I. A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule

µ, J. of Diff. Eq. (2014) [3], C. P. Koch, M. Lemeshko, D. Sugny, Schrödinger equation

Its controllability properties have been recently studied for small finite-dimensional subsystems ([4]), but a rigorous mathematical approach should be adopted for its corresponding Schrödinger PDE.

II. Asymmetric molecule
Its controllability properties are not known yet, the main difficulty being the non explicit structure of the spectrum. Anyway, one degenerate quantum number vanishes, due to the asymmetry, and this could seriously help the controllability of the system.

III. Infinite-dimensional chiral molecules
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Motivations and open questions

• Planar molecule
Approximate controllability of a planar molecule has been established in [1]. The Schrödinger equation

\[ \frac{\partial}{\partial t} \psi(t) = - \nabla^2 \psi(t) + \mu_1 \psi(t) \cos \theta + \mu_2 \psi(t) \sin \theta, \quad \psi(t) \in L^2(S^2). \]

• Linear molecule
Approximate controllability of a linear molecule has been established in [2]. The Schrödinger equation

\[ \frac{\partial}{\partial t} \psi(t, \theta, \phi) = - \Delta \psi(t, \theta, \phi) + \mu_1 \sin \theta \cos \phi + \mu_2 \sin \phi \cos \theta + \mu_3 \psi(t, \theta, \phi), \quad \psi(t) \in L^2(S^3). \]

• Symmetric molecule
Is a natural generalization of a linear molecule, one more degree of freedom. We characterized its controllability in terms of its dipole moment. This is done by applying Lie-Galerkin technique, analyzing the controllability of finite-dimensional subspaces and taking the limit under good resonance assumptions. This problem was an open question, for example, in [3].

State selection for asymmetric chiral molecules

A chiral molecule can be seen as a direct sum system \( H \oplus H' \), where \( H \) is the Hilbert space of a symmetric or asymmetric-top. The two dipole moments are \( \mu^x \) and \( \mu^y \), one component with changed sign. For example, \( \mu^x = (\mu_0, \mu_1, \mu_2)^T, \mu^y = (\mu_0, -\mu_1, \mu_2)^T \).

The system is chiral controllable if the three spectral gaps are all different and the Rabi frequencies of one right-circularly polarized electric field, excited at frequencies \( |j| + 1 \), \( |j| \), \( |j| - 1 \), \( j = \pm 1 \), \( \pm 2 \) and the other \( 2\pi/\omega \) oscillate at a frequency \( \omega \).

Theorem
If the three spectral gaps are all different and the Rabi frequencies of one right-circularly polarized electric field are all different, then this chiral system is state selective starting from the ground state.

We remark that here we are dealing with finite-dimensional controllability.

A numerical simulation
The previous Theorem has been tested and exploited in a numerical simulation by Prof. Koch’s group of Theoretical Physics in the University of Kassel, Germany, to obtain state selection using quantum optimal control.

Motivations and open questions

• Symmetric-top
We consider a permanent dipole moment \( \mu = (\mu_0, \mu_1, \mu_2)^T \) inside the molecule. \( e_1, e_2, e_3 \) is the fixed frame, \( b_1, b_2, b_3 \) are the moments of inertia of the molecule.

\[ \frac{\partial}{\partial t} \psi(t, \theta, \phi) = - \nabla \psi(t, \theta, \phi) + \frac{\mu_1}{\sin \theta} \psi(t, \theta, \phi), \quad \psi(t) \in L^2(S^3). \]

The eigenstates of \( H \) are given by the Wigner functions \( B_m^j = |j, m \rangle \). Three quantum numbers needed to figure out the motion: \( j \in \mathbb{N}, m = -j, \ldots, j \). The energy levels are given by

\[ E_j = \frac{(j + 1)}{2m}, \quad |j, m \rangle \leadsto |j, m \rangle = \frac{1}{\sqrt{2m + 1}} |j, m \rangle. \]

• Genuine symmetric-top
Is a symmetric-top which verifies \( \mu = (0, 0, \mu_2)^T \), that is, dipole component only on the symmetry axis. Due to Noether’s Theorem, we found

Theorem
The quantum number \( k \) is invariant in the controlled motion of the genuine symmetric-top. That is,

\[ L^2(S^2) \ni \psi(t) = \sum_{i=0}^\infty C_i \psi_{E_i} \ni \psi(t) \in \mathbb{H}, \quad m = -j, \ldots, j. \]

\[ \psi(t) \in \text{a decomposition in orthogonal invariant subspaces (and reachable sets).} \]

Driving all the transitions between the symmetric states, by exciting the polarizations at three different type of frequencies, we obtained

\[ \psi(t) = \sum_{i=0}^\infty C_i \psi_{E_i} \ni \psi(t) \in \mathbb{H}, \quad m = -j, \ldots, j. \]

The orthogonal accidentally symmetric-top
Its dipole is orthogonal to the symmetry axis, that is, \( \mu_1 = 0 \). Here we used a rotated version of the Wang states

\[ \psi_{B_{E_i}}(\theta) := \sum_{k=-1}^{1} a_{E_i}^{(k)} |j, k \rangle, \quad j \in \mathbb{N}, k = -1, \ldots, 1. \]

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