# 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 I: Polaron Formation – Self-Trapping Crossover

- Introduction
  - Motivation
  - Modelling
- Numerical approaches to the polaron problem
  - Exact diagonalisation & basis optimisation
  - Kernel polynomial method
  - Cluster perturbation theory
- Ground-state and spectral properties of Holstein polarons
  - Polaron formation
  - Dimensionality effects
  - Band dispersion
  - Electron-phonon correlations
  - Single particle spectral function
  - Phonon spectral function
  - Optical response

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

Polaronic effects in a great variety of (novel) materials:

- quasi-1D metals, MX chains, quantum spin-systems,...
- quasi-2D high-$T_c$ cuprates
- 3D charge-ordered nickelates
- colossal magneto-resistive manganites
- bulk novel semiconductors, excitonic insulators
- ...

Problem: Relevant energy scales are not well separated!

strongly correlated systems $\neq \sum$ weakly interacting parts
" the whole is greater than its parts"

$\hookrightarrow$ collective behaviour of electrons may be highly correlated on a macroscopic scale

$\hookrightarrow$ order phenomena and (spectacular) transport properties are intimately related

Challenge: Quantum dynamics of complex many-particle systems!

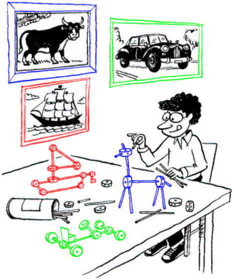
## Question

How to proceed?

physical system

$\Downarrow$

construction of minimal models



Dick Codor

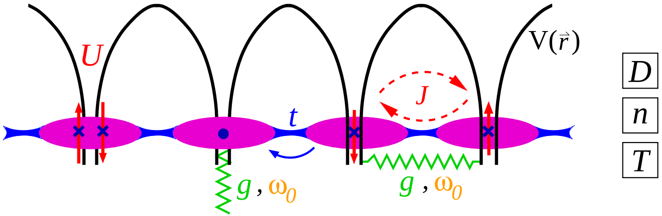
Hamiltonian

reliable theory and numerics

| ground state properties | thermodynamics, excitation spectra | dynamical correlation functions |
|---|---|---|
| $E_0$, $\|\psi_0\rangle$, $\langle\ldots\rangle_0$ | $E_n$, $Z$, $c_\nu$, ... | $\sigma(\omega)$, $\chi(q,\omega)$, ... |

$\hookrightarrow$ comparison with experiment

- Ingredients ?




$\hookrightarrow$ Interplay of charge, spin, orbital, and lattice degrees of freedom !

- Generic models? . . . **Holstein-Hubbard Hamiltonian**

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

- Problem: Not solvable even in 1D (also not for just one $e^-$ or at $n = 1$)!
- Approximations? Bad luck! “Standard” many-body techniques fail in most interesting cases... ☹

## Question

Way out?

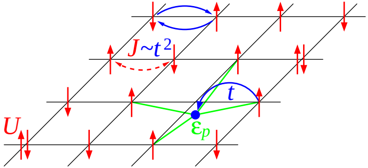
| Field Theory | (Statistical) DMFT | "Unbiased" Numerics |
|---|---|---|
| low D | high D | finite systems |

Here: Focus on numerical approaches...

- Exact Diagonalisation
  small systems, high energy resolution *but* thermodynamic limit?
- Density Matrix Renormalisation Group
  larger systems (1D) *but* dynamics, $T > 0$, 2D ...expensive!
- Quantum Monte Carlo
  large systems (1D-3D) *but* ..., very limited energy resolution (MaxEnt)!

# Hilbert Space

$\hookrightarrow$ Exact treatment of finite electron-phonon quantum systems:




Fermions: $4^N$ (Hubbard)

 $\rightarrow$ $3^N$ (t-J-model)

$n = 1$ $\rightarrow$ $2^N$ (Heisenberg)

Phonons: $D_p = \infty$ even for $1e^-$!

- boundary conditions: [anti] periodic ([A]PBC), open (OBC)
- symmetrized basis $(G(\vec{K}) = G_T \times G_L(\vec{K}) \times G_S)$ in the tensorial product Hilbert space of electrons and phonons:

$$\boxed{|b\rangle = \mathcal{P}_{\vec{K},rs}\{|e\rangle \otimes |p\rangle\}} \quad \text{with} \quad |e\rangle = \prod_{i=1}^{N} \prod_{\sigma=\uparrow,\downarrow} (c_{i\sigma}^{\dagger})^{n_{i\sigma,e}} |0\rangle_e$$

