomura, Okamoto, Voit,...)

$$\varepsilon_0(\infty) - \frac{E_0(N)}{N} = \frac{\pi}{3}\frac{u_\rho}{2}\frac{1}{N^2} \qquad \propto \text{ground-state energy}$$

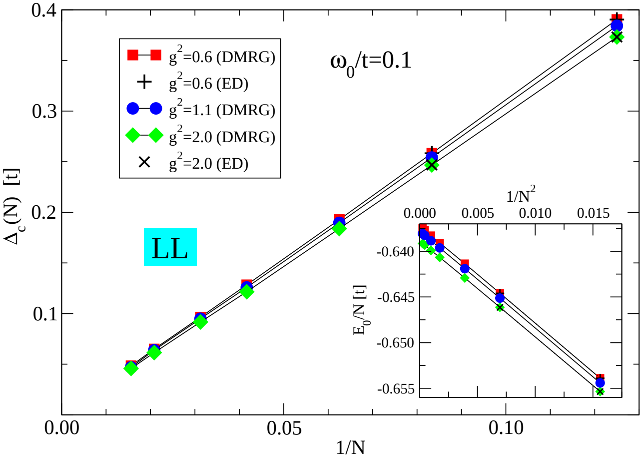
$$E_0^{(\pm 1)}(N) - E_0(N) = \pi\frac{u_\rho}{2}\frac{1}{K_\rho}\frac{1}{N} \qquad \propto \text{charge excitation gap}$$

Density Matrix Renormalisation Group:
systems with $N=128\ldots512$ accessible

$\hookrightarrow$ determination of (non-universal) K_ρ & u_ρ!



- Effects of EP coupling?

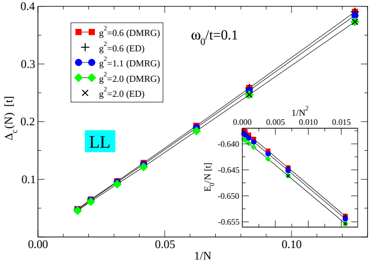


$\hookrightarrow$ scaling relations are still fulfilled almost perfectly – $\forall\alpha$!

(but, of course, they break down at large g^2)

Finite-size scaling

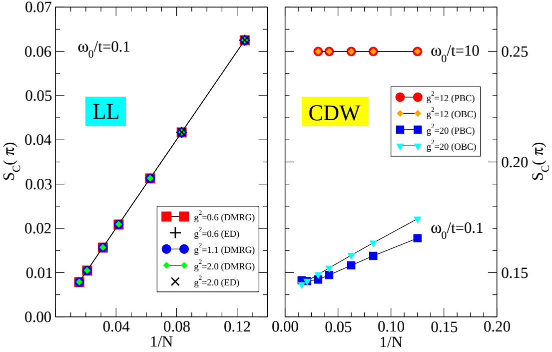
- Extraction of LL parameters:



g^2	$\omega_0/t = 0.1$		$\omega_0/t = 10.0$	
	K_ρ	$u_\rho/2$	K_ρ	$u_\rho/2$
0.6	1.031	~ 1	~ 1	0.617
2.0	1.055	0.995	0.949	0.146
4.0	1.091	0.963	0.651	0.028
	> 1		< 1	

$\hookrightarrow$ adiabatic regime: attractive interaction & weak u_ρ-renormalisation
anti-adiabatic regime: repulsive interaction & strong u_ρ-renormalisation!

- Charge structure factor at π: $$\boxed{S_c(\pi) = \frac{1}{N^2}\sum_{i,j}(-1)^j\langle(n_i-\tfrac{1}{2})(n_{i+j}-\tfrac{1}{2})\rangle}$$



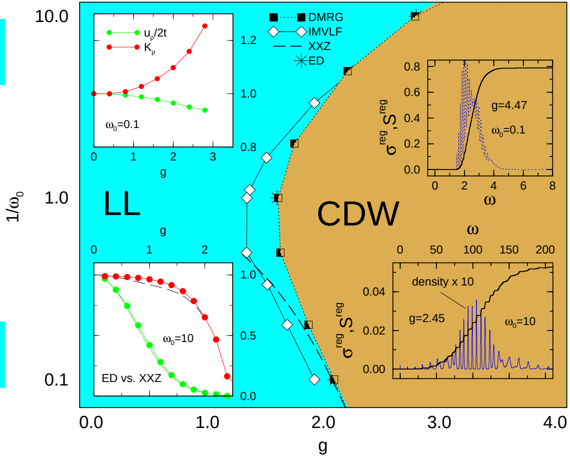
no LRO LRO

$\hookrightarrow$ existence of a Peierls-CDW phase above $g_c(\alpha)$!

