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Wall Induced-oscillations in Photo detachment of Homo Nuclear Diatomic Molecular Negative ion

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ABSTRACT: The Pd (Photodetachment) of a hydrogen molecular negative ions near a soft reflecting wall is being investigated theoretically, focusing on the differential and total Pd.CS (Photodetachment Cross Section) when the laser polarisation is along the molecular axis of the ion. Quantum interference becomes evident on the observable plane when the two components of the electron wave superimpose at a considerable distance and propagate outward. The investigation of these interferences contributes to improving our understanding of the structure of diatomic molecular negative ions. Wall-induced fluctuations are observed in the detached electron spectra. As the distance between the ion and wall (R) increases, the wall effect diminishes, and the results approach those of the Ions in free space, the oscillation amplitude in the Pd.CS decreases, and their frequency increases as both Walls (R) and the distance between the two opposing ion centers (d) increase. The oscillations eventually cease to exist, and the CS (cross-section) exhibits uniform behavior at tremendous values of R and $(R \to \infty, d \to \infty)$ resulting in the match to the Ions in free space.

Keywords: Pd. (Photodetachment), Wall-induced Oscillations, CS (Cross Section), Flux,

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Introduction:

A required field of study in quantum physics has always been the phenomenon of quantum interactions between tiny elements [1]. In addition to being an incredibly intriguing aspect of physics, the quantum interference of matter waves has a wide range of practical applications. The interference of Pd. electrons from negative Ions is a primary demonstration of this intriguing occurrence. The study of negative Ions has been vital in science in recent years [2]. Negative Ions are used in many different applications [3], particularly in electronegative gases and plasmas, which have many applications in surface processing, atmospheric chemistry, environmental sciences for disposal gas cleaning, and many others [4].

Negative ion research is an essential component of atomic and molecular physics. Negative ions are necessary for food preservation. Due to the effect of electronegative pollutants such as halocarbons on ozone depletion, the significance of this topic is widely acknowledged [5]. In high-voltage technology, electron-attaching gases are often used as insulators [6]. Negative Ions processes are essential in various modern application zones, including gas discharges. The attachment of electrons to molecules in electronegative gases reduces plasma conductivity and electrical current and can cause instabilities [7]. Negative ions can also be employed in the field-effect Transistors and thin film Transistors fabrication processes [8]. Negative-ion electrospray mass Spectrometry is an efficient method for analysing the composition of un-derivatised neutral oligosaccharides [9]. Because of the high vitality of accelerated particles, Van de Graaff electrostatic accelerators, which utilise negative ions, are still helpful in researching the spectra and

structures of atomic nuclei [10]. From 1983 to 1992, inductively coupled plasma mass spectrometry was studied to enable the use of negative atomic and molecular Ions for quantitative measurement. The investigation examined the structure of negative ion spectra, their strength in proportion to plasma and detecting parameters, an element interpretive framework, and the effects of structural anions and cations on analysis outcomes [11].

