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 II: Disorder, Correlation, and Finite-Density Effects

- Anderson localisation of polarons
  - Local distribution approach
  - Statistical DMFT
  - Holstein & Anderson regimes
  - Phase diagram
- Influence of electron correlations on polaron formation
  - (Jahn-Teller) polaron effects in CMR manganites
  - Hole-polarons in high-T_c cuprates
  - Bipolarons
- Polaron formation at finite carrier densities
  - Weak- and strong-coupling limits
  - Photoemission spectra and DOS of many-polaron systems (ic case)
  - Density-driven polaron-to-metal transition

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

Part I: Anderson localisation of polarons

motivation:

disorder "localisation"	$\rightleftharpoons$	EP coupling "self-trapping"

- quantum interference *vs* inelastic e^--ph scattering ?
- material imperfections *vs* itinerant polaron states ?
- transport properties, hopping conductivity $(T > 0)$?

problem: motion of a single e^- in a disordered deformable medium ...

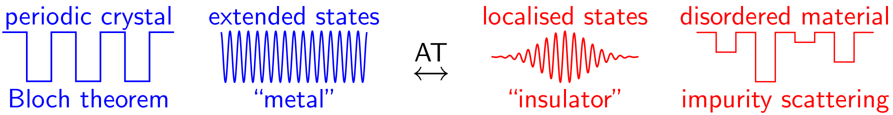
generic model:

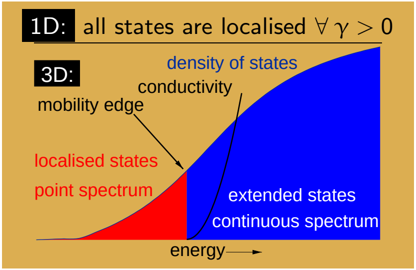
$$H = \sum_i \epsilon_i n_i - t \sum_{\langle i,j \rangle} c_i^\dagger c_j - g\,\omega_0 \sum_i (b_i^\dagger + b_i) n_i + \omega_0 \sum_i b_i^\dagger b_i$$

$$p(\epsilon_i) = \frac{1}{\gamma}\,\theta\left(\frac{\gamma}{2} - |\epsilon_i|\right)$$

Anderson Holstein Hamiltonian

Anderson localisation in a nutshell





Problem: Calculating quantities which characterise the localisation transition,

$|\psi(r)| \propto e^{-r/\lambda}$,

$\sigma_{dc} \propto \mathrm{Tr}[\hat{v}\,\mathrm{Im}\{\hat{G}\}\,\hat{v}\,\mathrm{Im}\{\hat{G}\}]$,

$P_{ij}(t \to \infty) \propto |\hat{G}^R_{ij}|^2, \ldots$

is an extremely difficult task, especially in the presence of interactions!

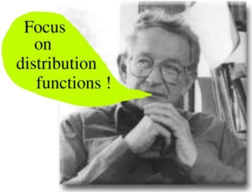
All simple attempts give diffusion!

Alice: "In our country… you'd generally get to somewhere else if you ran very fast for a long time as we've been doing."

Queen: "A slow sort of country! Now here, you see, it takes all the running you can do, to keep in the same place."

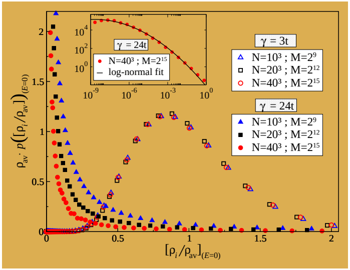
- How to proceed?

Most mean values, e.g. $\langle \text{DOS} \rangle$, contain almost no information about AT!



- LDOS: $\rho_i = \sum_{n=1}^{N} |\psi_n(\mathbf{r}_i)|^2 \delta(E - E_n)$
  - obtained efficiently by KPM
  - random sample generation $\rightsquigarrow p(\rho_i)$
  - distribution $p(\rho_i)$ critical at AT
  - $\gamma \nearrow$: normal $\rightarrow$ log-normal $\rightarrow$ singular

LDOS distribution density for $E = 0$:



- Characterisation of the distribution?

arithmetic mean $\rho_{av} = \langle \rho_i \rangle$ inappropriate
geometric mean $\rho_{ty} = \exp\langle \ln \rho_i \rangle$ suitable

$$\langle \ldots \rangle = \frac{1}{K_r K_s} \sum_{\text{samples}}^{K_r} \sum_{\text{sites}}^{K_s} \ldots$$

⇐ 3D simple cubic lattice:
typical values: $K_r \times K_s = 10^4 \times 100$

Statistical DMFT

- Localisation problem necessitates treatment of very large systems !?

