

## Molecular orientation effect on the photodetachment of a diatomic molecular anion

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**Abstract.** The interference effect in the photodetachment of a diatomic molecular anion is investigated theoretically for different molecular orientation by using the two-center model. An analytic formula is presented for the photodetached electron flux distribution at a given observation plane. Taking  $H_2^-$  as an example, we calculate the electron flux distribution and photodetachment cross section for arbitrary molecular orientation. The results show that the molecular orientation has great influence on the photodetachment of the diatomic molecular anion. At certain molecular orientation, the interference in the electron flux distribution is totally constructive; while at some other orientations, the interference is destructive. For molecular orientation along the laser light polarization, the oscillation amplitude in the photodetachment cross section is the largest; however, for the molecular orientation perpendicular to the laser light polarization, no oscillation appears in the cross section. Our studies suggest that we can control the photodetachment process of the molecular negative ion by changing the molecular orientation. Our researches will be helpful for the theoretical and experimental study of the photodetachment of molecular anion.

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**Key words:** molecular orientation, photodetachment, interference, two-center model.

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## 1 Introduction

During the past two decades, many researchers have studied the photodetachment of negative ion in various external fields [1-12]. As a simple one-center model system, the photodetachment of  $H^-$  ion have been investigated both theoretically and experimentally. It has been found that the photodetachment cross sections of  $H^-$  in external fields display oscillatory structures. Since the photodetachment cross section is proportional to

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the integrated outgoing electron flux across a large enclosure in which the bound  $H^-$  sits, therefore it is clear that the oscillation in the total cross section of  $H^-$  in external fields reflects the interferences in the spatial distribution of the electron flux. Recently, with the development of the molecular photodetachment microscopy, the photodetachment of negative molecular ion has attracted a lot of attention [13-15]. Since 2006, Afraq and Du have studied the photodetachment of a negative hydrogen molecular ion in the absence of external fields by using a two-centre model and discussed the interference effect of the nuclei [16-17]. In their works, they studied in great detail the dependence of the cross section on the distance between the two nuclei, photon energy and the laser polarization. Their results suggest when the molecular axis of the diatomic molecular anion is perpendicular to the laser polarization, the total photodetachment cross section is still smooth curve; while for the molecular orientation is parallel to the laser polarization, oscillation appears in the cross section. Based upon their work, we discussed the photodetachment of a diatomic molecular anion with the molecular axis orientation varied in a fixed plane [18]. Then what will happen for arbitrary spatial molecular orientation? None has given the discussion.

In this paper, by using the two-center model, we study the photodetachment of a diatomic molecular anion with arbitrary spatial molecular orientation. The two atomic centers in the diatomic molecular anion are assumed to interact with one another to an extent sufficient to establish two coherent sources of detached electrons. When interacting with a laser, each center is assumed to produce an outgoing wave similar to that in  $H^-$ . These outgoing waves propagate to large distances. Sufficiently far from the molecular anion, the wave propagates according to semiclassical mechanics, and it is correlated with classical trajectories. Two classical trajectories for a photodetached electron propagating along two distant paths starting from each center to an observation point produce the interference pattern in the electron flux distribution on the screen. The detached-electron flux on the screen can be calculated analytically. By integrating the detached-electron flux for all outgoing directions, we are able to calculate the photodetachment cross section with arbitrary molecular orientation.

## 2 Theoretical method

The schematic diagram of the system is shown in Fig. 1. Suppose the diatomic molecular anion is placed in the  $x$ - $y$ - $z$  plane. The two circles represent the two centers of the negative molecular ion,  $d$  is the distance between the two centers.  $\theta_D$  is the angle between the molecular axis and  $z$ -axis, and  $\varphi_D$  is the azimuth angle. The observation plane is placed perpendicular to  $z$ -axis and the laser light is polarized along the  $+z$ -direction.

As in Ref. [14], we assume that there is only one active electron in the molecular anion system and the active electron is loosely bound by a short-range, spherically symmetric molecular core potential  $V_b(r)$ , where  $r$  is the distance between the active electron and the origin of the system. Before photodetachment, the normalized wave