Optimal Control of Molecular Objectives: Quantum Computing and Cool Molecules

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Abstract. Shaped femtosecond laser pulses provide a flexible tool to achieve control even for complex molecular systems. We apply Optimal Control Theory (OCT) to find the optimal pulse shape for various molecular objectives. The optimization algorithms were extended to handle complex systems and to obtain experimentally feasible laser pulses. Furthermore we modified the standard OCT functional to handle multi target problems and provide counterintuitive STIRAP pulse sequences in the solution space. We these modifications we are able to design realistic and robust laser pulses for the given control tasks. Examples will be presented from two different areas: quantum computing and molecular cooling.

We proposed a new concept for molecular quantum computing defining molecular vibrations as qubits and shaped laser pulses as quantum gates addressing them. OCT is applied to realize these logic quantum gates. Results for global quantum gates will be presented and the question of decoherence in the selected computational sub-space will be addressed. The second example combines concepts of quantum optics with molecular physics to transfer an atomic into a molecular Bose-Einstein condensate (BEC) again with optimized laser fields. Solutions are found in the nanosecond as well as in the femtosecond regime.Both examples underline the wide range of possibilities of the optimal control approach.