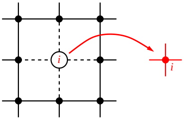
⤳ analytical approach: statistical Dynamical Mean Field Theory

probabilistic method based on the self-consistent construction of random samples for the distribution function of local physical quantities!

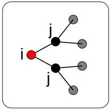
⤳ basic idea: mapping of the original model → ensemble of Anderson impurity models, where spatial fluctuations of, e.g., LDOS are taken into account by AAT but interaction is treated by DMFT (i.e. within $D = \infty$ approximation)!

Abou-Chacra, Anderson, Thouless: J. Phys. C 6, 1734 (1973)
Dobrosavljevič, Kotliar: Phys. Rev. Lett. 78, 3943 (1998)

cavity method



Bethe lattice



$t \to \tilde{t}/\sqrt{K}$

$$G_{ii}(z) = \left[z - \epsilon_i - \frac{\tilde{t}^2}{K} \sum_{j}^{K+1} G_{jj}^{(i)}(z) - \Sigma_{ii}(z) \right]^{-1}$$

$$\Sigma_{ii}(z) = \mathrm{CFE}\left[\varepsilon_p p\omega_0, z - \epsilon_i - p\omega_0, G_{jj}^{(i)}(z - p\omega_0) \right]$$

for details see: Bronold, Alvermann, HF: Phil. Mag. 84, 673 (2004)

Localisation criterion

- Self-consistent scheme?

(i) reinterpret the equations as self-consistency equations for random variables

$$G_{jj}^{(i)}(z - p\omega_0) = \text{function}[K \cdot \epsilon_j{}'s, K \cdot G_{jj}^{(i)}(z - \bar{p}\omega_0)'s, \ldots] \text{ with } p \leqslant \bar{p} \leqslant \widetilde{M}$$

(ii) solve the complicated stochastic recursion scheme for $N \times \widetilde{M}$ variables

$G_{jj}^{(i)}(z - p\omega_0)\ \forall\ z = \omega + i\eta$ by Monte Carlo sampling!

(typical array: # of sites $N = 50\,000$, # of virtual phonons $\widetilde{M} = 50$)

(iii) first row ($p = 0$) $\rightsquigarrow$ probability distribution of LDOS $p(\rho_i(\omega))$

Of course, dealing with distributions is a bit "unhandy";
LDOS distribution becomes singular at the AT! ☹

- Order parameter?

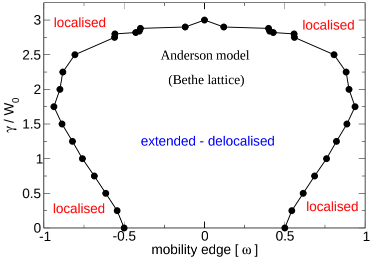
Anderson: Focus on typical quantities! $\rightsquigarrow$ possible localisation criterion

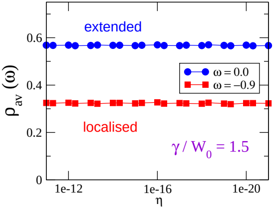
$$\boxed{\rho_{ty}(\omega) \to 0} \quad \text{while} \quad \boxed{\rho_{av}(\omega) > 0} \quad ?!$$

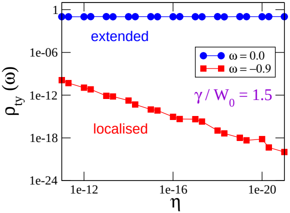
Order parameter

important point: limit $\eta \to 0$ has to be performed (numerically) in order to distinguish between extended & localised states!

phase diagram







(note the logarithmic scale!)