Ground-state phase diagram

attractive LL

repulsive LL



Peierls distorted state

metallic behaviour

activated transport

u_ρ, K_ρ

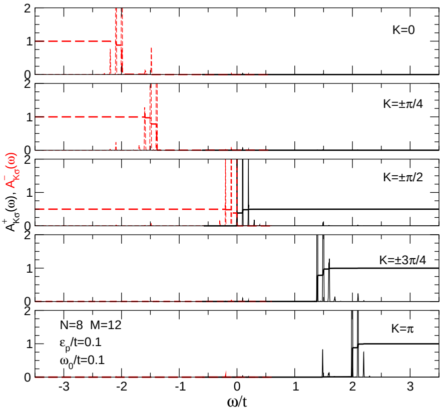
$\sigma^{reg}(\omega)$

Photoemission spectra I

- Injection/emission of electrons? ($c^{+}_{K\sigma} = c^{\dagger}_{K\sigma}$ - IPE; $c^{-}_{K\sigma} = c_{K\sigma}$ - PE; $\sigma \equiv \uparrow$)

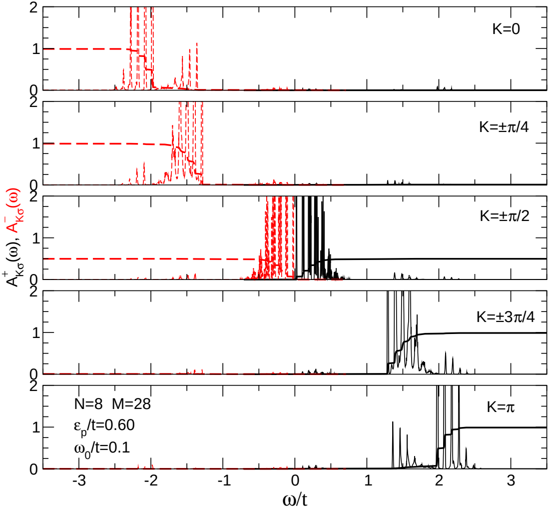
$$\boxed{A^{\pm}_{K\sigma}(\omega) = \sum_m |\langle \psi_m^{(N_{el}\pm 1)} | c^{\pm}_{K\sigma} | \psi_0^{(N_{el})} \rangle|^2 \delta[\omega \mp (E_m^{(N_{el}\pm 1)} - E_0^{(N_{el})})]}$$

- weak coupling:



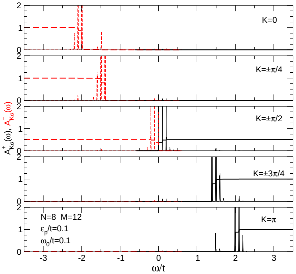
- metal
- QP peak
- phonon satellites

- critical coupling:



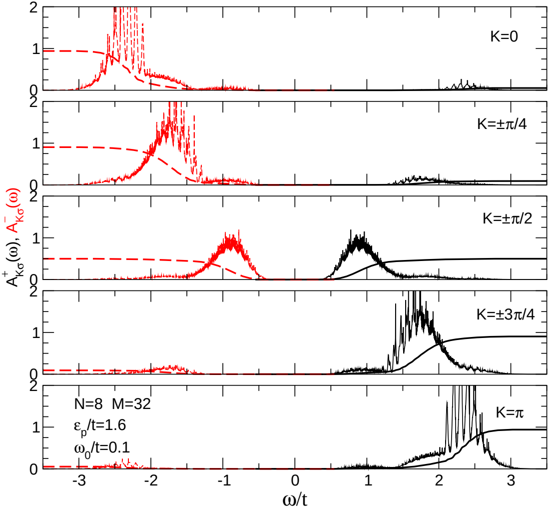
- gap feature emerges
- redistribution of QP weight
- phonon absorption bands

weak coupling:

