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[116] Mixed singlet and triplet two-hole states in Bi2Sr2CaCu2O8+δ unveiled by cluster modeling of the d-d excitations observed by Resonant Inelastic X-Ray Scattering

We studied the d-d excitations in $Bi_2Sr_2CaCu_2O_{8+}$ by Cu L_3 -edge Resonant Inelastic X-ray Scattering with azimuthal rotation of the polarizations in the sample space, and analyzed the experimental response with a single cluster model. Utilizing group theory classification to incorporate two-hole Coulomb interactions via a Green's function approach, the calculations suggest that the d-d excitations can be described by a two-hole ground state composed of a Hund's triplet mixed with a Zhang-Rice singlet state in all the studied doping regions. Our results highlight the existence of the spin-triplet two-hole state for doped cuprates, and that Hund's triplet physics could play a role in the optimally doped and over-doped regions.

Theoretical Work

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