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Superconductivity from repulsion in LiFeAs: novel s-wave symmetry and potential time-reversal symmetry breaking ILYA EREMIN, FE-LIX AHN, Institut für Theoretische Physik III, Ruhr-Universität Bochum, JO-HANNES KNOLLE, Max-Planck Institut für Physik komplexer Systeme Dresden, VLADIMIR ZABOLOTNYY, S. BORISENKO, Leibniz-Institut für Festkörperund Werkstoffforschung Dresden, P.O. Box 270116, D-01171 Dresden, Germany, RODERICH MOESSNER, Max-Planck Institut für Physik komplexer Systeme Dresden, BERND BUCHNER, Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, P.O. Box 270116, D-01171 Dresden, Germany, ANDREY CHUBUKOV, Department of Physics, University of Wisconsin-Madison, Madison, Wisconsin 53706, USA — Using the ten orbital tight-binding model, derived from the ab-initio LDA calculations and fitted to the ARPES experiments, we analyze the structure of the superconducting gap in LiFeAs. We treat superconductivity as quasi-2D and decompose the pairing interaction for various k_z cuts into s- and d-wave components. Analyzing the leading superconducting instabilities we find that in addition to the conventional s^{+-} -wave superconducting order parameter where the gap changes sign between electron and hole pockets LiFeAs possesses another instability where the superconducting gap also changes sign between two smaller inner hole pockets. This occurs due to relatively large repulsion between these two small pockets and also relatively weak interaction between outer and inner hole pockets. The sizes of the gaps on the inner hole pockets is larger than the average value of the superconducting gap on the outer hole pockets and electron pockets which agrees with experimental data. Depending on the input parameters this gap structure is either a leading instability in the s-wave channel or a subleading one to the usual s^{+-} .

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