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Optical response of many-polaron systems

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Abstract

Exact results for the density of states and the AC conductivity of the spinless Holstein model at finite carrier density are obtained combining Lanczos and kernel polynomial methods.

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Optical measurements have proved the importance of electron–phonon (EP) coupling and even polaron effects in several important classes of materials, including one-dimensional (1d) MX chains, quasi-2d cuprate superconductors, and 3d colossal magnetoresistance manganites. In all these materials, a noticeable density of (polaronic) charge carriers is observed, which puts the applicability of single-polaron theories into question, particularly in the region of intermediate EP coupling strength and phonon frequency.

Recently, the photoemission spectra of many-polaron systems have been investigated in the framework of the 1d spinless Holstein model

$$H = -t\sum_{\langle i,j\rangle} c_i^\dagger c_j + \omega_0 \sum_i b_i^\dagger b_i - g\omega_0 \sum_i \hat{n}_i (b_i^\dagger + b_i), \qquad (1)$$

describing tight-binding (t) electrons coupled locally (g) to Einstein phonons (ω_0), where $c_i^\dagger$ ($b_i^\dagger$) denote the corresponding fermionic (bosonic) creation operators, and $\hat{n}_i = c_i^\dagger c_i$. Most notably, provided that the EP coupling is not too strong, a density-driven crossover from large polarons to weakly dressed electrons has been found to occur [1]. In the meantime, this result was corroborated by cluster perturbation theory (CPT) [2].

Here, we use Lanczos diagonalization and kernel polynomial expansion methods [3] to study the (linear) optical response of a many-polaron system to an external (longitudinal) electric field, $\mathrm{Re}\,\sigma(\omega) = D\delta(\omega) + \sigma^{\mathrm{reg}}(\omega)$, the regular part of which is given by

$$\sigma^{\mathrm{reg}}(\omega) = \frac{\pi}{N}\sum_{m>0} \frac{|\langle 0|\hat{\jmath}|m\rangle|^2}{\omega_{m0}}\,\delta(\omega - \omega_{m0}), \qquad (2)$$

where $\omega_{m0} = E_m - E_0$, E_m ($|m\rangle$) are the eigenvalues (eigenstates) of our N-site coupled EP system with at most M phonons, and $\hat{\jmath} = iet\sum_i (c_i^\dagger c_{i+1} - c_{i+1}^\dagger c_i)$. In addition, we calculate the partial densities of states (DOS) $\rho^+(\omega)$ and $\rho^-(\omega)$, which are obtained from the k-integrated single-particle spectral functions

$$A_k^\pm(\omega) = \sum_m |\langle m^{(N_{\mathrm{el}}\pm 1)}|c_k^\pm|0^{(N_{\mathrm{el}})}\rangle|^2 \times \delta[\omega \mp (E_m^{(N_{\mathrm{el}}\pm 1)} - E_0^{(N_{\mathrm{el}})})], \qquad (3)$$

$c_k^+ = c_k^\dagger$, $c_k^- = c_k$, where $A_k^-(\omega)$ [$A_k^+(\omega)$] is related to the [inverse (I)] photoemission (PE) of an electron.

Fig. 1 displays selected numerical results for the optical properties of the 1d model (1) for $g^2 = 5$, $\omega_0/t = 0.4$ and various characteristic particle densities.

Starting with a *single electron* ($n = 0.1$), we notice from the DOS that there is a polaron feature at the Fermi level E_F (cf. the jump in the integrated DOS at E_F and the