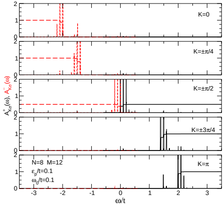


Photoemission spectra III

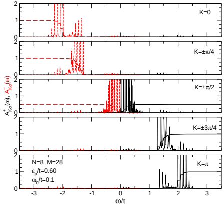
- strong coupling: finite gap $\rightsquigarrow$ CDW insulator



weak coupling:



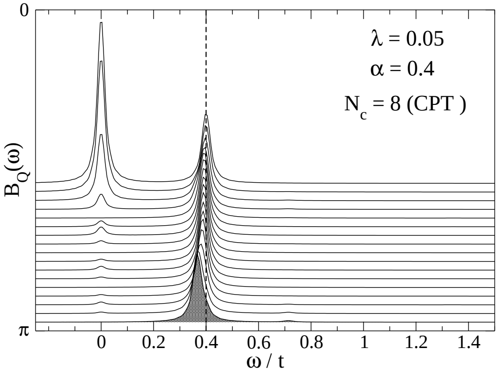
critical coupling:



- Renormalisation of phonon dispersion? $\boxed{D_Q(\omega) = 2\omega_0 \, \langle\langle x_Q ; x_{-Q} \rangle\rangle_\omega}$

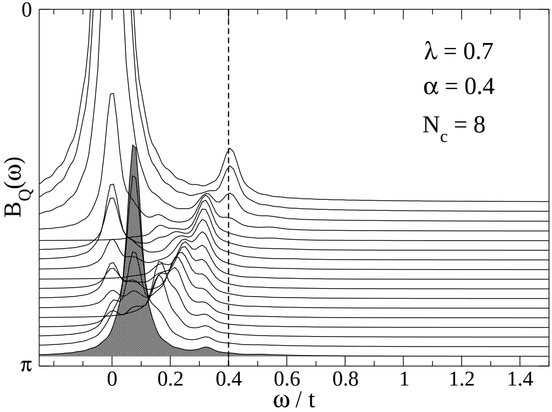
$$\text{(with } x_i = (b_i^\dagger + b_i)/\sqrt{2\omega_0}; \quad B_Q(\omega) = -\tfrac{1}{\pi}\mathrm{Im} D_Q(\omega))$$

- weak coupling:



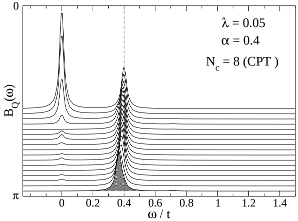
- $\widetilde{\omega}(Q) \simeq \omega_0$
- $K = 0$ "electron" state - phonon admixture

- $\lambda \rightarrow$ critical coupling:



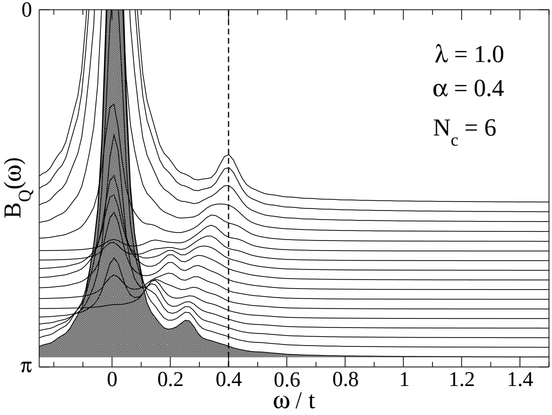
- zone boundary phonon becomes soft
- redistribution of phonon spectral weight

weak coupling:

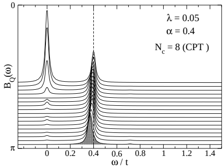


Phonon spectra - adiabatic case III

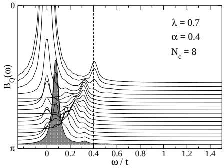
- strong coupling: CDW insulator



weak coupling:

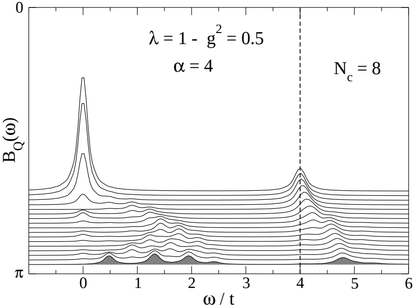


critical coupling:

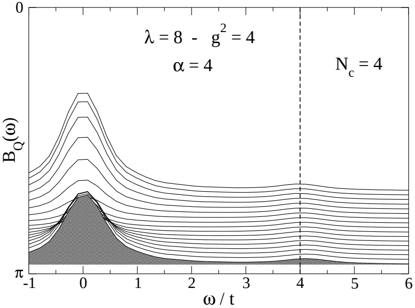


- doubling of Brillouin zone
- phonon hardening sets in

weak coupling



strong coupling

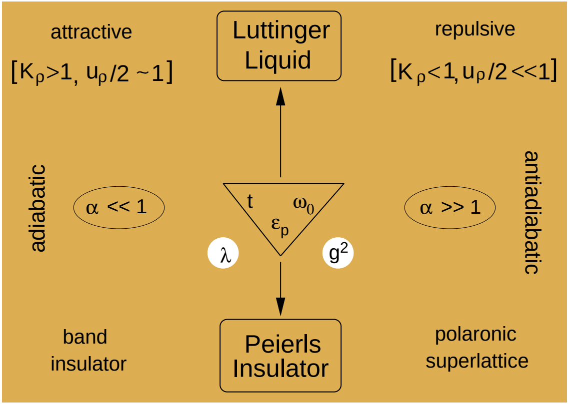


- signature of polaron band dispersion
- precursor of softening?

- almost perfect doubling
- dispersionless signature at ω_0

Hohenadler, Alvermann, HF: in preparation (2005)

Schematic phase diagram



- HF, Holicki, Weiße: Adv. Solid State Physics, 40 , 235 (2000)
- Sykora, Hübsch, Becker, Wellein, HF: Phys. Rev. B 71, 045112 (2005)
- HF, Wellein, Hager, Weiße, Becker, Bishop: Physica B 359-361, 699 (2005)

Part II: Insulator-Insulator Transition

(Peierls vs Mott)

simplest model: 1D Holstein Hubbard model at half-filling

$$H = \sum_{i\sigma} \epsilon_i n_{i\sigma} - t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - g\,\omega_0 \sum_{i\sigma} (b_i^{\dagger} + b_i) n_{i\sigma} + \omega_0 \sum_i b_i^{\dagger} b_i + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

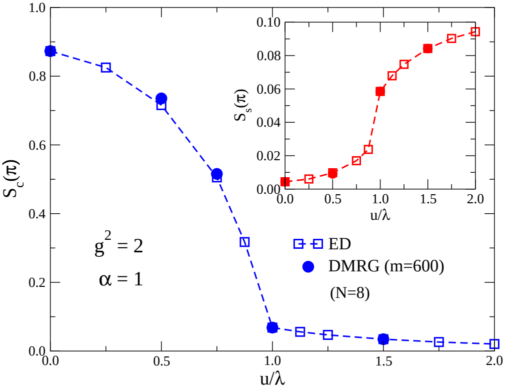
N sites, $N_{e\uparrow} = N_{e\downarrow} = N/2$ electrons, i.e. $n = 1$, dispersionless phonons, $T = 0$

parameters: $g^2 = \varepsilon_p/\omega_0$; $\lambda = \varepsilon_p/2t$, $\alpha = \omega_0/t$, and $u = U/4t$

Hardly any exact results!

- Suppression of CDW by Hubbard interaction?
- Increase of SDW? $S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$

$$\boxed{S_s(\pi) = \frac{1}{N^2}\sum_{i,j}(-1)^j \langle S_i^z S_{i+j}^z \rangle}$$

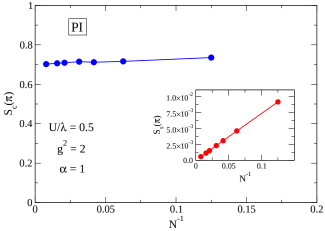


Yes! Finite-size effects?