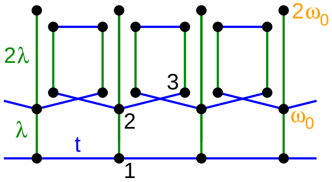
$$|p\rangle = \prod_{i=1}^{N} \frac{1}{\sqrt{m_{i,p}!}} (b_i^{\dagger})^{m_{i,p}} |0\rangle_p$$

$$n_{i\sigma,e} \in [0,1], \qquad e = 1, \ldots, D_e = \binom{N}{N_\sigma}\binom{N}{N_{-\sigma}},$$

$$m_{i,p} \in [0, \ldots, \infty], \; p = 1, \ldots, D_p = \infty$$

# Treatment of Phonons I

- unitary transformations (IMVLF)
  $\rightsquigarrow \Delta_i, \gamma, \tau^2$ (static displacement, polaron, squeezing effects)
  $\hookrightarrow$ average over transformed phonon vacuum $\rightsquigarrow H_e^{eff}$
  HF, Röder, Wellein, Mistriotis: PRB 51, 16582 ('95), ...
- "naive" Hilbert space truncation
  $|p\rangle$ with $m_p = \sum_{i=1}^{N} m_{i,p} \leqslant \widetilde{M} \rightsquigarrow D_p^{\widetilde{M}} = (\widetilde{M}+N)!/\widetilde{M}!N!$
  Bäuml, Wellein, HF: PRB 58, 3663 ('98), ...
- variational Hilbert space construction (VL)
  Ku, Trugman, Bonča: PRB 65, 174306 ('02), ...




basis:

$|1\rangle$ $e^-$ at site 0 with no phonon excitation
$|2\rangle$ $e^-$ and phonon at site 0
$|3\rangle$ $e^-$ at site 1 and one phonon at site 0

i.e., vertical bonds create or destroy phonons

generation $m$: act $m$ times with off-diagonal terms + all translations on an infinite lattice

# Treatment of Phonons II

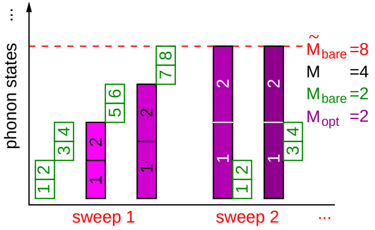
- phonon basis optimisation (density matrix based)

general state: $|\psi\rangle = \sum_{e=0}^{D_e-1} \sum_{p=0}^{D_p-1} C_{ep}^{\Psi}\{|e\rangle \otimes |p\rangle\}$

<u>idea:</u> construct optimised basis $|\tilde{p}\rangle = \sum_{p=0}^{D_p-1} \alpha_{p\tilde{p}}|p\rangle$ with $D_{\tilde{p}} < D_p$

by minimizing $\boxed{\| \, |\psi\rangle - |\tilde{\psi}\rangle \, \|^2 = 1 - \mathrm{Tr}\{\alpha\rho\alpha^\dagger\}}$ w. r. t. $\alpha$!

Weiße, HF, Wellein, Bishop: Phys. Rev. B 62, R747 (2000),. . .




<u>mixed phonon basis $\{|\mu\rangle\}$:</u>

$\{|\tilde{p}\rangle\}$, $1 \leqslant \mu \leqslant M_{opt}$; $\{|p\rangle\}$, $M_{opt} \leqslant \mu \leqslant M$

<u>sweep algorithm:</u>

(1) calculate $|\psi_n\rangle$ of H in terms of $\{|\mu\rangle\}$

(2) replace $\{|\tilde{p}\rangle\}$ with most important eigenstates of $\rho^{\psi}$

(3) change additional states $\{|p\rangle\}$ in the set $\{|\mu\rangle\}$

(4) orthonormalize $\{|\mu\rangle\}$ and return to (1)

What remains? Diagonalisation of large sparse Hermitian matrices!

- iterative subspace methods:

  (1) matrix $A \in \mathbb{R}^n \to$ projection on subspace $\bar{A}^k \in \mathbb{V}^k$ $(k \ll n)$

  (2) solution of eigenvalue problem in $\mathbb{V}^k$ using standard routines

  (3) extension of subspace $\mathbb{V}^k \to \mathbb{V}^{k+1}$ by $\vec{t} \perp \mathbb{V}^k \to$ (2)

  $\rightsquigarrow$ sequence of approximative inverses of problem matrix $A$

  - Lanczos (ED) technique: $H^D \to T^L$ Krylov subspaces $\rightsquigarrow$ $E_0$ , $|\psi_0\rangle$
    fast convergence for extremal eigenvalues ($D \lesssim 10^{11}$, $L = 100 \rightsquigarrow \Delta E_0 \lesssim 10^{-9}$)!
  - Jacobi Davidson algorithm $\rightsquigarrow$ $E_n$ , $|\psi_n\rangle$, up to $n \lesssim 30$ for $D \lesssim 10^7$

  $\Rightarrow$ basic computational requirement:

  highly efficient (parallel) matrix-vector multiplication

  make use of supercomputers!

$\hookrightarrow$ ground state, static correlation functions,. . . ☺, *but* what about dynamics?

