Control Problems for Schrödinger Equations and Hartree-Fock Systems

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Bastille day !

Outline

Motivation. Control

We can act on a closed quantum system via an electric field deriving from a potential performed for example by laser beams or a magnetic field (which will not be considered here).
Control problems for these systems ask the following questions : can we choose the external (electric) potential in order to obtain a “desired” behavior of the solution?
This has to be made precise.

Motivation. Control

Schrödinger equation (all constants are taken equal to one)

$$\begin{cases} i\partial_t \psi + \Delta\psi + V_0\psi + V_1\psi + ... = 0, & t \in (0,T) \\ \psi(t=0) = \psi_0, \end{cases}$$

V_0 internal potential : Coulombian attraction, harmonic oscillator,....
V_1 external potential (control)
.... : nonlinear terms etc.

Exact Controllability

Given an initial state ψ_0 and a target state ψ_1, can we find a potential V_1 such that

$$\psi(0) = \psi_0, \quad \text{and} \quad \psi(T) = \psi_1$$

Many mathematical difficulties. Very few results up to now.
One of the main directions of research. Hope for better results soon.....
K.Beauchard, C.Laurent, J-M.Coron, J.P.P., ...
Strange remark (for bounded domains) : only values of the potential near the boundary seem important.....
Approximate controllability using finite dimensional approximations : U. Boscain and collaborators.

Quantum Information Theory

Trapped ions or cubits (one or two) : two level system stabilized by a harmonic oscillator. Very rapidly oscillating potential with phase depending on the position.
How to drive a given initial data to a prescribed final state ?
Creation of quantum logic gates, etc.
Some work done on approximate controllability (P.Rouchon, S. Ervedoza-J.P.P.).

Quantum Chemistry

Breaking of molecules to obtain desired states, etc.
Many groups working on Optimal Control in these directions including numerical treatment.
H. Rabitz and collaborators.
C. Le Bris, E. Cances and collaborators.
G. Turinici and collaborators.
J.P.P.-L.Beaudouin for mathematical analysis.
Optimal Control : To minimize a functional in which enters the distance from the solution to the target at time T.
Here : case of a hydrogenoid atom subject to an external electric field.
First step : linearized model concerning the wave function of the electron, the position of the nucleus being prescribed, even if not fixed.
Second step ; coupled system electron-nucleus in the Hartree-Fock approximation.

Mathematical model I

Position of the nucleus : $a(t)$ given function.
Linear Schrödinger equation with Coulombian attraction from the nucleus and external electric potential.

$$\begin{cases} i\partial_t u + \Delta u + \dfrac{u}{|x-a(t)|} + V_1(x,t)u = 0, & (x,t) \in \mathbb{R}^3 \times (0,T) \\ u(x,0) = u_0(x), & x \in \mathbb{R}^3 \end{cases}$$

where the external electric potential V_1 takes its values in $\mathbb{R}$.
This equation preserves the L^2 norm for the solution.

Mathematical model I

Remarks :
-V_1 can be unbounded, for example if the electric field is constant....
-Even if $a(.)$ is very regular but not zero, if we take the derivative in time we have a very singular potential.....
We define

$$\begin{aligned} H_1 &= \left\{ v \in L^2(\mathbb{R}^3),\ \int_{\mathbb{R}^3} (1+|x|^2)|v(x)|^2\,dx < +\infty \right\} \\ H_2 &= \left\{ v \in L^2(\mathbb{R}^3),\ \int_{\mathbb{R}^3} (1+|x|^2)^2|v(x)|^2\,dx < +\infty \right\}. \end{aligned}$$

One can notice that H_1 and H_2 are respectively the images of H^1 and H^2 under the Fourier transform.

Result for Model I

We need a result of existence uniqueness and regularity for this equation (Beaudouin-Kavian-Puel)

Theorem

Let $T > 0$ be an arbitrary time and let a and the potential V_1 satisfy

$$\begin{aligned}
&a \in W^{2,1}(0,T),\\
&(1+|x|^2)^{-1} V_1 \in L^\infty((0,T)\times\mathbb{R}^3),\\
&(1+|x|^2)^{-1}\partial_t V_1 \in L^1(0,T;L^\infty) \ \ \textit{and}\\
&(1+|x|^2)^{-1}\nabla V_1 \in L^1(0,T;L^\infty).
\end{aligned}$$

for any $u_0 \in H^2 \cap H_2$, there exists a unique solution u with

$$u \in L^\infty(0,T;H^2\cap H_2) \ \ \textit{and} \ \ \partial_t u \in L^\infty(0,T;L^2)$$

In fact the solution is continuous with values in $H^1 \cap H_1$ and weakly continuous with values in $H^2 \cap H_2$.