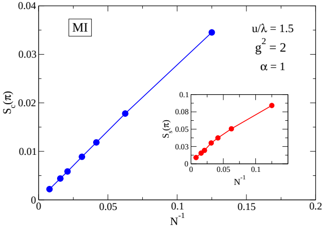
CDW-SDW TRANSITION

- Phase transition? $N \to \infty$! $\rightsquigarrow$ DMRG finite-size scaling necessary

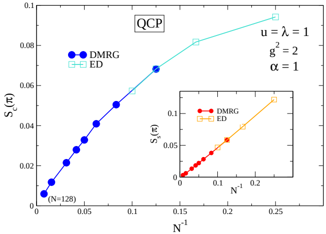
$\lambda > u$



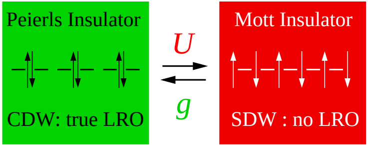
$\lambda < u$



critical ratio u/λ

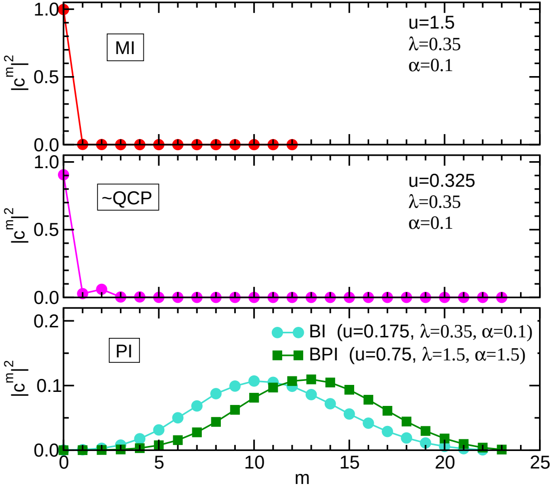


breaking of discrete symmetry



Phonon distribution

- Phonon "contribution" to the ground state?

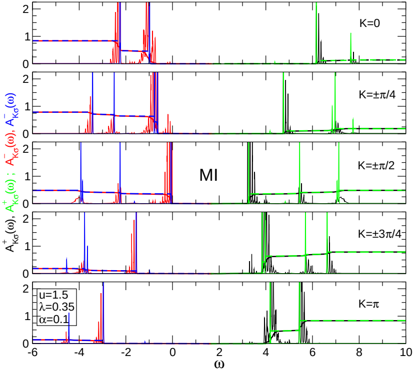


- MI: basically zero-phonon state (besides $Q = 0$ mode)
- QCP: increasing weight of multi-phonon states
- PI: Poisson-like distribution of phonons

Photoemission spectra I

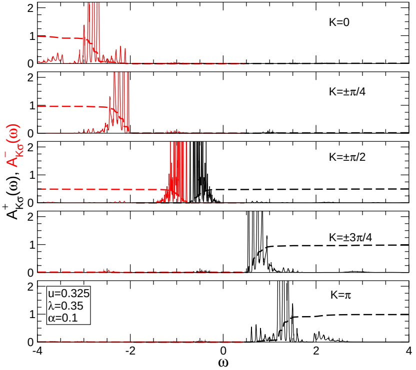
- Single-particle excitations?

Mott insulating regime $u/\lambda > 1$



- Mott-Hubbard correlation gap $\sim$ optical gap
- band renormalisation, phonon satellites
- "breather-like" excitations

Mott-to-Peierls transition $u/\lambda \simeq 1$

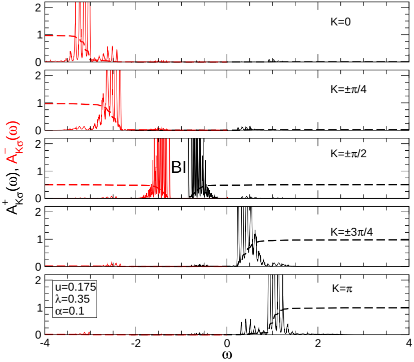


- gapless spin & charge excitations
- band width $\lesssim 4t$, broad (I)PE spectra
- uniform distribution of spectral weight

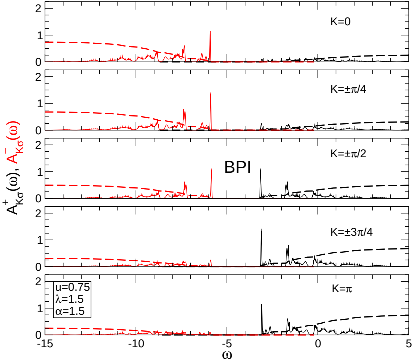
Photoemission spectra II

- CDW regime?

