

## Remarks on the controllability of the Schrödinger equation

Enrique Zuazua

ABSTRACT. Abstract: In this paper we present some results on the controllability of the Schrödinger equation. We first discuss the controllability of the linear equation with a control distributed along a subdomain or subset of the boundary of the domain where the equation holds. We also analyze some possible extensions to semilinear equations in which the nonlinearity involves the state equation but the control enters linearly in the system. We also study the model bilinear control problem arising in Quantum Chemistry and some issues related with the numerical approximation of the controls.

### 1. Introduction and problem formulation

In this article we report on some existing results on the controllability of Schrödinger equations. This has been a topic of research in which very intensive work has been done by many authors in the last fifteen years.

To fix ideas, let  $\Omega$  be a bounded, smooth domain of  $\mathbb{R}^n$  and let us consider the controlled linear Schrödinger equation:

$$(1.1) \quad \begin{cases} iy_t = \Delta y + v\chi_\omega & \text{in } \Omega \times (0, T), \\ y = 0 & \text{on } \partial\Omega \times (0, T), \\ y(x, 0) = y_0(x) & \text{in } \Omega. \end{cases}$$

Here  $y = y(x, t)$  is the *state* and  $v = v(x, t)$  is the *control*. Both are complex valued functions. The control is localized on the subdomain  $\omega$  of  $\Omega$  through  $\chi_\omega$ , the characteristic function of the set  $\omega$ .

System (1.1) is well-posed in  $L^2(\Omega)$ , with controls in  $L^2(\omega \times (0, T))$ . Indeed, for all  $y_0 \in L^2(\Omega)$  and  $v \in L^2(\omega \times (0, T))$  there exists a unique solution  $y \in C([0, T]; L^2(\Omega))$  of (1.1).

Here and in the sequel  $L^2(\Omega)$  and all other function spaces refer to spaces of complex-valued functions.

The control problem we shall address can be, roughly, formulated as follows: *To which extent can the solution  $y$  of (1.1) be perturbed by the action of the control  $v$  at a given final time  $t = T$  in order to reach a given final target?*

There are several ways of formulating this problem in a rigorous way. First of all, it can be formulated as an *Optimal Control* problem. To do that one fixes the final control time  $T$ , the target  $y_1 \in L^2(\Omega)$ , a positive number  $k > 0$  and considers the functional

$$(1.2) \quad J_k(v) = \frac{1}{2} \|y(T) - y_1\|_{L^2(\Omega)}^2 + \frac{k}{2} \|v\|_{L^2(\omega \times (0, T))}^2.$$

---

Supported by grant BFM2002-03345 of the MCYT (Spain) and the Networks "Homogenization and Multiple Scales" and "New materials, adaptive systems and their nonlinearities: modelling, control and numerical simulation (HPRN-CT-2002-00284)" of the EU..

The following minimization problem then arises naturally:

$$(1.3) \quad \begin{cases} \text{To find } v_k \in L^2(\omega \times (0, T)) \text{ such that} \\ J_k(v_k) = \min_{v \in L^2(\omega \times (0, T))} J_k(v). \end{cases}$$

Minimizing  $J_k$  introduces a compromise between achieving the goal of forcing the state  $y(T)$  to approximate the target  $y_1$  and penalizing the tendency of the control  $v$  to get too large. The penalty parameter  $k$  allows regulating that compromise. Obviously, letting  $k \rightarrow 0$ , one relaxes the constraint on the size of the control, while, when  $k \rightarrow \infty$ , one is relaxing the control requirement of making the state to get close to the target  $y_1$ .

It is easy to see that the minimum of  $J_k$  is achieved at a unique minimizer  $v_k \in L^2(\omega \times (0, T))$ . For, it is sufficient to observe that  $J_k$  is continuous, convex and trivially coercive from  $L^2(\omega \times (0, T))$  to  $\mathbb{R}$ .

However, when simply minimizing  $J_k$ , one does not answer to the following more quantitative version of the problem. What is the choice of the parameter  $k$  that guarantees that the state  $y_k(T)$  associated to the optimal control  $v_k$  is, at most, at a given distance from the target  $y_1$ ? Does this choice of  $k$  actually exist? If yes, once  $k$  is chosen, what is the size of the corresponding control  $v_k$ ?

In order to get more precise answers to these questions it is natural to look closer to the control problem by analyzing the controllability property. The Schrödinger equation is an infinite-dimensional, conservative, dynamical system and, accordingly, there are two different notions of controllability that should be distinguished:

- *Approximate controllability.* System (1.1) is said to be approximately controllable in time  $T$  if the set of reachable states starting from any  $y_0 \in L^2(\Omega)$ , when  $v$  ranges on  $L^2(\omega \times (0, T))$ , is dense in the state space  $L^2(\Omega)$ . In other words if, for any  $y_0, y_1 \in L^2(\Omega)$  and  $\varepsilon > 0$  there exists  $v \in L^2(\omega \times (0, T))$  such that the solution  $y$  of (1.1) satisfies

$$(1.4) \quad \|y(T) - y_1\|_{L^2(\Omega)} \leq \varepsilon.$$

- *Exact controllability.* System (1.1) is said to be exactly controllable in time  $T$  if, for any  $y_0, y_1 \in L^2(\Omega)$  there exists  $v \in L^2(\omega \times (0, T))$  such that the solution  $y$  of (1.1) satisfies

$$(1.5) \quad y(T) \equiv y_1.$$

As it is classical in control problems, these two control properties can be transformed into equivalent observability problems on the *adjoint system* (see [L]). The Schrödinger equation being time reversible, the adjoint equation may be replaced by the state equation itself without control, i.e.

$$(1.6) \quad \begin{cases} i\phi_t = \Delta\phi & \text{in } \Omega \times (0, T) \\ \phi = 0 & \text{on } \partial\Omega \times (0, T) \\ \phi(x, 0) = \phi_0(x) & \text{in } \Omega. \end{cases}$$

The approximate controllability property is then equivalent to the following uniqueness problem:

$$(1.7) \quad \phi \equiv 0 \text{ in } \omega \times (0, T) \implies \phi \equiv 0 \text{ everywhere?}$$

Using Holmgren's Uniqueness Theorem (see [Jh]) it is easy to see that this uniqueness property does indeed hold for all  $T > 0$  and for all open, non-empty subset  $\omega$  of  $\Omega$ . Thus, the Schrödinger equation (1.1) is approximately controllable for all  $T > 0$  with controls in any open, non-empty subset  $\omega$  of  $\Omega$ .

But, the approximate controllability property in itself does not provide much information since, in particular, it does not give any indication of what is the size of the control  $v_\varepsilon$  that is needed in order to achieve the  $\varepsilon$ -control property (1.4). In this sense the exact controllability property is much more satisfactory since:

- (a) When exact controllability holds, the controls  $v_\varepsilon$  such that (1.4) is satisfied, remain bounded as  $\varepsilon \rightarrow 0$  and in the limit (weakly in  $L^2(\omega \times (0, T))$ ) provide a control that fulfills the exact controllability property (1.5).
- (b) It allows obtaining upper bounds on the size of the controls needed to achieve the  $\varepsilon$ -control property (1.4). Indeed, exact controllability and the truncation of the Fourier representation of the solution allows to do that easily (we refer to [FCZ] for a similar result and argument in the context of the heat equation).

But, obviously, the exact controllability property is much harder to achieve. In fact, the exact controllability property is equivalent to the existence of a constant  $C = C(T) > 0$  such that the following inequality holds for every solution of (1.6):

$$(1.8) \quad \|\phi_0\|_{L^2(\Omega)}^2 \leq C \int_0^T \int_\omega |\phi|^2 dx dt.$$

This is the so-called *observability inequality*.

As we shall see below, in order for this inequality to be true, some geometric assumptions on the subdomain  $\omega$  where the control is supported are required.

