ÉCOLE DOCTORALE

Particules, hadrons, énergie et noyau: instrumentation, imagerie, cosmos et simulation (PHENIICS)

Title: Symmetry breaking and restoration for many-body problems treated on quantum computers

Keywords: Quantum Computation, Many-Body Problem, Symmetry Breaking/Symmetry Restoration.

Abstract: The Symmetry-Breaking/Symmetry-Restoration methodology is a well-established tool in many-body physics, which serves to enhance the approximation of a Hamiltonian's ground state energy within a variational framework. At its core, this technique involves intentionally breaking in the wave function ansatz the symmetries respected by the Hamiltonian during the search for the ground state. This process allows us to capture complex correlations between particles at a lower numerical cost compared to a symmetry-preserving framework. Given that the true ground state must be consistent with the problem symmetries, a symmetry-restoration step is a priori needed to project the symmetry-breaking ansatz back into the appropriate subspace of the total Hilbert space.

This thesis mainly investigates how to implement the symmetry-breaking/symmetry-restoration scheme using quantum computers. The Variational Quantum Eigensolver (VQE) is the quantum algorithm used for the variational component. Its goal is to prepare an approximation of the ground state using a parametric quantum state ansatz by minimizing the energy associated with the Hamiltonian. The Bardeen-Cooper-Schrieffer (BCS) ansatz was employed as a symmetry-breaking ansatz, and the applications were demonstrated using the pairing and Hubbard Hamiltonians. We also used the Jordan-Wigner transformation to encode the operators based on the Hamiltonians. With these elements, we can identify two ways of using the symmetry-breaking/symmetry-restoration process in conjunction with the VQE method: we can either vary the parameters of a symmetry-breaking ansatz before or after the symmetry restoration. The first approach is identified as Quantum Projection After Variation, while the latter is named Quantum Variation After Projection.

One of the achievements of this thesis is the development of diverse techniques for symmetry restoration. Some of them are based on the Quantum Phase Estimation (QPE) algorithm, including the Iterative QPE and Rodeo methods. We also investigated other techniques based on the quantum “Oracle” concept, such as the Oracle+Hadamard and Grover-Hoyer methods. The Linear Combination of Unitaries algorithm was used to either directly implement the projection or the oracle in the “Oracle”-based methods. We also adopt the Classical Shadow formalism to restore symmetries intending to optimize the quantum resources required for the symmetry-restoration step. The different methods for symmetry restoration are illustrated through the thesis for the particle number and total spin symmetries.

In the final part, we present hybrid quantum-classical techniques that can help extract valuable information about the low-lying spectrum of a Hamiltonian. Assuming we can accurately extract the Hamiltonian moments from their generating function using a quantum computer, we introduce two methods for spectra analysis: the t-expansion method, which combines imaginary time evolution and the Padé approximation, and the Krylov method, a quantum subspace expansion method that can provide information about the low-lying eigenvalues of the Hamiltonian and the evolution of the survival probability. Furthermore, we also present the Quantum Krylov method. This technique gives similar information to the Krylov method but without the need to estimate the Hamiltonian moments, a task that can be difficult on near-term quantum computers.