Control of the orientational and vibrational degrees of freedom of a quantum molecule

**Type de contrat:** CDD de la fonction publique  
**Niveau de diplôme exigé:** Thèse ou équivalent  
**Fonction:** Post-Doctorant

**A propos du centre ou de la direction fonctionnelle**

Inria, the French National Institute for computer science and applied mathematics, promotes “scientific excellence for technology transfer and society”. Graduates from the world’s top universities, Inria's 2,700 employees rise to the challenges of digital sciences. With its open, agile model, Inria is able to explore original approaches with its partners in industry and academia and provide an efficient response to the multidisciplinary and application challenges of the digital transformation. Inria is the source of many innovations that add value and create jobs.

**Mission confiée**

**Assignments:**
With the help of the team CAGE, the recruited person will be taken to master the Lie–Galerkin technique for control of quantum systems, and to adapt it to new applications in molecular dynamics.

**For a better knowledge of the proposed research subject:**
A state of the art of the techniques that will be used during the post-doc can be found in the following articles:


**Collaboration:**
The recruited person will be in connection with Domique Sungy who works at Université de Bourgogne.

**Principales activités**

The spirit of the project is to develop the Lie–Galerkin technique (developed by the members of the team and collaborators) and to exploit its advantages in applications to molecular dynamics. In particular, in the first part of the postdoc (Task 1 below) we want to study the controllability of models describing the orientation and alignment of nonsymmetric molecules. In Task 2 we consider the controllability of the internal degree of freedom (torsion, vibration, etc.) of a rotating molecule.

**Task 1.** One of the main advantages of the Lie–Galerkin technique is that the results apply to very general systems and in particular to those with strong spectral degeneracies and geometrically nontrivial state space. This is extremely helpful when studying molecular orientation. For linear molecules driven by linearly polarized laser fields in gas phase, alignment means an increased probability direction along the polarization axis and orientation requires in addition the same direction as the polarization vector. In the mathematical framework the problem is to control the Schrödinger equation on Riemannian manifolds such as $S^1$, $S^2$, or $SO(3).$ Geometric techniques have been successfully applied to prove the controllability of a symmetric molecule rotating on a plane [1] and in the space [2]. A mathematically challenging and physically relevant open problem we will address is the orientation of a nonsymmetric molecule, which is modeled by the Schrödinger equation on $SO(3).$ Since models for the evolution of the molecular orientation are physically realistic and verified experimentally, we can in this way evaluate the performance of our approach. Natural mathematical developments would be the extension of the controllability of the Schrödinger equation on a Lie group, or the case of a molecule presenting a “thin” degree of freedom. In the last case the free Hamiltonian contains a sub-Laplacian and it would be interesting to study both the free evolution (many questions are still open for the hypoelliptic Schrödinger equation) and the controllability. In order to tackle these problems we are going to exploit the Lie–Galerkin technique and to combine it with the generalized Fourier transform, which is a helpful tool to investigate the spectral properties of the Schrödinger operator when the state space is a Lie group.
Task 2. The fine comprehension of the interaction of a molecule with its environment passes through the study of even more complex models than those proposed in the previous task. The full models feature elementary nanomachines controlled by laser. In this direction, it is natural to study the control of internal molecular degrees of freedom, such as torsional and vibrational ones. Recent experimental results have shown the possibility to control the torsional dynamics by laser fields in complex molecules [3,4]. In [5] effective Hamiltonians describing the internal dynamics of such molecular systems (vibrational and torsional degrees of freedom) have been established. The system presents a rotational Hamiltonian coupled with a Hamiltonian accounting for the internal degrees of freedom. The mathematical problem is then to control simultaneously the two Hamiltonians. One of the main challenges is represented by the resonances among the eigenstates of the two Hamiltonians. To overcome these difficulties we are going to exploit the Lie–Galerkin Control Condition introduced in [2]. Its advantage is that, while in preceding results based on the Lie–Galerkin technique the only actions on the system obtained by resonance that are exploited for the controllability are those corresponding to elementary transitions between two eigenstates, no such a restriction is imposed in the Lie–Galerkin Control Condition. This feature allows to prove approximate controllability for systems presenting several resonances.


Compétences

Technical skills and level required: the candidate should have a strong background in geometric control both from the theoretical point of view (symplectic language, differential geometry, sub-Riemannian structures, Lie groups) and applications (even in areas different from quantum control).

Languages: English knowledge is mandatory

Relational skills: we expect the candidate to quickly integrate in the team Cage and also to interact with physicists with whom we collaborate

Avantages sociaux

- Subsidised catering service
- Partially-reimbursed public transport

Rémunération

- Location: Paris 12ème
- Gross Salary per month: 2 653€ brut/mensuel

Security and defense procedure:

This position is likely to be situated in a restricted area (ZRR), as defined in Decree No. 2011-1425 relating to the protection of national scientific and technical potential (PPST).

Authorisation to enter an area is granted by the director of the unit, following a favourable Ministerial decision, as defined in the decree of 3 July 2012 relating to the PPST. An unfavourable Ministerial decision in respect of a position situated in a ZRR would result in the cancellation of the appointment.