# Kernel Polynomial Method I

Spectral properties at T=0?

$$A^{\mathcal{O}}(\omega) = -\frac{1}{\pi}\lim_{\eta\to 0}\left\langle \psi_0 \left| \mathcal{O}^{\dagger} \frac{1}{\omega - H + E_0 + i\eta} \mathcal{O} \right| \psi_0 \right\rangle = \sum_n |\langle \psi_n|\mathcal{O}|\psi_0\rangle|^2 \delta[\omega - (E_n - E_0)]$$

complete spectrum !?

Way out: Kernel Polynomial & Maximum Entropy Methods

(1) expansion of $\delta[\ldots]$ – series in Chebyshev polynomials $T_m(x)$:

$$A^{\mathcal{O}}(x) = \frac{1}{\pi\sqrt{1-x^2}}\left(\mu_0^{\mathcal{O}} + 2\sum_{m=1}^{M=\infty} \mu_m^{\mathcal{O}} T_m(x)\right)$$

(2) determination of moments: $\mu_m^{\mathcal{O}} = \int_{-1}^{1} dx\, T_m(x) A^{\mathcal{O}}(x) = \langle \psi_0|\mathcal{O}^{\dagger} T_m(X)\mathcal{O}|\psi_0\rangle$

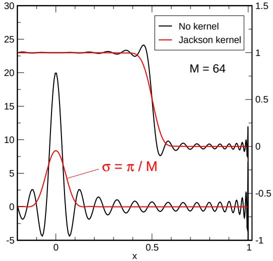
by iterative MVM, where $X = (H - b)/a$, i.e. $E_n \in [-1, 1]$ and $M < \infty$

(3) (FFT) reconstruction of $A^{\mathcal{O}}(x)$ from $M$ moments via linear approximation (KPM) or nonlinear optimisation procedure (MEM)

# Kernel Polynomial Method II

- problem: Gibbs oscillations,
  M finite $\rightsquigarrow$ truncation errors!

  solution: damping factors,
  e.g., Jackson or Lorentz kernels




- advantages of KPM:

| uniform reconstruction of spectra – gap features | high-resolution applications | CPU-time ($\propto$ MD) "trace" – average over $|r\rangle$ |
|---|---|---|

- recent improvements:

  generalisation to multivariate case $\rightsquigarrow$ calculation of finite-temperature (dynamical) correlation functions

  combination with other techniques
  (Cluster Perturbation Theory, Monte Carlo, . . .)

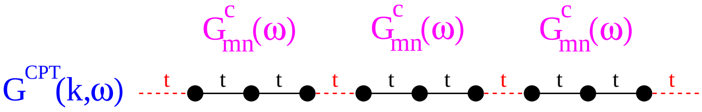
  Weiße, Wellein, Alvermann, HF: cond-mat/0504627 (review, many applications)

# KPM *vs* Lanczos recursion

| | Chebyshev | Lanczos |
|---|---|---|
| recursion | $\|\phi_0\rangle = \mathcal{O}\|0\rangle,\ \|\phi_1\rangle = \widetilde{H}\|\phi_0\rangle,\ \mu_0 = \langle\phi_0\|\phi_0\rangle$ <br> $\|\phi_{n+1}\rangle = 2\widetilde{H}\|\phi_n\rangle - \|\phi_{n-1}\rangle$ <br> $\mu_{2n+2} = 2\langle\phi_{n+1}\|\phi_{n+1}\rangle - \mu_0$ <br> $\mu_{2n+1} = 2\langle\phi_{n+1}\|\phi_n\rangle - \mu_1$ <br> • very stable $O(MD)$ <br> $M$ moments | $\|\phi_0\rangle = \mathcal{O}\|0\rangle/\beta_0,\ \beta_0 = [\langle 0\|\mathcal{O}^\dagger\mathcal{O}\ \|0\rangle]^{(1/2)}$ <br> $\|\widetilde{\phi}\rangle = H\|\phi_n\rangle - \beta_n\|\phi_{n-1}\rangle,\ \alpha_n = \langle\phi_n\|\widetilde{\phi}\rangle$ <br> $\|\widetilde{\phi}\rangle = \|\widetilde{\phi}\rangle - \alpha_n\|\phi_n\rangle,\ \beta_{n+1} = [\langle\widetilde{\phi}\|\widetilde{\phi}\rangle]^{(1/2)}$ <br> $\|\phi_{n+1}\rangle = \|\widetilde{\phi}\rangle/\beta_{n+1}$ <br> • tends to lose orthogonality <br> $O(MD)$ - $M$ MVM |
| reconstruction | Apply kernel : $\widetilde{\mu}_n = g_n\mu_n$ <br> FFT : $\widetilde{\mu}_n \to \widetilde{f}(\widetilde{\omega}_i)$ <br> Rescale : $f(\omega_i) = \dfrac{\widetilde{f}[(\omega_i - b)/a]}{\pi\sqrt{a^2 - (\omega_i - b)^2}}$ <br> • procedure is linear in $\mu_n$ <br> • $O(P\log(P))$ for $P$ points $\omega_i$ <br> • well defined resolution $\propto 1/M$ | $f(z) = -\dfrac{1}{\pi}\mathrm{Im}\dfrac{\beta_0^2}{z - \alpha_0 - \dfrac{\beta_1^2}{z-\alpha_1-\frac{\beta_2^2}{z-\alpha_2-\dots}}}$ <br> where $z = \omega_i + i\epsilon$ <br> • procedure is not linear in $\alpha_n$, $\beta_n$ <br> • $O(PM)$ for $P$ points $\omega_i$ <br> • $\epsilon$ somewhat arbitrary |