The ability of negative ions to cause positive biochemical changes in humans has been investigated. Breathing in harmful Ion-charged air can reduce stress, induce a joyful mood, and increase serotonin levels. Negative ions can also help the brain receives more oxygen, enhancing energy and alertness. In addition to being negative ions may offer protection against bacteria and toxins in the air, which can be beneficial for those with allergies and may also help to reduce respiratory irritations [12]. Studies have investigated negative ions' kinetics and surface physics, focusing on photoelectron release in the presence of a magnetic field, electric field, electronic gradient field, or metallic surfaces. Yang et al. [13] analysed the Pd. process near the interface using COT and derived an analytical expression for the Pd.CS. They found that, like an electron in an electric field, the Pd.CS contains a homogeneous background and sinusoidal oscillation. The interface has a significant impact on the Pd. process. Haneef et al. [14] were the first to use TIM to compute the Pd hydrogen negative ion.CS near a wall surface. Using COT, A. Afaq et al. [15] investigated photodetachment when a laser was polarised along the z-axis near an elastic surface. They believed electronic waves travelled from an image of the source beneath the surface, just like outgoing disconnected electron waves from the source. Then, they used TIM to determine the classical action for those paths followed by an electron perpendicular to the surface. They claimed that the curvature κ of the surface influences surface effects in the Pd.CS. Their results coincide with the plane wall case when the sphere's curvature is zero. Du and Delos [16] discussed the Pd.CS in the presence of an electric field. They used a quantum mechanical method to calculate the Pd.CS, employing a stationary-phase estimate and momentum-space wave distribution. Yang et al. [13] analysed the Pd. process near the interface using COT and derived an analytical expression for the Pd.CS. They found that, like an electron in an electric field, the Pd.CS contains a homogeneous background and sinusoidal oscillation. The interface has a significant impact on the Pd process. Haneef et al. [14] were the first to use TIM to compute the Pd hydrogen negative ion.CS near a wall surface. Using COT, A. Afaq et al. [15] investigated Pd. When a laser was polarised along the z-axis near an elastic surface, they believed that electronic waves travelled from a Wang et al. [17] used semiclassical theory and COT to establish a formula for calculating the Pd.CS in a microcavity. When an electron wave propagates in a closed orbit, the microcavity causes substantial oscillation in the Pd. CS. They show that the Pd.CS is greatly influenced by negatively charged ion orientation and polarisation angle. The Pd.CS peak after Fourier transformation correlates to each closed orbit's length.

Wang De-Hua [18] investigated the Pd.CS of ions close to an interface employs COT and a two-central model. The outcomes reveal that the Pd.CS is affected by the separation between two centres and the distance between molecular ion interfaces. At equilibrium distance and low photon energy, the Pd.CS of the near interface is twice that of one of the close interfaces, suggesting that interference is significant for the two centres. The Pd.CS of both interfaces is similar at high photon energies, indicating that the interference effect between their centres has died out. Haneef et al. [1] used a theoretical imaging approach

to calculate the Pd.CS and detachment electron flux near a soft reflecting surface. The oscillation highly influences the surface in the spectrum of a detached electron.

As the distance between the ion and a soft reflecting wall approaches infinity, the Pd.CS becomes half the original value when the Ions are close to the wall. Moreover, in free space, the Pd.CS is reduced to a two-centre system. Haneef and colleagues investigated an unnoticed oscillation in the Pd.CS of an ion located close to a soft reflecting wall. The study focused on the behavior of the Pd.CS molecule under a laser beam directed perpendicular to the molecule's axis of negative ions [3]. The same problem is addressed in this paper. We discuss the Pd.CS of an Ions near a soft reflecting wall surface, where the laser polarisation is parallel to the molecular axis of the negative ion. We report a significant extra oscillation induced in the Pd.CS of an ion near the soft reflecting wall surface. Our research will be beneficial in investigating the structure of diatomic negative ions near the surface and in ion traps.

Theory:

The schematic visualisation for Pd of negative Ions near an ideal reflecting wall with parallel laser polarisation direction is shown in Fig. 1. When laser light falls on the negative ion, the ion absorbs energy from the laser and ejects an extra loosely bound electron. The negative ion and its image behind the soft wall surface are the coherent source of detached electron waves.

The total wave function consists of two parts: one part of electron waves coming directly from the negative ion and another part of electron waves reflecting from the soft wall surface, which appears to come from the image of the negative ion behind the wall surface. The detached electron wave function is treated quantum mechanically to derive further the expression for the detached total and differential Pd.CS.

When a laser beam of specified energy strikes a homo-nuclear diatomic ion, it serves as a source (S) of detached wave electrons, which electrons thought to generate waves correlated with the detached electron. The reflective wall (W) has a soft surface and is positioned perpendicular to the axis of the source along the y-axis.

