Photoemission spectra of one and many polaron systems

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Overview

- single Holstein polaron
  - spectral function $A(k, \omega)$
  - kernel polynomial method (KPM)
  - cluster perturbation theory (CPT)
- single Holstein polaron in a disordered medium
  - intrinsically stochastic approach to disorder combined with DMFT
  - distribution of local DOS $\rho_i(\omega)$
  - cooperative effects: disorder $\leftrightarrow$ interaction
- many Holstein polarons
  - spectral function $A(k, \omega)$ away from half filling
  - QMC data

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Holstein model

electrons locally coupled to dispersionless Einstein phonons

one-dimensional spinless Holstein model:

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + \omega_0 \sum_i b_i^\dagger b_i - \sqrt{\omega_0 E_P} \sum_i \hat{n}_i (b_i^\dagger + b_i)$$

- parameters:
  - hopping integral: $t = 1$ (energy scale)
  - phonon frequency: $\overline{\omega}_0 = \omega_0 / t$
  - e-ph coupling: $\lambda = E_P / 2t$ or $g^2 = E_P / \omega_0$
- physics in a nutshell
  - polaron formation at sufficiently strong coupling
  - crossover large polaron — small polaron (1d)
  - half filling: quantum phase transition $\rightsquigarrow$ Peierls insulator
- spinful Holstein model at half filling:
  - competition Peierls insulator $\leftrightarrow$ Mott insulator

  (H. Fehske, talk next week – Correlation Days)

Kernel polynomial method

KPM: tailored for spectral information in different settings, e.g. spectral function for a single Holstein polaron

$$A(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\langle 0|c_k \frac{1}{\omega - H} c_k^\dagger|0\rangle$$

- expansion in Chebyshev polyn. $T_m(x) = \cos(m \arccos x)$

$$A(k,\omega) = \frac{1}{\pi\sqrt{1-\omega^2}}\left[\mu_0(k) + 2\sum_{m=1}^{\infty}\mu_m(k)T_m(\omega)\right]$$

  ▶ numerically stable, uniform convergence

- moments $\mu_m(k) = \langle 0|c_k\, T_m(H)\, c_k^\dagger|0\rangle$ from recursion

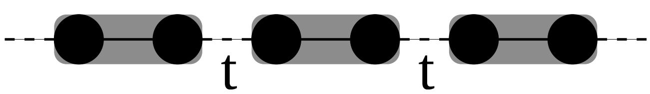
$$T_{m+1}(H) = 2HT_m(H) - T_{m-1}(H)$$

  ▶ numerically: dealing with finite systems
  ▶ (sparse) matrix-vector-multiplication

- how to deal with truncation of infinite series?
  ▶ convolution with appropriate kernel (e.g. Jackson kernel)

- straightforward combination with e.g. CPT

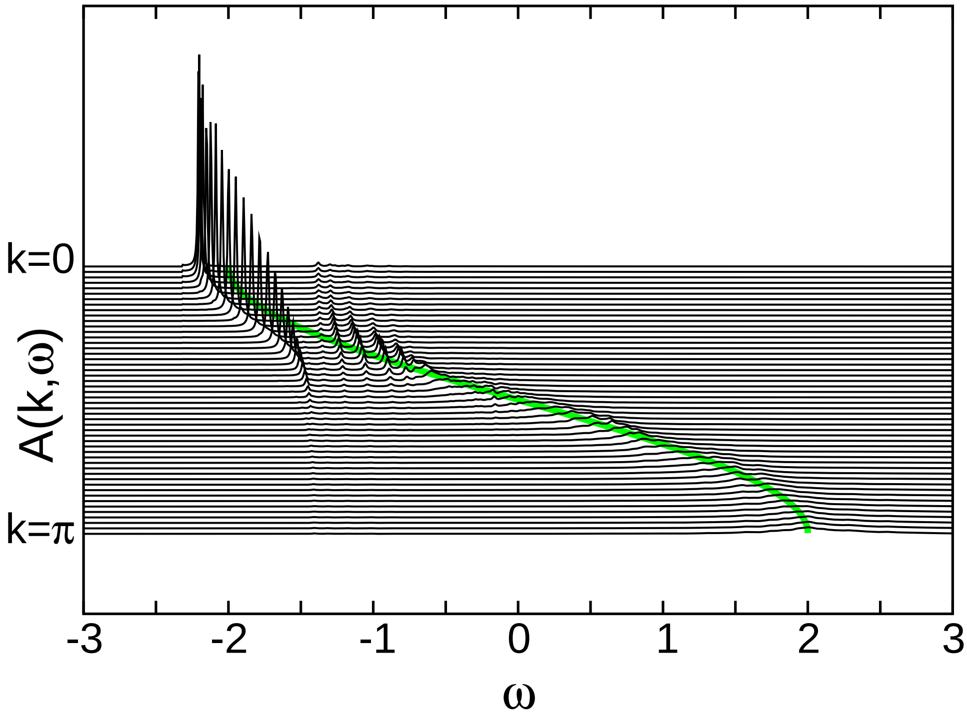
  ▶ use KPM for $G_{ij}^c(\omega)$ on a finite cluster
  ▶ reconstruct lattice Green function $G(k,\omega)$ via CPT



