Algorithm development for multi-dimensional and multi-particle simulation of quantum dynamics using NISQ devices

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One of the promising applications of quantum computing is a simulation of the dynamical processes of quantum systems, and several methods adopting quantum Fourier transform (QFT) have been proposed to simulate the dynamical processes of quantum systems in real space [1,2]. In order to perform a time propagation of a wave function of the system by QFT in which $\Theta(n^2)$ CNOT gates are used, we need to introduce $\Omega(n^2M)$ CNOT gates in the quantum circuit for the entire simulation, where n and M represent respectively the number of qubits and the number of time steps. Therefore, as long as noisy intermediate-scale quantum (NISQ) devices are adopted, it is not realistic to set the time step sufficiently short so that quantum dynamics can be simulated with a reasonable level of accuracy. Here, we propose an alternative approach to simulate quantum dynamics in real space on a NISQ device and demonstrate its performance for a one-dimensional one-particle system using *ibm_kawasaki* [3]. In this approach, the finite difference method is adopted to solve the Schrödinger equation and the wave function is represented by the one-hot encoding. The x coordinate is discretized by the 15 points, each of which is represented by one qubit. Consequently, a total of 15 qubits are used in quantum computing. The one-hot encoding results in the reduction of the number of CNOT gates from $\Omega(n^2M)$ to $O(nM)$, indicating that the numerical calculation on a NISQ device is expected to be less erroneous. The results of the time evolution of the wave packet of a particle in a one-dimensional harmonic potential are shown in Fig. 1. It is found that the results obtained by *ibm_kawasaki* agree well with those obtained by the simulator within the first few time steps, but the deviation becomes larger as the number of time steps increases.

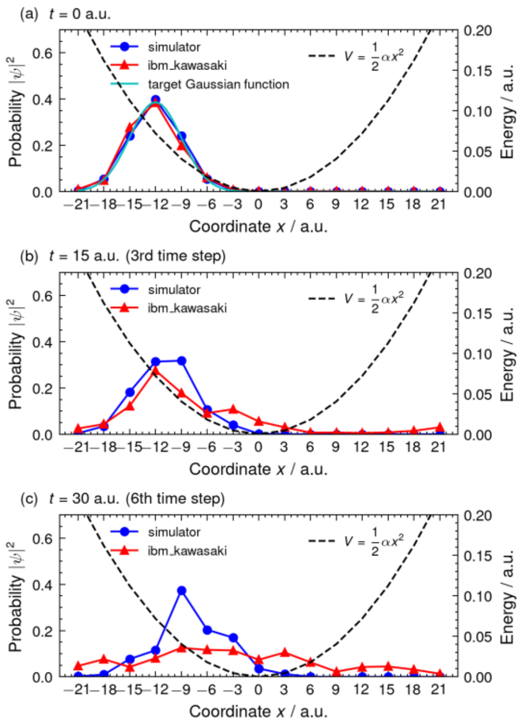

Fig. 1 Temporal evolution of $|\psi|^2$ at (a) $t = 0$ a.u., (b) $t = 15$ a.u., and (c) $t = 30$ a.u. obtained using a simulator with no noise (filled circles) and *ibm_kawasaki* (triangles). As the potential parameter, $\alpha = 0.001$ a.u. is adopted.

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