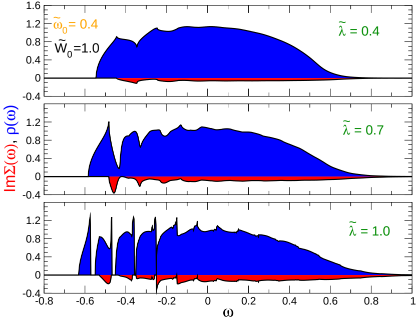
$\hookrightarrow$ $\rho_{ty} \to 0$ at $\gamma_c(\omega)$ – ρ_{ty} acts as a kind of order parameter ☺ !

DMFT DESCRIPTION

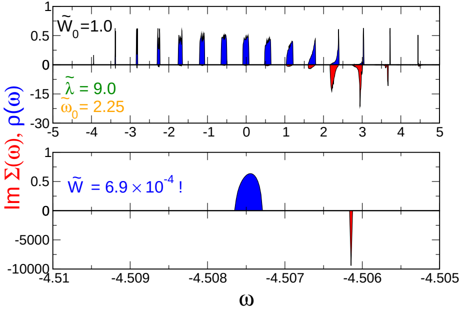
- Does DMFT capture main aspects of polaron physics? $D = \infty$?!

DOS, Bethe lattice with $K = 2$; no disorder ($\gamma \equiv 0$):

weak-to-intermediate coupling – adiabatic



strong coupling – anti-adiabatic



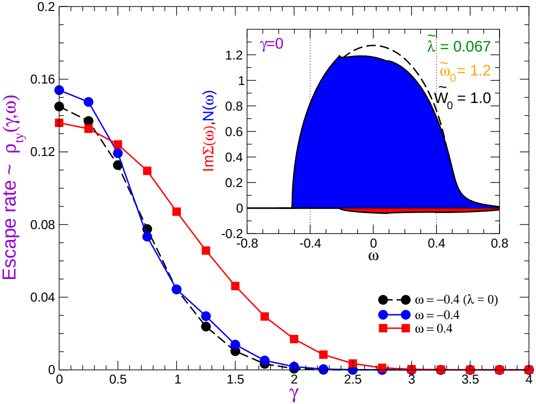
$\hookrightarrow$ polaron band formation, flattening, ... ✓

Escape rate I

- Measure for the itinerancy of a polaron state?

↪ tunnelling (escape) rate from a given site i:

(i) Weak EP coupling:

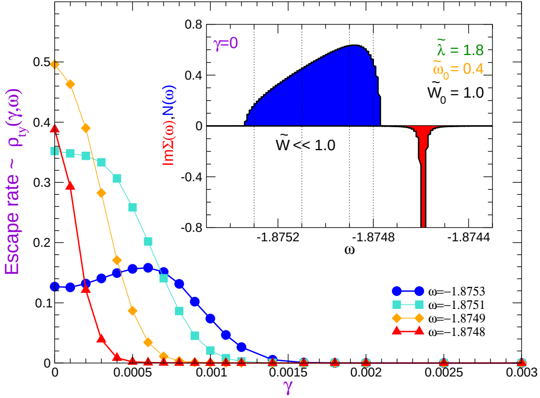


- different behaviour for energies below and above the optical phonon emission threshold!
- quantum interference needed for localisation is significantly suppressed by inelastic EP scattering!

↪ nontrivial interplay $\lambda \rightleftharpoons \gamma$

(ii) Strong EP coupling adiabatic regime:

rather "mobile" ("sluggish") states exist at the bottom (top) of the sub-band!



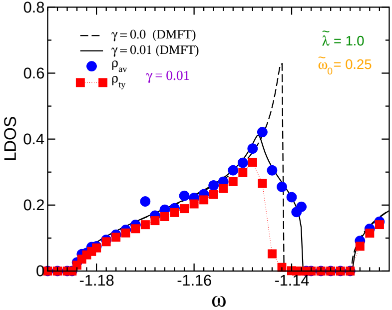
- $\widetilde{W} \ll \widetilde{W}_0 \rightsquigarrow$ extremely weak disorder leads to localisation!
- now the bottom states determine the critical disorder strength:

  $$(\gamma_c/\widetilde{W}) > (\gamma_c/\widetilde{W}_0)$$

↪ In this sense the adiabatic Holstein polaron is more difficult to localise than a bare electron!