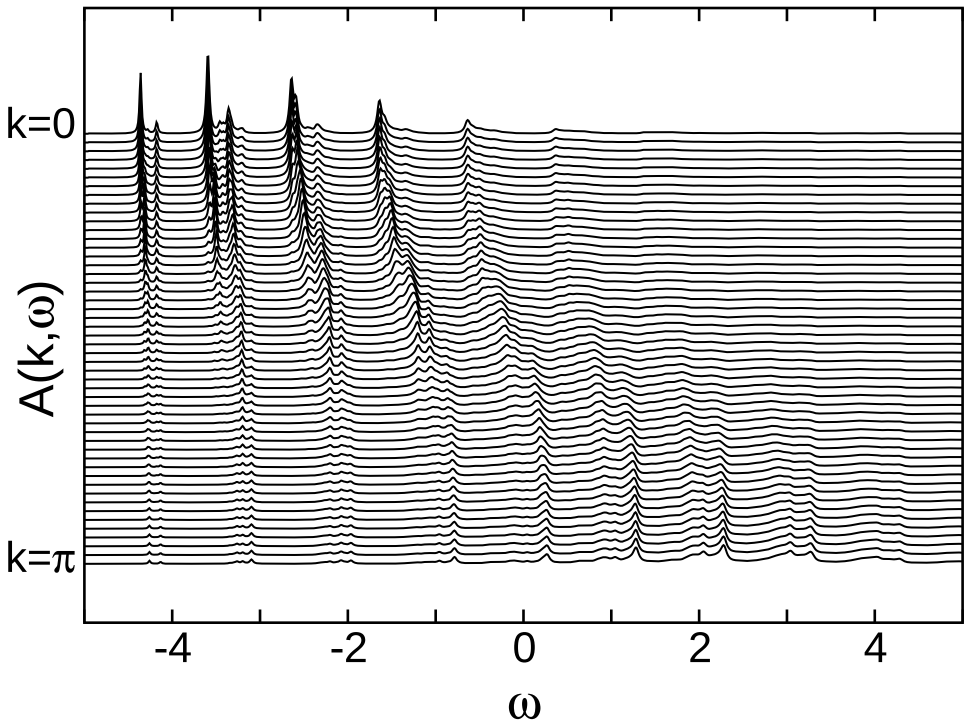
- further new applications: conductivity at finite temperatures (A. Weiße, talk next week – Correlation Days)

KPM+CPT for single Holstein polaron

weak coupling $\overline{\omega}_0 = 0.8, \lambda = 0.125$
$N = 16, M = 7$



intermediate coupling $\overline{\omega}_0 = 1.0, \lambda = 1.0$
$N = 6, M = 25$



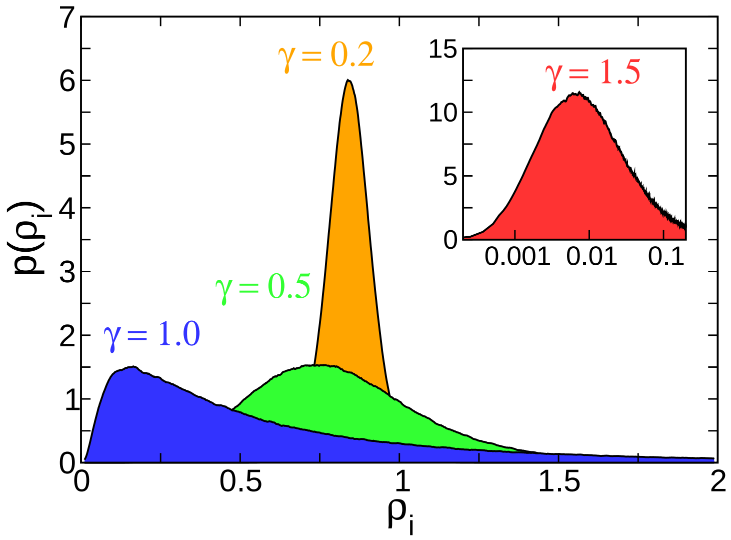
Holstein polaron + substitutional disorder