Estimate :
If for some $\alpha > 0$ and $\rho > 0$,

$$\Big|a\Big|_{W^{2,1}(0,T)} \leq \alpha \quad \textit{and}$$
$$\Big|(1+|x|^2)^{-1}V_1\Big|_{W^{1,1}(0,T,L^\infty)} + \Big|(1+|x|^2)^{-1}\nabla V_1\Big|_{L^1(0,T,L^\infty)} \leq \rho$$

then there exists a non negative constant $C_{T,\alpha,\rho}$ depending on T, α and ρ such that

$$\|u\|_{L^\infty(0,T;H^2\cap H_2)} + \|\partial_t u\|_{L^\infty(0,T;L^2)} \leq C_{T,\alpha,\rho}\|u_0\|_{H^2\cap H_2}.$$

Model I. Control

For every potential V_1 in a suitable class we have a solution.
Can we choose the potential such that the solution at time T has a desired property, for example to be as close as possible to a prescribed target u_1?
Exact controllability : can we obtain $u(T) = u_1$?
Very few results in this sense and only for the simplest cases : 1-d and without Coulombian potential (Beauchard, Beauchard-Laurent). This is a major direction of research.
Approximate controllability : can we obtain $u(T) - u_1$ as small as we want? Some results without singular potentials using Galerkin approximation and finite dimensional control (Boscain-Chambrion-Sigalotti and collaborators). Some results for systems modeling trapped ions with very rapidly oscillating potentials using approximate equations (Ervedoza-Puel).
For the present case, no result of controllability.

Model I. Bilinear Optimal Control

The electric potential V_1 is the control, and if $u_1 \in L^2$ is a given target, the problem reads:

$$\text{Find a minimizer } V_1 \in H \text{ for}$$
$$\inf\{J(V_1),\ V_1 \in H\}$$

where

$$H := \left\{ V,\ \left(1+|x|^2\right)^{-\frac{1}{2}} V \in H^1(0,T;W) \right\} \tag{1}$$

with W an Hilbert space such that $W \hookrightarrow W^{1,\infty}$,

$$J(V) = \frac{1}{2}\int_{\mathbb{R}^3} |u(T)-u_1|^2\,dx + \frac{r}{2}\|V\|_H^2 \text{ with } r>0,$$

Also find an optimality condition which can be interpreted..

Theorem

There exists an optimal control V_1 such that

$$J(V_1) = \inf_{V \in H} J(V)$$

and it satisfies the optimality condition:

$$\forall \delta V \in H, \quad r\langle V_1, \delta V \rangle_H = Im \int_0^T \int_{\mathbb{R}^3} \delta V(x,t) u(x,t) \bar{p}(x,t)\, dxdt$$

where u is solution of the state equation and p is solution of the adjoint problem

$$\begin{cases} i\partial_t p + \Delta p + \dfrac{p}{|x-a|} + V_1 p = 0 & \textit{in } \mathbb{R}^3 \times (0,T) \\ p(T) = u(T) - u_1 & \textit{in } \mathbb{R}^3. \end{cases}$$

Remark.

The previous Theorem relies essentially on the regularity result which has been obtained before. Also, we show that the mapping

$$V_1 \in H \to u(T) \in L^2$$

is differentiable.

If we consider the mapping with values in H^1 for example it is not clear that it is still differentiable....

Of course the proof starts by considering a minimizing sequence and then one has to prove "good" convergences in order to pass to the limit.

Interpretation

in the particular case when $W = H^3(\mathbb{R}^3)$:

$$\widetilde{H} = \left\{ V, \ \left(1 + |x|^2\right)^{-\frac{1}{2}} V \in H^1(0, T; H^3) \right\}.$$

Optimality condition:

$$\forall \delta V \in \widetilde{H}, \quad r\langle V_1, \delta V\rangle_{\widetilde{H}} = Im \int_0^T \int_{\mathbb{R}^3} \delta V u \overline{p} \, dx dt$$

In this particular case, if $V \in \widetilde{H}$, there exists $X \in H^1(0, T; H^3)$ such that $V = \left(1 + |x|^2\right)^{\frac{1}{2}} X$. Moreover, $X = (I - \Delta)^{-1} Y$ with $Y \in H^1(0, T; H^1)$.

