Quantum chemistry and control: theoretical, experimental and numerical challeges

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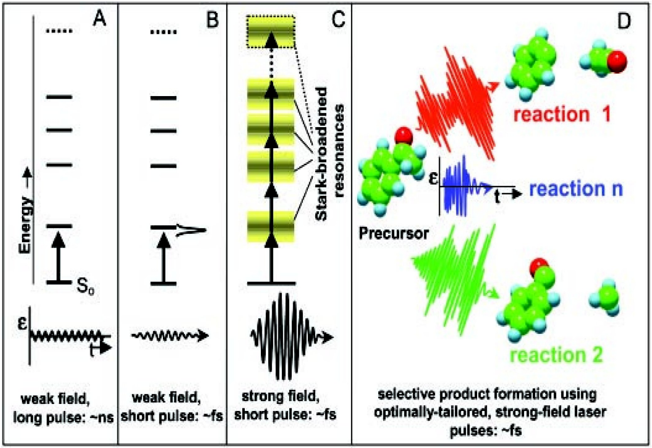


Figure: R. J. Levis, G.M. Menkir, and H. Rabitz. *Science*, 292:709–713, 2001

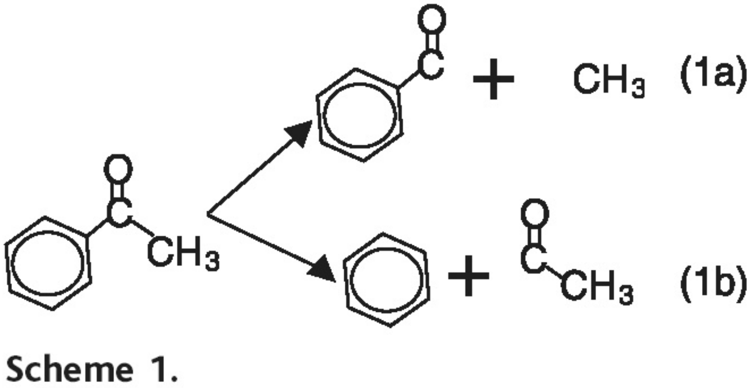
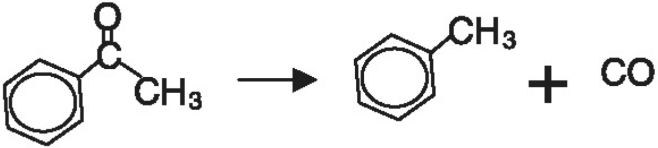


Figure: SELECTIVE dissociation of chemical bonds (laser induced).
Other examples: CF_3 or CH_3 from CH_3COCF_3 ...
(R. J. Levis, G.M. Menkir, and H. Rabitz. *Science*, 292:709–713, 2001).



Scheme 2.

Figure: Selective dissociation AND CREATION of chemical bonds (laser induced).

Other examples: CF_3 or CH_3 from CH_3COCF_3 ...

(R. J. Levis, G.M. Menkir, and H. Rabitz. *Science*, 292:709–713, 2001).

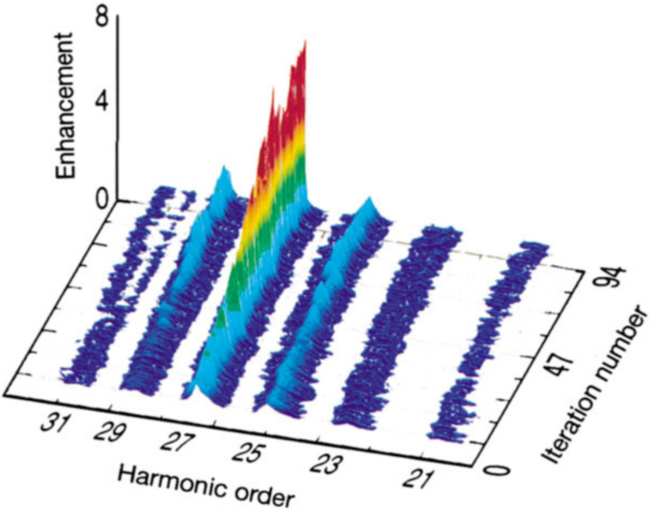


Figure: Experimental High Harmonic Generation (argon gas) obtain high frequency lasers from lower frequencies input pulses $\omega \longrightarrow n\omega$ (electron ionization that come back to the nuclear core) (R. Bartels et al. Nature, 406, 164, 2000).

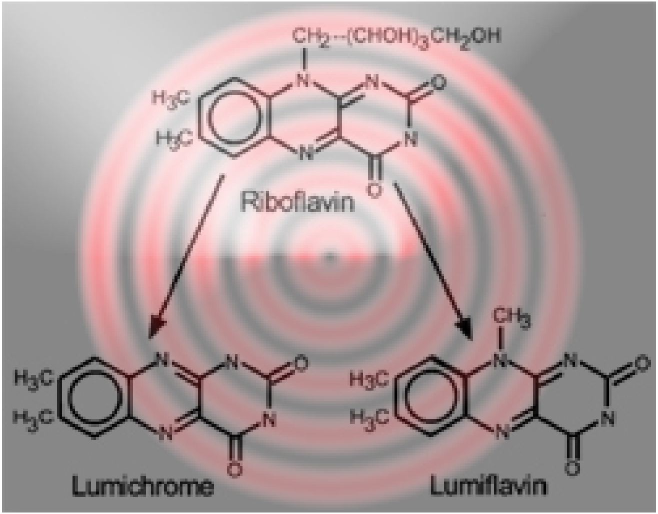


Figure: Studying the excited states of proteins. F. Courvoisier et al., App.Phys.Lett.

