Quantum computation of time-dependent dynamics of H_2^+ in intense laser fields by quasi-stationary Floquet approach

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Recent advances in quantum computing technologies brought revolutionary changes in computational studies in fundamental and applied research fields. Even though currently available noisy intermediate-scale quantum computers (NISQ) suffer from a variety of errors, recent pioneering studies have revealed that electronic structure of small-sized molecules and the vibrational levels of small molecular systems can be calculated using NISQ with acceptable accuracies after appropriate error mitigations. However, so far, no systematic studies of time-dependent molecular systems interacting with an external light field have been achieved by quantum computing. In the present study, we apply quantum computing to a hydrogen molecular ion, H_2^+, interacting with an intense laser field, forming light-dressed states, and show how the quantum computation can describe well the temporal evolution of the light-dressed potentials of H_2^+ based on the quasi-stationary Floquet formalism[1].

In the calculation of the time-dependent potential energy curves created via the dipole coupling between the $1s\sigma_g$ and $2p\sigma_u$ states of H_2^+, a method called the subspace-search variational quantum eigensolver (SSVQE)[2] is adopted. The results of the calculations are summarized in Fig. 1, in which the light-dressed potentials given at the respective laser field intensities. In each frame of the figure, the dotted lines represent the potential energy curves calculated using the classical computer and the solid lines represent those calculated by the *ibm_kawasaki*[3] quantum computer. As shown in the figure, the energy gap at the one-photon crossing of the light-dressed potentials are well reproduced by the quantum computation. The good agreement can be ascribed to the fact that the circuit is composed of only one qubit, so that the crosstalk errors with nearby qubits are sufficiently small.

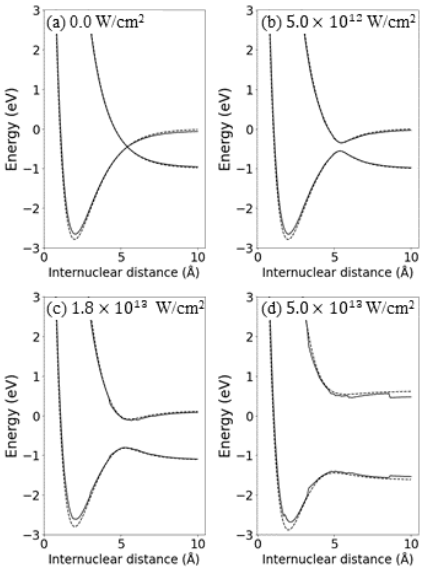

Fig. 1 Temporal evolution of the light-dressed potential energy curves created by the $1s\sigma_g$ and $2p\sigma_u$ states of H_2^+ calculated using a classical computer (dotted line) and the *ibm kawasaki* machine (solid line).

References:

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