But, in order to explain the connection between the controllability problem for (1.1) and the observability inequality (1.8) for the adjoint system (1.6) it is convenient to explain how (1.8) allows building the control for (1.1). To do that, we assume that the subset  $\omega$  of  $\Omega$  and the time  $T > 0$  are such that (1.8) holds. We fix the initial datum  $y_0 \in L^2(\Omega)$  of (1.1) to be controlled. Taking into account that the Schrödinger equation is time-reversible we may, without loss of generality, assume that the target  $y_1 \equiv 0$ . Thus, we look for the control  $v \in L^2(\omega \times (0, T))$  such that the solution of (1.1) satisfies

$$(1.9) \quad y(T) \equiv 0.$$

Multiplying in (1.1) by  $\bar{\phi}$ , integrating by parts in  $\Omega \times (0, T)$  and using the equations (1.6) that  $\phi$  satisfies we deduce that

$$(1.10) \quad \int_0^T \int_\omega v \bar{\phi} dx dt + i \int_\Omega y_0 \bar{\phi}_0 dx = i \int_\Omega y(T) \bar{\phi}(T) dx.$$

Taking real parts in (1.10) we deduce that

$$(1.11) \quad \operatorname{Re} \int_0^T \int_\omega v \bar{\phi} dx dt - \operatorname{Im} \int_\Omega y_0 \bar{\phi}_0 dx = -\operatorname{Im} \int_\Omega y(T) \bar{\phi}(T) dx.$$

Here and in the sequel  $\operatorname{Re}$  and  $\operatorname{Im}$  stand for the real and the imaginary part of a complex number.

On the other hand, when  $\phi_0$  runs over  $L^2(\Omega)$ ,  $\bar{\phi}(T)$  covers the whole space  $L^2(\Omega)$  too. Thus, (1.9) is equivalent to:

$$(1.12) \quad \operatorname{Im} \int_\Omega y(T) \bar{\phi}(T) dx = 0, \forall \phi \text{ solution of (1.6)},$$

or, equivalently,

$$(1.13) \quad \operatorname{Re} \int_0^T \int_\omega v \bar{\phi} dx dt - \operatorname{Im} \int_\Omega y_0 \bar{\phi}_0 dx = 0, \forall \phi \text{ solution of (1.6)}.$$

In (1.13) we identify the Euler-Lagrange equation associated with the minimization of the functional

$$(1.14) \quad J(\phi_0) = \frac{1}{2} \int_0^T \int_\omega |\phi|^2 dx dt - \operatorname{Im} \int_\Omega y_0 \bar{\phi}_0 dx.$$

The functional  $J : L^2(\Omega) \rightarrow \mathbb{R}$  is continuous and convex. Moreover,  $J$  is coercive because of the observability inequality (1.8). Thus,  $J$  achieves its minimum at a single point  $\psi_0 \in L^2(\Omega)$ . It is easy to

see that this minimum provides the control we are looking for. More precisely, if  $\psi_0$  is the minimum of  $J$  then  $v = \psi$ , where  $\psi$  is the solution of the adjoint system (1.6) with the minimizer  $\psi_0$  as initial datum, is the control we are looking for since (1.13) holds.

In the following section we shall briefly describe the existing positive and negative results on this matter. In section 3, we shall then comment on some possible extensions to the semilinear setting and, in particular, we shall mention some interesting open problems.

Most of the literature on the controllability of the Schrödinger equation has been written in the context of boundary control. Here we shall rather consider the case where the control acts in the interior of the domain to avoid unnecessary difficulties related with the solvability and well-posedness of boundary value problems.

In section 4 we shall discuss the bilinear control problem arising in Quantum Chemistry. We shall mainly indicate why the techniques developed in the previous sections on the classical linear controllability problem do not suffice to address this challenging mathematical open problem. Finally, in section 5 we shall comment on the problem of the numerical approximation of the control.

The interested reader is referred to the fundamental articles [BS], [PDR], [RVMK] and [SWR] for a complete discussion of the motivations and relevance of control problems in Quantum Chemistry. Before closing this introduction we would like to refer also to the survey articles [Zu3] and [Zu4] for the readers interested on the controllability theory for Partial Differential Equations.

### Acknowledgements

The author is grateful to the organizers of the workshop “Quantum Control: Mathematical and Numerical Challenges” of the CRM, for their kind invitation, warm hospitality and support.

## 2. Exact controllability of the Schrödinger equation

There are several results on the exact controllability of the Schrödinger equation (1.1). One of the most relevant ones is certainly that due to G. Lebeau [Le] which guarantees that the Geometric Control Condition (GCC) for the exact controllability of the wave equation is sufficient for the exact controllability of the Schrödinger equation (1.1) in any time  $T$ .

The GCC can be, roughly, formulated as follows (see [BLR]): The subdomain  $\omega$  of  $\Omega$  is said to satisfy the GCC in time  $T$  if and only if all rays of Geometric Optics that propagate inside the domain  $\Omega$  and bouncing on its boundary reach the control set  $\omega$  in time less than one.

This geometric property is extremely natural for the exact controllability of the wave equation (in which the velocity of propagation has been normalized to one) to hold. In fact, for the wave equation, it is a necessary and sufficient condition for exact controllability and, when it fails, one loses an infinite number of derivatives at the level of the space of controllable data.

The result by G. Lebeau [Le] indicates that, to some extent, the Schrödinger equation can be viewed as a wave equation with infinite speed of propagation. Indeed, the fact that the GCC is satisfied for some finite time  $T^*$  suffices for the exact controllability of the Schrödinger equation (1.1) to hold for all  $T > 0$ . The proof in [Le] is based on a dyadic decomposition of the Fourier representation of solutions of the Schrödinger equation which allows viewing them as superposition of an infinite sequence of solutions of wave equations with velocity of propagation tending to infinity.

A particular case of the result in [Le] was previously proved by E. Machtyngier in [Ma1] where the exact controllability property was proved with the multiplier techniques developed in [L]. Later, this result was extended and adapted to the problem of boundary feedback stabilization in [LT1] and [MaZ].

But, in fact, the Schrödinger equation is slightly better than a wave equation with infinite velocity of propagation from the point of view of controllability. Indeed, there are a number of results showing that, in

some situations in which the GCC is not fulfilled in any time  $T^*$ , one can still achieve very satisfactory results for the Schrödinger equation. Two of the most significant results in this direction are:

- The result by S. Jaffard [**Ja**] showing that, when the domain  $\Omega$  is a square, for any open non-empty subset  $\omega$  the exact controllability of the Schrödinger equation (1.1) holds in any time  $T$ , in the space  $L^2(\Omega)$  and with controls in  $L^2(\omega \times (0, T))$ .
- The result by N. Burq [**Bu**] showing that the Schrödinger equation in a perforated domain, despite of the existence of trapped rays bouncing back and forth in between two holes, can be controlled from a neighborhood of the exterior boundary in any Sobolev space  $H^\delta(\Omega)$  with  $\delta > 0$ .

Of course, none of these results is true for the wave equation. Indeed, as we said above, for the wave equation, as soon as one loses the GCC there is a defect of an infinite number of derivatives at the level of the space of controllable data (see [**R**] and [**McZ**]).

Rigorously speaking the results in [**Ja**] and [**Bu**] refer to the exact controllability of the plate equation with hinged boundary conditions. But, in fact, it is easy to transfer exact controllability results from one system to another (see, for instance, [**Le**]). This fact is simply based on the property that the operator  $\partial_t^2 + \Delta_x^2$  arising in plate equations can be decomposed as two conjugate Schrödinger operators:

$$(2.1) \quad \partial_t^2 + \Delta_x^2 = (-i\partial_t + \Delta_x)(i\partial_t + \Delta_x).$$

The exact controllability of the Schrödinger equation in some other cases in which the GCC fails has been studied in other articles too. We refer to B. Allibert [**A**] for the case of surfaces of revolution with control on one side of its lateral boundary and to G. Chen et al. [**Ch**] and J. Lagnese [**La**] for the analysis of the behaviour of the eigenfunctions on the disk, which allows giving negative results when the control acts in an interior subdomain without intersection with the exterior boundary.

