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Non-adiabatic transitions in a diatomic molecule under a bichromatic laser field

Edgar Barriga Aguirre [1†], Luis E. F. Foà Torres [2], Carlos Cárdenas Valencia[1]
[1] *Departamento de Física, Facultad de Ciencias, Universidad de Chile, Santiago, Chile.*
[2] *Departamento de Física, Facultad Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile.*
†edgar.barriga@ug.uchile.cl

Abstract

Degeneracies in molecular systems have been studied extensively in the last decades. This kind of singularity has profound impacts on the dynamics since non-adiabatic effects arise due to the coupling between the electronic and nuclear motion [1]. For an N-state system the non-crossing rule requires $(N-1)(N+2)/2$ conditions over internal coordinates to achieve a degeneracy point in configuration space. Despite this seemingly strong restriction conical intersections of more than two states have shown to be not just a curiosity but the rule [2]. The existence of degeneracies is not restricted to the field-free case. It has been shown that they can be created by external means [3,4].

In this work we show that by using a bichromatic radiation field a three-state degeneracy can be created in diatomic molecules. This situation is forbidden for field-free diatomic molecules due to the non-crossing rule. The threefold degeneracy comes along with novels kind of two-state intersections (also forbidden for field-free diatomic molecules). We study the effects of the polarization of the lasers in these different induced intersections between the potential energy surfaces. The system chosen is the Cs_2 molecule.

The time-dependent Hamiltonian is treated with the Many Mode Floquet Theory (MMFT) [5]. We use the MMFT formalism to calculate the long-time averaged transition probabilities. We found a non-trivial dependence of the relative phase in this observable. Our results establish a way that can be implemented experimentally to control the non-adiabatic dynamics in molecular systems through the relative phase.

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Referencess

[1] X. Zhu and D. R. Yarkony, Molecular Physics 114, 1983–2013 (2016).
[2] L. Shen, B. Xie, Z. Li, L. Liu, G. Cui, and W.-H. Fang, The Journal of Physical Chemistry Letters 11, 8490–8501 (2020)
[3] B. Garraway and S. Stenholm, Optics communications 83, 349–357 (1991)
[4] N. Moiseyev, M. Šindelka, and L. S. Cederbaum, Journal of Physics B: Atomic, Molecular and Optical Physics 41, 221001 (2008).
[5] T.-S. Ho, S.-I. Chu, and J. V. Tietz, Chemical Physics Letters 96, 464–471 (1983).