Photoemission spectra of many-polaron systems

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Motivation

- Polaronic carriers are expected to exist in a number of strongly correlated materials (e.g., colossal magnetoresistive manganites).
- Question: WHAT happens to polarons if their density is large enough so that individual quasiparticles would overlap?
- Even for the most simplified models no reliable analytical results exist in the adiabatic intermediate coupling regime.
- Numerical methods allow unbiased studies for realistic parameters.

Model

1D spinless Holstein Hamiltonian

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

$c_{i\sigma}^\dagger$: creates spinless fermion at site i
$b_i^\dagger$: creates phonon at site i
$\hat{n}_i$: electron occupation number, $\hat{n}_i = c_i^\dagger c_i$, $n_i = 0, 1$

Parameters:
t : nearest-neighbour hopping parameter
ω_0 : phonon energy
g : electron-phonon coupling strength, $g = \sqrt{E_\mathrm{p}/\omega_0}$

We use the dimensionless parameters

$$\lambda = \frac{E_\mathrm{p}}{2t} \quad \text{and} \quad \overline{\omega}_0 = \frac{\omega_0}{t}.$$

- Bipolarons suppressed by Coulomb repulsion, here: $U \to \infty$.
- Extended polaron state only exists in one dimension!
- We mainly consider $\overline{\omega}_0 < 1$ (adiabatic regime).

Methods

Quantum Monte Carlo (QMC)

- Grand-canonical method, free of autocorrelations.
- Based on Lang-Firsov transformed model.
- Finite temperature $k_\mathrm{B}T = \beta^{-1}$, Trotter discretization $\Delta\tau = 0.1$.
- Sign problem for intermediate λ and small $\overline{\omega}_0$ at low temperatures.
- Maximum entropy method required to get dynamic quantities.

Exact diagonalization (ED)

- Kernel polynomial method, parallel matrix-vector multiplication.
- Zero temperature.
- Analytical separation of symmetric phonon mode [2].
- Cutoff for maximal number of phonons.
- Maximum entropy method to maximize energy resolution [3].

Observables

Single-particle spectral function

$$A(k, \omega - \mu) = -\frac{1}{\pi}\mathrm{Im}\, G(k, \omega - \mu)\,.$$

at momentum k and energy $\omega - \mu$ (μ: chemical potential).
QMC can measure

$$G(k,\tau) = \langle c_k^\dagger(\tau) c_k \rangle = \int_{-\infty}^{\infty} d\omega \, \frac{e^{-\tau(\omega-\mu)} A(k, \omega - \mu)}{1 + e^{-\beta(\omega-\mu)}}\,,$$

$G(k,\tau)$ denotes imaginary-time Green function.
Single-particle density of states:

$$\rho(\omega - \mu) = -\frac{1}{\pi}\mathrm{Im}\, G(\omega - \mu)\,.$$

Kernel polynomial method yields approximation to

$$A^+(k,\omega) = \sum_l |\langle \Psi_{l,k}^{(N_e+1)} | c_{k-q}^\dagger | \Psi_{0,q}^{(N_e)} \rangle|^2 \, \delta[\omega - (E_{l,k}^{(N_e+1)} - E_{0,q}^{(N_e)})]\,,$$
$$A^-(k,\omega) = \sum_l |\langle \Psi_{l,k}^{(N_e-1)} | c_{q-k} | \Psi_{0,q}^{(N_e)} \rangle|^2 \, \delta[\omega + (E_{l,k}^{(N_e-1)} - E_{0,q}^{(N_e)})]\,,$$

where $\langle \Psi_{l,k}^{(N_e)} |$ and $E_{l,k}^{(N_e)}$ denote the lth eigenstate with momentum k and N_e electrons and the corresponding energy, respectively.

Weak coupling

[$N = 32$, $\beta t = 10$, $\overline{\omega}_0 = 0.4$, $\lambda = 0.1$]

Expect weakly dressed electrons, no polarons.

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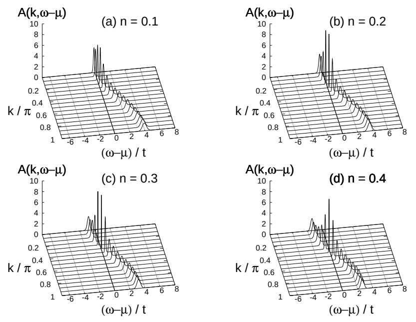
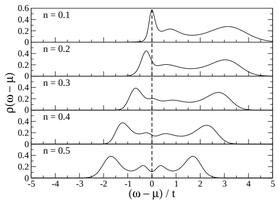
Spectral function (QMC)



- Free-electron-like spectra, bandwidth close to $4t$.
- Weak phonon signatures.