Therefore,

$$\langle V_1, \delta V\rangle_H = \langle X_1, \delta X\rangle_{H^1(0,T;H^2)} = \langle Y_1, \delta Y\rangle_{H^1(0,T;H^1)}$$

and on the one hand,

$$\begin{aligned}\langle Y_1, \delta Y\rangle_{H^1(0,T;L^2)} &= \int_0^T \int_{\mathbb{R}^3} (I - \partial_t^2) Y_1 \delta Y \\ &+ \int_{\mathbb{R}^3} \left(\partial_t Y_1(T)\delta Y(T) - \partial_t Y_1(0)\delta Y(0)\right).\end{aligned}$$

while on the other hand,

$$\begin{aligned}\langle \nabla Y_1, \nabla\delta Y\rangle_{H^1(0,T;L^2)} &= \int_0^T \int_{\mathbb{R}^3} -(I - \partial_t^2)\Delta Y_1 \delta Y \\ &+ \int_{\mathbb{R}^3} \left(\partial_t \Delta Y_1(0)\delta Y(0) - \partial_t \Delta Y_1(T)\delta Y(T)\right).\end{aligned}$$

We obtain

$$\langle Y_1, \delta Y\rangle_{H^1(0,T;H^1)} = \int_0^T \int_{\mathbb{R}^3} (I-\partial_t^2)(I-\Delta)Y_1\delta Y$$
$$+\int_{\mathbb{R}^3} \big(\partial_t(Y_1-\Delta Y_1)(T)\delta Y(T) - \partial_t(Y_1-\Delta Y_1)(0)\delta Y(0)\big).$$

The optimality condition becomes:

$$\forall \delta Y \in H^1(0,T;L^2),$$
$$r\int_0^T \int_{\mathbb{R}^3} (I-\partial_t^2)(I-\Delta)Y_1\delta Y\,dxdt + r\int_{\mathbb{R}^3} \partial_t(Y_1-\Delta Y_1)(T)\delta Y(T)\,dx$$
$$- r\int_{\mathbb{R}^3} \partial_t(Y_1-\Delta Y_1)(0)\delta Y(0)\,dx$$
$$= Im\int_0^T \int_{\mathbb{R}^3} u\overline{p}\sqrt{1+|x|^2}\,(I-\Delta)^{-1}\,\delta Y\,dxdt$$

and from an integration by parts, we obtain for all δY in $H^1(0, T; L^2)$,

$$
\begin{aligned}
& r \int_0^T \int_{\mathbb{R}^3} (I - \partial_t^2)(I - \Delta) Y_1 \delta Y \, dxdt \\
& + r \int_{\mathbb{R}^3} \big(\partial_t (Y_1 - \Delta Y_1)(T) \delta Y(T) - \partial_t (Y_1 - \Delta Y_1)(0) \delta Y(0) \big) \, dxs \\
& = Im \int_0^T \int_{\mathbb{R}^3} \delta Y (I - \Delta)^{-1} \left(u \bar{p} \sqrt{1 + |x|^2} \right) \, dxdt.
\end{aligned}
$$

It can be noticed that by some regularity arguments the right hand side has a meaning.

Thus, the optimality condition corresponds to the system:

$$\begin{cases} r(I-\partial_t^2)(I-\Delta)Y_1 = (I-\Delta)^{-1}\left(Im(u\overline{p})\sqrt{1+|x|^2}\right) & \text{in } \mathbb{R}^3 \times (0,T) \\ \partial_t(Y_1 - \Delta Y_1)(T) = \partial_t(Y_1 - \Delta Y_1)(0) = 0 & \text{in } \mathbb{R}^3. \end{cases}$$

where

$$V_1 = \left(1+|x|^2\right)^{\frac{1}{2}}(I-\Delta)^{-1}\ Y_1.$$

Mathematical Model II

On the one hand, since the nucleus is much heavier than the electrons, we consider it as a point particle which moves according to the Newton dynamics in the external electric field and in the electric potential created by the electronic density (nucleus-electron attraction of Hellman-Feynman type). We obtain a second order in time ordinary differential equation solved by the position $a(t)$ of the nucleus (of mass m).

