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Many-polaron problem by cluster perturbation theory

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Abstract

The carrier-density dependence of the photoemission spectrum of the Holstein many-polaron model is studied using cluster perturbation theory combined with an improved cluster diagonalization by Chebychev expansion.

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Polaronic quasiparticles originating from strong electron–phonon interaction play an important role in polar solids, including alkali halides, transition metal oxides/perovskites and, in particular, quasi one-dimensional (1D) materials such as MX chains, conjugated polymers or organic charge-transfer complexes. However, the theoretical description of the underlying models represents a challenging open problem.

Recently, significant effects of finite carrier density on the spectral properties of a polaronic system have been discovered for the spinless Holstein model [1], revealing the shortcomings of widely used single-polaron theories. The Hamiltonian of the 1D tight-binding (t) Holstein model reads

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

Here $c_i^\dagger$ ($b_i^\dagger$) creates a spinless fermion (a phonon) at lattice site i, and $\hat{n}_i = c_i^\dagger c_i$. The parameters are the adiabaticity ratio ω_0/t, and the dimensionless coupling constant $\lambda = E_\mathrm{p}/2t$, with the polaron binding energy E_p.

While existing work based on finite-cluster calculations was restricted either in energy or momentum resolution [1,2], the cluster perturbation theory (CPT, see Ref. [3] and references therein) yields accurate results in the thermodynamic limit.

Here, we calculate the zero-temperature Green function $G(k,\omega) = \langle\langle c_k; c_k^\dagger\rangle\rangle_\omega$ using CPT in combination with a Chebychev expansion technique [4]. The latter does not suffer from the shortcomings of other methods, and exploits the analytical separation of the symmetric phonon mode [5] in order to ensure well-converged results. Calculations have been done on parallel supercomputers, with the largest matrix dimension exceeding 10^{10}. Within CPT, the one-particle Green function is obtained from $G^{-1} = G^{(\mathrm{c})-1} - V$, where $G^{(\mathrm{c})}$ and V denote the corresponding real-space cluster Green function and the intercluster hopping matrix, respectively, and subsequent Fourier transformation [3].

A substantial dependence of the system properties on the band filling is expected for intermediate electron–phonon interaction, for which a large (extended) polaron state is known to exist in the single-electron case. By contrast, for strong coupling, the polaron size collapses to a single site, so that different carriers will not overlap (interact). Hence, we take $\lambda = 1$, the critical coupling for the large-to-small polaron cross-over in the adiabatic regime $\omega_0/t < 1$. Note

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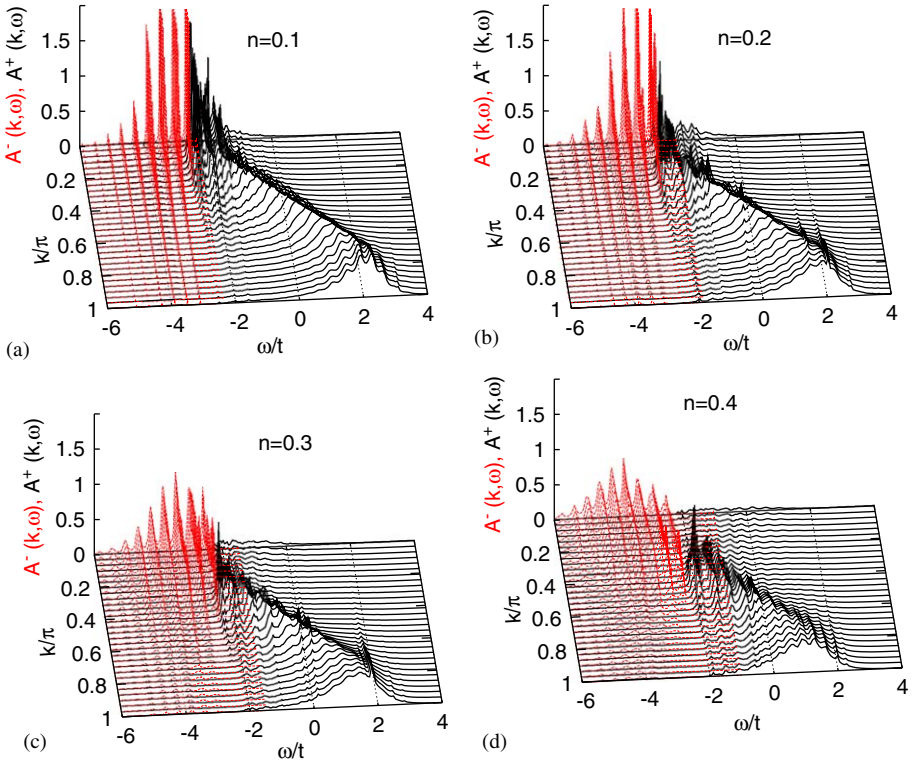

Fig. 1. One-electron spectral functions $A^{-}(k,\omega)$ (red dashed lines) and $A^{+}(k,\omega)$ (black solid lines) for different band fillings n. Here $\omega_0/t = 0.4$, $N = 10$ and $\lambda = 1$. (a) $n = 0.1$; (b) $n = 0.2$; (c) $n = 0.3$; (d) $n = 0.4$.

that the above-mentioned density effects are absent for $\omega_0/t \gg 1$ [1].

Fig. 1 shows results for the one-electron spectral functions $A^{\pm}(k,\omega) = -\mathrm{Im}\, G^{\pm}(k,\omega)/\pi$, where G^{-} (G^{+}) corresponds to the (inverse) photoemission part of G, for fixed cluster size $N = 10$.

In the low density case $n = 0.1$ (Fig. 1(a)), we can easily identify a (coherent) polaron band crossing the Fermi level E_F, the latter being situated at the point where A^{-} and A^{+} intersect. The band flattens at large k, as known from single-polaron studies. Below this band, there exist equally spaced phonon excitations with small spectral weight, which reflect the Poisson distribution of phonons in the one-electron ground state. Finally, above E_F, there is a broad incoherent band whose maximum follows closely the dispersion relation of free particles.

As the density n increases (Figs. 1(a)–(c)), the gap between the polaron band and the incoherent excitations is reduced, and the low-energy phonon peaks begin to broaden, until they have ultimately merged into a broad band for $n = 0.4$ (Fig. 1(d)). More importantly, for $n \gtrsim 0.3$, a polaron band can no longer be identified as incoherent excitations lie very close to the Fermi level. Finally, at $n = 0.4$, the spectrum consists of a broad main band of effective width $\approx 6t$ crossing E_F, as in a metallic system, and low-energy excitations are available. This indicates that the polaronic quasiparticles, existing at small n, have dissociated into dressed electrons due to mutual interaction. Therefore, the system can no longer be described in terms of small-polaron theory, as expected for intermediate electron–phonon coupling at large n.

To summarize, the density-driven cross-over from a polaronic system to one with moderately dressed electrons has been studied by means of CPT, whose unlimited momentum resolution significantly simplifies the interpretation compared to previous calculations [1]. Finally, the improvement of the cluster diagonalization represents an important step toward future studies of even more complex problems.

Acknowledgments

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