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Affiliation: Physics Department, Universidad Autonoma Metropolitana

Horacio Olivares-Pilon

Periodic Trajectories in Molecular Physics: The H_3^+ Molecule

Abstract

A molecule is a many-body quantum system consisting of electrons and nuclei. The well-established Born–Oppenheimer approximation enables the separation of electronic and nuclear motions, with the eigenvalues of the electronic Hamiltonian defining the corresponding potential energy surfaces. Within this quantum-mechanical framework, the rotational-vibrational spectrum of a molecule is obtained by solving the nuclear Schrödinger equation, using one of these electronic potential energy surfaces as the potential.

In the classical picture, instead, we can study the dynamics in terms of trajectories. In this talk, we present a study of closed periodic trajectories in the H_3^+ molecule. We will explore the rich variety of trajectories that arise and show how their properties give rise to a phenomenon of energy quantization.