More recently, L. Baudonin and J.P. Puel [**BP**], in the context of an inverse problem for the Schrödinger equation, have used Carleman inequalities to prove observability inequalities for Schrödinger equations with bounded potentials depending on the space variable  $x$ :

$$(2.2) \quad \begin{cases} i\phi_t = \Delta\phi + V\phi & \text{in } \Omega \times (0, T) \\ \phi = 0 & \text{on } \partial\Omega \times (0, T) \\ \phi(x, 0) = \phi_0(x) & \text{in } \Omega \end{cases}$$

with  $V = V(x) \in L^\infty(\Omega)$ . The geometric assumptions on the control/observation subdomain  $\omega$  are those one gets by multiplier techniques. More precisely, in [**BP**], the boundary observability problem is addressed and it is proved that

$$(2.3) \quad \|\phi(0)\|_{H_0^1(\Omega)}^2 \leq C(V, T) \int_0^T \int_{\Gamma_0} \left| \frac{\partial\phi}{\partial\nu} \right|^2 d\sigma dt$$

with  $\Gamma_0$  a subset of the boundary of the form

$$(2.4) \quad \Gamma_0 = \{x \in \partial\Omega : (x - x_0) \cdot \nu(x) > 0\},$$

for some  $x_0 \in \mathbb{R}^n$ , where  $\nu(x)$  denotes the unit outward normal to  $\Omega$  at  $x \in \partial\Omega$ .

Inequality (2.4) holds for all  $T > 0$  for the solutions of (2.2) in  $\Omega \times (0, T)$  with Dirichlet boundary conditions.

We refer also to [**LTZ**] for other independent results in this context where inequalities of the form (2.3) are derived in the case of potentials depending both on space and time and also for Neumann boundary conditions. The work in [**LTZ**] is based on the previous results by X. Zhang [**Zh**] on the plate model.

In view of (2.3) and using the arguments in [L] one can immediately deduce the following variant

$$(2.5) \quad \|\phi(0)\|_{H_0^1(\Omega)}^2 \leq C(V, T) \int_0^T \int_{\omega} |\nabla \phi|^2 dx dt,$$

where  $\omega$  is a neighborhood of  $\Gamma_0$  in  $\Omega$ , i.e.  $\omega = \Omega \cap \Theta$ , where  $\Theta$  is a neighborhood of  $\Gamma_0$  in  $\mathbb{R}^n$ .

The inequality (2.5) allows to get immediately the controllability of the corresponding Schrödinger equation in  $H^{-1}(\Omega)$  with a bounded potential  $V = V(x)$  and with controls in  $L^2(0, T; H^{-1}(\omega))$ .

It would be interesting to pursue the research in [BP] in the following directions:

- To derive the  $L^2$ -version of (2.5).
- To address the case of potentials  $V$  depending both in space and time and to do all this getting explicit bounds on the constants  $C(V, T)$  arising in the observability inequality. This is particularly relevant in the context of the control of semilinear problems.

The paper by K. D. Phung [Ph] is also worth mentioning. In [Ph] the author establishes the connections between the heat, wave and Schrödinger equations through suitable integral transformations. This allows him to get, for instance, estimates on the coast of approximate controllability for the Schrödinger equation when the GCC is not satisfied and also on the dependence of the size of the control with respect to the control time.

### 3. The semilinear Schrödinger equation

Let us now consider the semilinear Schrödinger equation

$$(3.1) \quad \begin{cases} iy_t = \Delta y + f(y) + v\chi_{\omega} & \text{in } \Omega \times (0, T) \\ y = 0 & \text{on } \partial\Omega \times (0, T) \\ y(0) = y_0 & \text{in } \Omega. \end{cases}$$

To simplify the presentation we assume that  $f$  is globally Lipschitz, i.e.

$$(3.2) \quad \exists L > 0 : |f(s_1) - f(s_2)| \leq L |s_1 - s_2|, \forall s_1, s_2 \in \mathbb{C}.$$

Under this assumption, system (3.1) is well posed in  $L^2(\Omega)$ . Therefore, the approximate and exact controllability problems make sense in this semilinear setting too.

It is not hard to see that, whenever the Schrödinger equation is exactly controllable, then the semilinear equation (3.1) is also exactly controllable provided the Lipschitz constant  $L$  is small enough. This can be done easily by using the fixed point theorem for contractive maps.

In order to deal with general globally Lipschitz nonlinearities, in [Zu1], a fixed point method was introduced in the context of the exact controllability of the wave equation. Later it was shown that the method does also apply to some slightly superlinear nonlinearities [Zu2] and in the context of the approximate controllability of the semilinear heat equation, [FPZ].

This fixed point argument is roughly as follows. To simplify the presentation we assume that  $f(0) = 0$  and we introduce the new nonlinearity:

$$(3.3) \quad g(s) = \begin{cases} f(s)/s, & s \neq 0 \\ f'(0), & s = 0. \end{cases}$$

Then, the equation in (3.1) reads

$$(3.4) \quad iy_t = \Delta y + g(y)y + v\chi_{\omega}.$$

Given any  $z \in L^\infty(0, T; L^2(\Omega))$  we introduce the linearized system

$$(3.5) \quad iy_t = \Delta y + g(z)y + v\chi_{\omega}.$$

Note that this corresponds to a linear Schrödinger equation with potential  $V_z = g(z)$ , which depends both on  $x$  and  $t$ . Moreover, in view of the globally Lipschitz assumption (3.3), it follows that

$$(3.6) \quad \|V_z\|_{L^\infty(\Omega \times (0, T))} \leq L, \quad \forall z \in L^\infty(0, T; L^2(\Omega)).$$

The method consists in building the nonlinear map

$$\mathcal{N} : L^\infty(0, T; L^2(\Omega)) \longrightarrow L^\infty(0, T; L^2(\Omega)) \\ z \longmapsto y_z$$

where  $y_z$  is the solution of (3.5) with the control  $v_z$  that fulfills the control requirements. In view of the fact that the potentials are uniformly bounded (see (3.6)), it is natural to expect the controls to be also bounded, and, consequently, the range of the nonlinear mapping  $\mathcal{N}$  to be a bounded set of  $L^\infty(0, T; L^2(\Omega))$ . Then, provided  $\mathcal{N}$  is compact, the Schauder fixed point Theorem provides the existence of a fixed point  $z = y$  and, by construction,  $y$  is a solution of (3.1) that fulfills the control requirements.

The compactness of  $\mathcal{N}$  is easy to prove in the context of the semilinear heat and wave equation. It is more difficult to achieve it for the Schrödinger equation because of the intrinsic lack of regularizing effect of this equation. But this difficulty could possibly be overcome by using a global version of the Inverse Function Theorem as in [LT2].

However, in order to conclude that the semilinear Schrödinger equation (3.1) is exactly controllable under the globally Lipschitz assumption (3.3) there is a need of proving a uniform observability inequality that, as far as we know, constitutes an open problem. To rigorously state this problem we consider the adjoint system (2.2) with potential  $V = V(x, t) \in L^\infty(\Omega \times (0, T))$  depending both on  $x$  and  $t$ .

It is very likely to expect that, for every  $T > 0$ , every open subset  $\omega$  of  $\Omega$  satisfying some suitable geometric property (for instance when  $\omega$  is a neighborhood of a subset of the boundary of the form  $\Gamma_0$  as in (2.4) and every  $R > 0$ , there exists a observability constant  $C_R = C(T, \omega, R) > 0$  such that

$$(3.7) \quad \|\phi(0)\|_{L^2(\Omega)}^2 \leq C_R \int_0^T \int_\omega |\phi|^2 dx dt$$

for every solution  $\phi$  of (2.2) with potential  $V = V(x, t)$  such that

$$(3.8) \quad \|V\|_{L^\infty(\Omega \times (0, T))} \leq R.$$

However, as far as we know, this uniform (with respect to the potential  $V$  as in (3.8)) observability inequality has not been proved in the literature.

