Strongly correlated materials via embedding methods: solving impurity models with a noisy quantum computer

Pauline Besserve[1,2*] and Thomas Ayral[1]
[1]*Atos Quantum Laboratory, Les Clayes-sous-Bois, France*
[2]*Centre de Physique Théorique, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France*

Modelling materials exhibiting strong electronic correlations is a notoriously difficult task as static mean field treatments are not able to capture typical many-body effects. A powerful way to address such systems are so-called embedding methods, retaining correlations on a few 'impurity' orbitals only. Yet, classical computers still reach their limits in this context as they are faced with either an exponential scaling or the fermionic sign problem.

In this work, we propose a hybrid quantum classical method to solve the two-dimensional Hubbard model using noisy quantum processors. We show that, by combining an advanced many-body embedding method, the Rotationally Invariant Slave Boson (RISB [1], equivalent to the Gutzwiller method [2] at the saddle-point level), and a variational algorithm, the Variational Quantum Eigensolver (VQE [3]), one can compute, even in the presence of quantum noise, and beyond a single impurity, the evolution of the quasiparticle weight as a function of the interaction strength. We go beyond previous works in this direction [4–6] by optimizing the use of quantum resources through the design of advanced variational states and an optimized orbital representation. This allows us to double the size of the impurity problem, reaching two impurities or equivalently eight qubits, while previous works were limited to two or four qubits. We carry out noisy simulations of the behavior of our hybrid method and show that it is robust to the noise levels that are reported on today's quantum processors. Finally, we argue that the method paves the way to larger impurity sizes and thus a controllable approximation of the solution to the Hubbard model.

[1] Frank Lechermann, Antoine Georges, Gabriel Kotliar, and Olivier Parcollet. Rotationally-invariant slave-boson formalism and momentum dependence of the quasiparticle weight. *Physical Review B*, 76(15):155102, October 2007. arXiv: 0704.1434.

[2] Nicola Lanatà, Yongxin Yao, Cai-Zhuang Wang, Kai-Ming Ho, and Gabriel Kotliar. Phase Diagram and Electronic Structure of Praseodymium and Plutonium. *Physical Review X*, 5(1):011008, January 2015.

[3] Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J. Love, Alán Aspuru-Guzik, and Jeremy L. O'Brien. A variational eigenvalue solver on a photonic quantum processor. *Nature Communications*, 5(1):4213, July 2014. Number: 1 Publisher: Nature Publishing Group.

[4] Trevor Keen, Thomas Maier, Steven Johnston, and Pavel Lougovski. Quantum-classical simulation of two-site dynamical mean-field theory on noisy quantum hardware. *arXiv:1910.09512 [cond-mat, physics:quant-ph]*, October 2019. arXiv: 1910.09512.

[5] I. Rungger, N. Fitzpatrick, H. Chen, C. H. Alderete, H. Apel, A. Cowtan, A. Patterson, D. Munoz Ramo, Y. Zhu, N. H. Nguyen, E. Grant, S. Chretien, L. Wossnig, N. M. Linke, and R. Duncan. Dynamical mean field theory algorithm and experiment on quantum computers. *arXiv:1910.04735 [cond-mat, physics:quant-ph]*, January 2020. arXiv: 1910.04735.

[6] Yongxin Yao, Feng Zhang, Cai-Zhuang Wang, Kai-Ming Ho, and Peter P. Orth. Gutzwiller Hybrid Quantum-Classical Computing Approach for Correlated Materials. *arXiv:2003.04211 [cond-mat, physics:physics]*, March 2020. arXiv: 2003.04211.

* pauline.besserve@atos.net