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Finite temperature dynamical density matrix renormalization group study of high-energy optical conductivity in high-Tc cuprates
SHIGETOSHI SOTA, RIKEN AICS, TOMONORI SHIRAKAWA, SEIJI YUNOKI, RIKEN AICS, RIKEN ASI, CREST — Synchrotron-based high-energy optical conductivity measurement has been proposed as an effective experimental means to investigate the magnetic correlations around doped carriers in strongly correlated materials. For example, very recent experiments on high-Tc cuprates have observed the surprisingly significant temperature dependence of the spectra for an energy region much higher than the value of the spin exchange ($\sim$ 125 meV) below room temperature. Motivated by these experiments, we here study the high-energy optical conductivity and its temperature dependence of an effective model for high-Tc cuprates using massively parallelized dynamical density matrix renormalization group (DMRG). To describe the Zhang-Rice singlet as well as the high-energy excitations properly, we employ a one-dimensional three-band Hubbard model describing a CuO_3 chain. Our finite-temperature dynamical DMRG calculations find the strong temperature dependence of the optical conductivity, which occurs over a wide range of the excitation energy. We attribute this anomalously strong spectral redistribution to a magnetic origin, thus indicating that the high-energy optical conductivity contains valuable information of spin dynamics.

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