In fact, it would be interesting to prove (3.7) with an explicit value on the observability constant  $C_R$ . Very likely,  $C_R$  will depend exponentially on  $R$  as it is the case in the context of the wave and the heat equation, and this may have important consequences for the controllability of the semilinear equation (3.1). Indeed, in [Zu2] and [FCZ] it has been proved that, because of this exponential dependence of the observability constant, the semilinear wave and heat equations are controllable for a class of nonlinearities that grow at infinity in some logarithmic superlinear way. It would be very interesting to see if this type of result holds also for the semilinear Schrödinger equation and, in particular, for the logarithmic nonlinear terms addressed in [C] and [CH] from the point of view of existence and uniqueness of solutions.

Obviously one expects all these results on the controllability of the semilinear Schrödinger equation to hold for any control time  $T > 0$ . In [FCZ] it was observed that, the infinite speed of propagation may help to control blowing-up evolution equations and it was proved that this does indeed happen for a class of blowing-up semilinear heat equations. It would be very interesting to see if this is also true for some blowing-up Schrödinger equations.

In the absence of blow-up phenomena, for instance, for nonlinear terms allowing global energy estimates, it is natural to expect local controllability results. To be more precise, one can expect that for any initial datum  $y_0 \in L^2(\Omega)$  and  $T > 0$  there exists  $\varepsilon > 0$  such that for all  $y_1 \in L^2(\Omega)$  with  $\|y_0 - y_1\|_{L^2(\Omega)} \leq \varepsilon$

there exists a control  $v \in L^2(\omega \times (0, T))$  such that the solution of (3.1) satisfies  $y(T) = y_1$ . It would be very interesting to prove this type of result for

power-like nonlinearities. But, due to the lack of regularizing effect of the Schrödinger equation, to do that one will need very likely to use the dispersive properties (the so-called Strichartz inequalities) of the Schrödinger equation. This was done recently in [DLZ] in the context of the wave equation when  $\omega$  is a neighborhood of the whole boundary  $\partial\Omega$ . In fact, in [DLZ], by combining this local controllability result with a stabilization property, it was proved that any initial and final states can be matched provided the control time is large enough. But, doing this for the Schrödinger equation constitutes an open problem.

#### 4. Bilinear control

Let us consider now the following bilinear control problem:

$$(4.1) \quad \begin{cases} iy_t = \Delta y + v(t)y & \text{in } \Omega \times (0, T) \\ y = 0 & \text{on } \partial\Omega \times (0, T) \\ y(0) = y_0 & \text{in } \Omega. \end{cases}$$

Here, once again,  $y$  is the state and  $v = v(t)$  is the control, that enters on the system as a time-dependent potential (and this makes the system under consideration to be bilinear). The control  $v$  is assumed to be independent of  $x$  and real-valued.

Multiplying in (4.1) by  $\bar{y}$  taking the imaginary part in the identity one obtains and integrating by parts, due to the fact that  $v$  is real-valued, we deduce that

$$(4.2) \quad \int_{\Omega} |y(x, t)|^2 dx = \int_{\Omega} |y_0(x)|^2 dx, \quad \forall 0 \leq t \leq T.$$

This clearly indicates that the initial datum determines the sphere of  $L^2(\Omega)$  in which the solution lives for all  $T > 0$ , regardless of the choice of the control.

The control problem we address consists, roughly, on determining the set of reachable states a given time  $T$ .

The same problem can be formulated for a wider class of Schrödinger equations and control mechanisms. In particular the problem makes sense for an equation of the form

$$(4.3) \quad iy_t = \Delta y + v(t)a(x)y \quad \text{in } \Omega \times (0, T),$$

where  $a$  is a given, real-valued smooth function. All solutions of (4.3) do satisfy the same constraint (4.2).

This type of system and controllability problem arises naturally in the context of Quantum Mechanical and molecular systems. In the bibliography at the end of this article we include some basic references on this topic.

One of the main differences of the problem under consideration (4.1) or (4.3) and the problems we have addressed above in which the control enters in the system in a linear way, is that, the structure of the reachable set depends very strongly on the initial datum  $y_0$ . Indeed, in view of (4.2), it is clear, for instance, that when  $y_0 \equiv 0$ , the only possible final target one may reach is  $y_1 \equiv 0$ . In fact, as pointed out in [Tu2], whatever the initial datum is, the set of reachable states has a dense complement in  $L^2(\Omega)$  (this was previously observed in [BMS] in the context of the bilinear control of beams).

In order to analyze the structure of the set reachable states it is natural to fix the control time  $T > 0$  and the initial datum to be controlled  $y_0 \in L^2(\Omega)$  and to consider the nonlinear map

$$(4.4) \quad \begin{cases} \mathcal{N} : L^2(0, T) & \longrightarrow & L^2(\Omega) \\ v & \longrightarrow & y(T), \end{cases}$$

where  $y$  is the solution of (4.1) (or (4.3)) with initial datum  $y_0$  and control  $v$ . Recall that in (4.4)  $L^2(0, T)$  stands for the space of real valued controls.



The map  $\mathcal{N}$  being nonlinear, it is natural to consider its linearization at  $v = 0$ . One obtains the system

$$(4.5) \quad \begin{cases} iz_t = \Delta z + w(t)\tilde{y} & \text{in } \Omega \times (0, T) \\ z = 0 & \text{on } \partial\Omega \times (0, T) \\ z(0) = 0 & \text{in } \Omega, \end{cases}$$

where  $\tilde{y}$  is the solution of the original system in the absence of control

$$(4.6) \quad \begin{cases} i\tilde{y}_t = \Delta\tilde{y} & \text{in } \Omega \times (0, T) \\ \tilde{y} = 0 & \text{on } \partial\Omega \times (0, T) \\ \tilde{y}(0) = y_0 & \text{on } \Omega. \end{cases}$$

With this notation

$$(4.7) \quad \langle DN(0), w \rangle = z(T),$$

where  $z$  solves (4.5).

In order to describe locally (for controls of small amplitude) the structure of the set of reachable states for the bilinear control problem (4.1) it is natural to first analyze it for the linearized system (4.5) and then apply the Inverse Function Theorem. This strategy was successfully pursued in [BMS] in the context of the beam equation.

In this way one is led to address the linear control problem (4.5). It is similar to those we have discussed in the previous sections except that:

- The control  $w$  in (4.5) is real-valued.
- The control  $w$  depends only on time.
- The control  $w$  acts on the system through a profile  $\tilde{y}$  which is in fact a solution of the Schrödinger equation (4.6).

The so-called HUM (Hilbert Uniqueness Method) developed by J.L. Lions in [L] can also be applied in this problem. The question is, once again, reduced to the obtention of a suitable observability inequality for the adjoint system (1.6). However, this time, the inequality of interest reads as follows:

$$(4.8) \quad \|\phi_0\|_*^2 \leq C \int_0^T \left| \operatorname{Im} \left( \int_{\Omega} \bar{\phi} \tilde{y} dx \right) \right|^2 dt.$$

The following comments are in order:

- The observed quantity is a weighted average of the solution  $\phi$  of the adjoint system. The weight  $\tilde{y}$ , which depends on  $x$  and  $t$ , is the solution of (4.6) and, consequently, is very sensitive to the initial datum  $y_0$  to be controlled. Consequently, the observability inequality one expects depends very strongly on the initial datum to be controlled, which is in agreement with the previously observed fact that the set of reachable states for (4.1) depends very strongly on the initial datum.
- The fact that the right hand side term in (4.8) defines a norm is far from being obvious. The underlying uniqueness problem now reads as follows:

$$(4.9) \quad \operatorname{Im} \left( \int_{\Omega} \bar{\phi} \tilde{y} dx \right) = 0, \quad \forall 0 \leq t \leq T \implies \phi \equiv 0?.$$

This problem does not enter in the class of Cauchy problems one may solve by means of Holmgren's Uniqueness Theorem.