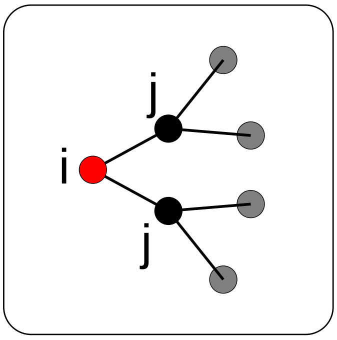
single polaron in a system with substitutional disorder

Anderson-Holstein model $\quad H = H_{Holstein} + \sum_i \varepsilon_i \, \hat{n}_i$

ε_i random on-site potentials, $p(\varepsilon_i) = \Theta(\gamma/2 - |\varepsilon_i|)$

- focus on distribution of local DOS $\rho_i(\omega)$
  - $\longrightarrow$ critical at the localization transition
  - $\longrightarrow$ $\rho_{\rm ave}(\omega) = \langle \rho_i(\omega) \rangle$ finite (non-critical)





- stochastic theory for distribution of $G_{ii}(\omega)$, (Abou-Chacra, Anderson, Thouless 1973)

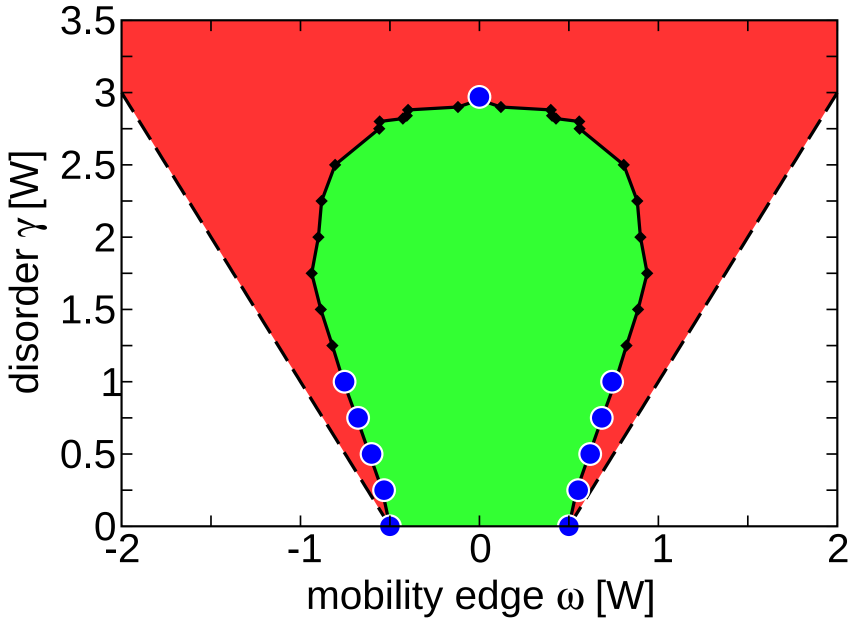
$$G_{ii}(\omega) = \left[\omega - \varepsilon_i - t^2 \sum_{j=1}^{K} G_{jj}(\omega) - \Sigma_{ii}(\omega) \right]^{-1}$$

- interaction via DMFT (Dobrosavljević & Kotliar 1998)

$$\Sigma_{ii}(\omega) = \Sigma_{ii}(\omega) \left[\omega - \varepsilon_i - t^2 \sum_{j=1}^{K} G_{jj}(\omega) \right]$$

