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Molecular quantum computation by using ultrashort intense laser pulses under the influence of non-Markovian dissipation YUKIYOSHI OHTSUKI, Tohoku University & JST-CREST — We numerically study molecular quantum computation by combining an ensemble of molecular states and shaped ultrashort intense laser pulses through a case study of Grover's quantum search algorithm, in which qubits are implemented in the vibrational states of I2. In the simulation, the Grover iteration is divided into two basis operations, the so-called oracle and the inversion about mean operation, which are realized by laser pulses designed by an optimal control method within the density matrix formalism. These pulses perform Grover iteration with high accuracy although the lack of extreme precision leads to a slight reduction in the population associated with the solution to the search problem. The accuracy of the Grover iteration is shown to be improved by the normalization with respect to the "qubit population." The relaxation effects on the accuracy of the computation are systematically examined by using the non-Markovian master equation with phenomenological relaxation parameters. The gate pulses are designed under the influence of non-Markovian dissipation, in which the pulse design equation is solved by a newly proposed iteration algorithm.

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