In fact, it is clear that (4.9) may not hold since  $\phi = \tilde{y}$  solves (1.6), is non-trivial when  $y_0 \neq 0$ , and the left hand side term in (4.9) vanishes. This fact is related with the constraint (4.2) that solutions of the bilinear system (4.1) satisfy. The range of  $\mathcal{N}$  is necessarily contained

in the sphere (1.2) and therefore one does not expect the range of its linearization to be full and this is precisely due to this lack of uniqueness that the solution  $\phi = \tilde{y}$  imposes.

In order to further understand inequality (4.8) and its possible variants, it is convenient to observe that there are many other solutions that are an obstacle for it to hold. To see this it is convenient to develop both  $\phi$  and  $\tilde{y}$  on the basis of eigenfunctions of the Laplacian

$$(4.10) \quad \begin{cases} -\Delta w_k = \lambda_k w_k & \text{in } \Omega \\ w_k = 0 & \text{on } \partial\Omega, k \geq 1. \end{cases}$$

It is well-known that  $\{w_k\}_{k \geq 1}$  can be chosen to constitute an orthonormal basis of  $L^2(\Omega)$ . In this way,  $\phi$  and  $\tilde{y}$  solutions of (4.6) and (1.6) respectively, can be written in the form

$$(4.11) \quad \tilde{y}(x, t) = \sum_{k \geq 1} y_{0,k} e^{i\lambda_k t} w_k(x); \quad \phi(x, t) = \sum_{k \geq 1} \phi_{0,k} e^{i\lambda_k t} w_k(x)$$

where  $\{y_{0,k}\}_{k \geq 1}$  and  $\{\phi_{0,k}\}_{k \geq 1}$  are respectively the Fourier coefficients of their initial data.

In view of this we have

$$(4.12) \quad \operatorname{Im} \left( \int_{\Omega} \bar{\phi} \tilde{y} dx \right) = \operatorname{Im} \left[ \sum_{k \geq 1} \bar{\phi}_{0,k} y_{0,k} \right] = \operatorname{Im} \left( \int_{\Omega} \bar{\phi}_0 y_0 dx \right).$$

According to the identity (4.12) it is clear that (4.9) fails whatever the initial datum  $y_0$  is. In fact, it is clear that the fact that  $\operatorname{Im} \left( \int_{\Omega} \bar{\phi} \tilde{y} dx \right)$  vanishes in a time interval  $[0, T]$  simply guarantees that the initial datum  $\phi_0$  of  $\phi$  is orthogonal to  $y_0$ .

Let us now discuss the more general control system (4.3). As we shall see, the degree of controllability of the system can be greatly improved by an appropriate choice of the control profile  $a$ .

When one considers the control mechanism in (4.3) with a different profile  $a(x)$ , the corresponding observability inequality reads

$$(4.13) \quad \|\phi_0\|_*^2 \leq C \int_0^T \left| \operatorname{Im} \left( \int_{\Omega} a(x) \bar{\phi} \tilde{y} dx \right) \right|^2 dt$$

and the underlying uniqueness problem is now as follows

$$(4.14) \quad \operatorname{Im} \left( \int_{\Omega} a(x) \bar{\phi} \tilde{y} dx \right) = 0, \quad 0 \leq t \leq T \implies \phi \equiv 0?$$

Again the solution  $\phi = \tilde{y}$  is an obstacle for this to hold since  $a = a(x)$  is real-valued.

To see whether there are other obstructions for (4.14) to hold, we can argue as above by means of Fourier series. This time we get

$$(4.15) \quad \operatorname{Im} \left( \int_{\Omega} a(x) \bar{\phi} \tilde{y} dx \right) = \operatorname{Im} \sum_{k,j=1}^{\infty} \bar{\phi}_{0,k} \tilde{y}_{0,j} e^{i(\lambda_j - \lambda_k)t} \alpha_{k,j}$$

where the infinite matrix  $(\alpha_{k,j})_{k,j \geq 1}$  is constituted by the elements

$$(4.16) \quad \alpha_{k,j} = \int_{\Omega} a(x) w_k(x) w_j(x) dx.$$

To simplify the discussion let us consider the particular case in which the initial datum  $y_0$  is such that

$$(4.17) \quad y_{0,1} \neq 0, \quad y_{0,j} = 0, \quad \forall j \geq 2$$

and the control profile  $a = a(x)$  satisfies

$$(4.18) \quad \alpha_{k,1} \neq 0, \quad \forall k \geq 1.$$

In this case the quantity under consideration can be rewritten as

$$(4.19) \quad \operatorname{Im} \left( \int_{\Omega} a(x) \bar{\phi} \tilde{y} dx \right) = \operatorname{Im} \left( \sum_{k=1}^{\infty} \bar{\phi}_{0,k} y_{0,1} \alpha_{k,1} e^{i(\lambda_1 - \lambda_k)t} \right) = \sum_{k \geq 1} (a_k e^{i\mu_k t} + b_k e^{-i\mu_k t})$$

with

$$(4.20) \quad \begin{cases} a_k = \frac{\alpha_{k,1}}{2} [\operatorname{Im}(\bar{\phi}_{0,k} y_{0,1}) - \operatorname{Re}(\bar{\phi}_{0,k} y_{0,1})] \\ b_k = -\frac{\alpha_{k,1}}{2} [\operatorname{Im}(\bar{\phi}_{0,k} y_{0,1}) + \operatorname{Re}(\bar{\phi}_{0,k} y_{0,1})], \end{cases}$$

and

$$(4.21) \quad \mu_k = \lambda_k - \lambda_1.$$

Thus, we are led to analyze non-harmonic Fourier series of the form

$$(4.22) \quad f(t) = \sum_{k \in \mathbb{Z}} c_k e^{i\omega_k t}$$

where  $\{\omega_k\}_{k \in \mathbb{Z}}$  is an increasing sequence of distinct real number such that

$$(4.23) \quad \omega_k \rightarrow \infty, k \rightarrow \infty; \quad \omega_{-k} \rightarrow -\infty, k \rightarrow -\infty.$$

The following classical result by Ingham plays a central role in the understanding of the behavior of these series (see [Y]):

*“Let us assume that the sequence  $\{\omega_k\}_{k \in \mathbb{Z}}$  is such that*

$$(4.24) \quad \omega_{k+1} - \omega_k \geq \gamma, \quad \forall k \in \mathbb{Z}$$

*for some gap number  $\gamma$ .*

*Then, for any  $T > 2\pi/\gamma$  there exist positive constants  $C_1, C_2 > 0$  depending on  $T$  such that*

$$(4.25) \quad C \sum_{k \in \mathbb{Z}} |c_k|^2 \leq \int_0^T |f(t)|^2 dt \leq C_2 \sum_{k \in \mathbb{Z}} |c_k|^2,$$

*for any function  $f$  as in (4.22).”*

Several variants of this inequality have been proved. In particular, it is well-known that the time  $T$  needed for (4.25) to hold depends only on the asymptotic gap of the sequence  $\{\omega_k\}_{k \in \mathbb{Z}}$  as  $|k| \rightarrow \infty$ , while the value of the constants  $C_1, C_2$  in (4.25) depends also on the minimal distance between consecutive values of the  $\omega_k$ 's too (see, for instance, [MiZ]). We also refer to [BKL] for a stronger generalization where a uniform gap condition is not required.

In our case

$$(4.26) \quad \omega_k = \mu_k = \lambda_k - \lambda_1, \quad k \geq 1, \quad \omega_{-k} = -\mu_k = \lambda_1 - \lambda_k.$$

Thus, the gap condition (4.24) is fulfilled in one space dimension. Indeed, when  $n = 1$  and, for instance,  $\Omega = (0, \pi)$ , we have  $\lambda_k = k^2$  and, consequently, (4.24) holds. In fact, the asymptotic gap

$$(4.27) \quad \gamma_{\infty} = \liminf_{|k| \rightarrow \infty} (\omega_{k+1} - \omega_k) = \infty.$$

Consequently, using the variant of Ingham's inequality in [MiZ] we deduce that the analogue of (4.25) holds for all  $T > 0$ .