Local density of states

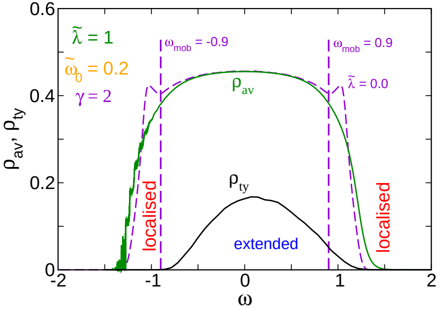
Holstein regime ("$\gamma \ll \widetilde{W}$")



- flattening strongly affects upper mobility edge

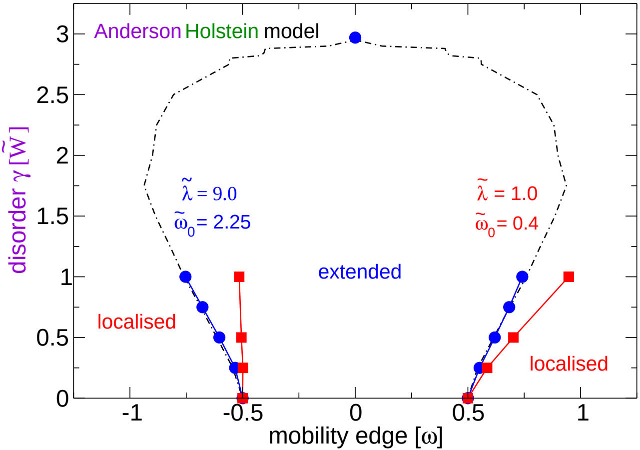
  disorder weakens band repulsion

Anderson regime ("$\gamma \gg W_0$")



- strongly localised polaron defect states at deep impurities

  $\rightsquigarrow$ independent boson model



- adiabatic weak-to-strong coupling regime: asymmetric mobility edges
- anti-adiabatic strong coupling regime: “internal polaron structure” irrelevant

Part II: Correlation Effects

so far: charge - lattice interaction

What about the interplay with other degrees of freedom?

spin - orbital

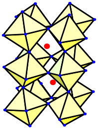
(escpecially important at finite n!)

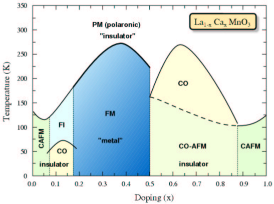
Polaronic effects in CMR manganites

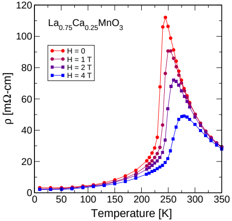
- What is interesting about manganites?

Mixed-valence manganese oxides $R_{1-x}A_xMnO_3$

(R = La, Pr, Nd ; A = Ca, Sr, Ba) $[R^{3+}Mn^{3+}, A^{2+}Mn^{4+}]$



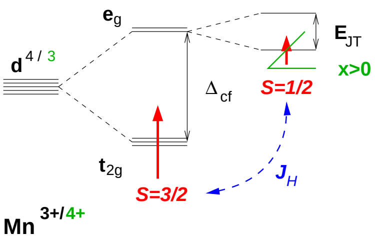




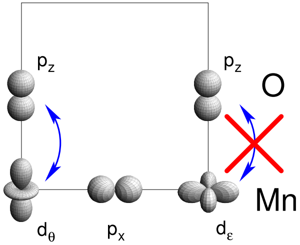
- colossal negative magneto-resistance near $T_c \rightsquigarrow$ enormous technological potential (sensors, spintronics)
- rich electronic, magnetic & structural phase diagram
- strong electron-phonon correlations
- relevance of orbital degrees of freedom

$\hookrightarrow$ challenge for solid state theory!