On the other hand, under the restricted Hartree-Fock formalism, we describe the behavior of the electrons by a wave function, solution of a time dependent Hartree-Fock equation. We can define it as a Schrödinger equation with a coulombian potential due to the nucleus, singular at finite distance, an electric potential corresponding to the external electric field, possibly unbounded at infinity (for example $V_1 = I(t).x$), and a nonlinearity of Hartree type in the right hand side. We want precisely to study the optimal control of the wave function of the electrons only, the control being performed by the electric potential.

We are in fact considering the following coupled system :

$$\begin{cases} i\partial_t u + \Delta u + \dfrac{1}{|x-a|} u + V_1 u = (|u|^2 \star \dfrac{1}{|x|}) u, & \text{in } \mathbb{R}^3 \times (0, T) \\ u(0) = u_0, & \text{in } \mathbb{R}^3 \\ m \ \dfrac{d^2 a}{dt^2} = \displaystyle\int_{\mathbb{R}^3} -|u(x)|^2 \nabla \dfrac{1}{|x-a|} \, dx - \nabla V_1(a), & \text{in } (0, T) \\ a(0) = a_0, \ \ \dfrac{da}{dt}(0) = v_0 \end{cases} \tag{2}$$

where V_1 is the external electric potential which takes its values in $\mathbb{R}$

We need a result of existence and regularity for this problem.

Theorem

We assume that T is a positive arbitrary time and the same hypothesis on V_1 plus

$$\nabla V_1 \in L^2(0,T; W^{1,\infty}_{loc}(\mathbb{R}^3)).$$

(We can take $V_1 \in H$).
If $u_0 \in H^2 \cap H_2$, a_0, $v_0 \in \mathbb{R}$, then the system has at least a solution

$$(u,a) \in \left(W^{1,\infty}(0,T;L^2) \cap L^\infty(0,T;H^2 \cap H_2)\right) \times W^{2,1}(0,T).$$

Remark
We have no proof of uniqueness up to now....

The proof of the existence and regularity result is not straightforward and requires first of all a result of local existence and in a second step a lot of estimates in order to show the global existence and regularity result.

The controllability problem for the previous system is completely out of reach at the moment and we will give a result of optimal control.
In the case where $a(.)$ is given and we only have a nonlinear Schrödinger equation, the result is similar to the one for the first model and we also have an interpretation of the optimality condition using and adjoint state.
In the case of the full coupled system, we willl give a result of existence for an optimal control but the optimality system is formal...
Let us formulate the optimal control problem.

if $u_1 \in L^2$ is a given target, find a minimizer $V_1 \in H$ for

$$\inf\{J(V_1),\ V_1 \in H\} \tag{3}$$

where the cost functionnal J is defined by

$$J(V_1) = \frac{1}{2}\int_{\mathbb{R}^3} |u(T) - u_1|^2\, dx + \frac{r}{2}\Big|V_1\Big|_H^2,\ r > 0, \tag{4}$$

where,

$$H = \Big\{V,\ \ (1 + |x|^2)^{-\frac{1}{2}}\, V \in H^1(0, T; W)\Big\}$$

and W is an Hilbert space such that $W \hookrightarrow W^{1,\infty}(\mathbb{R}^3)$.

We obtain the following result of existence for an optimal control.

Theorem

There exists an optimal control $V_1 \in H$ such that

$$J(V_1) = \inf\{J(V),\ V \in H\}$$

and for all δV in H,

In general we don't have a rigorous result for an optimality condition but this result can be proved if the system is decoupled and $a(.)$ is given.

