Outline for Quantum Computing Presentation 1

Content of Presentation

Breadth:

High-level overview of background:

First Principle Calculation:

The world around us is made of condensed matter, i.e. matter whose energy is low enough that it has condensed to form stable systems of atoms and molecules, usually in solid or liquid phases. The large variety of ways in which these systems can take form leads to a rich diversity of physical phenomena that is practically endless in scope.

Because of this, approaching the field of condensed matter physics from a theoretical or computational angle can be a very challenging task to undertake. For the most part, the way this is done is to pick a particular macroscopic phenomenon, which has been well studied experimentally, and to build empirical, or semi-empirical, models to describe the experimentally observed results. This often provides a good understanding of the physics of the system under study, and it is often possible to interpolate or extrapolate these models in order to predict the behaviour of systems under conditions not yet tested experimentally. However, due to the complexity of condensed matter systems, and the difficulty in building accurate models, the predictive power of such an approach can be severely limited.

The first principles approach to condensed matter theory is entirely different from this. It starts from what we know about all condensed matter systems - that they are made of atoms, which in turn are made of a positively charged nucleus, and a number of negatively charged electrons. The interactions between atoms, such as chemical and molecular bonding, are determined by the interactions of their constituent electrons and nuclei. All of the physics of condensed matter systems arises ultimately from these basic interactions. If we can model these interactions accurately, then all of the complex physical phenomena that arise from them should emerge naturally in our calculations.

The physics that describes the interaction of electrons and nuclei that is relevant to most problems in condensed matter is actually relatively simple. There are only two different types of particle involved, and the behaviour of these particles is mostly governed by basic quantum mechanics. What makes first principles calculations difficult is not so much the complexity of the physics, but rather the size of the problem in terms of a numerical formulation. The development of accurate and efficient theoretical and computational techniques for dealing with so many particles is therefore central to the ongoing research in this field.

Problem statement:

Exact first-principles calculations of molecular properties are currently intractable because their computational cost grows exponentially with both the number of atoms and basis set size.

Proposed quantum algorithm for quantum chemical calculations in a linear optic quantum computer. Obtaining the energies of the hydrogen molecule in a minimal basis.

Methodology:

1. Encoding a molecular wave function into qubits;
2. Simulating its time evolution using quantum logic gates;
3. Extracting the approximate energy using the phase estimation algorithm.

Major result:

Equal to the exact value of minimal basis, to a precision of ±2-20Eh

Depth:

Specific Algorithm:

IPEA

An algorithm to find eigenvalues for a Hermitian matrix. - relating to ground state energy of particles.

Evaluation and analysis:

Impacts on the research field:

Proposed an experiment to show that quantum computers can simulate particles.

Who should care:

Researcher in chemistry and quantum computing.

Why is this important:

Before this, simulating particle movement is just an idea. But this paper showed that with the development of quantum computers, we can simulate more complicated particles.

Is it believable:

Yes.

582 citations in 10 years

Limitations:

This is an experiment designed specifically to two-atom systems in the minimal basis. That's the simplest problem we can have. By doing this experiment, we can simply show that this system works, but how we can actually expand our result to complex problem is still unclear.

Quality of Presentation

Structure:

Outline the content of the talk?

Professional preparation and delivery:

Well rehearsed?
Slides well organized and clear?

Timing:

Fit properly in 30 mins?