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Ground-state and time-dependent properties of frustrated quantum antiferromagnets: from high-T_C superconductors to ultracold atoms

(M2 internship => PhD thesis project)

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Understanding the fundamental mechanisms underlain high critical temperature superconductivity (high-T_C SC) is one of the central problems in modern physics. Indeed, despite an impressive research effort carried on over the last three decades, crucial aspects such as how electronic correlations induce pairing of fermionic holes are still far from being fully clarified. In this respect, recent experimental developments open completely new intriguing perspectives. Specifically, ultracold atoms in optical lattices constitute a very promising setup to realize the properties of relevant Hamiltonians [1], also allowing for the estimates of time-dependent features of selected initial states. From a theoretical point of view, soon after the discovery of high-T_C SC in cuprates [2], the t-J model (tJM) has been proposed [3] as a minimal hamiltonian description of the physics of this compounds. The tJM, in the absence of holes (i.e., at half-filling) reduces to the spin-1/2 antiferromagnetic Heisenberg model (AHM) which captures essential traits of the insulating copper-oxide planes. The latter can turn superconducting when doped with mobile holes, whose presence is accounted in the tJM by adding to the AHM term a nearest-neighbor hole-hopping one. Despite its intuitive formulation, the study of the low temperature physics of the tJM, similarly to the case of the vast majority of strongly correlated frustrated/fermionic lattice models, remains a very challenging task. In fact, it lacks an analytical solution and standard unbiased numerical techniques based on computer simulations (e.g., Quantum Monte Carlo) cannot be adopted without uncontrolled approximations. An alternative viable option is provided by the variational approach, ultimately consisting in a parameterization (Ansatz) of the wave function (WF) in terms of adjustable coefficients. In this scheme, a fundamental bias is introduced by the adopted functional form for the Ansatz WF: a desirable one should therefore be systematically improvable, and able to capture the correct physics via a restricted number of variational parameters.

In this internship/thesis project we will focus on a general family of variational states known as Entangled-Plaquette-States (EPS) [4, 5], which has proven to give an accurate description of the ground-state of different frustrated quantum lattice models. In an EPS wave function, correlations between different groups of lattice sites, forming the so-called plaquettes, are explicitly encoded, and, being the various plaquettes entangled (i.e., overlapped) also those at distances exceeding the linear dimension of the plaquettes are generally well reproduced. Although the number of variational parameters scales exponentially with the number of sites included in a plaquette, accurate estimates are obtainable with plaquettes of manageable sizes. Furthermore, plaquettes can comprise sites at any chosen distance giving rise to an Ansatz potentially free of limitations in terms of its capability in describing long-range correlations and entanglement. For this reasons, the EPS WF also emerges as an appropriate tool to gain insight into out-of-equilibrium scenarios. It is indeed possible, in the context of the time dependent variational principle [6], to estimate the real-time dynamics of a non-eigenstate of a given Hamiltonian opening the possibility to investigate the time evolution of physical observables.

In this theoretical framework we can address a wide range of scientific questions of relevance to both condensed matter and atomic/molecular physics. For example:

1) How, in two spatial dimensions, frustration arising e.g., from competing interactions, particular lattice geometries or i(n a broad sense) from fermionic quantum statistics may suppress antiferromagnetic order leading to (novel) possibly disordered phases of matter at zero temperature ?

2) What are the dynamical properties of the state prepared by removing one or two electrons from the ground-state of the half-filled t-J model ?

3) What is the ground-state phase diagram of the t-J model at finite-hole concentration ?

The theoretical work will be conducted in collaboration with Tommaso Roscilde (ENS de Lyon) and Tommaso Comparin (ENS de Lyon), actively involved in the development and applications of the EPS Ansatz.

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