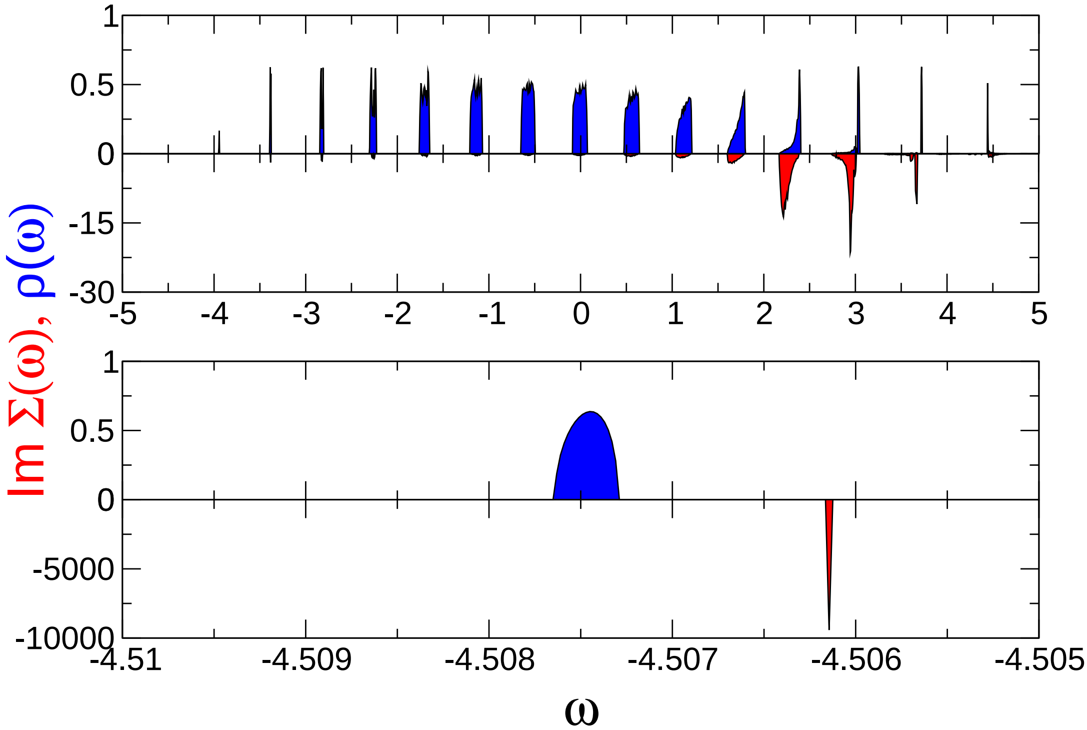
Localization of a Holstein polaron

mobility edges for the Anderson model (as in 3d)



DMFT $\Sigma_{ii}(\omega)$ for single Holstein polaron → CFE (Sumi 1974)

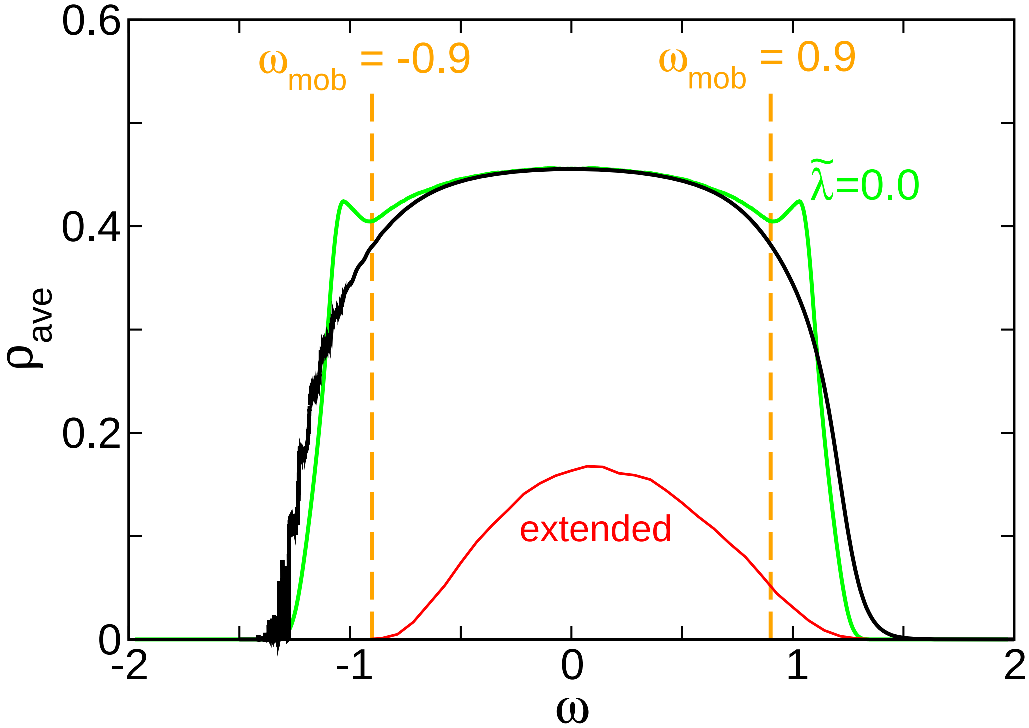
- localization transition in interaction renormalized band
  antiadiabatic strong coupling $\tilde{\omega}_0 = 2.25, \tilde{\lambda} = 9.0$