Formal Optimality System

A first step is to consider the functional

$$\begin{array}{rcl}\Phi : \widetilde{\mathcal{H}} & \longrightarrow & L^\infty(0,T;L^2(\mathbb{R}^3)) \times L^\infty(0,T) \\ V_1 & \longmapsto & (u(V_1), a(V_1)))\end{array}$$

Assuming that we have uniqueness of the solution of our system and assuming that Φ is differentiable, if we set $D\Phi(\delta V_1) = (z,b)$, then $(z(t,x), b(t))$ has to satisfy the following coupled system set in $\mathbb{R}^3 \times (0,T)$ with $V_0 = \dfrac{1}{|x-a|}$

$$\left\{\begin{array}{l} i\partial_t z + \Delta z + V_0 z + V_1 z = -\dfrac{\partial V_0}{\partial a} \cdot b\ u - \delta V_1 u \\ \qquad\qquad\qquad\qquad + (|u|^2 \star \dfrac{1}{|x|})z + 2(Re(u\bar{z}) \star \dfrac{1}{|x|})u, \\ m\ \dfrac{d^2 b}{dt^2} = -\displaystyle\int_{\mathbb{R}^3} |u|^2 \nabla \dfrac{\partial V_0}{\partial a} \cdot b - 2\int_{\mathbb{R}^3} Re(u\bar{z}) \nabla V_0 - \nabla \delta V_1(a) \\ \qquad\qquad\qquad\qquad - \nabla(\nabla V_1) \cdot b(a) \end{array}\right.$$

with initial conditions $z(0) = 0,\ b(0) = 0,\ \dfrac{db}{dt}(0) = 0$ and .

we can deduce the candidate adjoint system:

$$\begin{cases} i\partial_t p + \Delta p + V_0 p + V_1 p = (|u|^2 \star \dfrac{1}{|x|})p \\ \qquad\qquad\qquad\qquad +2i\ (Im(u\overline{p}) \star \dfrac{1}{|x|})\overline{u} - 2i\overline{u}\ \nabla V_0 \cdot \varrho, \\ p(T) = u(T) - u_1, \\ m\ \dfrac{d^2\varrho}{dt^2} = -\int_{\mathbb{R}^3} \dfrac{\partial V_0}{\partial a}\ Im(u\overline{p}) - 2\displaystyle\int_{\mathbb{R}^3} Re(\overline{u}\nabla u)\dfrac{\partial V_0}{\partial a} \cdot \varrho - \nabla(\nabla V_1)(a) \cdot \varrho, \\ \varrho(T) = 0,\ \dfrac{d\varrho}{dt}(T) = 0. \end{cases}$$

Therefore, the bilinear optimal control V_1 is the solution of a partial differential equation defined by variational formulation in the following way:

$$r\langle V_1, \delta V_1\rangle_{\widetilde{\mathcal{H}}} = \int_0^T\int_{\mathbb{R}^3} Im\left(u(t,x)\overline{p}(t,x)\right)\delta V_1(t,x)\,dxdt - \int_0^T \left\langle \varrho(t)\cdot\nabla\delta_{a(t)}, \delta V_1(t)\right\rangle\, dt.$$

As for the first model by choosing $W = H^3$ we can give an interpretation of the previous condition in terms of PDE for Y_1 such that

$$V_1(x,t) = \left(1+|x|^2\right)^{\frac{1}{2}}\left(I-\Delta\right)^{-1} Y_1(x,t) + E_1(t)$$

....

Thus, the optimality condition corresponds to the system:

$$\begin{cases} r\Big[(I-\partial_t^2)+(I-\Delta)\Big](I-\Delta)Y_1=(I-\Delta)^{-1}G & \text{in } \mathbb{R}^3\times(0,T) \\ \partial_t(Y_1-\Delta Y_1)(T)=\partial_t(Y_1-\Delta Y_1)(0)=0 & \text{in } \mathbb{R}^3 \\ r\left(E_1-\dfrac{d^2E_1}{dt^2}\right)=\int_{\mathbb{R}^3}G(x)\,dx & \text{in } (0,T) \\ \dfrac{dE_1}{dt}(T)=\dfrac{dE_1}{dt}(0)=0 & \end{cases}$$

where

$$\begin{aligned} G(x,t) \quad &= \quad Im\left(u(x,t)\overline{p(x,t)}\right)\sqrt{1+|x|^2} \\ &\quad -\varrho(t)\cdot\nabla\delta_{a(t)}(x)\sqrt{1+|a(t)|^2}+\frac{a(t)\cdot\varrho(t)}{\sqrt{1+|a(t)|^2}}\;\delta_{a(t)}(x) \end{aligned}$$

and

$$V_1(x,t)=\left(1+|x|^2\right)^{\frac{1}{2}}\left((I-\Delta)^{-1}\;Y_1(x,t)+E_1(t)\right).$$