

Density functional theory for painted potential quantum simulators

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Description:

The purpose of this *theory of condensed matter* physics PhD project is to study the properties of cold atoms in painted potentials, using advanced simulation techniques to identify novel quantum technologies, building on our previous experience in this area [1,3,4,5,6]. Cold atoms in painted potentials are important because they are uniquely programmable with the potential to lead to novel quantum technologies, such as quantum simulators [1,2]. We need to understand the properties of painted potential quantum simulators because they offer a new paradigm of programmability in quantum technology [3,4,5]. We need to identify contemporary condensed matter systems that would benefit from development as quantum simulators, so that new insight can be gained into complex materials that are either hard or impossible to simulate computationally. Moreover, we need to work closely with experimentalists to ensure that our calculations are relevant to real implementations of quantum simulators.

This project will apply advanced simulation techniques to painted potential quantum simulators, specifically a density functional theory methodology that will be developed in-house. You will carry out density functional calculations in order to determine the properties of cold atom quantum simulators. You will carry out analytic calculations to understand how the properties of the quantum simulator align with contemporary problems in condensed matter physics. You will work closely with our experimental cold atoms group to identify applications of your techniques to real quantum systems. In the process, you will develop skills in simulation techniques, computer programming and mathematical techniques, which are key to the theory of condensed matter, and also highly transferrable to a variety of different academic disciplines and other careers.

References:

1. Experimental demonstration of painting arbitrary and dynamic potentials for Bose–Einstein condensates. K Henderson, C Ryu, C MacCormick and M G Boshier. *New J. Phys.* Vol. 11 043030 (2009)
2. Quantum simulations with ultracold atoms in optical lattices. C. Gross and I. Bloch. *Science*, Vol. 357, 995-1001 (2017)
3. Cold-atom quantum simulator to explore pairing, condensation, and pseudogaps in extended Hubbard-Holstein models. J. P. Hague, P. E. Kornilovitch, and C. MacCormick. *Phys. Rev. A* Vol. 102, 033333 (2020)
4. Implementation strategies for multiband quantum simulators of real materials. J. P. Hague and C. MacCormick. *Phys. Rev. A*, Vol. 95, 033636 (2017)

Continued

5. Bilayer of Rydberg atoms as a quantum simulator for unconventional superconductors. J. P. Hague, C. MacCormick. Phys. Rev. Lett. Vol. 109 (2012) 223001
6. Quantum simulation of electron-phonon interactions in strongly deformable materials. J.P. Hague, C. MacCormick. New Journal of Physics Vol. 14 (2012) 033019

Qualifications required:

Good first degree in physics or possibly related subject where quantum mechanics has been studied (e.g. applied mathematics, chemistry), preferably at master's level.