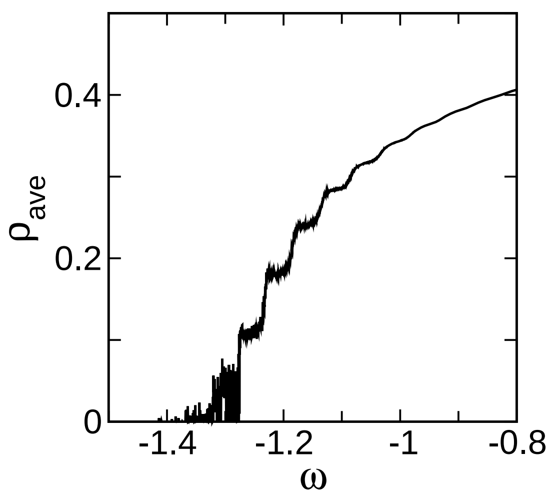


Beyond renormalization: cooperative effects

- polaron-like defect states (cf. Anderson 1972)
  - upper mobility edge: interaction weakens localization
  - lower mobility edge: polaron formation
  - strongly localized polaron states at deep impurities
  - density of states ⇝ independent boson model

disorder $\gamma = 2.0$ e-ph-coupling $\tilde{\omega}_0 = 0.2, \quad \tilde{\lambda} = 0.75$





The many polaron problem

- motivation:
  e.g. CMR materials call for many polaron description

- almost no analytical/numerical results are available *away* from half filling
  ▶ need to fill a gap

- expectation (intermediate coupling, adiabatic regime)

  ▶ low density: large polarons

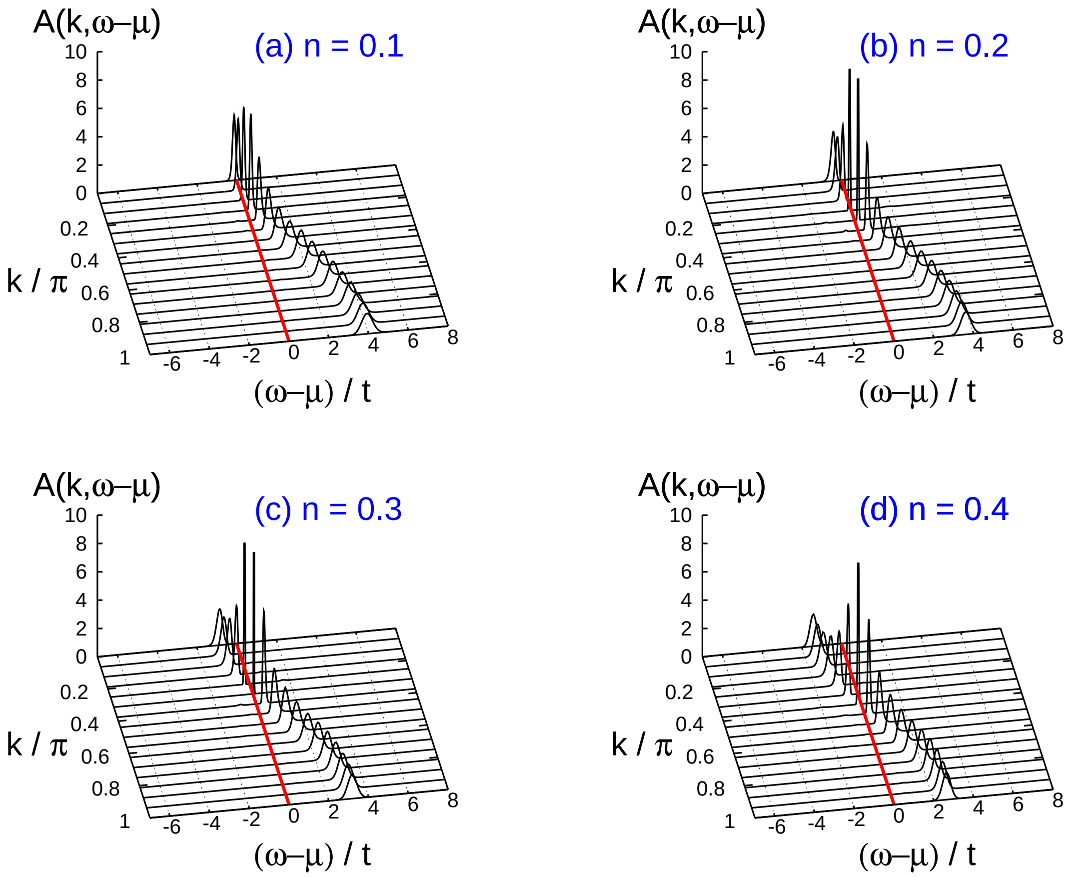
  ▶ high density: phonon clouds overlap $\longrightarrow$ dissociation of polarons