adiabatic case: $\alpha \ll 1$



anti-adiabatic case: $\alpha \gg 1$



- dispersion $\propto \epsilon_k$ + gap feature
- phonon softening: $\widetilde{\omega}_\pi \to 0$

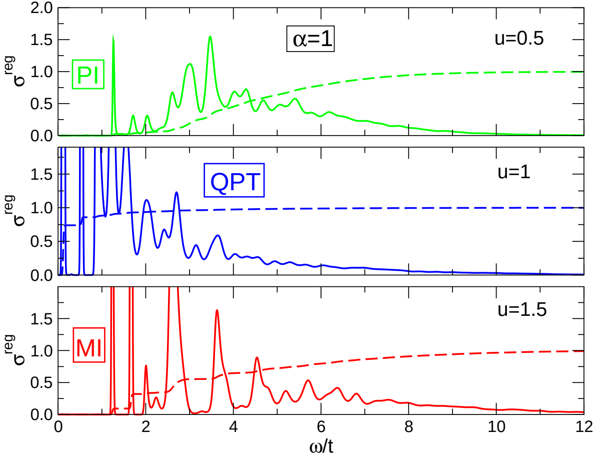
$\hookrightarrow$ "normal" Peierls band insulator

- low-weight dispersionless band
- + ordering

$\hookrightarrow$ polaronic superlattice

- Signatures of the PI-MI QPT in the optical conductivity?

  EP coupling fixed ($\lambda = 1$, $\alpha = 1$) – increasing Hubbard interaction:



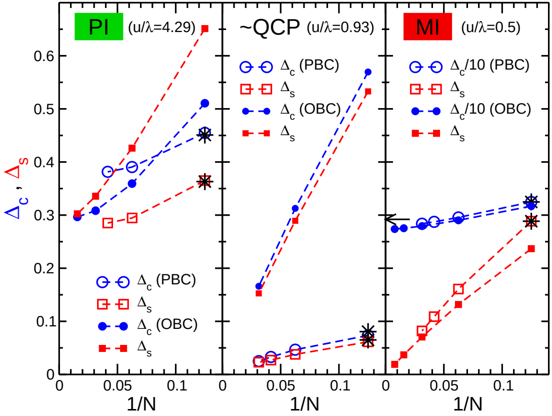
- $(u/\lambda)_c \rightsquigarrow$ optical gap $\Delta_{opt} = 0$, metal!? Drude-weight ill-defined!

Many-body excitation gaps

- Proof of spin-charge separation? $\rightsquigarrow$ DMRG finite-size scaling of

charge gap: $\boxed{\Delta_c = E_0^{(N_{el}+1)}(\tfrac{1}{2}) + E_0^{(N_{el}-1)}(-\tfrac{1}{2}) - 2E_0^{(N_{el})}(0)}$

spin gap: $\boxed{\Delta_s = E_0^{(N_{el})}(1) - E_0^{(N_{el})}(0)}$ (both including lattice relaxation!)



✓

- $(u/\lambda)_c$ – level crossing $\leftrightharpoons$ symmetry change?

  - HHM - invariant with respect to inversion at site i

    inversion symmetry (parity) operator: $\boxed{\hat{P} c_{i\sigma} \hat{P}^\dagger = c_{N-i\sigma}}$ $(i = 0, 1, \ldots, N-1)$

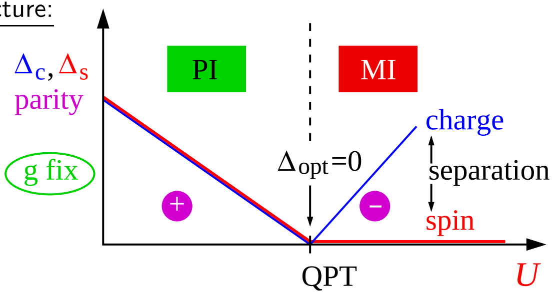
  - Hubbard model on finite lattices ($N = 4L$; PBC):

