Superconductivity and Orbital Selectivity in a three-orbital Hubbard model for the iron pnictides: interplay of correlation and band structure

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The complexity of the interplay between various interaction mechanisms present in an iron-pnictide superconductor (IBS) makes it difficult to predict the behavior of the system [1],[2]. The particular multi-orbital structure and the interaction in the electronic system may be the trigger of the superconductive order. We focus on a 3-orbital tight-binding model that reproduces qualitatively the Fermi surfaces typical of the IBS, to which local interactions are added as with intra/inter-orbital Coulomb interaction (U/U') and Hund's coupling (J) [3],[4].

We perform a non-perturbative study thanks to a Variational Monte Carlo method which captures spatial correlations and can address superconductivity directly in two dimensions. The work aims to understand the behavior of the model for different doping values and how the different parts of the Hamiltonian influence the physics of the system. At fixed J/U for different hole doping values, the system transits to an orbital selective phase, for large enough values of the Coulomb repulsion. Orbital selectivity does not occur in the absence of Hund's coupling J and is characterized by having two of the three orbitals half-filled. Our most important finding is that, for certain doping values, orbital selectivity is accompanied by the emergence of superconductivity, mainly in the orbital with more than one electron per site. In the absence of Hund's coupling, also superconductivity is absent. Finally, we show that a realistic tight-binding model is necessary to obtain the correct symmetry of the superconducting gap.

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