

Theoretical Study of Resonant Inelastic X-ray Scattering Spectrum in Nickelates

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The two-dimensional nickelate $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$ has received special attention as a reference system of high- T_c cuprates. The undoped nickelate ($x = 0$) has the charge-transfer gap in the optical conductivity. Upon doping of holes, a broad spectrum appears in the gap. We have shown theoretically that the broad spectrum comes from excitations to the low spin states.¹ In the Ni K -edge resonant inelastic X-ray scattering (RIXS) measurement, the momentum-resolved charge excitations are obtained.² In this study, we examine theoretically the RIXS spectra on nickelates by using numerically exact diagonalization techniques on the two-band Hubbard model. We also calculate other spectra such as the dynamical charge density function and discuss what excitations appear in the RIXS spectrum.

¹K. Tsutsui, W. Koshibae, and S. Maekawa, *Phys. Rev. B* **59**, 9729 (1999).

²E. Collart *et al.*, *Phys. Rev. Lett.* **96**, 157004 (2006); S. Wakimoto *et al.*, *Phys. Rev. Lett.* **102**, 157001 (2009); L. Simonelli *et al.*, *Phys. Rev. B* **81**, 195124 (2010).