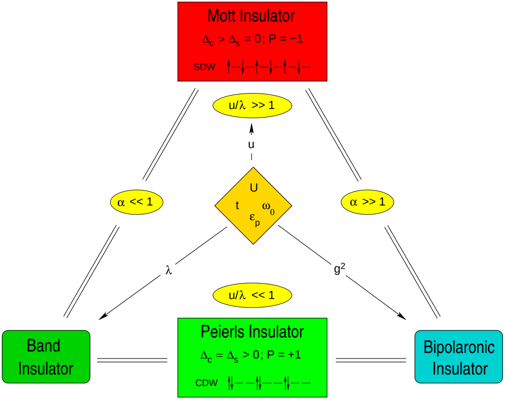
    $P=1$ for $U = 0$ & $P = -1$ $\forall U > 0$

  - Holstein Hubbard model: σ^{reg} points parity change out!

    $|\psi_0\rangle$ by ED $\rightsquigarrow$ $P=1$ for $U < U_c$!

physical picture:





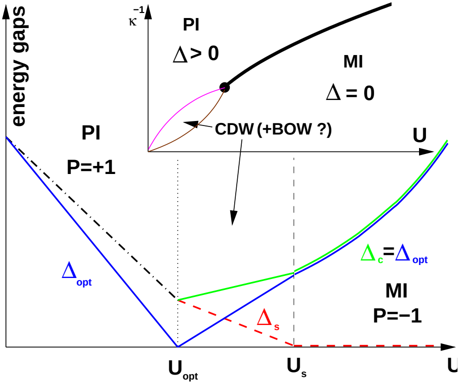
HF, Wellein, Hager, Weiße, Bishop: Phys. Rev. B 69 , 165115 (2004),. . .

Experimental relevance? $\rightsquigarrow$ quasi-1D MX solids (M=Pt,Pd,Ni - X=Cl,Br,I)!

- "Frozen phonons" $(\omega = 0)$?

$$\boxed{H_{t-U} - \sum_{i\sigma} \Delta_i n_{i\sigma} + \frac{K}{2} \sum_i \Delta_i^2}$$

schematic phase diagram:

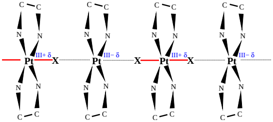


Maybe two (continuous) transitions at weak EP couplings !?

HF, Kampf, Sekania, Wellein, Eur. Phys. Jour. B 31, 11 (2003),...

Intrinsic localised vibrational modes

Pt-Cl MX-chain: CDW



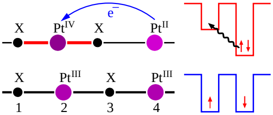
Peierls-Hubbard model

EP-coupling

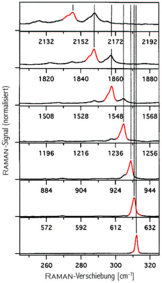
$$\propto \lambda_R (b_R + b_R^\dagger)(n_{e,2} - n_{e,4})$$

non-linear dynamics!

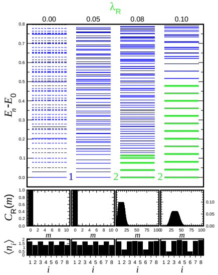
IVCT gap $\simeq$ 2.4 eV



resonance raman spectra



JADA diagonalisation



$\rightsquigarrow$redshift of overtones!

$$r_n = \frac{n\,\omega_R^{(1)} - \omega_R^{(n)}}{\omega_r^{(1)}}$$

n	$r_n^{\text{exp.}}$	$r_n^{\text{theo.}}$
2	0.4	0.4
3	1.1	1.1
4	2.4	2.5
5	4.6	4.7
6	7.7	7.5
7	11.6	11.2

✓

Swanson et al. PRL 82, 3288   HF et al PRB 63, 245121

“Message”

Strongly correlated electron-phonon systems

$\rightsquigarrow$ remarkable variety of

interesting physical phenomena & theoretical problems

$\hookrightarrow$ great challenge!

- numerical study of simplified (but generic) model Hamiltonians on finite lattices $\hookrightarrow$ powerful tool to address this field
- ground state and spectral properties of the 1D Holstein (Hubbard) model are understood to a large extent, but
- what about $0 < n < 1$ (including the spin degrees of freedom), $D > 1$, $T > 0$, ...?

There is still a lot of work to be done!