# Cluster Perturbation Theory

- Green function $G(k,\omega)$ on infinite lattice $(N=\infty)$?




- We have: Green function $G^{c}_{mn}(\omega)$ on finite cluster(s) of $N_c$ sites (OBC) !
- 1st order perturbation in $V = \sum - \overset{t}{-} -$

$$G^{(1)}_{ij}(\omega) = G^{c}_{ij}(\omega) + \sum_{rs} G^{c}_{ir}(\omega) V_{rs} G^{(1)}_{sj}(\omega)$$

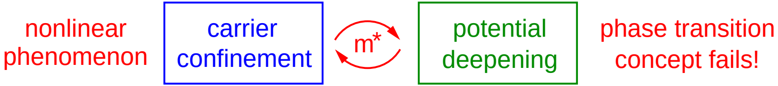
$$G^{(1)}_{mn}(K,\omega) = \left( \frac{G^{c}(\omega)}{1 - V(K) G^{c}(\omega)} \right)_{mn} \qquad (K = N_c k)$$

- Fourier transform: $G^{CPT}(k,\omega) = \frac{1}{N_c} \sum_{m,n=1}^{N_c} G^{CPT}_{mn}(K,\omega) e^{-ik\cdot(m-n)}$

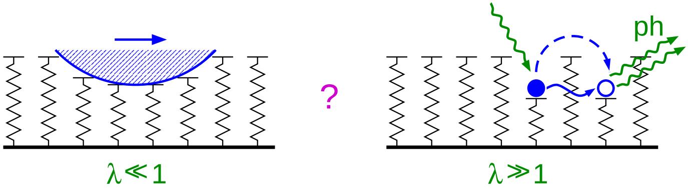
# Polaron Problem I

Questions:

- Polaron formation: Nature of "self-trapping" transition?




- Crossover regime: Polaron transport?




- Influence of dimensionality? ...

# Polaron Problem II

Simplest case: Single electron Holstein model

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

Physics is governed by two parameter ratios:

- phonon frequency *vs* electron transfer amplitude $\alpha = \omega_0 / t$
  - $\rightsquigarrow$ retardation effects
  - $\rightsquigarrow$ adiabatic regime ($\alpha \ll 1$) $\Leftrightarrow$ anti-adiabatic regime ($\alpha \gg 1$)
- EP interaction: $\lambda = \varepsilon_p / 2Dt$ or $g^2 = \varepsilon_p / \omega_0$ $\quad \varepsilon_p$ – polaron binding energy
  - $\rightsquigarrow$ weak- ($\lambda \ll 1$) $\Leftrightarrow$ strong-coupling ($\lambda \gg 1$) regime
  - $\rightsquigarrow$ few- ($g^2 < 1$) $\Leftrightarrow$ multi-phonon ($g^2 \gg 1$) regime

Focus on:

A. Ground-state properties

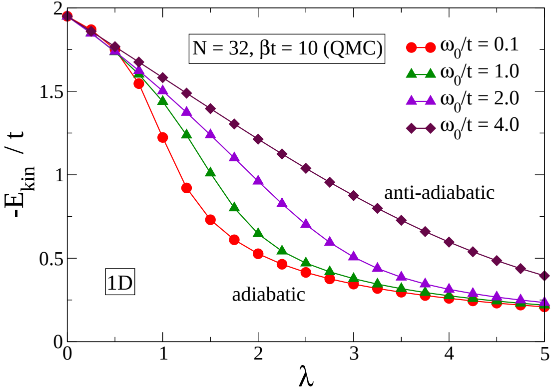
B. Spectral properties

Most interesting: Intermediate frequency and coupling regime!

