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Symmetry of spin excitation spectra in 122-ferropnictides¹

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We have studied the symmetry of spin excitation spectra in 122-ferropnictide superconductors by comparing the results of first-principles calculations with inelastic neutron scattering (INS) measurements on Ni- and Co-doped BaFe_2As_2 samples close to the optimal doping level, which exhibit neither static magnetic phases nor structural phase transitions. In both the normal and superconducting (SC) states, the spectrum does not follow the $I4/mmm$ space group of the crystal, but instead inherits its symmetry from the unfolded Brillouin zone of the Fe- sublattice. This is manifest both in the in-plane anisotropy of the normal- and SC-state spin dynamics and in the out-of-plane dispersion of the spin-resonance mode and the SC spin gap. The in-plane anisotropy is temperature-independent and can be qualitatively reproduced in normal-state density-functional theory calculations without invoking a symmetry-broken (“nematic”) ground state that was previously proposed as an explanation for this effect. Below the SC transition, the energy of the magnetic resonant mode, as well as its intensity and the SC spin gap, inherit the normal-state intensity modulation along the out-of-plane direction. Apparently, it can be traced back to the three-dimensional band structure and the superconducting gap, both of which were reported to disperse along the out-of- plane direction.

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