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The iron pnictides and chalcogenides, a DMFT perspective

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The complex multi-band nature of iron pnictides and chalchogenides makes the interplay of superconductivity with spin and orbital dynamics very intriguing, leading to very material dependent magnetic excitations, and pairing symmetries. We use the first-principles Dynamical Mean Field method, including ab-initio determined two-particle vertex function, to study the spin dynamics and superconducting pairing symmetry in a large number of iron-based superconductors. In iron compounds with high transition temperature, we find both the dispersive high-energy spin excitations, and very strong low energy commensurate or nearly commensurate spin response, suggesting that these low energy spin excitations play the dominat role in cooper pairing. We find three closely competing types of pairing symmetries, which take a very simple form in the space of active iron $3d$ orbitals, and differ only in the relative quantum mechanical phase of the xz, yz and xy orbital contributions. The extensively discussed s^{+-} symmetry appears when contributions from all orbitals have equal sign, while the opposite sign in xz and yz orbitals leads to the d wave symmetry. A novel orbital antiphase s^{+-} symmetry emerges when xy orbital has opposite sign to xz and yz orbitals. We propose that this orbital-antiphase pairing symmetry explains the puzzling variation of the experimentally observed superconducting gaps on all the Fermi surfaces of LiFeAs. This novel symmetry of the order parameter may be realized in other iron superconductors.