INTERNSHIP PROPOSAL

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Elucidating strongly correlated materials with noisy quantum computers

Strongly correlated materials are, by definition, materials for which easy classical computational approaches, such as mean-field theory, break down: they are typically unable to explain the exotic quantum phases---superconductivity, charge-density waves, Mott insulators---that these materials display. To explain those phenomena, exponentially costly, yet highly optimized, algorithms (Lanczos method, Monte-Carlo approaches, tensor-network methods) have been developed over the years, but still fail to reach physically interesting regimes due to their cost.

Quantum computers have been proposed to circumvent this exponential hurdle: thanks to their quantum properties, they provide, at least on paper, fast (polynomial) algorithms to tackle strongly correlated materials. In reality, however, the levels of noise inherent to current and near-term quantum processors severely challenge the promises of quantum computing, despite fast-paced progress in the number and quality of available qubits, with qubit numbers in the 10-100 range and gate error rates of about 0.1%. Thus, in practice, it is nowadays still better to use classical algorithms than quantum ones to elucidate the properties of strongly correlated materials.

The goal of this internship is to develop algorithmic methods to extend the reach of classical algorithms thanks to quantum algorithms. The approach will be to identify the most promising candidates on both---classical and quantum---sides and devise hybrid methods that play on their respective strengths. A typical first direction will be the use of (classical) embedding methods such as Dynamical Mean Field Theory (or simplified versions [1]) to reduce the problem to a smaller effective problem called an impurity problem. This impurity problem will then be solved with quantum algorithms (possibly supplemented with classical algorithms, for instance tensor networks as in [2], or Monte-Carlo algorithms as in [3]). Error mitigation techniques could be used to alleviate the effects of noise. The intern will benefit from high-performance computing power thanks to access to the Eviden Qaptiva platform, with large-scale simulation of noisy quantum computers, among others.

P. Besserve, T. Ayral, Physical Review B 105, 115108 (2022)
B. Anselme-Martin et al., arXiv:2305.19231 (2023)
W. Huggins et al., Nature 603, 416 (2022)

Condensed Matter Physics: YES Quantum Physics: YES Soft Matter and Biological Physics: Theoretical Physics:

NO YES