Iron-Based Superconductors: Space Group Symmetry, Spin-Orbit Coupling, and the Low Energy Effective Action

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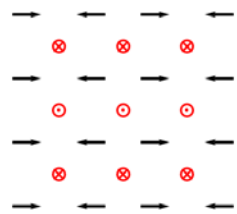
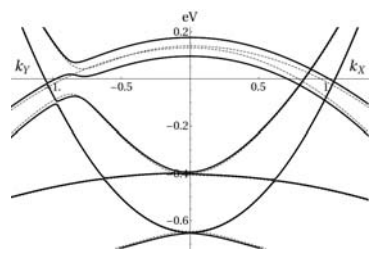
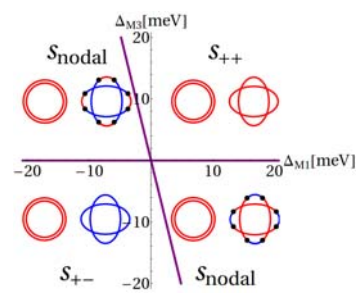
Introduction/Abstract

A common feature in the band structure of iron-based superconductors are hole bands at □ and electron bands at M point in the Brillouin zone (BZ) close to the Fermi level. Using the Luttinger method of invariants, we construct a low-energy effective theory for these states. The method of invariants allows us to readily include the spin-orbit (SO) effect, which is significant for iron. Our symmetry analysis allows us to classify spin density wave (SDW) order parameters and study their physical consequences on the low-energy spectrum. We find that the SO effect leads to the locking of the spin direction along high-symmetry lines and to induced magnetic moment on pnictogen atoms (Fig. 1). Plotting the dispersion, we find that the nodal SDW is unstable due to the SO effect (Fig. 2). This claim is rigorously proven using Wigner-von Neumann type of symmetry arguments. A similar analysis is performed for the A_{1g} (s-wave) superconducting (SC) state. In the absence of spin orbit, the SC order parameter is spin-singlet characterized by three parameters. The spectral gap is anisotropic on the hole Fermi surfaces (FS), and anisotropic on the electron FS's. The relative values of the three parameters determine whether the SC state is s_{++}, s_{+-} or nodal-s wave state (Fig. 3). In the presence of SO coupling, there are additional, spin-triplet, pairing terms characterized by two more parameters. This results in the anisotropy of the spectral gap on both hole and electron FS's.



Results and Conclusions

In this work we construct the low-energy effective theory for iron-based superconductors. We study the irreducible representations of iron-based superconductors space group P4/nmm. This space group is non-symmorphic, leading to double degeneracy of all single-particle states and order parameters whose momentum is at the edge of the BZ. The low-energy states are therefore given by a six component spinor: 2 components representing the degenerate hole states at □, and 4 components for two doublets at M point. The resulting Hamiltonian acquires a block diagonal form allowing analytic approach to problems in iron-based superconductors, in contrast to any multi-orbital model. The parameters of the low-energy effective theory are obtained by matching the dispersion to 5- and 8-orbital models. Without the SO effect, the ground state spectrum has Dirac points and lines of degeneracy. The SO effect lifts these degeneracies at all points in the BZ and each band has only Kramers degeneracy; the exception is M point where each state must be 4-fold degenerate. The collinear SDW order lowers the symmetry and removes this 4-fold degeneracy. This state, while odd under the time-reversal (TR), is even under the product of the TR and inversion, thus preserving the Kramers degeneracy for each band. We show that, in the presence of SO coupling, the dispersion of collinear SDW cannot have Dirac points at any point in the BZ, thereby ruling out the nodal SDW state (Fig. 2). We also analyze coplanar SDW, where we find the Kramers degeneracy to be violated. The superconductivity is analyzed within the framework of the low-energy effective theory. All possible pairing terms are classified according to their symmetry and we concentrate on A1g (s-wave) pairing terms. In the absence of the SO effect, there are three such terms, representing pairing strength for the one doublet at □ and two doublet states at M, respectively. This pairing leads to isotropic and equal spectral gap for both hole FS's. The spectral gap for electron FS's is anisotropic and, depending on the relative strength of the pairing strengths, the SC state is s_{++}, s_{+-} or nodal-s wave state (Fig. 3). The SO effect introduces additional, spin-triplet, pairing terms. The spin-triplet pairing term for the states at □ point leads to anisotropy of the spectral gap on hole FS's. The spin-triplet pairing term for the states at M point contributes to already present anisotropy of the spectral gap on electron FS's. However, since the SO effect reconstructs the electron FS's, the anisotropy qualitatively changes from 2- to 4-fold.