

# Seminari Informal de Matemàtiques de Barcelona

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**Speaker:** Henar Hernández Mendiola.  
**Universitat:** Universidad Politécnica de Madrid.

**Data:** divendres 31 de maig de 2013.  
**Horari:** 15:15, *coffee break*; 15:30, xerrada.  
**Lloc:** Aula IMUB (al terrat), Facultat de Matemàtiques de la UB.

**Títol:** Influence of a laser pulse on the isomerization dynamics of the LiNC/LiCN molecular system.

**Resum:** The Transition State Theory allows us to obtain kinetic information about molecular systems without knowing the whole Potential Energy Surface. It is necessary to obtain a dividing surface on the phase space. The equator of the dividing surface corresponds to the so called “activated complex”. Once it is known it makes possible to obtain the gap time distributions, the reactive density of states, or the reactive flux across it and so, to calculate reaction rates. Such a dividing surface can be calculated even if the Hamiltonian function depends on time. That fact enables us to include laser-pulse perturbations [1], and so to study its effect on the dynamics and kinetics of molecular systems. We study the isomerization process for the molecular system LiNC/LiCN. A general way to write the Hamiltonian function is:

$$H(R, \theta, p_R, p_\theta, t) = H_0(R, \theta, p_R, p_\theta) + R\xi(t) \cos \alpha$$

where  $H_0(R, \theta, p_R, p_\theta)$  is the Hamiltonian of the isolated system,  $R, \theta$  are the Jacobi coordinates,  $p_R, p_\theta$  are the conjugated momenta,  $\alpha$  is the angle between the C-N and  $\xi(t)$  the pulse and is the function that simulates the electromagnetic pulse. The mathematical equation that describes the pulse has been taken from Ref. 1. It depends on some parameters such as the period of the perturbation, the amplitude or the frequency. The main goal of this project is to study the influence of that parameters on the dynamical geometric objects near the dividing surface (transition state, normally hiperbolic invariant manifold and its stable and unstable manifolds) and on the kinetic data mentioned before.

[1] S. Kawai, A. D. Bandrauk, C. Jaffé, T. Bartsch, J. Palacián, T. Uzer, Transition state theory for laser-driven reactions. J. Chem. Phys. 126, 164306 (2007).

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**Qui som?** El SIMBa és un seminari jove organitzat per estudiants de doctorat de matemàtiques. Està dirigit a estudiants de doctorat, de màster i, fins i tot, dels darrers cursos de grau. El nostre objectiu és donar a conèixer la recerca que estem fent, així com adquirir coneixements d’altres àrees de les matemàtiques diferents de la pròpia. Més informació a <http://euclides.imub.ub.es/simba>.