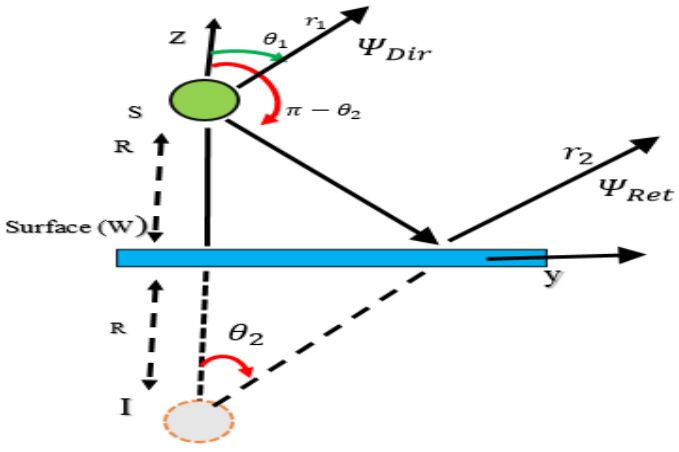


Fig. 1: The schematic representation for Pd of H_2^- near a soft wall surface with a parallel laser beam. The green circle shows the negative Ions, the grey ring is the image that appears behind the Wall, and (W) indicates the Wall surface.

The source (S) is on the z-axis, while the distance between the source and the soft reflecting wall is R atomic units. The green dotted line shows the orientation of laser polarisation, which is parallel to the z-axis. There are two components to a detached electron wave Ψ_{Dir}

and Ψ_{Ret}, which are represented in Fig. 1. There is a Ψ_{Dir} direct part of the wave that comes directly from the source, and the return part of the wave Ψ_{Ret} that appears to be reflected from the wall and seems to be coming from the image (I) behind the wall. Let there be a wave Ψ_{Dir} associated with a loosely bound electron detached from the source H_2^- after being absorbed by laser light.

This wave makes an angle θ_1 with the z-axis. Half of the total wave is not reflected from any wall and goes directly to a considerable distance, making the angle θ_1 smaller than π that with the z-axis. The other portion of the detached electron wave first moves toward the reflecting wall while forming an angle θ_2 larger than π with the z-axis. Following this, the mirrored electron wave from the wall surface moves toward the screen, which is positioned L atomic units away from the system. We can observe that two distances, r_1 and r_2, are covered by Ψ_{Dir} and Ψ_{Ret}, respectively, towards the observatory screen. The observatory screen is placed perpendicular to the diatomic molecular axis. The outgoing detached electronic wave Ψ at a considerable distance from the H_2^- ion is a linear combination of two waves given by [1];

$$\Psi = \Psi_{Dir} + \Psi_{Ret} \quad (1)$$

The spherical coordinates of the detached electron for the source (S) are (r_1, θ_1, ϕ_1), and the spherical coordinates of the detached electron after reflecting off the wall surface to form an image (I) behind the wall surface (r_2, θ_2, ϕ_2) are known. The first propagation towards the wall introduces a minus sign due to the detached electron wave's p-symmetry, while the reflecting wall introduces an additional phase (r_2, θ_2, ϕ_2) to the wave Ψ_{Ret}.

The expression of total direct detach electronic wave without any wall is given by Afaq and Due [19]:

$$\Psi_{Dir}\ (r_1, \theta_1, \phi_1) = U(k, \theta_1, \phi_1)\sqrt{2}\ cos\left(\frac{kdcos\theta_1}{2}\right)\frac{exp(ikr_1)}{r_1} \quad (2)$$

In the presence of a wall surface, the additional phase induced in the wave which falling on it then the reflected part Ψ_{Ret} is given as [18]:

$$\Psi_{Ret}\ (r_2, \theta_2, \phi_2) = U(k, \pi - \theta_2, \phi_2)\sqrt{2}\ cos\left(\frac{kdcos\theta_2}{2}\right)\frac{exp\left(i(kr_2 - \mu\frac{\pi}{2}\right)}{r_2} \quad (3)$$