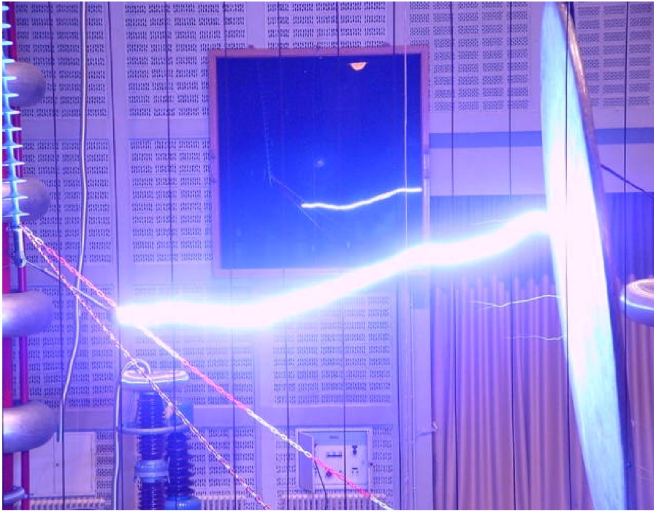


Figure: thunder control : experimental setting ; J. Kasparian Science, 301, 61 – 64 team of J.P.Wolf @ Lyon / Geneve , ...

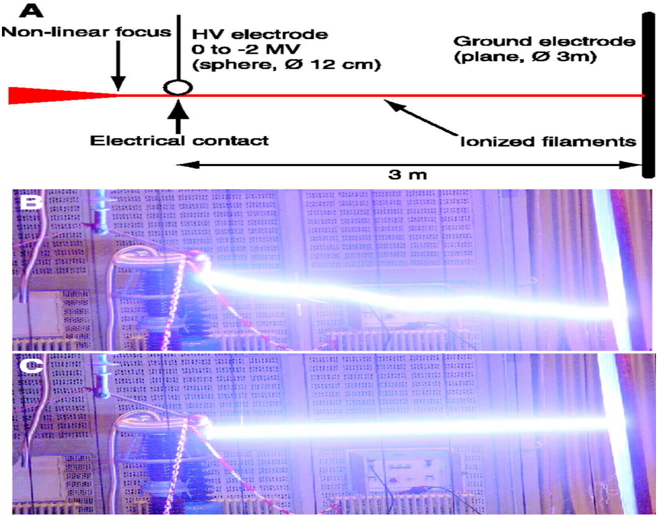


Figure: thunder control : (B) random discharges ; (C) guided by a laser filament ; J. Kasparian Science, 301, 61 – 64 team of J.P.Wolf @ Lyon / Geneve , ...

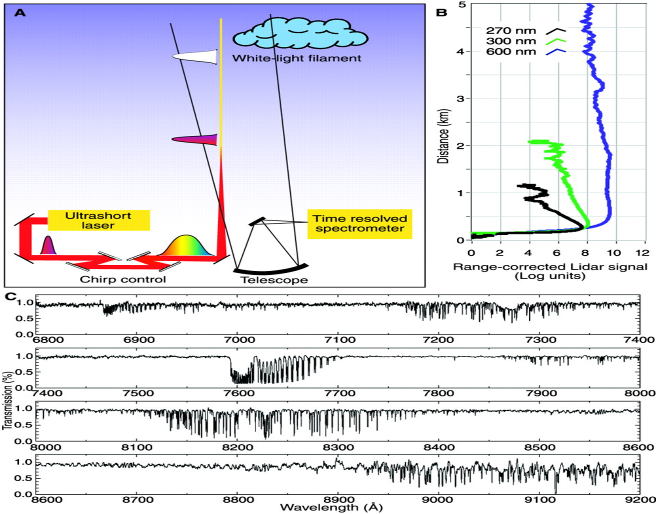


Figure: LIDAR = atmosphere detection; the pulse is tailored for an optimal reconstruction at the target : 20km = OK ! ; J. Kasparian Science, 301, 61 – 64

