# Optimal Control of Wave-Packets: a Semiclassical Approach

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The control of the quantum dynamics of molecules, atoms, clusters, and chemical reactions is of great interest in chemical physics. Many of the existing methodologies currently used to attain controlled quantum dynamics employ the interaction of tailored light pulses with the molecule. Assuming that the light intensity is so low(High) that its coupling to matter only leads to adiabatic(nonadiabatic) Dynamical processes in the molecule. In both processes we can exploit the time-frequency coherence of light to actively interfere with the quantum state of the molecule to achieve a given control target [1]. The optimal control of the molecular state is performed by coupling a set of time-dependent control functions to the time-dependent Schrödinger equation of the closed molecular system. The optimal time-dependence of these control functions is reached by optimizing a cost functional, in a Hilbert space of a dimensionality that grows exponentially with the number of imposed constraints. Consequently, computational costs for finding the shape of the optimal pulse increase significantly as more constraints to the light parameters (amplitude, frequency, intensity, and polarization) are imposed. As a result, performing controlled dynamics with this methodology is limited only to very small molecular systems.

We have proposed recently An alternative way to find the optimal pulse-shaping, which has a weaker dependence on Hilbert spaces. Our proposal combines Herman-Kluk propagator to determine the optimal pulse shape and split-operator method to evaluate the time-propagation of the wavepacket, bypassing the numerical optimization step involved in traditional optimal control methodologies. As a result, we observed a dramatic reduction in the scaling of the pulse shape generation step.

We expect that our approach can be used to perform controlled wave-packet dynamics of bigger molecular systems at fractions of the computational costs of conventional methods. We anticipate that the proposed methodology may be applied in studies related to: the suppression of quantum chaos; the design of quantum error correction protocols; the implementation at the quantum level of closed-loop control through the terms of the stability matrix involved in the calculation of the time sliced Herman-Kluk prefactors, the quantum information processing via controlled rotational wave-packet dynamics, and the optimal control of nonradiative decay processes via conical intersections.

## References

[1] David J. Tannor, Stuart A. Rice, J. Chem. Phys, 83(10), 15.