Density of states (QMC)



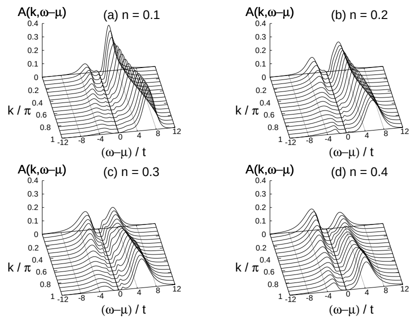
- Large spectral weight at μ for low densities.
- Tendency toward Peierls-insulating state at $n = 0.5$ ($T > 0$!).

Strong coupling

[$N = 32$, $\beta t = 10$, $\overline{\omega}_0 = 0.4$, $\lambda = 2.0$]

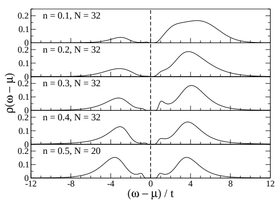
Small polarons, little overlap even for large n.

Spectral function (QMC)



- Exponentially small weight at Fermi level for all n (polaron band).
- Large high-energy incoherent features, reflecting the phonon distribution.

Density of states (QMC)



- Half-filled band: particle-hole symmetry, Peierls insulator with polaronic superlattice.

Intermediate coupling

[$N = 10$, $\beta t = 10$, $\overline{\omega}_0 = 0.4$, $\lambda = 1.0$]

At low densities: large polarons extending over more than one site; notably overlap with increasing carrier density
→ dissociation → new quasiparticles

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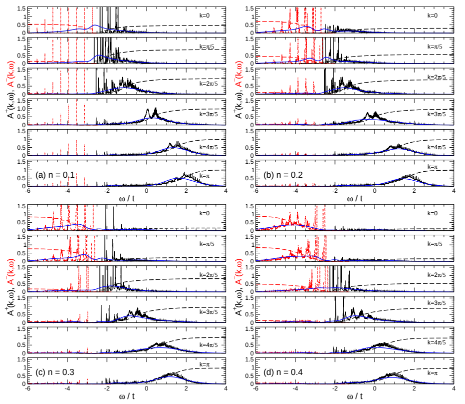
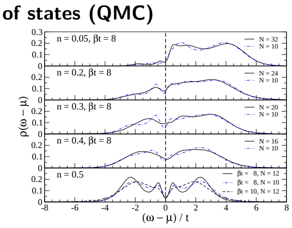
Spectral function (ED + QMC)



- $n = 0.1$: polaron band at Fermi level, flattening at large k.
- Incoherent part closely follows free dispersion.
- ↑ n: polaronic peaks broaden and merge to broad band at $n = 0.4$.
- $n = 0.4$: rather 'normal' metallic behaviour!
- Good agreement between QMC (blue) and ED.

Density of states (QMC)



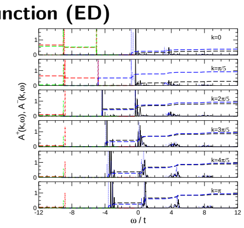
- Little weight at μ for $n = 0.1$, but increases with n due to dissociation of polarons.
- $n = 0.5$: charge-density-wave order sets in, weight at μ suppressed!
- $T > 0$: phonon excitations at $|\omega - \mu| \approx 2.5\omega_0$.

Nonadiabatic strong-coupling regime

[$N = 10$, $\overline{\omega}_0 = 4.0$, $\lambda = 2.0$]

Again consider critical coupling for small-polaron crossover ($g = 1$).

Spectral function (ED)



- Spectra mainly unchanged going from $n = 0.1$ (red/black) to $n = 0.3$ (green/blue).
- Polaronic carriers also at large fillings in nonadiabatic regime.

Conclusions

- Adiabatic intermediate coupling regime: Large polarons dissociate at large carrier densities.
- Crossover from a polaronic to a metallic system.
- Single-polaron theories not suitable at finite doping.

References

[1] Hohenadler et al., cond-mat/0412010
[2] Sykora et al., PRB **71**, 045112 (2005)
[3] Bäuml et al., PRB **58**, 3663 (1998)

Acknowledgments

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