Dynamics of Similar Quantum Systems

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Abstract

This talk is divided into two parts.

The first part presents an experimental paradigm, Optimal Dynamic Discrimination (ODD), of using shaped laser pulses to optimally discriminate similar quantum systems [1-4]. It is based on optimal control principles with the aid of closed loop learning algorithms. Simulations are carried out with a mixture of three similar species manipulated with shaped ultrafast laser, using static signals and time series signals, in the presence of detrimental factors such as environmental decoherence, laser noise, signal detection error and limited signal detection resolution. Numerical results not only demonstrate the capability of the ODD, but also show that ODD operates by drawing on constructive and destructive interference effects. The ODD principle has been successfully applied in two recent experiments [5,6].

The second part introduces a recently developed fast algorithm for evaluating the differences in the dynamics of similar quantum systems [7,8]. It is based on a semiclassical estimation of quantum fidelity, dephasing representation (DR). Its efficiency and accuracy have been demonstrated using the vibrational spectrum of H_2 and the photodissociation spectrum of CO_2 molecules. With DR, the accuracy of the quantum dynamics on an approximate PES can be estimated without actually running the quantum dynamics and without the need for a potential energy surface (PES) grid. Hence it can be used during the initial phase of a quantum dynamics simulation to decide whether the method chosen to compute a PES allows for a dynamics of the desired accuracy.

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