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Doctoral Dissertation Assesment Report

Quantum computing approach to non-relativistic and relativistic molecular energy calculations

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One of the promising roles of (future) quantum computers is in quantum simulation. Even though it seems quantum systems should be well suited to simulate other quantum systems, this is often surprisingly difficult. Libor Veis shows us how one can utilize a quantum computer for interesting applications in quantum chemistry. The thesis is a very well organized and written (small typos and corrections will be communicated to the author separately). It starts with an introduction to quantum computing, algorithms and quantum chemical computation, and with the main body of the text built on three papers by the author (as first author) and collaborators.

The first three chapters form the theoretical basis of the thesis. There is a nice introduction to quantum computing, complexity and physical realizations. We learn about quantum algorithms (mainly the Quantum Fourier Transform), and especially phase estimation (PEA). Then the focus turns on quantum full configuration interaction method (qFCI) for calculating the molecular energies (polynomially scaling in the quantum case, exponentially in the classical case). There are three important building blocks. First, we must map the molecular Hamiltonian to a spin Hamiltonian of the quantum computer (requiring a reasonable mapping and lots of classical precalculation). Second, we try to prepare a suitable initial state (e.g. adiabatically). Third, we need to simulate a unitary transformation corresponding to time evolution (according to the Schrödinger equation) for a chosen time interval. This is the unitary on which we perform phase estimation.

The fourth and fifth chapter contain the results of classical simulations of the quantum computer (up to 15 qubits) running the above described algorithms. First, for a non-relativistic example of methylene, and then for the relativistic Hamiltonian of SbH. Especially the last result is groundbreaking, and has a promising experimental proposal described in Section 5.4. Such quantum simulations allow us to explore the FCI energies for ranges of parameters (e.g. molecular distances, angles), resulting in an energy landscape useful for understanding chemical reactions.

The thesis follows a clear, focused line of research concerning a hot topic (molecular energy calculations on a quantum computer), with novel interesting results. The work done here goes far beyond the seminal works in the field [ref. 10-12], and therefore, I recommend the dissertation to be recognized with a PhD. degree.

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Finally, let me add a few questions and remarks for the thesis defense.

Following up on the discussion in Section 1.4, I would like to hear a little more about "Hamiltonians typically occuring in chemical physics", and good-enough approximate solutions, as these seem essential as a basic step for later computations.

My most pressing questions are about Section 2.4 and the success probability. Is it the probability of getting a correct phase (for some eigenstate), or is it the probability of projecting to a desired eigenstate in the first place? Can we make this process unambiguous, i.e. identify when we have arrived at a trustworthy result? Are the ways of amplifying success probabilities even if the original p is less than 0.5? What is the meaning of the inset in Fig.2.11? How can one guarantee the same initial state preparation in the B-version of the iterative PEA? These questions also apply to Section 4.4. What does success/failure of the method mean there?

At the end of Section 3.1, there is a discussion of different mapping schemes. Is what we are doing here in some way crude, meaning that another mapping would naturally result in local interactions, implying local gates in the PEA?

In Section 3.2.1, it is not clear that the QMA-complexity manifests itself in a small gap. Small gaps for adiabatic state preparation can appear simply because we have chosen our initial Hamiltonian badly, or just happened to walk on an unlucky path.

In Fig.3.1, how do we evaluate the success probability of the adiabatic preparation and subsequent IPEA?

Would you gain anything by using higher-order Trotter approximations in (3.6)?

Section 4.1 would benefit from a short explanation of the multireference character of the lowest state of CH_2 and why it is interesting. Did you also try adiabatic preparation for the initial states here?

Finally, what is the bottleneck of the presented methods, the IPEA or the initial state preparation? Do you have an intuition about when ASP should work well and when not?