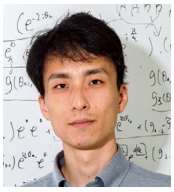
Next-generation information processing, Drug discovery/material design

Developing quantum algorithms for materials simulation



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Researchmap https://researchmap.jp/kosuke-mitarai?lang=en

Abstract

Quantum computers leverage the principles of quantum mechanics to perform computations that are impossible for classical computers. The hardware behind quantum computing is advancing rapidly, and I am confident that in the near future, quantum computers will solve problems that have long remained unsolvable. My research focuses on accelerating the practical applications of quantum computers through the development of software and algorithms. In particular, I am dedicated to creating algorithms that take full advantage of quantum computing's unique capabilities to simulate the microscopic world, including molecules, atoms, and electrons.

Background & Results

Quantum computers have the potential to simulate materials with an unprecedented level of accuracy, something classical computers could not achieve. My goal is to develop quantum algorithms that can predict the properties of materials with precision, provide insights into why these properties arise, and offer guidance for material design—all without requiring physical synthesis. If successful, this approach would have a profound impact on chemistry and physics, where material design is still largely based on experimental methods.

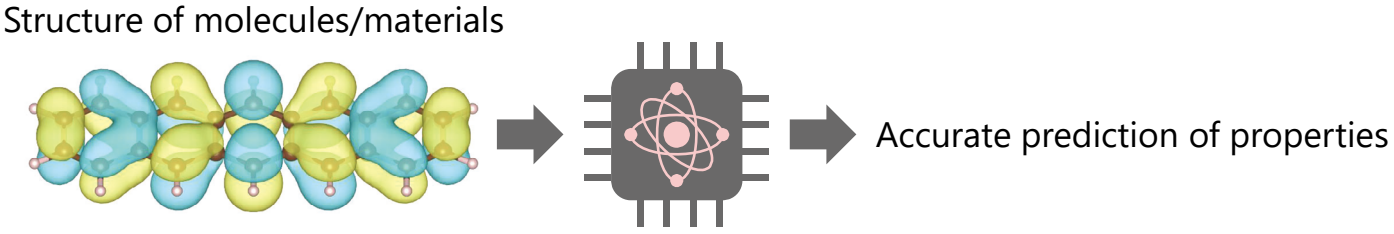
Significance of the research and Future perspective

One of my key research outcomes is the development of a computational approach called Quantum Selected Configuration Interaction (QSCI). This method enhances the traditional configuration interaction techniques used in classical computing by integrating quantum computational data, allowing for even greater precision. By relying on classical computers for most of the heavy lifting and using quantum computers to supplement calculations, QSCI reduces the computational burden on the quantum side, making it feasible to run on today's quantum hardware. In fact, IBM has applied our method to perform calculations on systems involving tens of electrons using currently available quantum devices [arXiv: 2405.05068v1].

While various methods have been proposed to simulate quantum systems on today's hardware, our approach offers two major advantages:

1. It significantly reduces the computational load placed on quantum computers.
2. Previous methods required additional quantum calculations to extract properties beyond energy, whereas our approach handles these calculations classically, improving efficiency.

Additionally, I am exploring algorithms designed for future large-scale quantum computers. One notable achievement is the development of a perturbative algorithm for quantum computation. Perturbation theory, a widely used technique in classical computing, approximates the behavior of a physical system by incrementally introducing small interactions. Our algorithm is the first to implement perturbative calculations on quantum computers, and we have also provided an analysis of the required quantum resources and computational time. Incorporating perturbation theory will enhance the interpretability of quantum simulation results, and we plan to further refine this approach to tackle more realistic physical systems.



Patent
Treatise Mitarai, Kosuke; Toyoizumi, Kiichiro; Mizukami, Wataru. Perturbation theory with quantum signal processing. Quantum. 2023, 7, 1000. doi: 10.22331/q-2023-05-12-1000
Kanno, Keita; Kohda, Masaya; Imai, Ryosuke et al. Quantum-Selected Configuration Interaction: classical diagonalization of Hamiltonians in subspaces selected by quantum computers. arXiv: 2302.11320 (2023). doi: 10.48550/arXiv.2302.11320
URL
Keyword quantum computer, ab-initio calculation, quantum chemistry calculation, material designs, quantum algorithms