The given expression involves the variable k, equal to the square root of 2 times the detached electron energy E. The quantities $U(k, \theta_1, \phi_1)$ and $U(k, \pi - \theta_2, \phi_2)$ represent the angular polarisation factors, and they can be expressed in the following way [1].

$$U(k, \theta_1, \phi_1) = Ccos\theta_1; \quad U(k, \pi - \theta_2, \phi_2) = -Ccos\theta_2 \quad (4)$$

The normalisation constant is denoted by B, and its value is 0.31552. The variable kb is related to the binding energy of the H^- Ions and is given by the expression $E_b = \frac{k_b^2}{2}$. The presentation also involves the variable k and a constant C, defined as $C = 4kB/(k_b^2 + k^2)^2$. These relationships are described in reference [20]. To determine the wave function. It is necessary to solve Equations respectively (1), (2), (3), and (4).

$$\Psi = Ccos\theta_1\sqrt{2}\ cos\left(\frac{kdcos\theta_1}{2}\right)\frac{exp(ikr_1)}{r_1} - Ccos\theta_2\sqrt{2}\ cos\left(\frac{kdcos\theta_2}{2}\right)\frac{exp\left(i(kr_2 - \mu\frac{\pi}{2})\right)}{r_2}$$

In this scenario, a soft wall surface is considered, with a value of μ equal to 1, as stated in Ref. [21]. The distances r_1 and r_2 are much larger than the separation between the molecular Ions and the wall surface. Thus a large distance approximation can be applied to simplify the detach electron wave function. To streamline the phase term, the approximations $r_1 \approx r - RCos\theta$ and $r_2 \approx r + RCos\theta$ are used, while all other terms can be

approximated as $r_1 \approx r_2 \approx r, \theta_1 \approx \theta_2 \approx \theta,$ and $\phi_1 \approx \phi_2 \approx \phi$. By applying these approximations, the given equation can be simplified as follows.

$$\Psi = 2\sqrt{2}\, C \frac{e^{i(kr+\frac{\pi}{4})}}{r} cos\theta\, cos\left(kR\, cos\theta + \frac{\pi}{4}\right)\, cos\left(\frac{kdcos\theta}{2}\right) - - - - - - - - (5)$$

The given equation describes the wave function of an outwardly propagating Pd electronic wave generated by a molecule source of negatively charged hydrogen ions near a soft wall.

Electron Flux

Electron flux refers to the number of electron waves approaching a screen per unit area. In other words, it quantifies the amount of electron wave that reaches an observatory screen. The calculation of electron flux involves using a widely known formula that can be found in any quantum mechanics textbook.

$$j(r, \theta, \phi) = \frac{i}{2}(\Psi \Delta \Psi^* - \Psi^* \Delta \Psi) - (6)$$

If we are concerned with the radial direction, then the formula mentioned above can be expressed as [1]:

$$j(r, \theta, \phi) = \frac{i}{2}\left(\Psi \frac{\partial \Psi^*}{\partial r} - \Psi^* \frac{\partial \Psi}{\partial r}\right) - - - - - - - - - - - - - - - - - - - (7)$$

The complex conjugate of the resultant wave function $\Psi^*$is given by

$$\Psi^* = 2\sqrt{2}\, C \frac{e^{-i(kr+\frac{\pi}{4})}}{r} cos\theta\, cos\left(kR\, cos\theta + \frac{\pi}{4}\right)\, cos\left(\frac{kdcos\theta}{2}\right)$$

By using Equations (5) and (6) and the value of Ψ^*, we can calculate the total electron flux

$$j_r(r, \theta, \phi) = \frac{2kC^2\, cos^2\theta}{r^2}(1 - sin\,(2kRcos\theta))\,\big(1 + cos(kdcos\theta)\big) - - - (8)$$

Here, the entire distribution of detached electrons near a soft wall in the radial direction. Equation (8) calculates the flux in the direction normal to the examination plane, allowing us to determine the flux in that direction. In the case of a parallel laser, such that $\hat{r}.\hat{n} = cos\theta$, the following applies:

$$j_z(r, \theta, \phi) = \frac{2kC^2\, cos^3\theta}{r^2}(1 - sin\,(2kRcos\theta))\,\big(1 + cos(kdcos\theta)\big) - - - - - (9)$$