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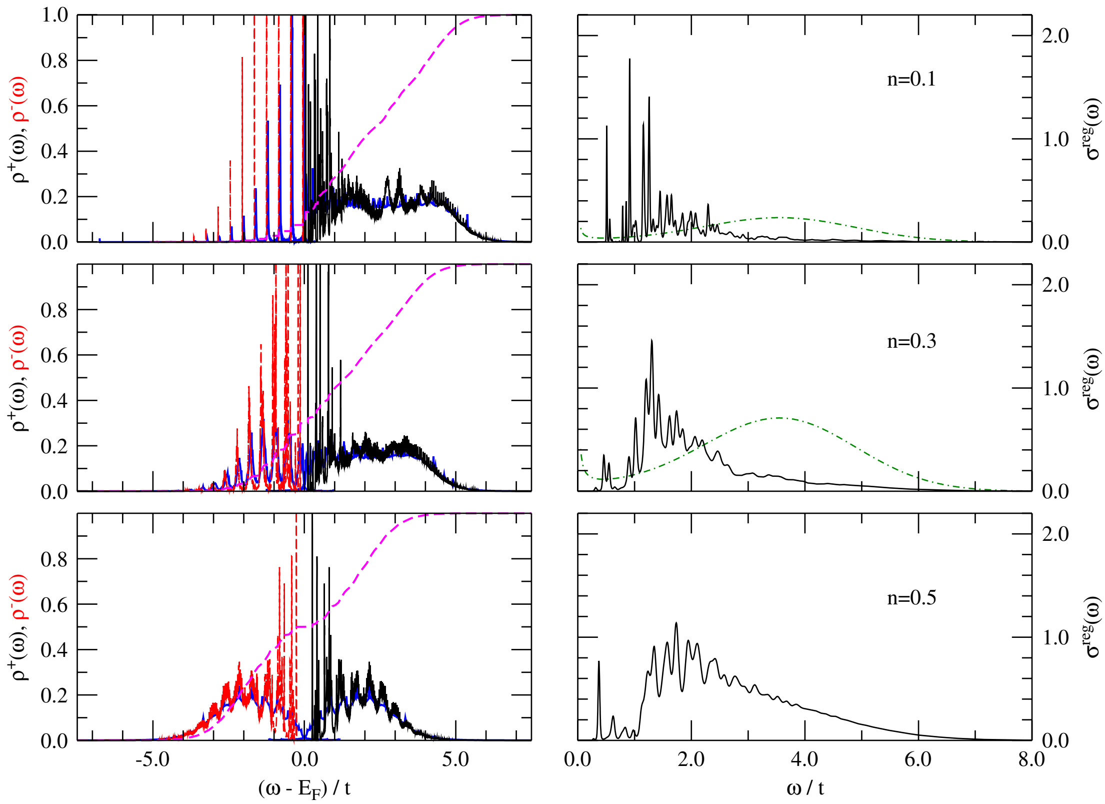

Fig. 1. (Color online) Left panel: Single-particle DOS $\rho^-(\omega)$ (red dashed lines) and $\rho^+(\omega)$ (black solid lines) for $g^2 = 5$, $\omega_0/t = 0.4$, and particle densities $n = 0.1$ (one electron), $n = 0.3$, and $n = 0.5$ (half filling). Results are for a ten-site system with periodic boundary conditions and $M \leqslant 15$ dynamical phonons. The homogeneous $q = 0$ lattice displacement was treated separately [5], leading to truncation errors $< 10^{-4}$. Dashed (magenta) lines give the integrated DOS. CPT data for $\rho^{\pm}(\omega)$ included for comparison (blue lines) were partly extracted from [2]. Right panel: Regular part of the optical conductivity $\sigma^{\rm reg}(\omega)$. (Green) dashed–dotted lines: analytical strong-coupling result $\sigma^{\rm reg}(\omega) = \sigma_0\, n\,(\omega_0 g)^{-1}\,\omega^{-1}\,\exp[(\omega - 2g^2\omega_0)/(2g\omega_0)]^2$ ($\sigma_0 = 8$) [4].

negligible spectral weight of $\rho^-(\omega < E_{\rm F})$). However, in view of the intermediate EP coupling strength chosen, $\lambda = g^2\omega_0/2t = 1$, the polaron is rather extended (large). Consequently, the polaron band is not far separated from incoherent excitations, and $\sigma^{\rm reg}(\omega)$ strongly deviates from the analytical strong-coupling result. In particular, the maximum in $\sigma^{\rm reg}$ occurs well below the small polaron value 4λ.

At *finite carrier density*, the system shows diffusive transport. The polarons are dissociated and the remaining electronic quasiparticles are scattered by virtual phonons. The peaks in the PE part of the spectrum, which for $n = 0.1$ had reflected the Poisson-like distribution of phonons in the ground state, now broaden significantly, and ultimately merge with the IPE part into a wide incoherent band (see also the continuous increase of the integrated DOS) [1].

In the *half-filled band case*, the model has a symmetry-broken insulating charge-density-wave ground state accompanied by a distortion of the lattice. This is because the EP coupling exceeds the critical interaction strength for the Peierls instability: $g > g_{\rm c}(\omega_0/t = 0.4) \simeq 1.9$ [5]. Accordingly, we find a gap feature in the DOS and a clear optical absorption threshold. Note that the CPT does not reproduce the very small gap in the DOS, as it "interpolates" between the wavevectors of the finite cluster.

In conclusion, increasing the particle density in the 1d spinless Holstein model at intermediate EP coupling strengths, we observe a crossover from a polaronic system to a metal composed of weakly dressed electronic quasiparticles and finally to a Peierls insulator at half filling. These transitions are reflected in significant changes of the optical spectra.

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