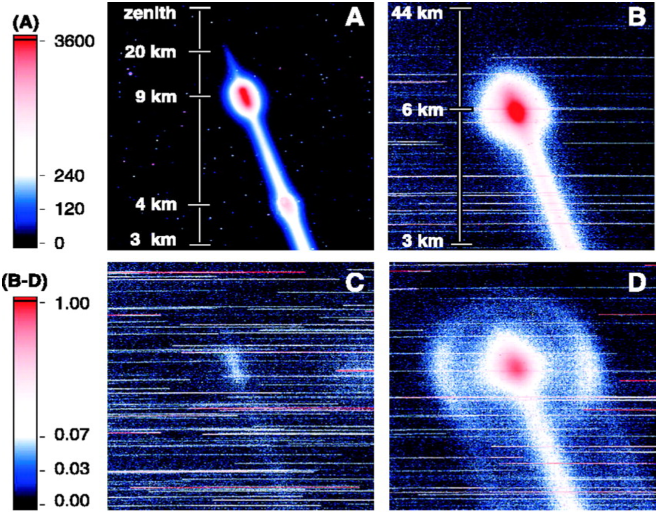


Figure: Creation of a white light of high intensity and spectral width ; J. Kasparian Science, 301, 61 – 64

Other applications

- EMERGENT technology
- creation of particular molecular states
- long term: logical gates for quantum computers
- fast “switch” in semiconductors
- ...

Outline

Single quantum system, bilinear control

Time dependent Schrödinger equation

$$\begin{cases} i\frac{\partial}{\partial t}\Psi(x,t) = H_0\Psi(x,t) \\ \Psi(x,t=0) = \Psi_0(x). \end{cases} \quad (1)$$

Add external BILINEAR interaction (e.g. laser)

$$\begin{cases} i\frac{\partial}{\partial t}\Psi(x,t) = (H_0 - \epsilon(t)\mu(x))\Psi(x,t) \\ \Psi(x,t=0) = \Psi_0(x) \end{cases} \quad (2)$$

Ex.: $H_0 = -\Delta + V(x)$, unbounded domain
Evolution on the unit sphere: $\|\Psi(t)\|_{L^2} = 1, \ \forall t \geq 0.$

Controllability

A system is controllable if for two arbitrary points Ψ_1 and Ψ_2 on the unit sphere (or other ensemble of admissible states) it can be steered from Ψ_1 to Ψ_2 with an admissible control.

Norm conservation : controllability is equivalent, up to a phase, to say that the projection to a target is $= 1$.

Galerkin discretization of the Time Dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(x,t) = (H_0 - \epsilon(t)\mu)\Psi(x,t)$$

- basis functions $\{\psi_i; i = 1, ..., N\}$, e.g. the eigenfunctions of the H_0: $H_0\psi_k = e_k\psi_k$
- wavefunction written as $\Psi = \sum_{k=1}^{N} c_k\psi_k$
- We will still denote by H_0 and μ the matrices $(N \times N)$ associated to the operators H_0 and μ : $H_{0\,kl} = \langle\psi_k|H_0|\psi_l\rangle$, $\mu_{kl} = \langle\psi_k|\mu|\psi_l\rangle$,

Lie algebra approaches

To assess controllability of

$$i\frac{\partial}{\partial t}\Psi(x,t) = (H_0 - \epsilon(t)\mu)\Psi(x,t)$$

construct the "dynamic" Lie algebra $L = Lie(-iH_0, -i\mu)$:

$$\begin{cases} \forall M_1, M_2 \in L,\ \forall \alpha, \beta \in \mathbf{R} : \alpha M_1 + \beta M_2 \in L \\ \forall M_1, M_2 \in L, [M_1, M_2] = M_1 M_2 - M_2 M_1 \in L \end{cases}$$

Theorem If $L = u(N)$ or $L = su(N)$ (the (null-traced) skew-hermitian matrices) then the system is controllable.

• (Albertini & D'Alessandro 2001) Controllability also true for L isomorphic to $sp(N/2)$ (unicity).
$sp(N/2) = \{M : M^* + M = 0, M^t J + JM = 0\}$ where J is a matrix unitary equivalent to $\begin{pmatrix} 0 & I_{N/2} \\ -I_{N/2} & 0 \end{pmatrix}$ and $I_{N/2}$ is the identity matrix of dimension $N/2$

Beyond bilinear setting: questions

- what about the system

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + \epsilon(t)\mu_1 + \epsilon(t)^2\mu_2\right]\Psi(x,t). \tag{3}$$

How is the controllability changed due to the constraint that the second control be the square of the first ?

- same for (rigid rotor interacting with linearly polarized pulse)

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + \epsilon(t)\mu_1 + \epsilon(t)^2\mu_2 + \epsilon(t)^3\mu_3\right]\Psi(x,t). \tag{4}$$

- same for (rigid rotor interacting with two-color linearly polarized pulse)

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + (E_1(t)^2 + E_2(t)^2)\mu_1 + E_1(t)^2\cdot E_2(t)\mu_2\right]\Psi(x,t). \tag{5}$$

Beyond bilinear setting

Theorem (G.T. 2005)

Consider the system

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + F_1(\epsilon(t))\mu_1 + \ldots + F_L(\epsilon(t))\mu_L\right]\Psi(x,t). \quad (6)$$

Suppose that the family $\{1, F_1, \ldots, F_L\}$ *is linearly independent and denote by* $L_{iH_0, i\mu_1, \ldots, i\mu_L}$ *the Lie algebra spanned by the matrices* $iH_0, i\mu_1, \ldots, i\mu_L$. *Then a sufficient condition for wave-function controllability of the equation* (6) *is*

$$L_{iH_0, i\mu_1, \ldots, i\mu_L} = su(N) \text{ or } u(N). \quad (7)$$

Remark : more precise results available (cf paper)

Remark : $\epsilon(t) \in \mathbb{R}^n$ (arbitrary n).