The term $\frac{2kC^2\, cos^3\theta}{r^2}$ represents the free-space electronic flux of the H^- Ions. Equation (9) provides the total electron flux observed on the screen in spherical coordinates. We can replace the spherical coordinates with Cartesian coordinates by assuming cylindrical symmetry, which allows us to represent the detached electronic flux at any position (x, y) on the screen using a Cartesian system [22, 23].

$$j_z(x, y) = \frac{kC^2L^3}{(\rho^2 + L^2)^{\frac{5}{2}}}(1 + \cos(A) - \sin(B) - \cos(A)\sin(B)) - - - - - - (10)$$

Where $A = \frac{kdL}{(\rho^2+L^2)^{\frac{1}{2}}}$ and $B = \frac{2kRL}{(\rho^2+L^2)^{\frac{1}{2}}}$.

Photo-Detachment Cross Section (Pd.CS)

To calculate the Pd.CS, we consider a very large spherical surface r that encloses our system. The differential CS is given by [15]:

$$\frac{d\sigma(q)}{ds} = \frac{2\pi E_{ph}}{c} \overrightarrow{J_r}.\hat{n} \quad ----------(11)$$

The speed of light is represented by the variable c and has an atomic unit value of around 137. The energy of incident photons, denoted by E_{ph}, is the sum of the photon energy E and the binding energy E_b. Equation (10) uses the variables q, n, and ds to denote a point on a surface, the average external vector at that point, and the differential area on a spherical surface, respectively. Specifically, ds is given by the expression $ds = r^2 sin\theta d\theta d\varphi$ [24].

To calculate the overall Pd.CS, we integrate the differential CS over the spherical surface, resulting in the following equation [20]:

$$\sigma(q) = \int_{\Gamma} \frac{d\sigma(q)}{ds} ds \quad ----------(12)$$

$$\sigma(E) = \frac{4\pi k E_{ph} C^2}{c} \int_0^{2\pi} \int_0^{\pi} cos^2\theta (1 - sin\,(2kRcos\theta))\ (1 + cos(kdcos\theta))\ sin\theta d\theta d\phi$$

Solving the integral above using Mathematica results in a large expression that consists of various trigonometric functions, as shown below:

$$\sigma(E) = \sigma_o(E)\Big(1 + \sigma(k\,d) - \sigma(2kR) + \sigma\big(k(d+2R)\big) - \sigma\big(k(d-2R)\big)\Big) ----(13)$$

$$\sigma_o(E) = \frac{8\pi^2 k E_{ph} C^2}{3c}$$

$$\sigma(k\,d) = \frac{3(2dk\cos[dk] + (-2 + d^2k^2)\sin[dk])}{d^3k^3}$$

$$\sigma(2kR) = \frac{3(-1 + (1 - 2k^2R^2)\cos[2kR] + 2kR\sin[2kR])}{4k^3R^3}$$

$$\sigma\big(k(d+2R)\big) = \frac{6 + 3(-2 + k^2(d+2R)^2)\cos[k(d+2R)] - 6k(d+2R)\sin[k(d+2R)]}{2k^3(d+2R)^3}$$

$$\sigma\big(k(d-2R)\big) = \frac{6 + 3(-2 + k^2(d-2R)^2)\cos[k(d-2R)] - 6k(d-2R)\sin[k(d-2R)]}{2k^3(d-2R)^3}$$

