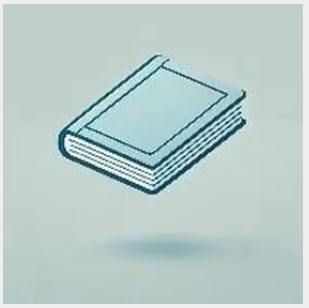
Huh / Kwon / Batista

Quantum Algorithms for Molecular Systems



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Quantum computing is revolutionizing our approach to solving complex problems in physics, chemistry, and biology. Among its most promising applications is the ability to determine quantum ground states—essential for understanding the fundamental properties of molecular systems, materials, and quantum systems. Historically, accessing these ground states has been computationally challenging, particularly for large and complex systems. Existing resources often focus on specific algorithms in isolation, leaving readers without a broader context or comparative insights. This book not only introduces the theoretical underpinnings of quantum algorithms but also provides practical guidance on their implementation and use cases (within budget). The chapters cover a broad spectrum of quantum algorithms for quantum state preparation, including foundational techniques like the Quantum Phase Estimation (QPE) and Variational Quantum Eigensolver (VQE), as well as advanced approaches such as the Quantum Krylov Subspace Diagonalization (QKSD), Quantum Filter Diagonalization (QFD), and quantum filter approaches. The text also provides other methods like Quantum Imaginary Time Evolution (QITE), resonant transition method, and dissipative quantum algorithm. Quantum Algorithms for Molecular Systems is primarily intended for researchers in the fields of quantum computing and quantum chemistry, with a particular focus on quantum algorithms for noisy intermediate-scale quantum (NISQ) computers and early fault-tolerant quantum computing (EFTQC). It is especially tailored to graduate students and post-doctoral fellows seeking to gain a strong foundation in the concepts and applications of quantum computing for chemistry. Additionally, researchers working on eigenvalue problems will benefit from the methodologies and insights provided.

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