Summit to: Atomic Scale and Quantum Mechanics

Quantum Algorithm for Multi-Slice Method

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EXTENDED ABSTRACT: Recently, there has been a dramatic increasing interest in quantum computing. It is an important topic how to apply quantum computing to practical physical simulation. In this work, we present a quantum algorithm for multi-slice method, which is based on quantum circuit model, to simulate electron wave function propagation and diffraction in thick specimens. To achieve this, we replace the core of classical multi-slice method to a quantum version. Especially, we replace classical fast Fourier transform (FFT), which is the most time-consuming part of the classical algorithm, to quantum Fourier transform (QFT), gaining an exponential speedup. Furthermore, with the size N of the system simulated increasing, comparing with $O(N)$ bits that are needed for classical algorithm, we only need $O(\log N)$ qubits for the quantum algorithm by taking advantage of entanglement of qubits. To verify the feasibility of the quantum algorithm, we simulated quantum circuit on classical computer to implement the quantum algorithm, and successfully obtained the results of electron density distribution and electron diffraction pattern for Au crystal as shown in figure 1 and figure 2 for example, which completely agree with those obtained by classical algorithm for multi-slice method. This work may indicate the possibility of applying quantum computing to electron wave function simulation and achieving quantum advantage in this method.

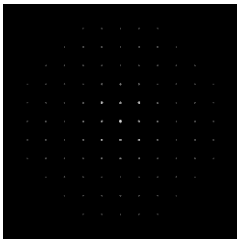

Figure 1. Electron diffraction pattern of Au crystal

Keywords： quantum algorithm; quantum computing; electron wave function simulation

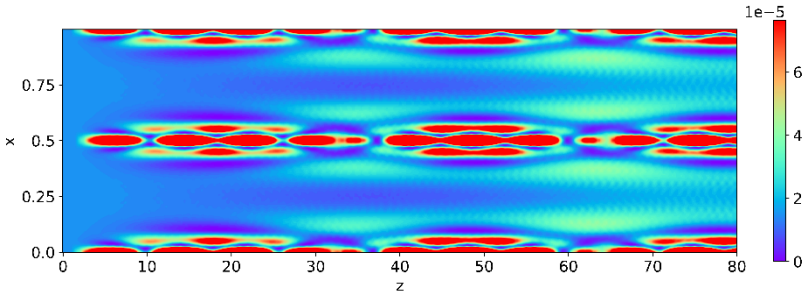

Figure 2. Cross sectional view of electron density distribution in Au crystal, the electron beam is in z axis direction.

BIOGRAPHY

Y.C. Wang has completed his Bachelor degree in 2018 from University of Science and Technology of China. And now he is pursuing PhD under Prof. Z.J. Ding.

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