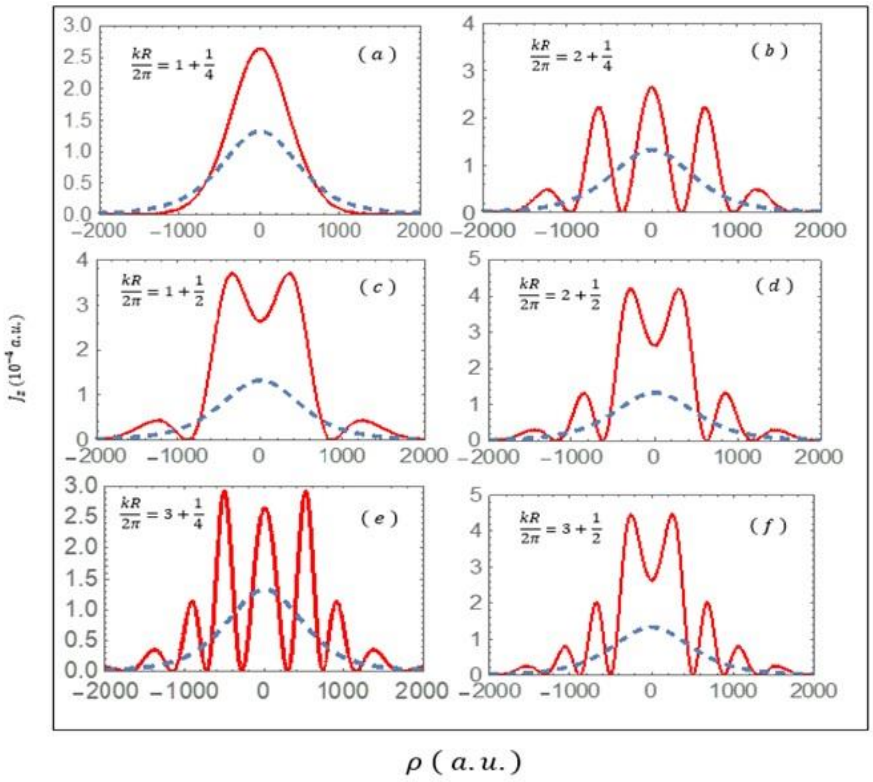
Equation (13) describes the total Pd.CS of the H_2^- molecular negative Ions near a soft wall surface that reflects light with a parallel polarisation direction. The term $\sigma_o(E)$ represents the Pd.CS of the H^- Ions in free space, while $\sigma_o(E)\big(1 + \sigma(kd)\big)$ represents the Pd.CS of the H_2^- Ions in free space with additional terms to account for the wall effect. As R approaches infinity, the terms $\sigma(2kR)$, $\sigma\big(k(d+2R)\big)$, and $\sigma\big(k(d-2R)\big)$ become very small and can be neglected. Therefore, the equation reduces to $\sigma_o(E)\big(1 + \sigma(kd)\big)$, which represents the Pd.CS of the H_2^- Ions in free space [25]. When both R and d approach infinity, the equation reduces to the expression for the Pd.CS of the H^- negative Ions in free space [26].

Results and Discussions

Figure. 2 depicts the detached electron flux pattern for parallel laser light, which was obtained using Eq. (10). The pattern exhibits a strong interference pattern observed at different distances between the wall and Ions (R), and the detached-electron flux is

represented in the figure.The interference pattern observed in Fig. 2 is caused by the interference of two detached electron waves, where one electron wave is emitted directly from the source, and the other wave is reflected from the soft wall surface, appearing to originate from the image of H_2^- behind the wall surface. The interference pattern depends on the values of$kR \geq \pi$, where when kR is an odd integral multiple of half of π, a peak at the centre of the screen is observed due to constructive interference of the two detached electronic waves.

Fig. 2: The distribution of electron flux for the detached electrons of the H_2^- Ions near the soft wall surface is shown by the solid red line, while the flux of detached electrons of



H^- in free space is indicated by the dotted blue line. The parameters L=1000, d=1.14 in atomic units, and $E_{ph} = 1\ eV$ are fixed, and different values of parameter R are used, namely: (a) R=60, (b) R=105, (c) R=70, (d) R=117, (e) R=152, and (f) R=164 in atomic units.

