

Optical and spectral properties of the t - J Holstein model

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Submitted : 29-08-2008

Keywords : t - J -Holstein model, spectral functions, optical conductivity

We develop an efficient numerical method for the description of a single-hole motion in the antiferromagnetic background. The method is free of finite-size effects and allows calculation of physical properties at an arbitrary wavevector. Methodical increase of the functional space leads to results that are valid in the thermodynamic limit. In the case of the t - J model we found good agreement with cumulant expansion, exact-diagonalization approaches on finite lattices as well as self-consistent Born approximations. The method allows a straightforward addition of other inelastic degrees of freedom, such as lattice effects. Our results for spectral functions as well as quasiparticle weight of the t - J -Holstein model are in agreement with diagrammatic Monte Carlo method. Calculated spectral functions in Fig (a) in the strong coupling limit reproduce well the waterfall structure seen in ARPES spectra on $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$.

We also compute the charge stiffness and optical conductivity of the t - J Holstein model, Fig (b). Coherent hole motion is most strongly influenced by the electron-phonon coupling within the physically relevant regime of the exchange interaction. Optical conductivity in the crossover to the strong coupling regime shows a two-peak structure. The low-frequency peak represents the excitation of the first string state, while the higher-frequency peak corresponds to the mid infrared band, broadened and renormalized by phonon excitations. Results are in agreement with recent optical measurements.

We furthermore extend the existing method to computation of the bipolaron. We discuss the shape of the magnetic bipolaron and the condition for the formation of the bound state.

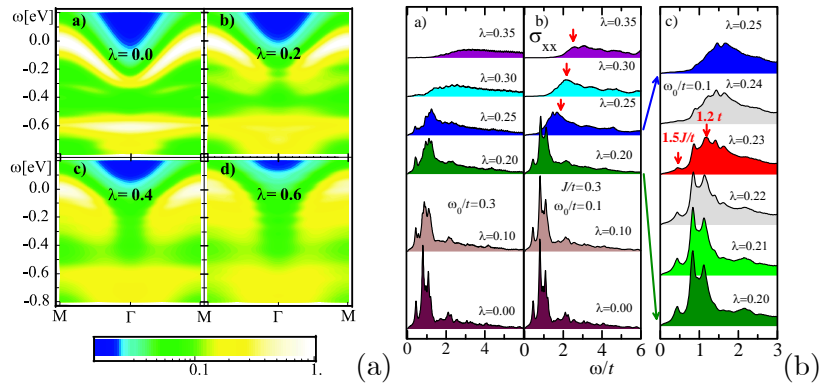


Figure 1: (a) Intensity plots of $A_{\mathbf{k}}(\omega)$ for the TJHH model ($J/t = 0.4$, $t'/t = -0.34$, $t''/t = 0.23$ and $t = 0.375\text{meV}$.) at different values of electron-phonon coupling strength λ and phonon frequency $\omega_0/t = 0.2$ and (b) σ_{xx} for the t - J -Holstein model.