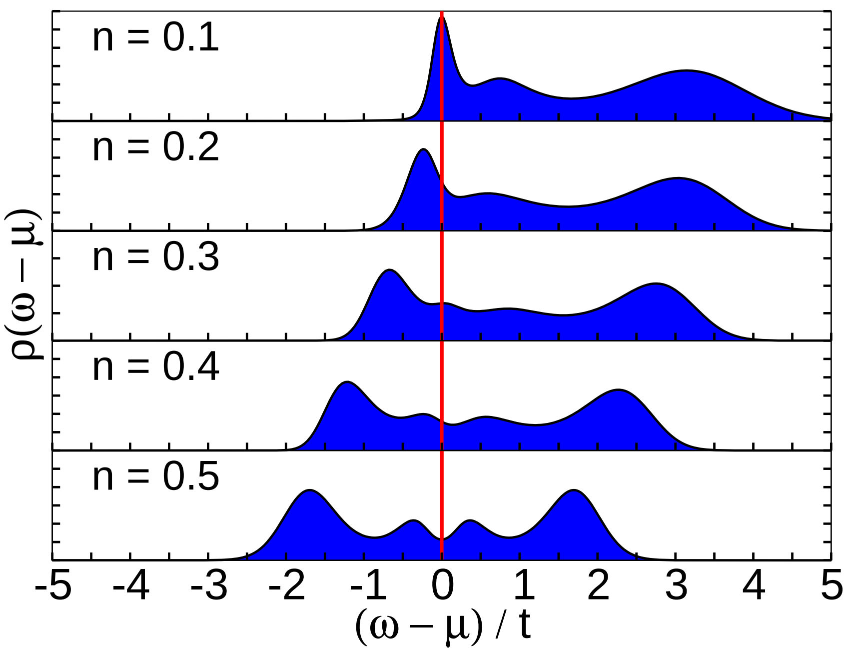
▶ density driven crossover from polaronic to metallic behaviour

- first data by Martin Hohenadler et. al. (*cond-mat 0412010*)
  ▶ QMC + Lang-Firsov-transformation, ED
  (poster next week – Correlation Days)

weak coupling

$$\overline{\omega}_0 = 0.4 \qquad \lambda = 0.1$$
$$N = 32, \quad \beta t = 8 \ldots 10$$