Conversely, when kR an integral multiple of π, the peaks are not centred, indicating destructive interference. Fig. 2 displays the detached electron flux pattern, exhibiting different peaks at different kR values. Eq. (13) shows that this interference effect is caused by the sizeable trigonometric function terms in the expression, which leads to extra oscillations in the Pd.CS. The total Pd.CS, which is greatly dependent on the distance between the ion and wall R, incidence photon energy, and interatomic distance d, is plotted in Fig. 3.

The large trigonometric functions in the expression produce significant oscillations in the Pd.CS. The red line in the graph represents the Pd.CS of H_2^- Ions near the soft wall, and the blue dotted line represents the Pd.CS of H_2^- Ions in free space. At significant photon energy limits, the Pd.CS of H_2^- Ions near the wall approaches that of the Pd.CS of H_2^- Ions in free space. The soft wall introduces extra oscillations in the Pd.CS for parallel laser polarisation. We plot the graph for different values of R, ranging from 10 to 1000 atomic units, and observe that the extra oscillations induced by the wall decrease as the distance between the Ions and Wall (R) increases.

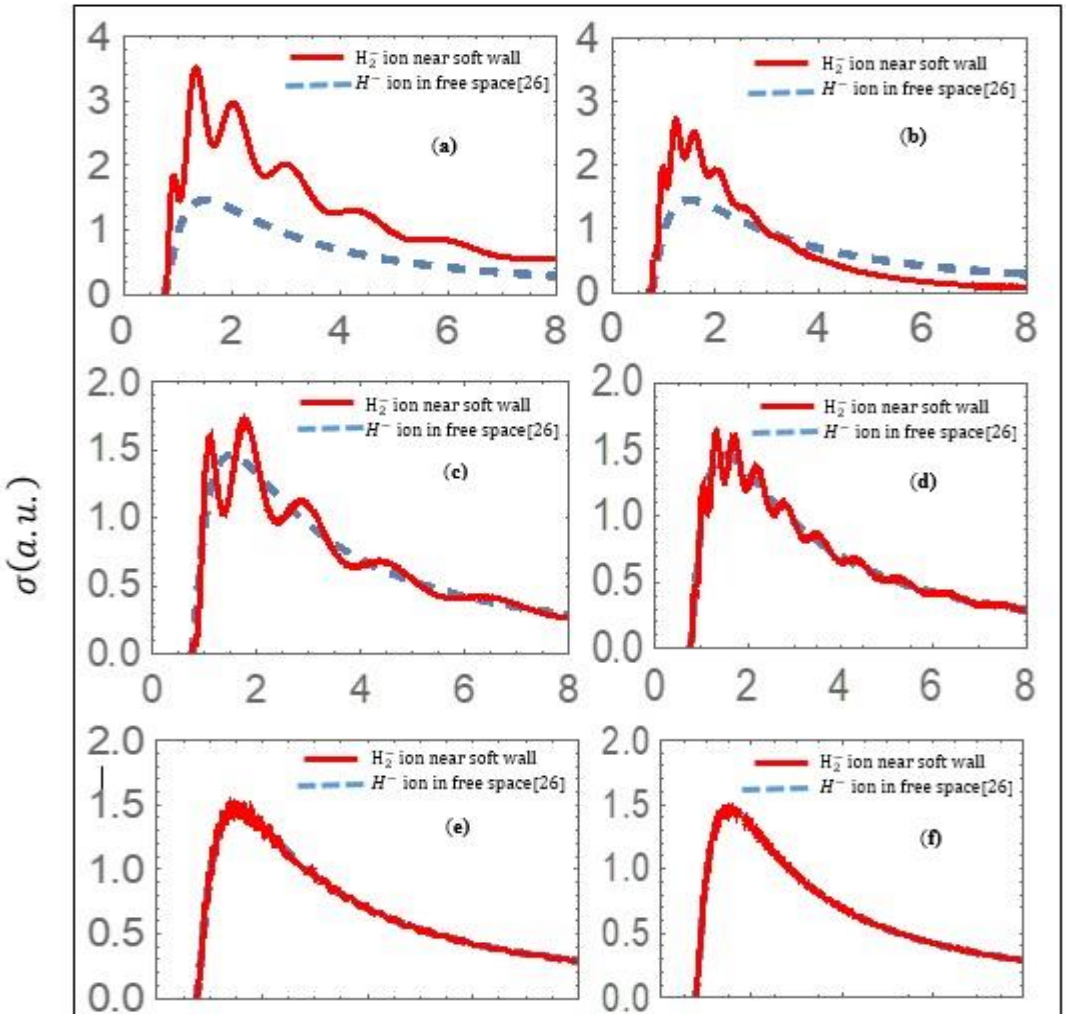


Fig. 3: Comparison between the Pd.CS of the homo-nuclear diatomic hydrogen

Fig. 4: A comparison between the H_2^- Ions near the soft wall and H^- Ions in free space [26]. The red line shows the CS of H_2^- Ions near the smooth wall and the dashed line shows the CS of H^- Ions in free space at different values of d and R. (a) R=30 and d=1.15 (b) R=50 and d=5 (c) R=500 and d= 50 (d) R=800 and d=100 (e) R=1000 and d= 300 (f) R=2000 and d=500 in atomic units.

As the distance, R, between the Ions and the wall increases, the amplitude of the extra oscillation decreases, but there is a simultaneous increase in the oscillation frequency. The additional oscillations in Pd.CS is reduced to almost zero in a considerable distance between the Ions and Wall. In this scenario, the system behaves as if it is in free space, as the reflected wall effect becomes negligible. This decrease in the Pd.CS can be attributed to the absence of the reflected wall effect. This phenomenon has been previously reported in reference [25].

