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.

Key words: electron-phonon interaction, cluster perturbation theory
PACS: 71.27.+a, 63.20.Kr, 71.10.-w, 71.38.-k

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

\[
H = -t \sum_{i<j} c_i^\dagger c_j + \omega_0 \sum_i b_i^\dagger b_i - \sqrt{E_p \omega_0} \sum_i \hat{n}_i (b_i^\dagger + b_i).
\]

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 \(\omega_0/t\), and the dimensionless coupling constant \(\lambda = E_p/2t\), 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 [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 \(G^{-1} = G^{(c)^{-1}} - V\), where \(G^{(c)}\) 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 that the abovementioned density effects are absent for \(\omega_0/t \gg 1\) [1].

Figure 1 shows results for the one-electron spec-
The relation of free particles.

The band whose maximum follows closely the dispersion relations is reduced, and the low-energy phonon peaks between the polaron band and the incoherent excitations is available. This indicates that the 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].

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.

This work was supported by the FWF project P15834, the DFG through SPP1073, and KONWIHR. M. H. is grateful to HPC-Europa.

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