Beyond bilinear setting: applications

- By the Thm. since $1, \epsilon, \epsilon^2$ are independent the system

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + \epsilon(t)\mu_1 + \epsilon^2(t)\mu_2\right]\Psi(x,t). \tag{8}$$

is controllable under the same circumstances as

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + \epsilon_1(t)\mu_1 + \epsilon_2(t)\mu_2\right]\Psi(x,t). \tag{9}$$

with ϵ_1 and ϵ_2 independent controls. The fact that ϵ^2 in μ_2 is both positive and constraint by ϵ in μ_1 does not play any role for controllability.

Beyond bilinear setting: applications

- same for

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + \epsilon(t)\mu_1 + \epsilon(t)^2\mu_2 + \epsilon(t)^3\mu_3\right]\Psi(x,t). \quad (10)$$

- same for

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left[H_0 + (E_1(t)^2 + E_2(t)^2)\mu_1 + E_1(t)^2 \cdot E_2(t)\mu_2\right]\Psi(x,t). \quad (11)$$

Remark F_k need not be smooth ! For instance $F(\epsilon)$ can be $M \cdot sgn(\epsilon)$.

Outline

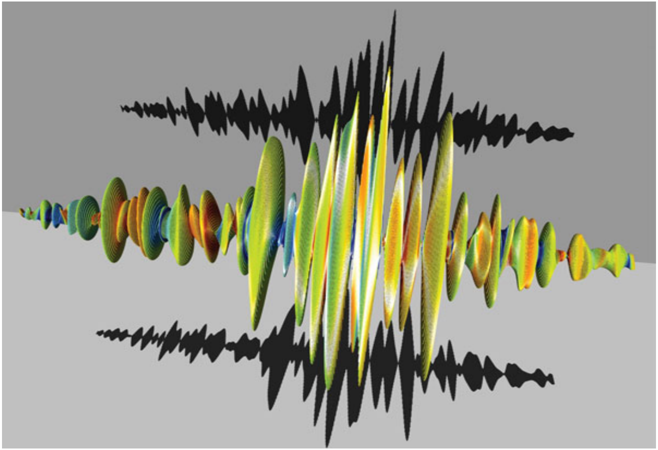


Figure: Polarization-shaped pulse, optimized for the ionization of potassium molecules. Ellipses represent the amplitude of the electric field, colours indicate different frequencies; Yaron Silberberg, Nature 430, 624-625 (2004)

Optimal Control formulation

Evolution equation:

$$i\frac{\partial}{\partial t}\Psi(x,t) = (H_0 - \epsilon(t)\mu)\Psi(x,t) \tag{12}$$

• optimal control: quality of a control expressed through a objective functional to optimize (maximize)
$J(\epsilon) = \langle\Psi(T)|O|\Psi(T)\rangle - \alpha\int_0^T \epsilon^2(t)dt$
Examples (O = projection to state ψ_{target}) Definition $< f|O|g > = < f, Og >$.
$J(\epsilon) = 2\Re\langle\psi_{target}|\psi(\cdot,T)\rangle - \int_0^T \alpha(t)\epsilon^2(t)dt$
$J(\epsilon) = 2 - \|\psi_{target} - \psi(\cdot,T)\|^2_{L^2} - \int_0^T \alpha(t)\epsilon^2(t)dt$

Standard optimization procedure

- construction of an extended objective functional i.e., add constraints through an *adjoint state* $\chi(x,t)$

$$J(\epsilon) = \langle \Psi(T)|O|\Psi(T)\rangle - \alpha \int_0^T \epsilon^2(t)dt$$
$$-2Re \int_0^T \left\langle \chi(x,t), \left\{ \frac{\partial}{\partial t} + i \cdot [H_0 - \epsilon(t)\mu] \right\} \Psi(x,t) \right\rangle$$

Partial derivatives

$$\frac{\delta J(\epsilon)}{\delta \epsilon} = -2\alpha\epsilon(t) - 2\mathrm{Im}\left\langle \chi|\mu|\Psi\right\rangle(t)$$

Euler-Lagrange critical point equation

$$\begin{cases} i\frac{\partial}{\partial t}\Psi(x,t) = (H_0 - \epsilon(t)\mu)\Psi(x,t) \\ \Psi(x, t=0) = \Psi_0(x) \end{cases}$$

$$\begin{cases} i\frac{\partial}{\partial t}\chi(x,t) = (H_0 - \epsilon(t)\mu)\chi(x,t) \\ \chi(x, t=T) = O\Psi(x,T) \end{cases}$$

$$\alpha\epsilon(t) = -\mathrm{Im}\,\langle\chi|\mu|\Psi\rangle\,(t)$$

- Chose a numerical algorithm to update the field $\epsilon(t)$, e.g.,

$$\epsilon^{n+1} = \epsilon^n + \frac{\delta J(\epsilon^n)}{\delta\epsilon} \tag{13}$$

slow convergence $\Longrightarrow$ complicated objective functional surface

Recent works by Alfio Borzi: functional surface seems to be very flat with many almost optimal regions.