strong coupling

$$\overline{\omega}_0 = 0.4 \qquad \lambda = 2.0$$

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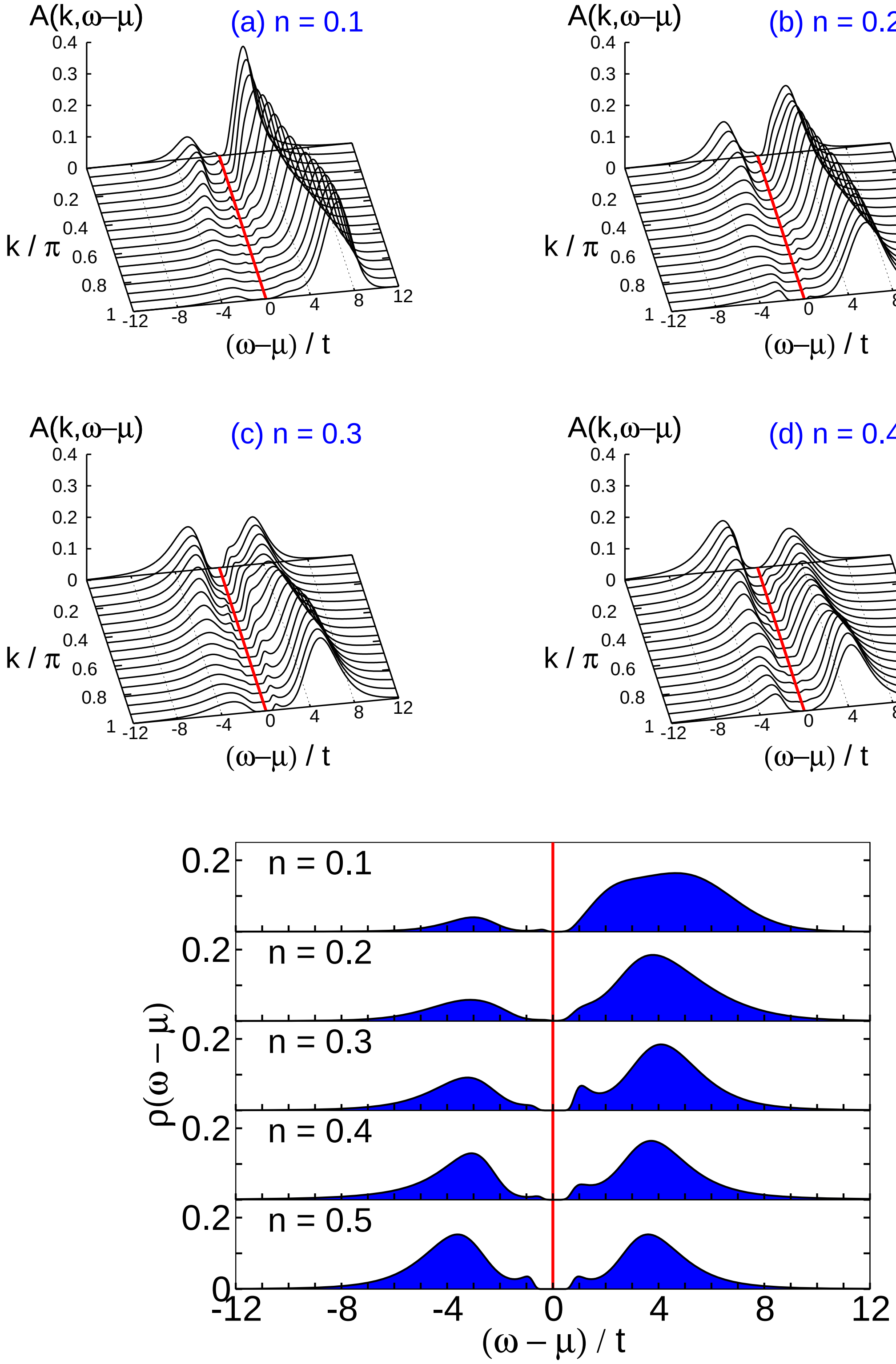
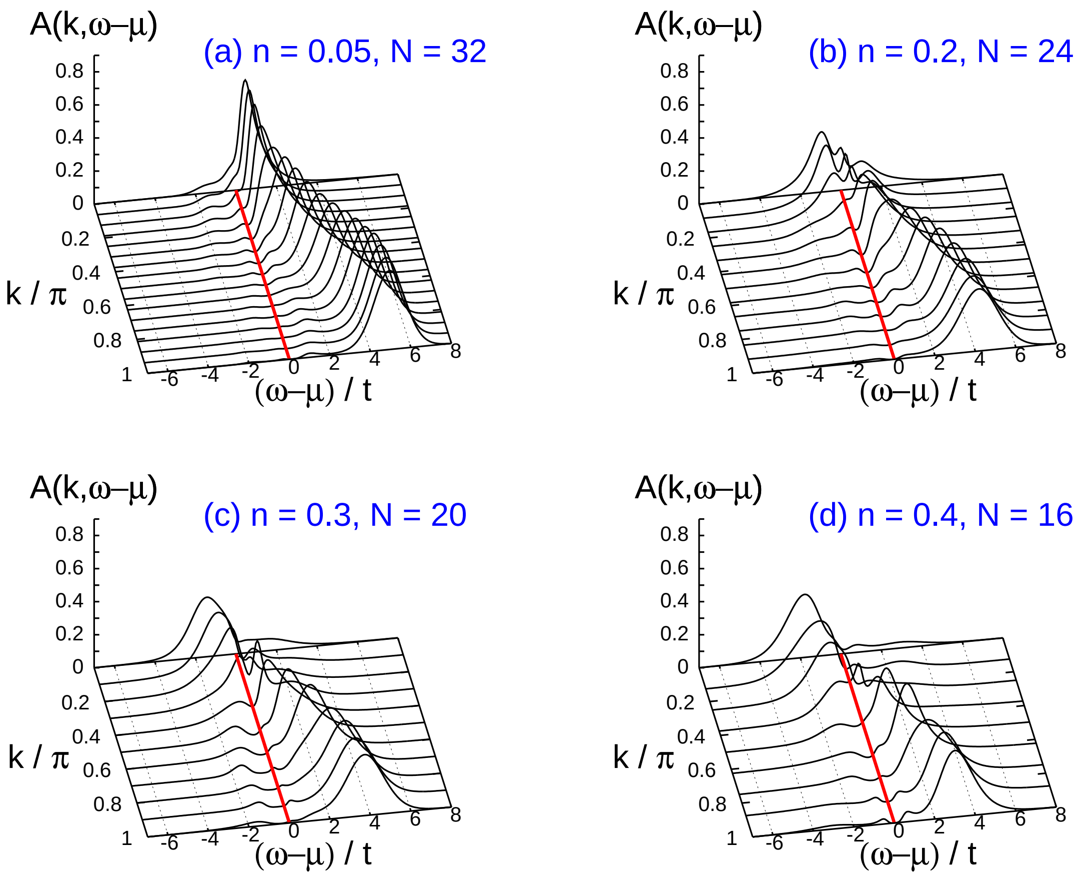
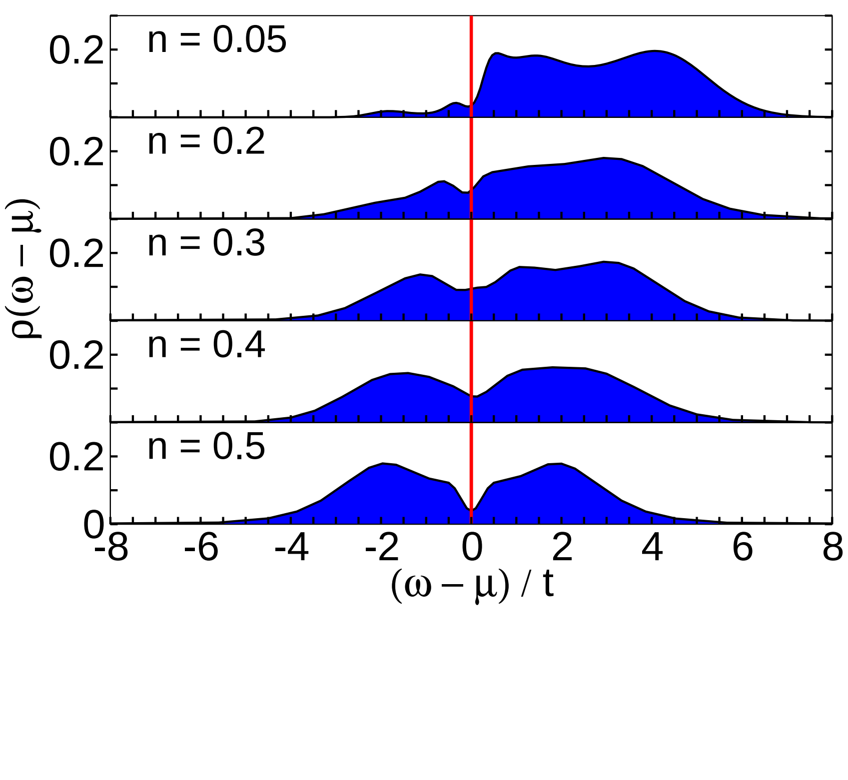


intermediate coupling

$$\overline{\omega}_0 = 0.4 \qquad \lambda = 1.0$$

$$N = 20 \ldots 32, \quad \beta t = 8 \ldots 10$$





Conclusions and Outlook

- KPM: thermodynamic and spectral properties
  - efficient: uniform convergence $\rightsquigarrow$ high resolution
  - reliable: numerical stability
  - combination with other techniques possible (CPT,MC,. . .)
  - correlation functions at zero and finite temperatures

- disordered interacting electron-phonon-system
  - stochastic approach to localization
  - interaction via DMFT
  - localization of Holstein polaron
  - cooperative effects: rich physics, non-universality

- many Holstein polarons away from half filling
  - (inverse) photoemission spectra (QMC/ED)
  - density driven crossover "polaronic" $\longrightarrow$ "electronic" QP

- work in progess
  - spinful polarons away from half filling: KPM + . . .
  - electronic and phononic correlation functions

- project: bringing together all aspects,
  e.g. with regard to CMR materials

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