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Correlation-enhanced odd-parity inter-orbital singlet pairing in LiFeAs REZA NOURAFKAN, Universite de Sherbrooke, GABI KOTLIAR, Rutgers University, A.-M. S. TREMBLAY, Universite de Sherbrooke — The rich variety of iron-based superconductors and their complex electronic structure lead to a wide range of possibilities for gap symmetry and pairing components. We solved, in the two-Fe Brillouin zone, the full frequency-dependent linearized Eliashberg equations to investigate spin-fluctuations mediated Cooper pairing for LiFeAs . The magnetic excitations were calculated with the random phase approximation on a correlated electronic structure obtained with density functional theory and dynamical mean field theory. The interaction between electrons through Hund's coupling promotes both the intra-orbital $d_{xz(yz)}$ and the inter-orbital magnetic susceptibility. As a consequence, the leading pairing channel, conventional s^{+-}, acquires sizeable inter-orbital $d_{xy} - d_{xz(yz)}$ singlet pairing with odd parity under glide-plane symmetry. The combination of intra- and inter-orbital components makes the results consistent with available experiments on the angular dependence of the gaps observed on the different Fermi surfaces [1]. We also explain the difference in pairing symmetry between LiFeAs and LiFeP [2].
[1] R. Nourafkan, G. Kotliar, and A.-M.S. Tremblay, Phys. Rev. Lett. **117**, 137001 (2016). [2] R. Nourafkan, Phys. Rev. B **93**, 241116(R) (2016)

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