Compute the optimal field $\epsilon(t)$ (Krotov cf. Tannor et. al 1992):
$(\chi^{k-1}, \epsilon^{k-1}, \Psi^{k-1}) \to (\chi^k, \epsilon^k, \Psi^k)$

$$\begin{cases} i\frac{\partial}{\partial t}\Psi^k(x,t) = (H_0 - \epsilon^k(t)\mu)\Psi^k(x,t) \\ \Psi^k(x, t=0) = \Psi_0(x) \end{cases} \tag{14}$$

$$\epsilon^k(t) = -\frac{1}{\alpha}\mathrm{Im}\langle\chi^{k-1}|\mu|\Psi^k\rangle(t) \tag{15}$$

$$\begin{cases} i\frac{\partial}{\partial t}\chi^k(x,t) = (H_0 - \epsilon^k(t)\mu)\chi^k(x,t) \\ \chi^k(x, t=T) = O\Psi^k(x,T) \end{cases} \tag{16}$$

In practice solve the equations (14)-(15) by propagating the non-linear equation

$$\begin{cases} i\frac{\partial}{\partial t}\Psi^k(x,t) = (H_0 + \frac{1}{\alpha}\mathrm{Im}\langle\chi^{k-1}|\mu|\Psi^k\rangle(t)\mu)\Psi^k(x,t) \\ \Psi^k(x, t=0) = \Psi_0(x) \end{cases} \tag{17}$$

Zhu & Rabitz formulation (1998)

$$\begin{cases} i\frac{\partial}{\partial t}\Psi^k(x,t) = (H_0 - \epsilon^k(t)\mu)\Psi^k(x,t) \\ \Psi^k(x,t=0) = \Psi_0(x) \end{cases}$$

$$\epsilon^k(t) = -\frac{1}{\alpha}\mathrm{Im}\langle\chi^{k-1}|\mu|\Psi^k\rangle(t)$$

$$\begin{cases} i\frac{\partial}{\partial t}\chi^k(x,t) = (H_0 - \tilde{\epsilon}^k(t)\mu)\chi^k(x,t) \\ \chi^k(x,t=T) = O\Psi^k(x,T) \end{cases}$$

$$\tilde{\epsilon}^k(t) = -\frac{1}{\alpha}\mathrm{Im}\langle\chi^k|\mu|\Psi^k\rangle(t)$$

THEOREM (W. Zhu and H. Rabitz. *J. Chem. Phys.*, 109:385–391, 1998.) Suppose O is a semi-positive definite (auto-adjoint) operator. Then for any $k \geq 0$: $J(\epsilon^{k+1}) \geq J(\epsilon^k)$, i.e. there is an improvement in the functional at any iteration.

A general class of algorithms (Y.Maday & G.T. 2002)

$$\begin{cases} i\frac{\partial}{\partial t}\Psi^k(x,t) = (H_0 - \epsilon^k(t)\mu)\Psi^k(x,t) \\ \Psi^k(x,t=0) = \Psi_0(x) \end{cases} \tag{18}$$

$$\epsilon^k(t) = (1-\delta)\tilde{\epsilon}^{k-1}(t) - \frac{\delta}{\alpha}\mathrm{Im}\langle\chi^{k-1}|\mu|\Psi^k\rangle(t) \tag{19}$$

$$\begin{cases} i\frac{\partial}{\partial t}\chi^k(x,t) = (H_0 - \tilde{\epsilon}^k(t)\mu)\chi^k(x,t) \\ \chi^k(x,t=T) = O\Psi^k(x,T) \end{cases} \tag{20}$$

$$\tilde{\epsilon}^k(t) = (1-\eta)\epsilon^k(t) - \frac{\eta}{\alpha}\mathrm{Im}\langle\chi^k|\mu|\Psi^k\rangle(t) \tag{21}$$

Particular cases: Zhu & Rabitz for $\delta = 1$ and $\eta = 1$; Krotov (Tannor et al. 1992) for $\delta = 1$ and $\eta = 0$.

THEOREM If O is an hermitian observable semi-positive definite then, for any $\eta, \delta \in [0, 2]$ $J(\epsilon^{k+1}) \geq J(\epsilon^k)$.

$$J(\epsilon^{k+1}) - J(\epsilon^k) =$$
$$\left\langle \Psi^{k+1}(T) - \Psi^k(T) | O | \Psi^{k+1}(T) - \Psi^k(T) \right\rangle +$$
$$\alpha \int_0^T (\frac{2}{\delta} - 1)(\epsilon^{k+1} - \tilde{\epsilon}^k)^2 + (\frac{2}{\eta} - 1)(\tilde{\epsilon}^k - \epsilon^k)^2$$