When the distance between the two centers (d) in a negative molecular H_2^- Ions becomes very large, the Ions dissociate into an H^- Ions. As a result, the interference effect due to two centres on the total cross-section disappears, leading to non-oscillatory behavior [26]. In this scenario, the total, partial cross-section approaches that of a single centre hydrogen negative Ions in free space. This observation highlights the importance of the distance between the centers on the behavior of negative molecular Ions.

Conclusion

In the above discussion, we discuss the analysis of oscillations in the Pd. Sy spectra of a diatomic molecular negative Ions (H_2^-) near a soft surface using a TIM are summarised. A soft surface induces a significant interference pattern in the detached electron flux. The value of kR determines the interference pattern observed in the electron flux spectra during Pd. When kR is an odd integral multiple of half of π, it leads to constructive interference and centred peaks. However, when kR is an integral multiple of π, it results in destructive interference and off-centred peaks. It was found that the Pd.CS of H_2^- Ions near the soft wall are more significant than the CS of H_2^- Ions in space, as reported in previous research [25].

The study showed that when the laser polarisation is parallel to the molecular axis of H_2^- Ions near the soft wall, it causes significant oscillations in the Pd.CS. Furthermore, the study examined the impact of the inter-ion surface distance on the overall Pd.CS and discovered that the amplitude of oscillations decreased as the distance between the Ions and Wall increased. For tremendous values of R, the result is identical to that of the negative Ions in free space. In addition to the amplitude of oscillations in the Pd.CS decreases, and their frequency increases as the distance between the Ions and Wall (R) and the inter-atomic distance (d) growth. The oscillations cease to exist, and the CS exhibits smooth behavior at tremendous values of R and d, which is the same as that of the H^- Ions in free space. The result of this study can offer essential insights for investigating the structure and dynamics of negative diatomic molecular Ions. The authors hope that this result will guide future experiments involving the Pd. of negative Ions near soft surfaces, cavities, and Ion traps.

Author's Contribution: M.A. conceived the idea, designed the simulated work, and acquired the data. M.A. and A.A. executed the simulated work, analysed and interpreted the data, and wrote the initial draft. A.A. and S.R. provided language and grammatical edits and made critical revisions.

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