# Kinetic Energy

- Mobility of an electron?

$$E_{kin} = -t \sum_{\langle ij \rangle} \langle (c_i^\dagger c_j + \mathrm{H.c.}) \rangle$$



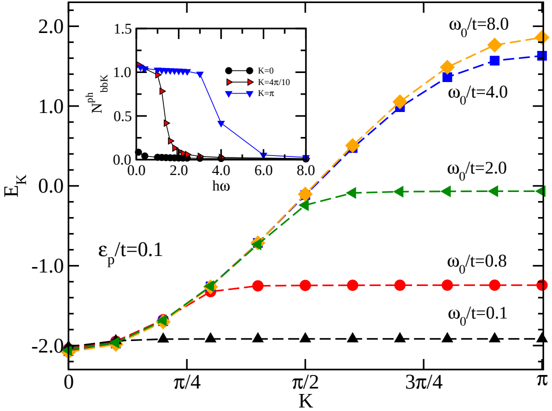

- $E_{kin}$ is suppressed by EP coupling
- rather smooth decay in the anti-adiabatic regime
- $\omega_0/t < 1 \rightsquigarrow \exists\, \lambda_c \sim 1$

  $\hookrightarrow$ polaron formation

. . . , Hohenadler, Evertz, von der Linden: Phys. Rev. B 69, 024301 (2004),. . .

- Band description?

  (i) weak coupling case:




Wellein, HF: Phys. Rev. B 56, 4513 (1997)

1D, N=20, ED:

- main panel:

  band dispersion $E_K$

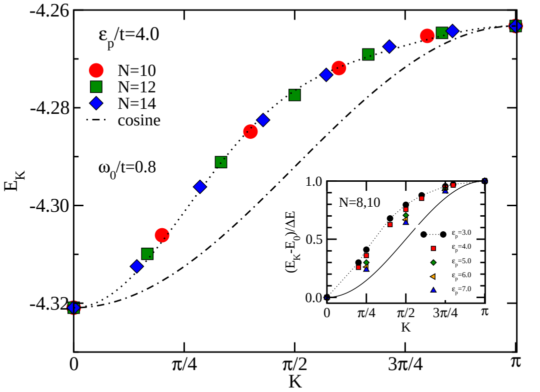
  - nearly unaffected cosine near $K = 0$
  - phonon intersects at $\omega_0$

  $\rightsquigarrow$ "flattening" near $K = \pi$

- inset:

  $N_K^{ph} = \sum_i \langle \psi_{0,K} | b_i^\dagger b_i | \psi_{0,K} \rangle$

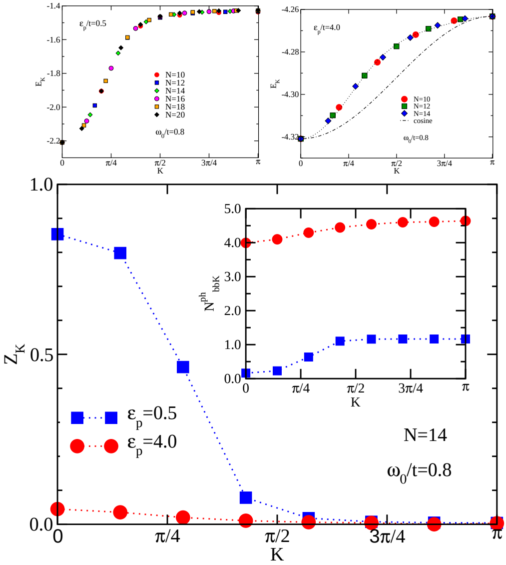
(ii) strong coupling case:




- well separated quasi-particle band: "coherent" bandwidth $4t \gg \Delta E_K \gtrsim 10\Delta E_K^{(LF)}$ $\Delta E_K^{(LF)} = 4Dt\exp[-g^2]$
- deviation from rescaled cosine: EP coupling induces longer ranged hopping processes
- inset: $\lambda \gg 1 \rightarrow$ LF result

$\hookrightarrow$ small polaron $\leftrightharpoons$ (still) itinerant quasi-particle at T=0!

2D case: HF, Loos, Wellein: Z. Phys. B 104 (1997)




single-particle spectral function:

$$A_K(E) = \sum_n |\langle \psi^{(1)}_{n,K} | c^\dagger_K | 0 \rangle|^2 \, \delta(E - E^{(1)}_n)$$

$\hookrightarrow$ K-resolved spectral weight

$$Z^{(c)}_K = |\langle \psi^{(1)}_{0,K} | c^\dagger_K | 0 \rangle|^2$$

- weak coupling:

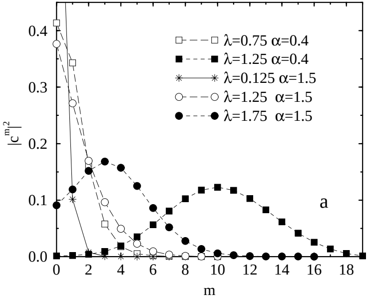
  $Z^{(c)}_K \lesssim 1$ near band centre
  $\Leftrightarrow$ “electronic” QP
  $Z^{(c)}_K \ll 1$ near band edge
  $\Leftrightarrow$ “phononic” QP

- strong coupling:

  $Z^{(c)}_K \ll 1 \; \forall \; K$
  $\Leftrightarrow$ “polaronic” QP

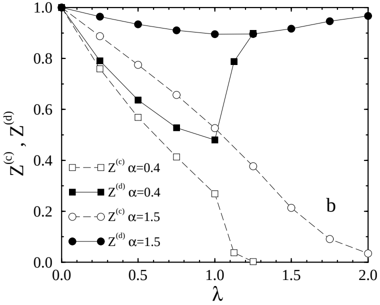
# Phonon distribution - QP weight

- Weight of the m-phonon state in the ground state $|c^m|^2(\widetilde{M})$:




- Construction of QP operators?

$$d^\dagger_{\vec{K}} = \sqrt{\frac{1}{N}} \sum_{i=1}^{N} e^{i\vec{K}\vec{R}_i} c^\dagger_i \sum_{m=0}^{\widetilde{M}} \sqrt{\frac{|c^m(\widetilde{M})|^2}{m!}} \left(b^\dagger_i\right)^m$$



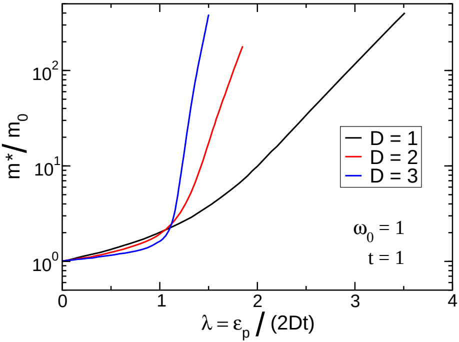

- $\lambda \gg 1, g^2 \gg 1 \rightsquigarrow$ importance of multi-phonon states
- "correct" polaron operators (d) $\rightsquigarrow$ quasi-particle weight $Z^{(d)}_{\vec{K}=0} \to 1$

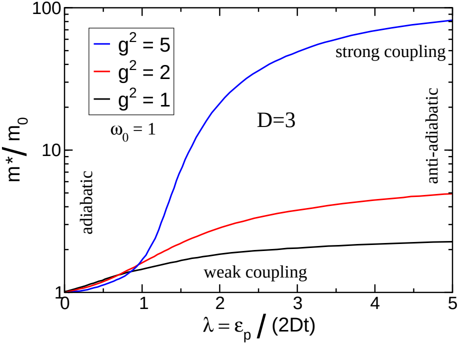
HF, Loos, Wellein: Z. Phys. B 104 (1997)

2D HM (N=10, K=0)

- Mass renormalisation? $1/m^* = \partial^2 E_{\vec{K}} / \partial \vec{K}^2|_{|\vec{K}| \to 0}$

(note that $[m^*]^{-1}$ differs from $Z_{\vec{K}=0}$ by the $\vec{K}$ dependence of the self-energy)




- polaron crossover at about $\lambda \sim 1$ ($g^2 \sim 1$) is much sharper in higher D !
- crossover region: $(m_0/m^* - Z_0)/Z_0 \lesssim 20\%$ (2 %) in 1D (3D) !

(SCPT: $Z^{(c)}_{K=0} = m_0/m^* = \exp[-g^2]$)

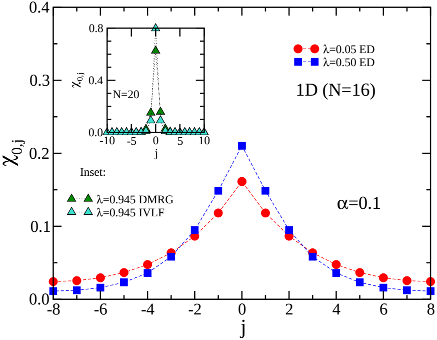
Ku, Trugman, Bonča: PRB 65, 174306 ('02) (agreement with DMFT? sc case ✓)

# Electron-Lattice Correlations I

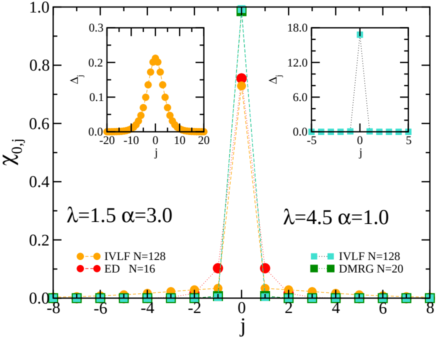
- Spatial extension of polarons?