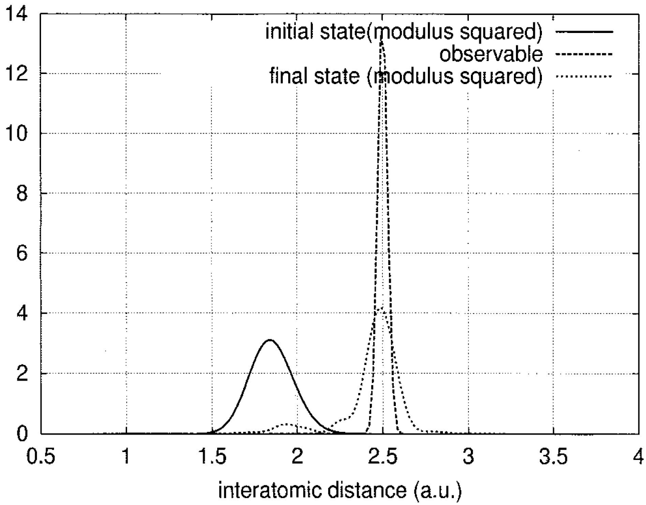


Figure: Successful quantum control for the localization observable.

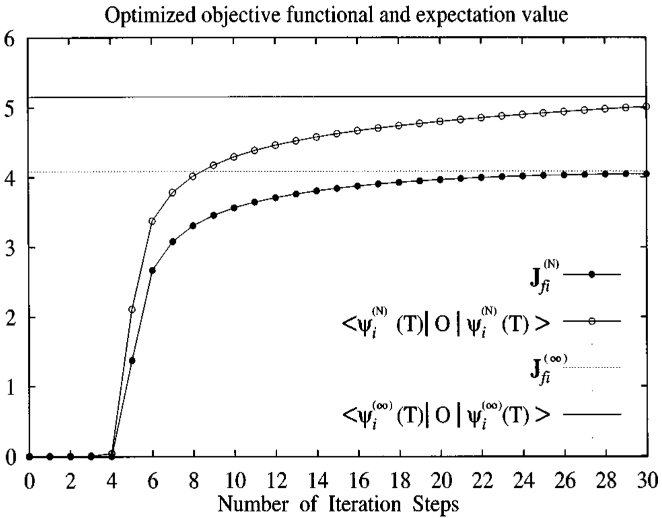


Figure: Typical monotonic convergence; two regions are obtained: initial finding of a descent direction (exploration) followed by the optimization step (exploitation).

Nonlinear situations: Euler-Lagrange

Quadratic intensity and quadratic penalization in ϵ:
$J(\epsilon) = \langle \Psi(T) | O | \Psi(T) \rangle - \alpha \int_0^T \epsilon^2(t) dt$
Critical point equations :

$$\begin{cases} i \frac{\partial}{\partial t} \Psi(x,t) = (H_0 - \epsilon^2(t)\mu)\Psi(x,t) \\ \Psi(x, t=0) = \Psi_0(x) \end{cases}$$

$$\begin{cases} i \frac{\partial}{\partial t} \chi(x,t) = (H_0 - \epsilon(t)^2\mu)\chi(x,t) \\ \chi(x, t=T) = O\Psi(x,T) \end{cases}$$

$$\alpha\epsilon(t) = -\epsilon(t) \mathrm{Im} \langle \chi | \mu | \Psi \rangle (t)$$

Remark: we obtain no useful formula to iterate on $\epsilon^k \longrightarrow \epsilon^{k+1}$!!

Nonlinear situations: Euler-Lagrange

3rd order intensity and quadratic penalization in ϵ:
$J(\epsilon) = \langle \Psi(T)|O|\Psi(T)\rangle - \alpha \int_0^T \epsilon^2(t)dt$
Critical point equations :

$$\begin{cases} i\frac{\partial}{\partial t}\Psi(x,t) = (H_0 - \epsilon^3(t)\mu)\Psi(x,t) \\ \Psi(x,t=0) = \Psi_0(x) \end{cases}$$

$$\begin{cases} i\frac{\partial}{\partial t}\chi(x,t) = (H_0 - \epsilon^3(t)\mu)\chi(x,t) \\ \chi(x,t=T) = O\Psi(x,T) \end{cases}$$

$$\alpha\epsilon(t) = -\epsilon^2(t)\mathrm{Im}\left\langle \chi|\mu|\Psi\right\rangle(t)$$

Remark: formula $\epsilon(t) = -\frac{\alpha}{\mathrm{Im}\langle\chi|\mu|\Psi\rangle(t)}$ may be unstable
Remark: we obtain no monotonicity if we just plug the formula to iterate on $\epsilon^k \to \epsilon^{k+1}$!!

Nonlinear situations: J. Salomon, C. Dion, G.T. for quadratic control

Let us consider $H(t) = BJ^2 - \mu_0 E(t) + \mu_1 E^2(t)$ and Ψ^k, χ^k the direct and respectivelly adjoint states.
Then the update formula

$$E(t) = -\frac{\mathrm{Im}\left\langle \Psi^k | \mu_0 | \chi^{k-1} \right\rangle (t)}{2\mathrm{Im}\left\langle \Psi^k | \mu_1 | \chi^{k-1} \right\rangle (t) - \alpha} \tag{22}$$

gives a monotonic algorithm (after computations).