As a consequence of this, under the assumptions (4.17) and (4.18), in one space dimension, we deduce that (4.13) holds for all  $T > 0$  and a suitable observability constant  $C = C(T) > 0$ , where the semi-norm  $\|\cdot\|_*$  is as follows:

$$(4.28) \quad \|\phi_0\|_*^2 = |y_{0,1}|^2 \sum_{k \geq 2} |\alpha_{k,1}|^2 |\phi_{0,k}|^2 + |\alpha_{1,1}|^2 |\operatorname{Im}(y_{0,1} \bar{\phi}_{0,1})|^2.$$

Several remarks are in order:

- We observe a difference in (4.28) when comparing the components  $k = 1$  and  $k \geq 2$ . Indeed, for the component  $k = 1$  we only get an estimate on  $\operatorname{Im}(y_{0,1} \bar{\phi}_{0,1})$ . This is due to the fact that  $\mu_1 = 0$ .  
This clearly indicates that  $\|\cdot\|_*$  is a semi-norm but not a full norm. This is so since  $\|\cdot\|_*$  has in its kernel the initial data  $\phi_0$  which are of the form  $\phi_0 = y_0 = y_{0,1} w_1(x)$ . This fact is in agreement with the observation we made above in the sense that the uniqueness property (4.14) does never fully hold.
- The semi-norm in (4.28) degenerates as  $y_{0,1} \rightarrow 0$ . This is in agreement with the fact that, when the initial datum  $y_0 \equiv 0$ , the systems under consideration (both the bilinear and the linearized one) are not controllable at all in the sense that the only reachable final state is the identically zero one.
- The norm in (4.28) depends on the sequence of coefficients  $\{\alpha_{k,1}\}_{k \geq 1}$ . Recall that

$$\alpha_{k,1} = \int_{\Omega} a(x) w_k(x) w_1(x) dx.$$

Then, as soon as  $a \in L^2(\Omega)$  we also have  $aw_1 \in L^2(\Omega)$  and, consequently,  $\{\alpha_{k,1}\} \in \ell^2$ . This shows that the semi-norm  $\|\cdot\|_*$  in (4.28) is weaker than the  $L^2(\Omega)$ -norm. Furthermore, it gets weaker and weaker as the control profile  $a$  becomes more and more smooth.

- The assumptions (4.17) and (4.18) guarantee, in one space-dimension, that the kernel of  $\|\cdot\|_*$  is one-dimensional. Of course, in general, this kernel could be of higher dimension. Roughly speaking, this corresponds to the existence of directions in  $L^2(\Omega)$  in which the control mechanism is inefficient.

To better understand these issues it is interesting to see how the observability inequality (4.13) with  $\|\cdot\|_*$  as in (4.28) can be used to derive controllability results for the linearized system (4.5).

This time, the initial datum of  $z$  in (4.5) being identically zero, it is natural to reach a non-trivial final target  $z_1 \in L^2(\Omega)$ . In other words, we look for a real-valued control  $w = w(t)$  such that the solution  $z$  of (4.5) satisfies

$$(4.29) \quad z(T) = z_1.$$

Identity (1.10) with  $v = w\tilde{y}$ , applied to (4.5) yields

$$(4.30) \quad \int_0^T w(t) \left( \int_{\Omega} \tilde{y} \bar{\phi} dx \right) dt = i \int_{\Omega} z(T) \bar{\phi}(T) dx.$$

Taking imaginary parts in this identity we deduce that

$$(4.31) \quad \int_0^T w(t) \operatorname{Im} \left( \int_{\Omega} a(x) \tilde{y} \bar{\phi} dx \right) dt = \operatorname{Re} \int_{\Omega} z(T) \bar{\phi}(T) dx.$$

Combining (4.29) and (4.31) we identify the Euler-Lagrange equations associated with the minimization of the functional

$$(4.32) \quad J(\phi_0) = \frac{1}{2} \int_0^T \left| \operatorname{Im} \left( \int_{\Omega} a(x) \tilde{y} \bar{\phi} dx \right) \right|^2 dt - \operatorname{Re} \int_{\Omega} z_1 \bar{\phi}(T) dx.$$

The functional  $J : L^2(\Omega) \rightarrow \mathbb{R}$ , is once again, continuous and convex. Thus, in order to minimize it, it is sufficient to prove that it is coercive. At this point we have to use the observability inequality (4.13). But, taking into account that the kernel of  $\|\cdot\|_*$  is non-trivial, the coercivity of  $J$  can not be achieved in the whole space  $L^2(\Omega)$ . In fact,  $J$  is only coercive in the orthogonal complement of  $y_0^\perp$ , i.e., in the vector space of the initial data  $\phi_0$  for which  $\operatorname{Re} \int_{\Omega} y_0 \bar{\phi}_0 dx = 0$ . But, moreover, as we pointed out above, taking into account that the semi-norm  $\|\cdot\|_*$  is weaker than the  $L^2(\Omega)$ -one, the coercivity does not hold in the  $L^2(\Omega)$ -norm, but rather in the canonical norm of the Hilbert space

$$(4.33) \quad H = \left\{ \phi_0 = \sum_{k \geq 1} b_k w_k(x) : \sum_{k \geq 1} |b_k|^2 \gamma_k < \infty, \phi_0 \in y_0^\perp \right\}$$

where the positive weights  $\gamma_k > 0$  are those arising in the definition of (4.28).

Minimizing  $J$  in  $H$  we do get a minimizer  $\psi_0 \in H$ . The control

$$(4.34) \quad w = \operatorname{Im} \int_{\Omega} a(x) \tilde{y} \bar{\psi} dx$$

(where  $\psi$  is the solution of the adjoint system with the minimizer  $\psi_0$  as initial datum) is then such that (4.31) holds for every  $\phi$  solution of the adjoint system with initial datum in  $H$ . Obviously, because of the constraint that  $\phi_0 \in y_0^\perp$  in  $H$ , we do not quite get the target (4.29) fully but rather the fact that

$$(4.35) \quad \pi z(T) = \pi z_1,$$

where  $\pi$  denotes the projection on the orthogonal complement of  $\mathcal{S}(T)y_0 = \tilde{y}(T)$ .

Obviously, this is related with the fact that all the solutions of the bilinear control problem are trapped in the sphere (4.2) which makes the control requirement (4.35) to be optimal.

In order for the functional to be well-defined in  $H$  one needs  $z_1$  to belong to its dual space  $H'$ . On the other hand, taking into account that the semi-norm  $\|\cdot\|_*$  is weaker than the  $L^2(\Omega)$ -one, the space  $H$  is strictly greater than the corresponding projection of  $L^2(\Omega)$  and therefore  $H'$  is strictly smaller.

All this indicates that, in the best case, (4.35) can only be achieved for a space of targets strictly smaller than  $L^2(\Omega)$  (roughly speaking, constituted by functions which are smoother than  $L^2(\Omega)$ ). Moreover this space turns out to be smaller and smaller when the control profile becomes more and more smooth.

Once this is done, one can get local controllability results for the bilinear control problem by combining the one we have proved for the linearized system and the Inverse Function Theorem. In this way we conclude that, under the assumptions (4.17)-(4.18), in one space dimension, we can control the bilinear system (4.1) to the intersection of the sphere (4.2) with a  $\varepsilon$ -neighborhood in  $H'$  of the final state  $\tilde{y}(T)$  that the equation reaches naturally in the absence of control.

The interested reader is referred for details to the paper by J. Ball et al. [BMS] on the controllability of a bilinear beam model.

