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Controllability and Trajectory Generation for Quantum Systems

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The laser control of chemical reactions is today a reality. Many experiments, carried out by many groups of researchers and in many different contexts and settings have demonstrated the feasibility of controlling the evolution of a quantum system using a laser field. The problem of dissociating a molecule along a prescribed channel, i.e. into prescribed channels ($ABC \rightarrow A + BC$, rather than $AB + C$, see [M. Shapiro and P. Brumer, J.Chem.Phys. 1993]), the alignment and orientation of a molecular system (as preliminary step toward a given chemical reaction [J.J. Larsen et al., Phys.Rev.Lett., 1999]), the control of some quantum devices (ion trap, quantum electrodynamics in cavity, ...) and etc, are some of the issues which has already been looked by chemists and physicists.

A standard modelling for the problem of the laser control of a molecular system involves the time-dependent Schrdinger equation

$$\iota\hbar\frac{\partial}{\partial t}\Psi = H_0\Psi - u(t)\mu\Psi$$

where $\Psi(t,.)$ describes the state of the system at time t. Here H_0 is the internal Hamiltonian, μ the coupling dipole moment and $u(t)$ is the external field intensity (H_0 and μ are self-adjoint operators defined on the Hilbert space where the system is defined).

A first approach for treating this model consists in decomposing the system on a finite dimensional modal approximation, so that H_0 and μ are changed to $n \times n$ Hermitian matrices. The controllability of such a system has been widely studied via the Lie algebra of commutativity of H_0/ι and μ/ι (see e.g. [H. Sussmann and V. Jurdjevic Journal of Differential Equations 1972],[Ramakrishna et al., Phys. Rev. A 1995] [G. Turinici and H. Rabitz, J. Phys. A 2003]). The important and not obvious problem then is to generate trajectories for such a finite dimensional system: optimal control (see e.g. [M. Zhu and H. Rabitz, J. Chem. Phys. 1998], [G. Turinici and Y. Maday J. Chem. Phys. 2003]),

Evolutionary algorithms (see e.g. [C. LeBris, H. Rabitz and G. Turinici, Phys. Rev. E, 2004.]), and some classical methods of dynamical systems (see e.g. [M. Mirrahimi and P. Rouchon, NOLCOS 2004], [W. Zhu and H. Rabitz, J. Chem. Phys. 2003]) are some of possible approaches in this direction.

Finally a very important issue to be explored in this domain correspond to the study of the control problem in its PDE configuration. A lot of works are to be done in this area: giving a mathematical sense to the controllability which interests the chemists or physicists, adapting different techniques of trajectory generation and studying well-posed ness of the problems, ... (see e.g. [E. Cances et al CRAS 2000], [L. Baudouin and J.P. Puel, Preprint UVSQ, 2004] and [K. Beauchard and J.M. Coron, Preprint Université d'Orsay, 2004]).