Nonlinear situations: polynomial case of Ohtsuki and Nagakami

Let us consider $H(t) = \sum_{m=0}^{M} H_m E^m(t)$ and Ψ_1^k, ..., Ψ_m^k; χ_1^k, ..., χ_m^k direct and respectively adjoint states with the following rules (for situation $M = 2$ i.e. $H(t) = H_0 + E(t)H_1 + E(t)^2 H_2$):

- χ_1^k is propagated with $H(t) = H_0 + \frac{\bar{E}_1^k + E_2^{k-1}}{2} H_1 + \bar{E}_1^k \cdot E_2^{k-1} H_2$ and $\bar{E}_1^k$ is from the critical point formula with E_2^{k-1} on the right side

- Ψ_1^k is propagated with $H(t) = H_0 + \frac{E_1^k + E_2^{k-1}}{2} H_1 + E_1^k \cdot E_2^{k-1} H_2$ and E_1^k is from the critical point formula with E_2^{k-1} on the right side

Nonlinear situations: polynomial case of Ohtsuki and Nagakami

- χ_2^k is propagated with $H(t) = H_0 + \frac{\bar{E}_2^k + E_1^k}{2} H_1 + \bar{E}_2^k \cdot E_1^k H_2$ where $\bar{E}_2^k$ is from the critical point formula with E_1^k on the right side

- Ψ_2^k is propagated with $H(t) = H_0 + \frac{E_1^k + E_2^k}{2} H_1 + E_1^k \cdot E_2^k H_2$ and E_2^k is from the critical point formula with E_1^k on the right side

Then the resulting algorithm is monotonic algorithm (after computations :-)).

Nonlinear situations: polynomial case with different functional : M. Lapert, R. Tehini, G.T., D. Sugny

Let us consider $H(t) = \sum_{m=0}^{M} H_m E^m(t)$ and introduce in the cost functional the term $\int_0^T E^{2n}(t)$ instead of the classic $(n = 1)$ term. Set the following:
$E^k(t) =$ ...(equation involving $E^k(t)$, $E^{k-1}(t)$, χ^{k-1} and the current $\Psi^k(t)$) (cf. paper, eq 24) .

Then the resulting algorithm is monotonic algorithm (after computations :-)).

Remark: only one direct and adjoint iteration, but at the price of modifying the cost functional.

Nonlinear situations: construction and insights

Let us consider $H(t) = H(\epsilon(t))$ and compute $J(\epsilon') - J(\epsilon)$ for $J(\epsilon) = \langle \Psi(T), \Psi_{target} \rangle - \alpha \int_0^T \epsilon^2(t)dt$

$$J(\epsilon') - J(\epsilon) = -\int_0^T \langle \chi, [H(\epsilon'(t)) - H(\epsilon(t))]\Psi \rangle + \alpha(\epsilon'(t)^2 - \epsilon(t)^2)dt \tag{23}$$

It can be proved that the term is (under suitable conditions) of the form $J(\epsilon') - J(\epsilon) = -\int_0^T \Delta(\epsilon', \epsilon) \cdot (\epsilon'(t) - \epsilon(t))dt$ thus in order to be monotonic it is enough to choose $\Delta(\epsilon', \epsilon) = \theta(\epsilon'(t) - \epsilon(t))$.

Convergence of Lyapunov algorithms (joint works with M. Mirrahimi, P. Rouchon)

Let us consider $V(t) = \|\psi(t) - \psi_{target}(t)\|^2$ with $\psi_{target}(t)$ a stationary state i.e. $i\frac{\partial}{\partial t}\psi_{target}(x,t) = H_0\psi_{target}(x,t)$

$$\frac{dV}{dt} = 2\epsilon(t) Im\langle \mu\psi, \psi_{target}\rangle \tag{24}$$

e.g. $\epsilon(t) = -a Im\langle \mu\psi, \psi_{target}\rangle$ $(a \geq 0)$ $\frac{dV}{dt}$ will be negative thus the Lyapunov function V decreases.
Remark: we can characterize the limit points by computing all derivatives of V which have the form $Im\langle [H_0 ... [H_0, \mu] ...]\psi, \phi\rangle$.

Interpretation of monotonic and tracking algorithms

$J(\epsilon, \psi, \chi) = 2\Re\langle\psi_{target}|\psi(., T)\rangle - \int_0^T \alpha(t)\epsilon^2(t)dt$
$-2\Re \int_0^T \langle\chi(., t)|\partial_t + iH - \mu\epsilon(t)|\psi(., t)\rangle dt$

Euler-Lagrange equations:

$$\nabla_\chi J \rightarrow \begin{cases} i\frac{\partial}{\partial t}\psi(x,t) = (H - \varepsilon(t)\mu(x))\psi(x,t) \\ \psi(x, t=0) = \psi_0(x) \end{cases}$$

$$\nabla_\psi J \rightarrow \begin{cases} i\frac{\partial}{\partial t}\chi(x,t) = (H - \varepsilon(t)\mu(x))\chi(x,t) \\ \chi(x, t=T) = \psi_{target}(x) \end{cases}$$

$$\nabla_\epsilon J \rightarrow \quad \alpha(t)\varepsilon(t) = -\Im < \chi(., t)|\mu|\psi(., t) >$$

Interpretation of monotonic and tracking algorithms

At time t, "best guess for a solution" is $\overline{\epsilon} = \epsilon \cdot \chi_{[0,t]} + \epsilon_{ref} \cdot \chi_{[t,T]}$.