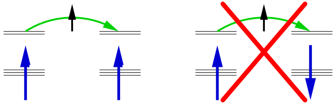
- electronic structure ($U \gg 1$)



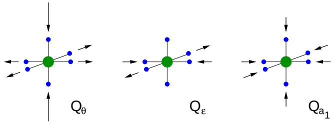
- orbitals (anisotropic hopping)



- ferromagnetic double exchange ($J_h > 1$)



- phonons (JT & breathing)



Weiße, HF: New. J. Phys. (Focus Review), 6, 158 (2004)

$$H = \sum_{i,\delta} R_\delta \left(H^{1,z}_{i,i+\delta} + H^{2,z}_{i,i+\delta} \right) + H^{ep}$$

$$H^{1,z}_{i,j} = -\frac{t}{4}\left(a_{i,\uparrow} a^\dagger_{j,\uparrow} + a_{i,\downarrow} a^\dagger_{j,\downarrow} \right) d^\dagger_{i,\theta} n_{i,\varepsilon} d_{j,\theta} n_{j,\varepsilon} + \text{H.c.} \quad \propto \text{doubleexchange}$$

$$\begin{aligned} H^{2,z}_{i,j} = {} & t^2 \frac{\vec{S}_i \vec{S}_j - 4}{8} \left[\frac{(4U + J_h) P^\varepsilon_i P^\theta_j}{5U(U + \frac{2}{3} J_h)} + \frac{(U + 2J_h) P^\varepsilon_i P^\varepsilon_j}{(U + \frac{10}{3} J_h)(U + \frac{2}{3} J_h)} \right] - t^2 \frac{\vec{S}_i \vec{S}_j + 6}{10(U - 5J_h)} P^\varepsilon_i P^\theta_j \\ & + t^2_\pi \frac{\vec{S}_i \vec{S}_j - 3}{3} \left[\frac{(U - 2J_h)(R_x(P^\varepsilon_i P^{a2}_j) + R_y(P^\varepsilon_i P^{a2}_j))}{\frac{19}{3} J_h (2U - \frac{7}{3} J_h)} + \frac{(U + \frac{5}{3} J_h)(R_x(P^\theta_i P^{a2}_j) + R_y(P^\theta_i P^{a2}_j))}{\frac{13}{3} J_h (2U - J_h)} \right] \\ & + t^2_\pi \frac{\vec{S}_i \vec{S}_j - 4}{8} \left[\frac{R_x(P^\varepsilon_i P^\varepsilon_j) + R_y(P^\varepsilon_i P^\varepsilon_j)}{U + 8J_h/3} + \frac{R_x(P^\theta_i P^\theta_j) + R_y(P^\theta_i P^\theta_j)}{U + 2J_h} \right. \\ & \left. + \frac{(2U + \frac{14}{3} J_h)(R_x(P^\varepsilon_i P^\theta_j) + R_y(P^\varepsilon_i P^\theta_j))}{(U + 4J_h)(U + \frac{2}{3} J_h)} \right] + t^2 \frac{\vec{S}_i \vec{S}_j - 3}{32 J_h} P^\varepsilon_i P^{a2}_j + t^2_\pi \frac{\frac{4}{9} \vec{S}_i \vec{S}_j - 1}{U + \frac{4}{3} J_h} P^{a2}_i P^{a2}_j + \text{H.c.} \end{aligned}$$

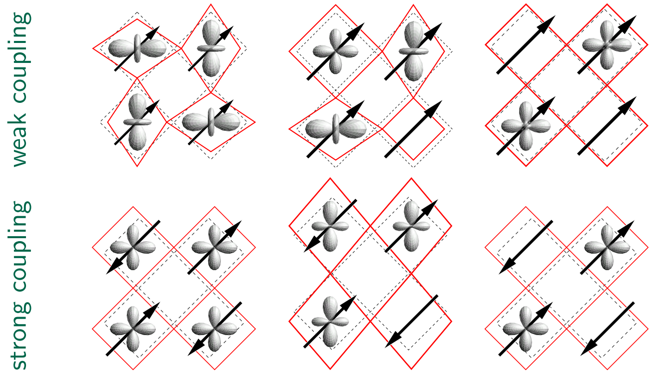
$$\begin{aligned} H^{ep} = {} & g \sum_i \left[(n_{i,\varepsilon} - n_{i,\theta})(b^\dagger_{i,\theta} + b_{i,\theta}) + (d^\dagger_{i,\theta} d_{i,\varepsilon} + d^\dagger_{i,\varepsilon} d_{i,\theta})(b^\dagger_{i,\varepsilon} + b_{i,\varepsilon}) \right] \\ & + \tilde{g} \sum_i (n_{i,\theta} + n_{i,\varepsilon} - 2n_{i,\theta} n_{i,\varepsilon})(b^\dagger_{i,a_1} + b_{i,a_1}) + \omega \sum_i \left[b^\dagger_{i,\theta} b_{i,\theta} + b^\dagger_{i,\varepsilon} b_{i,\varepsilon} \right] + \tilde{\omega} \sum_i b^\dagger_{i,a_1} b_{i,a_1} \end{aligned}$$

