

Abstract Submitted  
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**Effect of inter-mode anharmonicities on accuracy of gates in a two-qubit system of vibrational eigenstates.**<sup>1</sup> MEIYU ZHAO, DMITRI BABIKOV, Marquette University, Chemistry Department, Milwaukee, Wisconsin — We propose a quantum computer in which the qubits are implemented using the vibrational modes of a polyatomic molecule and the gates are applied using the optimally shaped femto-second infrared laser pulses. In order to study this system theoretically we developed a two-qubit model based on the normal vibration modes approximation afforded by the very low vibrational excitation regime. Optimal control theory and numerical time-propagation of the vibrational wavepackets are employed. One focus of this work is on understanding how the intra- and inter-mode anharmonicities affect the accuracy of quantum gates in such a system. Another emphasis is on achieving a proper control over the relative phase between the vibrational qubit states.

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