Forward objective functional (easily to compute at time "t"):
$i\frac{\partial}{\partial t}\psi_{ref}(x,t) = (H - \epsilon_{ref}(t)\mu)\,\psi_{ref}(x,t)$, $\psi_{ref}(T) = \psi_{target}$.

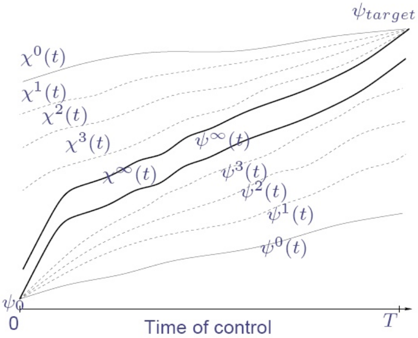
$$J_{fwd}(\epsilon, t; \epsilon_{ref}) = \int_0^t \alpha\epsilon^2(t)dt + \int_t^T \alpha{\epsilon_{ref}}^2(t)dt + \|\psi_{ref}(t) - \psi(t)\|^2.$$

Theorem (G.T., Proc. 44th IEEE CDC-ECC Sevilla, Spain, Dec. 2005. ; G. T., J. Salomon, J. Chem. Phys. 124:074102 (2006).): $J(\overline{\epsilon}) = J_{fwd}(\epsilon, t; \epsilon_{ref})$.

Decisions on the optimality of some control can be made locally e.g. by monotonic algorithms that ensure $J_{fwd}(\epsilon, t; \epsilon_{ref})$ is decreasing locally in time.

Interpretation of monotonic and tracking algorithms

Evolving state ψ^k approaches monotonically reference ψ^k_{ref}. No optimization during the backward propagation (i.e. $\tilde{\varepsilon}^{k+1} = \epsilon^{k+1}$), imply $\|\psi^{k+1}_{ref} - \psi^{k+1}\| = cst$. The shrinking distance between the two trajectories ensures the progression of the quality functional toward optimal values. The optimal couple of trajectories will be a tube whose nonzero width is related to the driving laser field fluence penalty α.



Outline

Robustness to noise (joint work with Adrian Zalinescu, Iasi)

SDE ("random laser" approach)

$$i d\Psi(x,t) = (H_0 - \epsilon(t)\mu)\Psi(x,t)dt - \sigma\mu\Psi(x,t)dW_t \tag{25}$$

Goal: maximize the functional (OCT)

$$J(\varepsilon) := \mathbb{E}\left\langle \Psi(T) \left| O \right| \Psi(T) \right\rangle - \alpha \int_0^T \varepsilon^2(t)\, dt.$$

The associated backward SDE is

$$\begin{aligned} i d\chi(x,t) &= \left[(H_0 - \varepsilon(t)\mu)\chi(x,t) - \sigma\mu Z(x,t) \right] dt - iZ(x,t)\, dW_t \\ \chi(x,T) &= O\Psi(x,T). \end{aligned} \tag{26}$$

The term Z makes χ adapted with respect to the filtration generated by W_t.

Robustness to noise

$$id\Psi^k(x,t) = \left(H_0 - \varepsilon^k(t)\mu\right)\Psi^k(x,t)\,dt - \sigma\mu\Psi^k(x,t)\,dW_t;$$
$$\Psi^k(x,0) = \Psi_0(x);$$
$$\varepsilon^k(t) := (1-\delta)\tilde{\varepsilon}^{k-1}(t) - \frac{\delta}{\alpha}\mathbb{E}\,\mathrm{Im}\left\langle\chi^{k-1}|\mu|\Psi^k\right\rangle(t);$$
$$id\chi^k(x,t) = \left[\left(H_0 - \tilde{\varepsilon}^k(t)\mu\right)\chi(x,t) - \sigma\mu Z^k(x,t)\right]dt - iZ^k(x,t$$
$$\chi^k(x,T) = O\Psi^k(x,T)$$
$$\tilde{\varepsilon}^k(t) := (1-\eta)\varepsilon^k(t) - \frac{\eta}{\alpha}\mathbb{E}\,\mathrm{Im}\left\langle\chi^k|\mu|\Psi^k\right\rangle(t).$$

Theorem (G.T. & A. Zalinescu 08)

The algorithm is monotonic i.e. $J(\epsilon^{n+1}) \geq J(\epsilon^n)$.

Numerical problem: computation of the conditional expectation to

Convergence of the algorithms (joint work with Catalin Lefter, Iasi

• Question : for $H = H_0 + \epsilon\mu + \epsilon^2\alpha$ does a Lyapunov type control converges, and to what ?
• this is a follow-up of a work with Mazyar Mirrahimi for the linear case (Lyapounov formulation), but same arguments fail (despite the fact that controllability is the same !);