Quantum Monte Carlo simulations for unconventional superconductors

Type of research: Theoretical/numerical

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The development of appropriate microscopic models is essential to elucidate the normal-state properties and the pairing mechanism of unconventional superconductors [1]. Typical examples are given by Copper-oxide materials, such as doped La_2CuO_4 and $YBaCu_3O_7$, but also include **Iron-based superconductors**, like doped LaFeAsO, $BaFe_2As_2$, and FeSe. In all these cases, a relatively high critical temperature can be obtained by chemical substitutions that effectively change the electron density in active Copper/Iron layers or by applying an external pressure. In particular, Iron-based superconductors are well known for their complex interplay between orbitals, spins, and lattice degrees of freedom and the competition between antiferromagnetism and superconductivity. These materials are mostly metallic and, therefore, good starting points are **effective low-energy models** that capture the electronic states near the Fermi level and their mutual interactions. However, in contrast to Cuprates, in Iron-based compounds, orbital fluctuations among the d shell of Iron atoms remain large down to low temperatures/energies. This fact implies that any effective model must necessarly contain orbital degrees of freedom, which are subject to Hubbard (density-density) and Hund (spin-spin) interactions, resulting in a rather complex lattice model. Furthermore, in similar electronic models, spin-orbit coupling may also lead to topological superconductivity, hosting exotic excitations (e.g., Majorana fermions) [2]. Finally, the role of **phonons** (that play a central role in the old theory developed by Bardeen-Cooper-Schrieffer for standard superconductors) has not been fully elucidated in both Cuprates and Iron-based superconductors.

The aim of the project is to investigate lattice models in which charge, spin, orbital, and lattice degrees of freedom are entangled together to find under which conditions superconductivity may emerge, determining the symmetry of the superconducting order parameter. Typical microscopic models are given by **two- or three-orbital Hubbard models on a two-dimensional square lattice**, with realistic band structures. The role of phonons may be considered in simplified one-orbital systems, to study the interplay and competition between superconductivity and charge-density waves within Su-Schrieffer-Heeger model, also in presence of a sizable electron-electron repulsion. These calculations are particularly relevant to identify the fundamental mechanisms leading to different phases of matter (superconductivity, charge/spin order...) and to describe a large variety of materials where electrons in d shells are the leading actors to determine the ultimate physical behavior [3].

This work is based upon **Jastrow-Slater wave functions** [4], which include electron correlations on top of a Slater determinant. Here, electron pairing can be easily included, as in the Resonating Valence Bond (RVB) states introduced long time ago by Anderson [5]. This approach allow one to have a rather flexible tool to describe a large variety of quantum states and predict the correct ground-state properties. Given the intrinsic strong-coupling character of the physical problem, these wave functions cannot be handled without an intensive numerical approach. Therefore, **quantum Monte Carlo methods** are necessary to treat the strong correlations beyond any mean-field or perturbative approaches. Thanks to significant methodological developments in quantum Monte Carlo methods, it is now possible to efficiently optimize many-body states [4]. Furthermore, the stability and the accuracy of these optimized wave functions can be further assessed by using improved projection Monte Carlo techniques. In this way, the Monte Carlo approach is really becoming competitive with standard methods used in the recent past.

Possible topics that will be considered along the Ph.D. work are:

- Determination of the ground-state phase diagram (including superconductivity and magnetism) of generic two- and three-orbital Hubbard models.
- Study of the interplay between charge/spin inhomogeneities and superconductivity due to the electron-phonon coupling.
- Study of the effect of a large spin-orbit coupling and the possibility to stabilize topological insulators and/or superconductors.
- Improvement of the present Jastrow-Slater wave functions by including the so-called backflow correlations in multi-orbital models.

The Ph.D. student will acquire skills for dealing with **strongly-interacting models on the lattice**, mainly by learing and using **numerical methods** (like exact Lanczos diagonalizations and variational/projection quantum Monte Carlo). At the end of the project, he is expected to pursue an independent reseach in the field, joining leading groups in the rest of the world.

Federico Becca's publications on the subject (and beyond) may be found at:

`http://www-dft.ts.infn.it/∼becca/`

Part of the work can be done in collaboration with **Dr L.F. Tocchio (Politecnico Torino)** and **Prof. S. Sorella (SISSA)**.

[1] D.J. Scalapino, Rev. Mod. Phys. **84**, 1383 (2012).

[2] M. Sato and Y. Ando, Rep. Prog. Phys. **80**, 076501 (2017).

[3] See for example, P. Fazekas, *Lecture Notes on Electron Correlation and Magnetism* (World Scientific, 1999).

[4] F. Becca and S. Sorella, *Quantum Monte Carlo Approaches for Correlated Systems* (Cambridge University Press, 2017)

[5] P.W. Anderson, Science **235**, 1196 (1987).