Quantum Monte Carlo simulations for highly-frustrated magnets

Type of research: Theoretical/numerical

Proponent: Federico Becca (UniTS)

For most of the last century, condensed matter physics has been dominated by the Landau's symmetry breaking theory. In this respect, by lowering the temperature, almost all forms of matter reorganize in order to generate some kind of long-range order (well known examples are given by the gas-liquid-solid transition or the paramagnetic-ferromagnetic one). However, in the recent past, there is a clear evidence for several cases that escape this standard description and keep a disordered nature down to very low temperatures. Exotic physical behaviors originate from quantum fluctuations that can be further enhanced by the competition among different kind of interactions (among spin, orbital and lattice degrees of freedom). This competition goes under the name of **frustration** and may eventually impede long-range ordering of the system [1]. The prototypical example is the Mott insulator that does not show any broken symmetry, including magnetic ordering. **Quantum spin liquids** form a novel class of matter where, despite the existence of strong exchange interactions, spins do not order down to zero temperature. The most striking aspects of these unconventional states are the presence of topological order (i.e., a robust ground-state degeneracy that is not related to any local order parameter) and the existence of fractional excitations (i.e., low-energy excitations having quantum numbers that are non-integer multiples of those of the constituents) [2]. Another remarkable feature is the appearence of gauge degrees of freedom, which emerge within their low-energy description, as exemplified within the Kitaev model [3].

The aim of the project is to investigate lattice models, which may describe realistic materials but still consider a restricted number of relevant low-energy degrees of freedom. The typical example is given by **Hubbard or Heisenberg models on generic D-dimensional lattices**. However, several materials require more complicated effective models with spin-orbit interactions, giving rise to Hamiltonians where spins and orbitals are highly entangled. In particular, we would like to consider Heisenberg-like models in presence of strong anisotropies on frustrated two-dimensional lattices (triangular, Kagome...), which are relevant to a variety of materials that show unconventional low-temperature properties, such as $YbMgGaO_4$ or $ZnCu_3(OH)_6Cl_2$. In addition, Kitaev-like interactions have been proved to be important in a wide range of compounds, including Na_2IrO_3 and α-Ru_3. Finally, the anisotropic Heisenberg model on the pyrochlore lattice represents a particularly challenging example, in which a quantum spin liquid has been proposed and whose low-energy description can be captured by an effective theory that is similar to quantum electrodynamics.

The paradigm of our approach is based upon the definition of correlated **Resonating Valence Bond (RVB) wave functions**. These states contain the most profound character of pure quantum phases, being described by a superposition of configurations in which spins form singlets but change partner from one configuration to the other. The RVB idea roots back to the original Pauling's theory of the chemical bond and it has been reformulated by Anderson to describe spin liquids and high-temperature superconductors [4]. Given the intrinsic strong-coupling character of the physical problem, RVB wave functions cannot be handled without an intensive numerical approach. In this regard, **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 [5]. 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:

- Characterization of the ground-state properties of Kitaev-Heisenberg models on various two-dimensional lattices.
- Magnetization curve and possible spin-liquid phases in presence of an external magnetic field (especially in the Kitaev model).
- Computation of the dynamical structure factor for frustrated spin models and characterization of the spin-liquid spectrum.
- Development of a variational quantum Monte Carlo methods to evaluate finite-temperature properties and comparison with available experiments.

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 **Prof. S. Sorella (SISSA)**. Collaborations with **Prof. R. Valenti (Frankfurt)** or **Prof. D. Poilblanc (Toulouse)** are also possible along the project.

[1] C. Lacroix, P. Mendels, and F. Mila, *Introduction to Frustrated Magnetism: Materials, Experiments, Theory* (Springer, 2013).

[2] L. Savary and L. Balents, Rep. Prog. Phys. **80**, 016502 (2017).

[3] A. Kitaev, Ann. Phys. **321**, 2 (2006).

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

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