The analysis carried out above, based on the use of the Fourier series developments and Ingham-like inequalities, has been partially successful to deal with the bilinear control problem but has also serious limitations. The main ones are as follows:

- The analysis above is based on the assumption (4.17). The situation is much more complex when the initial datum has more than one non-vanishing Fourier component. As far as we know this case has not been addressed in the literature.
- Gap conditions of the form (4.24) hold, typically, only in one space dimension. Indeed, according to Weyl's Theorem, the eigenvalues of the Laplacian  $\{\lambda_k\}_{k \geq 1}$  behave asymptotically as  $C(\Omega)k^{n/2}$  when  $k \rightarrow \infty$  ( $n$  being the space dimension) for a suitable constant  $C(\Omega)$  depending on the geometry of the domain  $\Omega$ . This excludes the possibility of having a gap property of the form (4.24) for  $n \geq 3$  and makes the case of the dimension  $n = 2$  to be critical.
- One can get weaker controllability results under weaker spectral assumptions by replacing Ingham's Theorem by a consequence of Beurling-Malliavin's Theorem (see [HJ]). According to it if the sequence  $\{\omega_k\}_{k \in \mathbb{Z}}$  is such that

$$(4.36) \quad \#\{|\omega_k| \leq \mu\} \leq 2d\mu + O(\mu^\alpha)$$

as  $\mu \rightarrow \infty$  with  $0 < \alpha < 1$  and some  $d > 0$ , then for all  $T > 2\pi d$  and  $m \in \mathbb{Z}$  there exists  $\gamma_m > 0$  such that

$$(4.37) \quad \gamma_m |c_m|^2 \leq \int_0^T |f(t)|^2 dt,$$

for every function  $f$  as in (4.25).

Obviously, Ingham's inequality (4.37) is stronger than (4.25) since it provides a global information on the coefficients  $\{c_k\}_{k \in \mathbb{Z}}$ . But assumption (4.36) is weaker than the gap condition (4.24) or (4.27). At this point the work by Baiocchi et al. [BKL] is worth mentioning since it may help on getting explicit estimates on the constants  $\gamma_m$  in (4.30) and this may be relevant to obtain explicit estimates on the observability space  $H$  and its dual  $H'$ , the space of controllable data.

Nevertheless, according to Weyl's Theorem, one may not expect (4.36) to hold except for dimensions  $n = 1, 2$ .

Summarizing, the use of classical results on nonharmonic Fourier series may allow obtaining inequalities of the form (4.13) in some particular situations. But, as far as we know, this issue has not been completely explored in the literature.

In this section we have formulated the problem of bilinear controllability for the Schrödinger equation and we have described the method, introduced in [BMS] in the context of beam equations, consisting on linearizing the system and then applying classical results on non-harmonic Fourier series to solve the linearized control problem.

However, as we have seen, this approach may only lead to local controllability results and can only be applied in very particular situations that require important restrictions on the initial datum  $y_0$  to be controlled, the control profile  $a = a(x)$  and the spectrum of the Laplacian.

This approach has not been fully developed in the literature except for some particular cases ([TT]). It seems that new tools are needed for a complete understanding of this challenging problem of bilinear control for Quantum mechanical systems.

## 5. Numerical approximation results

As far as we know, there are two types of relevant results in the literature on the controllability of numerical approximation schemes for the Schrödinger equations under consideration:

- Numerical approximation schemes for the linear Schrödinger equations (see [LZ], [Ma] and [Zu5]).

- Finite-dimensional Galerkin approximations of the bilinear control problem for the Schrödinger equation ([**RSDRP**] and [**Tu**]).

Let us briefly discuss these issues.

Concerning the controllability of the classical numerical approximation schemes for the linearized Schrödinger equation the following is known:

- In [**LZ**] it was proved that the boundary controls for the space semi-discretizations of the one-dimensional beam equation converge to the boundary control of the continuous beam model. This is true despite of the oscillatory behavior of the controls at high frequencies, because of the dispersive properties of the beam equation for which the results are significantly better than for the wave equation (where it is by now well-known that the controls may diverge as the mesh-size tends to zero (see [**Zu6**])). The results in [**LZ**] do apply to the Schrödinger equation too.
- In [**Ma**] a discrete Wigner measure theory has been developed to analyze the propagation of energy for solutions of numerical approximation schemes for wave-like equations. These results allow, in particular, to develop sharp Fourier filtering techniques to obtain uniform (with respect to the mesh-size) observability and controllability results. In [**Ma**] it has been also proved that, proceeding as in [**Le**], by means of a semi-classical reduction, as soon as the numerical schemes for the wave equation are uniformly (with respect to the discretization parameter) observable/controllable, then the corresponding numerical schemes for the Schrödinger equation have the same property in an arbitrarily small control time.

These results concern the controllability property of the linear Schrödinger equation analyzed in Section 2. As far as we know nothing is known about the controllability of the numerical approximation schemes for the semilinear Schrödinger equations in Section 3.

The same can be said about the bilinear control problems discussed in Section 4. However, the key remark in [**LZ**] may be relevant at this respect in one-dimensional problems. Indeed, in [**LZ**] it was pointed out that the spectra of the three-point finite-difference approximations of the Laplacian in  $1 - d$  fulfill the asymptotic gap condition (4.27), uniformly on the parameter  $h$  of the space discretization. As pointed out in [**LZ**], this allows applying Ingham's inequality uniformly with respect to the parameter  $h$ , both in what concerns the time  $T > 0$  (which can be taken arbitrarily small) and the constants entering in the inequality (4.25). Accordingly, pursuing this approach, one may expect in those cases that the method described in Section 3 does provide local controllability results for the bilinear control problem (4.3), the same to be true for the finite-difference space semi-discretizations, uniformly on the parameter  $h$ . One can then expect that, as  $h \rightarrow 0$ , the controls of the semi-discrete system converge to those of the continuous Schrödinger equation. But a detailed analysis of this issue remains to be done.

Concerning the controllability of finite-dimensional Galerkin approximations of the bilinear Schrödinger control problem several works are worth mentioning. Following the fundamental works by A. Peirce et al. [**PDR**], the finite-dimensional bilinear controllability problem has been analyzed by V. Ramakrishna et al. in [**RSDRP**] by Lie group techniques and by G. Turinici et al. in [**Tu**] by means of graph theory tools. These articles provide a full description of the controllability properties of the Galerkin approximations.

However, nothing is known about the behavior of the controls as the dimension of the Galerkin basis tends to infinity and, thus, when the finite-dimensional system approximates the Schrödinger equation. From a mathematical point of view this is a very challenging (and very likely difficult) open problem in this area.

## References

- [A] Allibert, B. *Contrôle analytique de l'équation des ondes et de l'équation de Schrödinger sur des surfaces de révolution*. Comm. Partial Differential Equations 23 (1998), no. 9-10, 1493–1556.

