Ab Initio Quantum Chemistry Methods, Computational Complexity, and Quantum Computation - DRAFT

Jacob P. Portes

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Abstract

The Self Consistent Field (SCF), Configuration Interaction (CI), and Multi-Configuration Self-Consistent Field (MCSCF) algorithms are introduced with an emphasis on computational cost and convergence. Second quantization notation is included where relevant. Recent efforts at polynomial cost full-CI via quantum phase estimation are explained.

1 Introduction

While much of the original motivation for quantum computation came from computationally difficult problems in chemistry and physics, most of the theoretical work of the past 30 years has focused on specialized algorithms in discrete algebra (for example, quantum factoring and quantum search algorithms). More recently, however, there has been a growing interest in quantum numerical methods for the simulation of physical systems such as multi-electron atoms and molecules. Many of these types of problems classically require exponential execution time relative to the number of interacting particles; quantum mechanically however, it has been shown that some of these problems can be executed in polynomial time.

Although these results are somewhat encouraging, they are certainly not panaceas to the many issues that plague computational quantum chemistry. This paper attempts to briefly outline a smattering of both classic-computational and quantum-computational algorithms for chemical simulation with a focus on theoretical motivation, convergence, and cost. We first introduce the traditional Self Consistent Field (SCF), the Configuration Interaction (CI), and the Multi-Configuration Self-Consistent Field (MCSCF) methods, including second quantization notation where relevant. We emphasize that while the best SCF procedures have third-order polynomial cost, and the best CI procedures have exponential cost, CI is often desired due to better convergence and accuracy. This explains why recent attempts to simulate electronic structure Hamiltonians using quantum computers focus on CI and not SCF. In the second part of this paper, we explain how polynomial cost CI is cleverly achieved by using quantum phase estimation, in recent efforts by Lloyd, Aspuru-Guzik, Whitfield, and others. We tentatively conclude, however, that the various (seemingly) necessary physical assumptions at the foundations of the abovementioned methods still

make third and fourth order polynomial cost prohibitively inefficient for all but the smallest multi-atomic and multi-molecular systems, and that convergence issues stemming from these assumptions only add insult to the injury.