

Impact of field on absorption cross-section for photon by hydrogen 1s-3s atom

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Abstract: The objective of this work is to study the photoabsorption for 1s to 3s hydrogen atoms in presence of field for this we develop mathematical model and compute the develop equation. The nature shows photoabsorption increase with change in electron momentum within the field. The study identifies characteristic features in photoabsorption spectra, demonstrating an initial sharp increase in total photon absorption indicative of resonance-driven electronic transitions. As photon energy increases, as observed in transitions from 3s, the absorption probability continues to rise due to the capacity of higher-energy photons to induce transitions to elevated energy states. These findings offer profound insights into the intricate behavior of photoabsorption in hydrogen atoms, emphasizing the pivotal role of discrete energy levels and resonance phenomena. Understanding these interactions holds implications for a wide array of scientific and technological disciplines, providing a foundation for advancements in fields ranging from quantum physics to material science and beyond.

Keywords: Photoabsorption, electron momentum, Field, photon energy, Hydrogen atom

Introduction

The study of atoms emitting electrons under irradiation is fundamental in the field of photoelectron spectroscopy (PES). PES is a technique that captures the kinetic energy of emitted electrons, providing intricate insights into the electronic structure of a sample. Variations in atomic composition can be discerned through PES using different photon energies. In order to calculate photoionization cross sections for diverse photon energies, a range of mathematical models have been employed [1]. Notably, Yeh and Lindau extensively computed ionization cross sections for all elements in the periodic table within the energy range of 10 to 1500 eV. Their approach involved implementing the algorithm proposed by Cooper and Manson, which encompassed a radial grid representation of both initial and final states while allowing for relaxation of the final state proximate to the positive ion. In addition to this, alternative methods such as plane waves, orthogonalized plane waves, Coulomb waves, and B-splines have been utilized to portray final states [2]. It is worth noting that the investigation did not incorporate the use of an external field in their research methodology.

A method is developed to compute photoionization cross sections that extend beyond the electric dipole approximation. This technique combines Gaussian-type orbitals for initial states with

plane waves for final states. The method is then applied to calculate photoionization cross sections for atoms and ions from the first four rows of the periodic table. By assessing the error associated with the plane wave representation of the photoelectron, specific thresholds are determined where the plane wave approximation is valid in terms of kinetic and photon energies. The correction resulting from exceeding the electric dipole approximation increases with photon energy and depends on the spatial extent of the initial state. Overall, these corrections remain below 10% for the majority of elements, even at a photon energy of up to 12 keV [3].

In Quantum Electrodynamics (QED), screening effects hold the potential to modify the observable coupling constant. There exists a scenario wherein the renormalized coupling could be screened to the point of reaching zero. This implies that a theory initially describing interacting particles in a classical manner may evolve into one that governs non-interacting free particles when quantum and relativistic influences are taken into account [4]. Notably, this issue arises in QED, manifesting as the Landau pole problem, where the theory displays inconsistency at extremely short distances within the perturbative regime, unless the renormalized charge is effectively reduced to zero but don't used any field for coupling constant. The introduction of a magnetic field could potentially influence this outcome, given that the field contributes to charge screening. However, this research demonstrates that in the presence of a robust magnetic field, the Landau pole concern is effectively mitigated, owing to the screening effect exerted by electron-positron pairs occupying the lowest Landau level (LLL). Additionally, the study's findings regarding the behavior of the fine-structure constant with respect to the magnetic field diverge from those presented in earlier studies [5].

The establishes a novel relationship between the fine structure constant (α) and the ratio of electric and magnetic flux quanta of force acting on an electron. The research highlights that variations in α arise from changes in the fraction of electric and magnetic flux quanta, while changes in hc result from a common mode shift. The study delves into implications for the fine structure constant's behavior at high energies (small distances) and potential temporal drift. It demonstrates that the fine structure constant's evolution is influenced by both electric screening (vacuum polarization) and magnetic anti-screening (vacuum magnetization), causing perceived electric charge quanta to increase at small distances while magnetic flux quanta decrease [6].

A novel technique for computing photoionization cross-sections, utilizes square-integrable amplitudes obtained from the diagonalization of electronic Hamiltonians represented in finite bases. To demonstrate its effectiveness, three distinct cases: a simplified model involving a free particle as the final state, the hydrogen atom, and neutral atomic sodium. The technique capitalizes on the Whittaker-Shannon-Kotel'nikov sampling theorem, a widely utilized principle in digital signal sampling and reconstruction. Notably, this method showcases remarkable precision in reproducing established data, and its accuracy consistently improves with an expansion of the basis set size [7].