Short-range correlations

- exact cluster calculations → correlation functions → SRO patterns

($U = 6$eV, $J_H = 0.7$eV, $t = 3t_\pi = 0.4$eV, $\omega_0 = \tilde{\omega}_0 = 0.07$eV, $g/\omega_0 = 0.5 \ldots 3$)

doping: $x = 0$ $x = 0.25$ $x = 0.5$



EP interaction → orbital order → spin order → transport

Percolative mixed-phase description

- Description of CMR effect?

  experiment: spatial coexistence of conducting and insulating regions both above and below T_c

  - theory: . . . , phase separation approaches, ... ?

↪ proposal: two-phase scenario with percolative characteristics!

$$\boxed{\pi^{(f)} = \pi^{(p)} = \pi_{eq}}$$

- FM metallic component

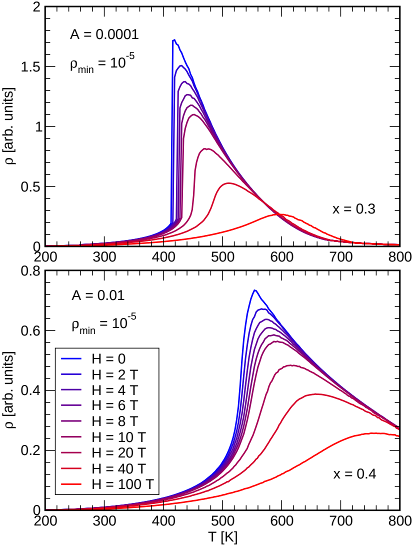
  $\rho^{(f)} = \frac{B}{x^{(f)}}(\rho_S + \rho_{min})$

- polaronic insulating component

  $\rho^{(p)} = \frac{A}{\beta x^{(p)}}\rho_S \exp(-\beta\epsilon_p)$

$\rho_S = \rho_S[S, z, B_S(z), \coth[S, z]\,]$

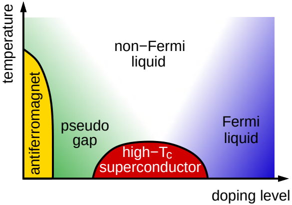
Weiße, Loos, HF: PRB 68, 024402 (2003)



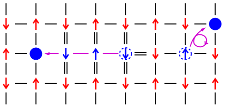
Hole polarons in high-T_C cuprates

- Why should EP coupling effects be of particular importance in high-T_C cuprates?

schematic phase diagram for, e.g., quasi-2D $La_{2-x}Sr_xCuO_4$



(doped) holes in AFM background



spin-bag "magnetic polaron"

effective low-energy Hamiltonian for CuO_2-planes:
Holstein t-J model

$$H = -t \sum_{\langle ij\rangle \sigma} \left(\tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + \mathrm{H.c.} \right) + J \sum_{\langle ij\rangle} \left(\vec{S}_i \vec{S}_j - \tfrac{1}{4} \tilde{n}_i \tilde{n}_j \right) - g\omega_0 \sum_i \left(b^{\dagger}_i + b_i \right) \left(1 - \tilde{n}_i \right) + \omega_0 \sum_i \left(b^{\dagger}_i b_i + \tfrac{1}{2} \right)$$

- $J = 4t^2/U$ - relevant energy scale for "coherent" hole motion
- magnetic "pre-localisation" of holes strengthens the effect of the hole-phonon interaction $\lambda_{eff} \sim \varepsilon_p / E_{kin}$!

