Abstract Submitted
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Correlation-enhanced odd-parity inter-orbital singlet pairing in the iron-pnictide superconductor LiFeAs[1] REZA NOURAFKAN, Université de Sherbrooke, GABRIEL KOTLIAR, Rutgers University, A.-M. S. TREMBLAY, Université 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. Here we solve in the 2-Fe Brillouin zone the full frequency-dependent linearized Eliashberg equations for LiFeAs with spin-fluctuation mediated pairing interactions. The magnetic excitations are calculated with the random phase approximation on a correlated electronic structure obtained with density functional theory and dynamical mean field theory. Correlations induce long-lived local moments with orbital-dependent dynamics. The interaction between electrons through Hunds coupling promotes both the intra-orbital $d_{xz(yz)}$ and the inter-orbital magnetic susceptibility. As a consequence, the leading pairing channel acquires sizeable inter-orbital d_{xy}-$d_{xz(yz)}$ singlet pairing with odd parity under glide-plane symmetry. These components reduce the superconducting gap magnitude induced by the intra-orbital components of the gap function at the electron pockets intersection where the Fe-d t_{2g} orbitals strongly mix. 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.

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