- [BKL] Baiocchi, C., Komornik, V., Loreti, P. *Ingham-Beurling type theorems with weakened gap conditions*, Acta Mathematica Hungarica, 97(1): 55-95.
- [BMS] Ball, J. M.; Marsden, J. E.; Slemrod, M. *Controllability for distributed bilinear systems*. SIAM J. Control Optim. 20 (1982), no. 4, 575-597.
- [BLR] Bardos, C., Lebeau, G. and Rauch, J. (1992). *Sharp sufficient conditions for the observation, control and stabilization of waves from the boundary*, SIAM J. Cont. Optim., **30**, 1024-1065.
- [BP] Baudouin, L. and Puel, J. P. (2002). *Uniqueness and stability in an inverse problem for the Schrödinger equation, Inverse problems, to appear*.
- [BS] P. Brumer and M. Shapiro, *Laser control of chemical reactions*, Scientific American, 1995, pp. 34-39.
- [Bu] Burq, N. *Contrôle de l'équation des plaques en présence d'obstacles strictement convexes*. Mém. Soc. Math. France (N.S.) No. 55 (1993).
- [C] T. Cazenave, *An introduction to nonlinear Schrödinger equations*, Textos de Métodos Matemáticos, 22, Instituto de Matemática, Universidad Federal de Rio de Janeiro, 1989.
- [CH] T. Cazenave and A. Haraux, *Equations d'évolution avec nonlinéarité logarithmique*, Ann. Fac. Sci. Toulouse, **2** (1980), 21-51.
- [Ch] Chen, G.; Fulling, S. A.; Narcowich, F. J.; Sun, S. *Exponential decay of energy of evolution equations with locally distributed damping*. SIAM J. Appl. Math. 51 (1991), no. 1, 266-301.
- [DLZ] B. Dehman, G. Lebeau and E. Zuazua, *Stabilization and Control of the semilinear subcritical wave equation potential*, Annales Ecole Normale Supérieure de Paris, to appear
- [FPZ] C. Fabre, J. P. Puel and E. Zuazua, *Contrôlabilité approchée de l'équation de la chaleur semilinéaire*, C. R. Acad. Sci. Paris. 315. 807-812. 1992.
- [FCZ] E. Fernández-Cara and E. Zuazua, *The cost of approximate controllability for heat equations: The linear case*, Advances Diff. Eqs., 5 (4-6) (2000), 465-514.
- [FCZ] E. Fernández-Cara and E. Zuazua, *Null and approximate controllability for weakly blowing up semilinear heat equations*, Annales de l'IHP. Analyse non linéaire, 17 (5) (2000), 583-616.
- [Ge] Gérard, P. (1991). *Microlocal defect measures*, Comm. P.D.E., **16**, 1761-1794.
- [HJ] Haraux, A., and Jaffard, S. (1991). *Pointwise and spectral controllability for plate vibrations*, Revista Matemática Iberoamericana, **7** (1), 1-24.
- [Ja] Jaffard, S. *Contrôle interne exact des vibrations d'une plaque carrée*. C. R. Acad. Sci. Paris Sr. I Math. 307 (1988), no. 14, 759-762.
- [Jh] F. John, *Partial Differential Equations*, (4. ed), Springer, 1982.
- [K] Kime, K. *Simultaneous control of a rod equation and a simple Schrödinger equation*. Systems Control Lett. 24 (1995), no. 4, 301-306.
- [La] Lagnese, J. *Control of wave processes with distributed controls supported on a subregion*. SIAM J. Control Optim. 21 (1983), no. 1, 68-85.
- [LT1] Lasiecka, I.; Triggiani, R. *Optimal regularity, exact controllability and uniform stabilization of Schrödinger equations with Dirichlet control*. Differential Integral Equations, 5 (1992), no. 3, 521-535.
- [LT2] Lasiecka, I.; Triggiani, R. *Exact controllability of semilinear abstract systems with application to waves and plates boundary control problems*. Appl. Math. Optim. 23 (1991), no. 2, 109-154.
- [LTZ] Lasiecka, I. and R. Triggiani and X. Zhang (2002). *Nonconservative Schrödinger equations with unobserved Neumann B. C.: Global uniqueness and observability in one shot*. Preprint, 2002.
- [Le] G. Lebeau, *Contrôle de l'équation de Schrödinger*, J. Math. Pures Appl., **71** (1992), 267-291.
- [LZ] León, L. and Zuazua, E. (2002). *Boundary controllability of the finite-difference space semi-discretizations of the beam equation*, ESAIM:COCV, A Tribute to Jacques-Louis, Tome 2, 827-862.
- [LTRR] B. Li, G. Turinici, V. Ramakrishna, and H. Rabitz. *Optimal dynamic discrimination of similar molecules through quantum learning control*. Journal of Physical Chemistry B, 106(33):8125-8131, 2002.
- [L] J.-L. Lions, *Contrôlabilité exacte, stabilisation et perturbations de systèmes distribués. Tome 1*. RMA **8**, Paris, 1988.
- [Ma1] Machtyngier, E. *Contrôlabilité exacte et stabilisation frontière de l'équation de Schrödinger*. C. R. Acad. Sci. Paris, Sr. I Math., 310 (1990), no. 12, 801-806.
- [Ma2] Machtyngier, E. (1994). *Exact controllability for the Schrödinger equation*, SIAM J. Control and Optimization, 32 (1), 24-34.
- [MaZ] E. Machtyngier and E. Zuazua, *Stabilization of the Schrödinger equation*. Portugaliae Mathematica, 51 (2) (1994), 243-256.
- [Ma] Macià, F. (2002). *Propagación y control de vibraciones en medios discretos y continuos*, PhD Thesis, Universidad Complutense de Madrid.



- [McZ] F. Macià and E. Zuazua, *On the lack of controllability of wave equations: a gaussian beam approach*, *Asymptotic Analysis*, **32** (1) (2002), 1-26.
- [MiZ] Micu, S. and Zuazua, E. (1997). *Boundary controllability of a linear hybrid system arising in the control of noise*, *SIAM J. Cont. Optim.*, **35**(5), 1614-1638.
- [PDR] Peirce, A., Dahleh, M., Rabitz, H., 1988. *Optimal control of quantum mechanical systems: Existence, numerical approximations, and applications*. Phys. Rev. A 37, 4950–4964.
- [Ph] Phung, K.D. *Observability and control of Schrödinger equations*. (English. English summary) SIAM J. Control Optim. 40 (2001), no. 1, 211–230.
- [R] Ralston, J. (1982) *Gaussian beams and the propagation of singularities*. *Studies in Partial Differential Equations*, MAA Studies in Mathematics, **23**, W. Littman ed., pp. 206-248.
- [RVMK] Rabitz, H., de Vivie-Riedle, R., Motzkus, M., Kompa, K., 2000. *Wither the future of controlling quantum phenomena?* *Science*, 288, 824–828.
- [RSDRP] Ramakrishna, V., Salapaka, M., Dahleh, M., Rabitz, H., Pierce, A. (1995) *Controllability of molecular systems*. Phys. Rev. A, **51** (2), 960–966.
- [R1] Russell, D. L. (1978). *Controllability and stabilizability theory for linear partial differential equations. Recent progress and open questions*. *SIAM Rev.*, **20**, 639-739.
- [SWR] Shi, S., Woody, A., Rabitz, H., 1988. *Optimal control of selective vibrational excitation in harmonic linear chain molecules*. J. Chem. Phys. 88, 6870–6883.
- [TT] Takahashi, T and Tucsnak, M, *Private communication*.
- [Tu] Turinici, G. and Rabitz H. (2001). *Quantum Wavefunction Controllability*. Chem. Phys. **267**, 1-9.
- [Tu2] Turinici, G. (2000). *Controllable quantities for bilinear quantum systems*. *Proceedings of the 39th IEEE Conference on Decision and Control*, Sydney Convention & Exhibition Centre, 1364-1369.
- [Y] Young, R. M. (1980). *An Introduction to Nonharmonic Fourier Series*, Academic Press, New York.
- [Zh] Zhang, X. (2001). *Exact controllability of the semilinear plate equation*. *Asymptot. Anal.* **27**, 95–125.
- [Zu1] E.Zuazua, *Exact boundary controllability for the semilinear wave equation*, in *Nonlinear partial differential equations and their applications*, Collège de France Seminar, Vol. X (Paris, 1987-1988), Pitman Res. Notes Math. Ser., **220**, Longman Sci. Tech., Harlow, 1991, pp. 357–391.
- [Zu2] E.Zuazua, *Exact controllability for semilinear wave equations in one space dimension*, *Ann. Inst. H. Poincaré Anal. Non Linéaire*, **10** (1993), pp. 109–129.
- [Zu3] Zuazua, E. (1998). *Some problems and results on the controllability of partial differential equations*, *Progress in Mathematics*, **169**, Birkhäuser Verlag, pp. 276-311.
- [Zu4] Zuazua, E. (2002). *Controllability of Partial Differential Equations and its Semi-Discrete Approximations*. *Discrete and Continuous Dynamical Systems*, **8** (2), 469-513.
- [Zu5] E. Zuazua, *Propagation, Observation, Control and Numerical Approximation of Waves*, preprint, 2002.
- [Zu6] E. Zuazua, *Boundary observability for the finite-difference space semi-discretizations of the 2 – d wave equation in the square*, J. Math. pures et appl., 78 (1999), 523-563.

DEPARTAMENTO DE MATEMÁTICAS, UNIVERSIDAD AUTÓNOMA, 28049 MADRID, SPAIN

E-mail address: [enrique.zuazua@uam.es](mailto:enrique.zuazua@uam.es)