$\hookrightarrow$ tendency towards lattice polaron formation is enhanced in strongly correlated electron systems

Bäuml, Wellein, HF: Phys. Rev. B 58, 3666 (1988)

Bipolaron Formation

- Will two (opposite-spin) electrons share a common lattice distortion?

Holstein Hubbard model:

$$H = -t \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$- g\,\omega_0 \sum_{i\sigma} (b_i^{\dagger} + b_i) n_{i\sigma} + \omega_0 \sum_{i} b_i^{\dagger} b_i$$

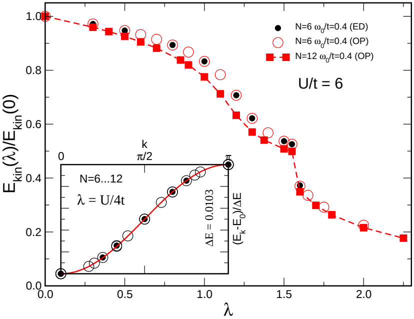
- λ, g enhance double occupancy
- U suppresses double occupancy
- phonon frequency?

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

  $\boxed{U_{eff} = U - 4t\lambda}$ (LF)

  $\alpha < 1$ retardation:

  $\hookrightarrow$ extended electron bound-states?



- kinetic energy:

  $\lambda \nearrow$: strong reduction of E_{kin}
  two successive "transitions"

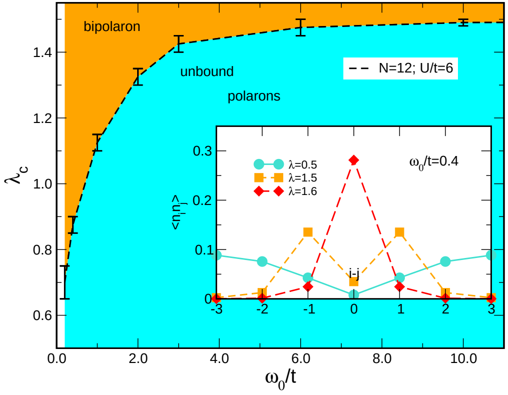
- bipolaron band dispersion:

  cosine shaped for $U_{eff} = 0$

Phase diagram

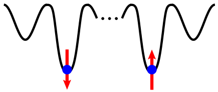
- Critical coupling for bipolaron formation?

binding energy $\boxed{\Delta = E_0(2) - 2E_0(1)} \to 0$

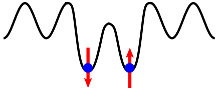


$\lambda, g^2 \nearrow$:

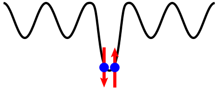
- unbound polarons



- mobile intersite bipolaron



- self-trapped on-site bipolaron



$\hookrightarrow$ pronounced retardation effects!

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

Part III: Finite-Density Effects on Polaron Formation

starting point: 1D spinless fermion Holstein model

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

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

previous results:

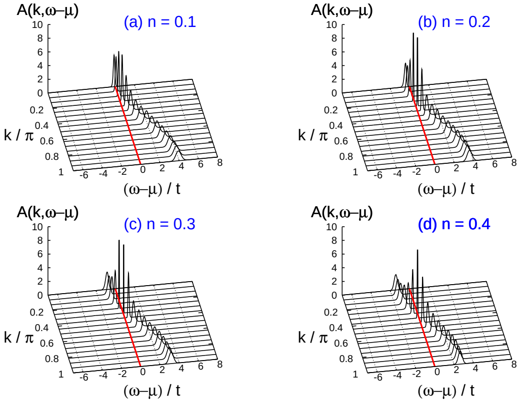
- for a single particle we observed a transition from a large polaron ("quasi-free" electron) to a small polaron with increasing EP coupling strength, at least in 1D
- in the intermediate coupling regime $\lambda \simeq 1$, $g^2 \simeq 1$, the size of the polaron was strongly dependent on the phonon frequency:
    - $\alpha \ll 1$: rather extended distortion
    - $\alpha \gg 1$: localised distortion
- focusing on the intermediate coupling adiabatic regime we expect strong density-effects due to a possible overlap of phonon clouds!