$$\chi_{0,j} = \frac{\langle n_0 (b^\dagger_{0+j} + b_{0+j}) \rangle}{2g \langle n_0 \rangle}$$

weak coupling - adiabatic




strong coupling - non-adiabatic



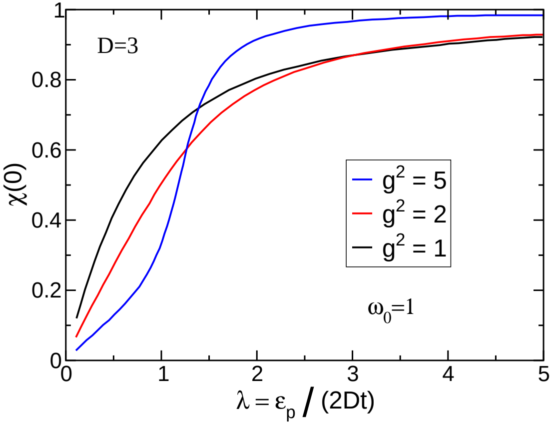

- crossover from large to small size polarons (1D)
- static displacement fields: $\Delta_i = \Delta_0 \operatorname{sech}^2[\lambda_{eff}\, i]$

Wellein, HF: PRB 58, 6208 (1998)

# Electron-Lattice Correlations II

- On-site electron-phonon correlation?

$$\chi(0) = \langle \psi_0 | n_0 (b_0^\dagger + b_0) | \psi_0 \rangle$$




$\hookrightarrow$ strong enhancement of $\chi(0)$ at the polaron "transition"!

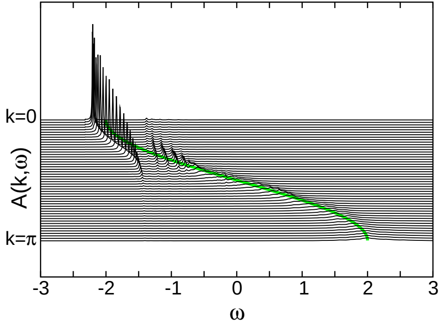
# Electron spectral function

- Inverse photoemission spectra? $\boxed{A(k,\omega) = -\frac{1}{\pi}\text{Im}\langle 0|c_k R c_k^\dagger|0\rangle}$

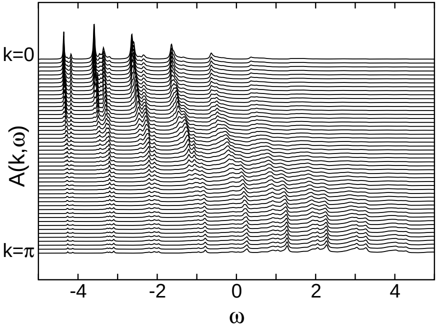
$R = [\omega - (H - E_0)]^{-1}$ (resolvent); transitions between different particle sectors

very recent CPT+KPM results ($N_c^{max} = 16$, $\widetilde{M}^{max} = 25, M = 2048$):

weak-coupling ($\lambda = 0.25$, $\alpha = 0.8$)




strong-coupling ($\lambda = 2$, $\alpha = 1.0$)

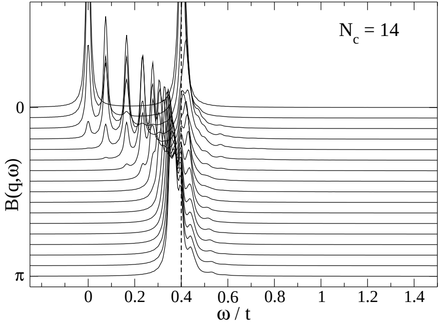



pronounced QP peak $\rightarrow$ intersection of phonon $\rightarrow$ broad incoherent feature

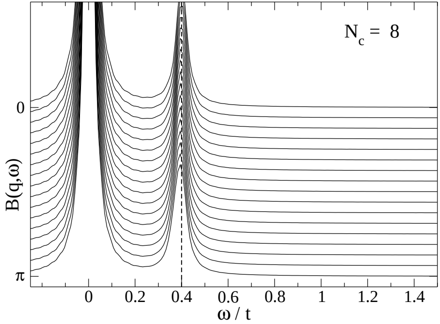
small polaron QP $\rightarrow$ sequence of absorption bands separated by $\omega_0$

- Phonon spectra? $B(q,\omega) = -\frac{1}{\pi}\mathrm{Im}\langle\psi_0^{(1)}|(b_q + b_q^\dagger)\, R\,(b_{-q} + b_{-q}^\dagger)|\psi_0^{(1)}\rangle$

weak-coupling ($\lambda = 0.5,\ \alpha = 0.4$)




strong-coupling ($\lambda = 2,\ \alpha = 0.4$)




signature of weakly dressed electron & flattening effect

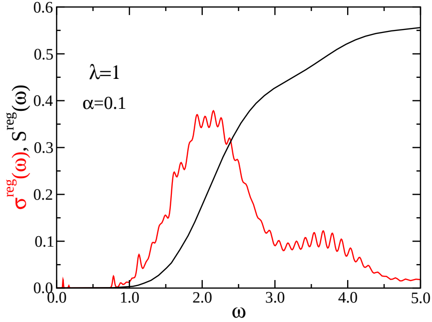
signature of dispersionless small polaron & bare phonon excitation

