Physica A 449 (2016) 101–110

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Controlling dissociation by trapping trajectories in highly energetic states

A.K. de Almeida Jr. [a], R. Egydio de Carvalho [a,*], E.F. de Lima [b]

[a] *Universidade Estadual Paulista-UNESP, Rio Claro-SP, Brazil*
[b] *Universidade Federal de São Carlos-UFSCAR, São Carlos-SP, Brazil*

HIGHLIGHTS

- A particle is trapped in a state outside the potential well.
- The trap is a non-linear resonance island.
- Chaotic and point attractors prevent the particle photo-dissociation.
- Dissipation inhibits photo-dissociation for energies above the dissociation threshold.
- The model used is the perturbed Morse oscillator.

ARTICLE INFO

Article history:
Received 17 December 2015
Available online 4 January 2016

Keywords:
Morse potential
Non-linear resonance
Dissociation
Dissipation
Attractors

ABSTRACT

We consider the non-linear dynamics of a polar diatomic molecule under the action of laser–field interactions and in the presence of a dissipation mechanism, described by the classical damped and driven one-dimensional Morse oscillator. In the absence of laser fields and dissipation, the phase space consists of a negative-energy bound region and a positive-energy dissociative region. Laser–molecule interaction changes the phase space allowing transitions from the bound to the dissociative region through chaotic routes. We show that for a spatially dependent dipole force, resonances with positive energies allow the trapping of trajectories in pseudo-bound states. We also show that, upon the introduction of dissipation, there exist non-trivial point attractors as well as chaotic attractors, which capture the trajectories in pseudo-bound states. Consequently, in addition to the parameters associated with the laser–molecule interaction, the amplitude of the dissipation acts as a control parameter of the photo-dissociation dynamics.

1. Introduction

Forced and dissipative non-linear oscillators can model a variety of important phenomena. One example is the damped and driven Morse oscillator, which can model vibrational excitations, breaking of a chemical bond of a polyatomic molecule by laser fields, multiphoton excitations and dissociation of hetero-nuclear diatomic molecules in a gaseous cell under high pressure [1–3].

In the absence of interactions with time-dependent external fields as well as dissipation, the Morse oscillator phase space can be divided into two parts: the bound region with negative energies and the unbound, or dissociative region with positive energies. The interaction of the unperturbed oscillator with an external driving field alters the phase space permitting

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* Corresponding author.
E-mail addresses: fenixcinza@yahoo.com.br (A.K. de Almeida Jr.), regydio@rc.unesp.br (R. Egydio de Carvalho), eflima@ufscar.br (E.F. de Lima).

http://dx.doi.org/10.1016/j.physa.2015.12.109

transitions from the bound to the unbound region through chaotic trajectories [4–8]. This photo-dissociation process can be regarded as a half collision, which is a particular case of chaotic scattering [9–15]. Although the majority of contributions investigating the Morse oscillator have been carried out for non-dissipative cases, including classical, semi-classical and quantum approaches [4–8,16–18], there are nevertheless, a number of works with the dissipative Morse oscillator. For instance, in Ref. [19] the bi-stable and chaotic behavior of the system were studied, while in Ref. [20] bifurcations and fixed-point diagrams for two damping constants were investigated, and in Ref. [21] the analytic structure of the Morse oscillator was considered. A detailed study of this system considering the variation of five parameters was performed in Ref. [22]. More recently, a study on the control of the chaotic dynamics through slaver–master feedback scheme has been presented in Ref. [23]; and in Ref. [24] investigations about vibrational resonances for the damped Morse oscillator driven by bi-harmonic forces were carried out. A common feature in all these works is that the periodic forcing of the oscillator is independent of the position.

The interaction energy of a polar diatomic molecule under the action of a laser–field depends on the permanent dipole function of the molecule as well as on the laser time-dependent electric field. A linear dipole function, which may be valid for small oscillation amplitudes, implies a force that is independent of the relative distance of the atomic pair. However, realistic molecular permanent dipoles generally have non-linear spatial behavior, leading to a force acting on the molecule which does depend on the inter-nuclear distance [25–27]. There is, in fact, an increasing interest in studying the role of the dipole function in controlling the dynamics of molecular systems [28,29]. We have investigated in previous works how this spatial dependence of the dipole influences the dissociation dynamics [30–32]. We have shown that the spatial variation of the dipole function through controllable parameters has a considerable impact in the system dynamics, inhibiting dissociation for some values of these parameters.

In the present work, we consider the classical damped Morse oscillator driven by a space-dependent and time-periodic force. In particular, we investigate the role played by a parameter related to the spatial shape of dipole function and by a parameter that dictates the dissipation strength. The paper is organized as follows. In Section 2, we describe the model system. In Section 3, we present and discuss the results of the calculations. Finally the conclusions are drawn in Section 4.

2. The Morse system, the laser field perturbation and dissipation

We consider the dynamics of polar diatomic molecules interacting with a laser–field, described by the classical driven one-dimensional Morse oscillator. In considering this model, we are neglecting both rotational and electronic excitations of the molecule. Although this approximation might be fulfilled by appropriate experimental apparatus, for instance by applying short linearly-polarized laser pulses in the infrared domain, the main reason for considering a non-perturbed Hamiltonian with one degree of freedom is that it captures the essence of the Physics involved in the breaking of the chemical bond, allowing us to focus on the relative distance of the nuclei.

For the non-dissipative case, the total Hamiltonian describing the system can be written in two parts. The first one is the Hamiltonian $H_0(x, p)$ which describes the unperturbed relative motion of the nuclei [5–8].

$$H_0(x, p) = \frac{p^2}{2} + \frac{1}{2}\left(\mathrm{e}^{-2x} - 2\,\mathrm{e}^{-x}\right), \tag{1}$$

where x stands for the inter-nuclear distance and p for the molecule momentum. If the molecule energy is negative, it is in the bound energy region, while for positive energies, it is in the unbound region. Both regions are separated by the limiting energy, $E = 0$, which corresponds to a separatrix curve in the phase space. Therefore, the bound energies correspond to libration tori and the unbound energies correspond to rotation tori in the phase space of the system governed by Eq. (1).

The second term, $H_1(x, t)$, is the perturbation accounting for the laser–molecule interaction,

$$H_1(x, t) = -\varepsilon(t)\mu(x, \eta), \tag{2}$$

where $\varepsilon(t)$ is the time-dependent external laser electric field and $\mu(x, \eta)$ is the non-linear dipole function of the molecule. The external laser field represents a monochromatic pulse, acting during an adjustable time interval T, given by

$$\varepsilon(t) = \varepsilon_0 \sin(\omega t), \tag{3}$$

with ε_0 and ω being the field amplitude and its frequency, respectively. The dipole function was taken from previous work [30],

$$\mu(x, \eta) = \frac{\sin\left[\eta\ (x + x_e)\right] \mathrm{e}^{-\xi\ (x+x_e)^4}}{\eta}, \tag{4}$$

where η and ξ are dimensionless adjustable parameters, x_e is related with the minimum of the Morse potential but is also adjustable. η plays the role of a deformation parameter introducing oscillations on the dipole function as it increases [30]. As η decreases, it is possible to model other known dipole functions, as for instance the one of the HF molecule. For small enough values of η, $\mu(x, \eta)$ does not oscillate in space and the mechanism of photo-dissociation can be explained through the splitting of the separatrix. Large values of η imply in oscillatory forms for $\mu(x, \eta)$, which can lead to a regularization of the phase space and consequently to the inhibition of dissociation.