Type-II Ising Pairing in Centrosymmetric Superconductors: Insights from First-Principles Calculations

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Abstract. The immunity of Ising superconductors to external magnetic fields arises from the spin-locking of paired electrons to an intrinsic Zeeman-like field [1]. In non-centrosymmetric crystalline materials, spin-momentum locking leads to type-I Ising pairing, where the direction of the intrinsic field can be inferred from spin expectation values. Conversely, in centrosymmetric crystals, electron spins locked to orbitals can form type-II Ising pairs, consisting of spin-orbit split doublets [2]. Due to time-reversal symmetry, these doublets remain spin-degenerate, making it challenging to determine the spin polarization of bands and the direction of spin-orbit fields.
In this work, we present an efficient approach for identifying Ising pairing in type-II Ising superconductors through first-principles calculations. By analyzing the anisotropy of the spin-mixing parameter and spin-orbital splittings, we extract the strength and direction of intrinsic Zeeman fields, which can be directly linked to the upper critical field Bc2. To complement our first-principles findings, we employ group theory to construct a detailed framework for spin-orbit coupling and spin mixing in the relevant bands forming Fermi pockets.
Our theoretical predictions for Bc2 in $PdTe_2$ align remarkably well with experimental values, demonstrating the robustness of our method in identifying Ising pairing [3]. Notably, contrary to conventional expectations based on spin-orbit locking, not all spin-orbit split doublets actively contribute to Ising pairing.

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