- Optical conductivity? $\sigma^{reg}(\omega) = \frac{\pi}{N} \sum_{m \neq 0} \frac{|\langle \psi_0 | \hat{\jmath} | \psi_m \rangle|^2}{E_m - E_0} \delta[\omega - (E_m - E_0)]$

current operator $\hat{\jmath} = i\, e t \sum_i (c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i)$ connects different parity sectors

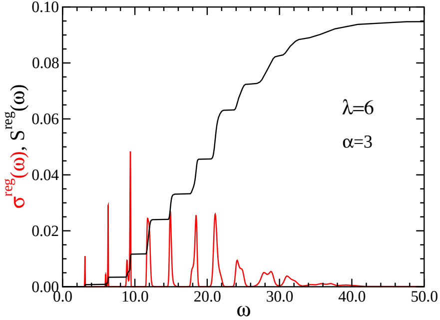
integrated spectral weight: $S^{reg}(\omega) = \int_0^\infty d\omega' \sigma^{reg}(\omega')$

intermediate coupling - adiabatic




asymmetric line-shape

strong coupling - anti-adiabatic



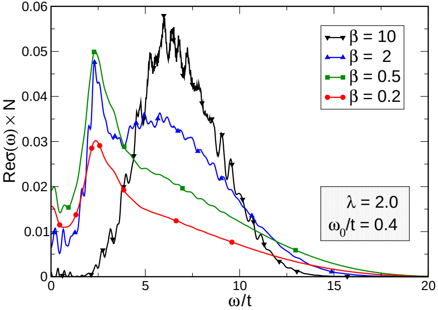

$\sim$ symmetric absorption maximum $\lesssim 2\varepsilon_p/t$

- Thermally activated transport in polaronic systems?

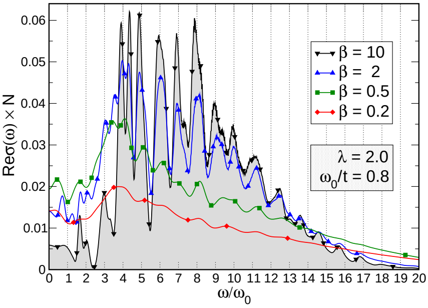
$$\mathrm{Re}\sigma(\omega) = \frac{\pi}{NZ}\sum_{m,n}^{\infty} \frac{e^{-\beta E_n} - e^{-\beta E_m}}{E_m - E_n} |\langle n|\hat{\jmath}|m\rangle|^2 \, \delta(\omega - (E_m - E_n))$$

$\hookrightarrow$ application of 2D KPM - Schubert, Wellein, Weiße, HF: cond-mat/0505447

strong-coupling adiabatic




non-adiabatic



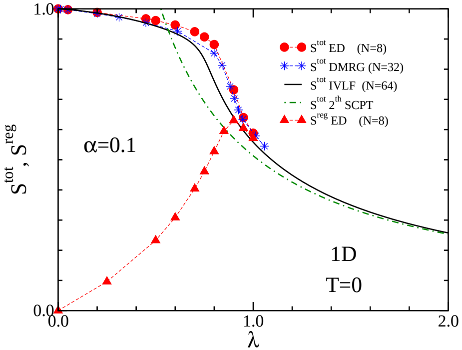

coherent transport strongly suppressed T $\nearrow$

2t-feature – "adiabatic" barrier $\sim \varepsilon_p/2 - t$

pronounced sub-band transitions

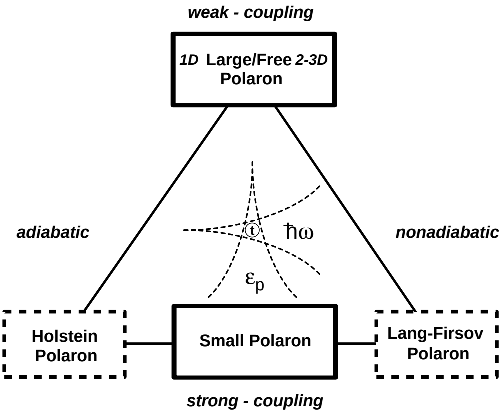
$\Leftrightarrow$ multi-phonon absorption/emission

- Sum rules? Decomposition of $\mathrm{Re}\sigma(\omega) = D\delta(\omega) + \sigma^{reg}(\omega)$ (D - Drude weight)!
  - $\int_0^\infty \omega \mathrm{Re}\sigma(\omega) d\omega = \frac{\pi e^2}{N} \langle 0|\hat{j}^2|0\rangle$ ✓
  - $-\frac{E_{kin}}{2} = S^{tot} = \frac{D}{2\pi e^2} + S^{reg}(\infty)$




crossover regime ⇋ regular part of $\mathrm{Re}\sigma(\omega)$ strongly enhanced!

- Schematic "phase" diagram of the single-electron Holstein model:




open questions: disorder, finite density, correlations. . . ? $\rightsquigarrow$ next talk!