$\hookrightarrow$ Is there a density-driven crossover from "polaronic" to "electronic" QP?

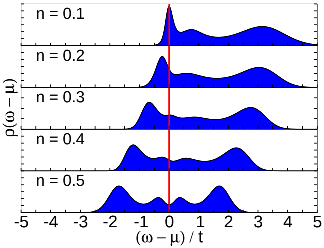
- Weak EP coupling:

$\lambda = 0.1$, $\alpha = 0.4$ – QMC results for $N = 32$, $\beta t = 8 \ldots 10$

single-particle spectral function



density of states



- pronounced QP peak $\forall n$
- gap feature develops for $n \to 0.5 \Leftrightarrow$ CDW (see next lecture . . .)

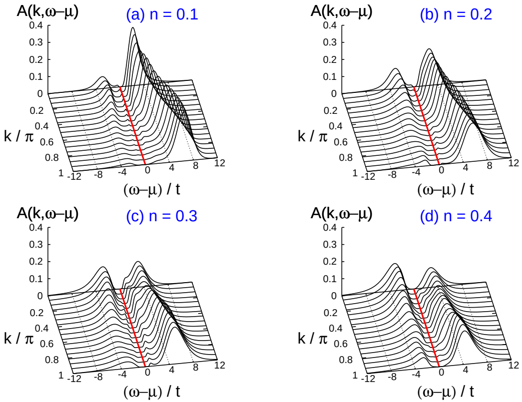
$\hookrightarrow$ dressed "electronic" QPs!

Many Polaron Problem II

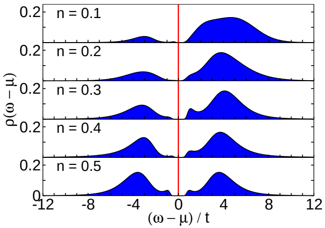
- Strong EP coupling:

$\lambda = 2.0$, $\alpha = 0.4$ – QMC results for $N = 32$, $\beta t = 8 \ldots 10$

single-particle spectral function



density of states



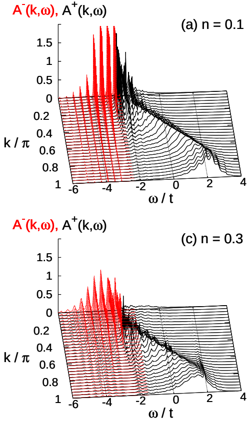
- exponential small spectral weight at μ $\forall n$
- QP band - "gap" - broad incoherent feature

$\hookrightarrow$ small polaron QPs!

Many Polaron Problem III

- Photoemission spectra at intermediate EP coupling?

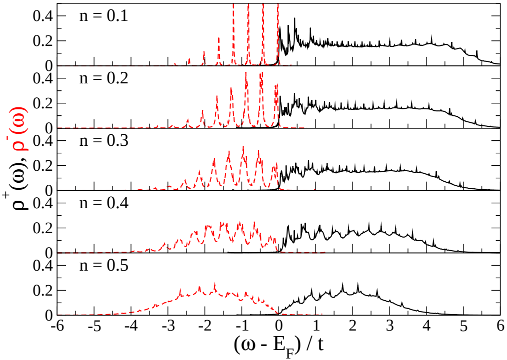
$\lambda = 1.0$, $\alpha = 0.4$ – CPT results for $N_c = 10$ and $T = 0$



$\hookrightarrow$ polaron band merged with incoherent excitations at about $n = 0.3 \dots 0.4$!

Many Polaron Problem IV

- Density of states:



$n \nearrow$: little weight at E_F (polaron) → "metallic" DOS at E_F (polaron dissociation)
→ pseudo-gap - precursor of CDW (∃ for $\lambda > \lambda_c$; see next talk...)

↪ crossover polaronic - metallic behaviour!

Hohenadler, Neuber, von der Linden, Wellein, Loos, HF: Phys. Rev. B 71, xxx (2005).
Hohenadler, Wellein, Alvermann, HF: cond-mat/0505559