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Improper s-wave symmetry for the electronic pairing in iron-based superconductors by first-principles calculations MICHELE CASULA, CNRS and Université Pierre et Marie Curie, Paris, France, SANDRO SORELLA, SISSA, Trieste, Italy — By means of space-group symmetry arguments, we argue that the electronic pairing in iron-based high temperature superconductors shows a structure which is a linear combination of planar s-wave and d-wave symmetry channels, both preserving the 3-dimensional A_{1g} irreducible representation of the corresponding crystal point-group. We demonstrate that the s- and d-wave channels are determined by the parity under reflection of the electronic orbitals through the iron planes, and by improper rotations around the iron sites. We provide evidence of these general properties by performing accurate quantum Monte Carlo ab-initio calculations of the pairing function for a FeSe lattice. In order to achieve a higher resolution in momentum space we introduce a BCS model that faithfully describes our QMC variational pairing function. This allows us to provide a k-resolved image of the pairing function, and show that non-isotropic contributions in the BCS gap function are related to the improper s-wave symmetry. Our theory can rationalize and explain a series of contradictory experimental findings, such as the observation of twofold symmetry in the FeSe superconducting phase and the s-to-d-wave gap transition in $BaFe_2As_2$ under K doping.

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