Do we really need Quantum Computers to simulate Quantum Chemistry?

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Abstract

The accurate calculation of the ground state of many-electron systems has been the central goal of quantum chemistry for the last 80 years. Exact methods, such as full CI, can only be applied to systems of a few electrons and it has long been assumed [1] that larger fermionic systems will only be simulated exactly on powerful "quantum computers".
Here we argue that this is not the case for a large class of realistic electronic systems, with up to ~50 electrons. The ground state of these fermion systems can be calculated using a very simple stochastic algorithm [2,3,4], based on a population dynamics of a set of *annihilating* walkers of positive and negative sign in the space of the Slater determinants of the system. We show that this algorithm can be used to solve difficult fermion systems to unprecedented accuracy, as exemplified by a recent application to the ionisation potential of the first row (3d) transition metal atoms [5]. Furthermore, we show that a replica trick allows the unbiased calculation of two-particle correlation functions [6], as well as excited states.

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[5] R Thomas, GH Booth, A Alavi, Phys Rev Lett, 114, 033001 (2015)
[6] C Overy, GH Booth, N Blunt, JJ Shepherd, A Alavi, J Chem Phys, 141, 244117, (2014)

Ali Alavi is a Director at the Max Planck Institute for Solid State Research in Stuttgart, and Professor of Theoretical Chemistry at the University of Cambridge. His research interests have spanned classical molecular dynamics simulation, density functional theory, surface chemistry and heterogeneous catalysis, and since about 2003, quantum simulations. With his group, he tries to understand how the various sign problems that arise in fermion systems can be solved, and how to do accurate electronic structure calculations, particularly in systems in which electronic correlations are strong.