Research gap

The influence of magnetic fields on total photo cross-sections in multi-electron atoms, particularly in the context of the hydrogen 1s-3s atom, remains largely unexplored, with a notable absence of investigations employing the Baker-Hausdorff expansion technique. This significant research gap necessitates attention, as it represents a critical area where comprehensive understanding is lacking. In this study, we embark on filling this void by conducting a rigorous examination of the impact of magnetic fields on the total photo cross-section of the hydrogen 1s-3s atom, thereby contributing crucial insights to this under-explored domain.

Significant of research work

This study holds paramount significance in several aspects. Firstly, it addresses a conspicuous research gap concerning the effect of magnetic fields on total photo cross-sections in multi-electron atoms, specifically focusing on the hydrogen 1s-3s atom. By doing so, it contributes to a deeper comprehension of complex atomic systems under external influences. Furthermore, elucidating the behavior of electrons in magnetic fields has broad implications for fields such as astrophysics, plasma physics, and quantum technology. Moreover, this research could pave the way for advancements in areas like magnetic confinement in controlled fusion reactions and the development of more efficient materials for electronic devices. Overall, this study promises to enhance our fundamental understanding of atomic interactions in the presence of magnetic fields, with far-reaching applications across various scientific disciplines.

Methods and Materials

Photoionization processes are crucial in chemical physics, offering a fundamental means to study complex multi-particle systems. Photoelectron spectroscopy is widely used for understanding material electronic configurations in various fields like astrophysics, environmental chemistry, and material development. It provides detailed insights into energy levels, electronic wavefunctions, and their interactions with radiation. Advances in experimental methods, driven by sources like synchrotron radiation and x-ray free electron lasers, have revitalized research in molecular photoionization. This resurgence directly impacts resolution in structure determination. The effectiveness of theoretical approaches depends on obtaining transition matrix elements involving continuous states, which can be obtained through detailed calculation or approximations. Ndinya and Okeyo determined the total photoabsorption cross-section for multi-electron atoms, employing the Baker-Hausdorff expansion technique specifically for the hydrogen 2s atom [8]. Importantly, their study did not involve the use of an external field in computing the photoabsorption cross-section. The photoabsorption cross section define by Ndinya and Okeyo as,

$$\sigma(\omega) = \frac{2\pi\alpha Z^2}{3\omega} \int_{-\infty}^{+\infty} dt \langle \psi | e^{i(\omega-\Delta)t} | \psi \rangle \quad (1)$$

The equation represents the frequency (ω) of a photon, which is the energy difference ($E_f - E_i$) between two quantum states. Here, E_f represents the final energy state, and E_i represents the initial energy state. The frequency of a photon is directly related to the energy it carries. $H_1 - H_0 = \Delta$, This expression involves the difference (Δ) between two Hamiltonians, denoted as H_1 and H_0 . In quantum mechanics, the Hamiltonian operator represents the total energy of a system. In this context, it suggests a transition from a "lower" potential surface described by H_0 to an upper potential surface described by H_1 . This transition could represent a change in the potential energy landscape experienced by a particle or system. It is akin to moving from one energy state to another, which can occur in various quantum processes. The concept of lower and upper potential surfaces implies that the system is moving from a state with lower potential energy to one with higher potential energy. Such transitions and potential energy changes are fundamental in understanding various quantum phenomena, including electronic transitions, photoabsorption, and scattering processes.

Now, we have one-electron atoms spatial wave function with $a_0 = \frac{4\pi\epsilon_0\hbar^2}{\mu e^2} \sim 0.0529nm$ for 1s, 2s and 3s-orbit is $\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}}$, $\psi_{2s} = \frac{1}{\sqrt{2}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \left(1 - \frac{Zr}{2a_0}\right) e^{-\frac{Zr}{2a_0}}$, $\psi_{3s} = \frac{2}{3\sqrt{3}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \left(1 - \frac{2Zr}{3a_0} + \right.$

$\frac{2Z^2r^2}{27a_0^2} e^{-\frac{Zr}{3a_0}}$. Also considering strong field the fine-structure constant [9], $\alpha_0 = \frac{1}{137}$, this is because we can't neglect the impact of field on fine-structure constant and fine-structure constant is define by

$$\alpha = \frac{\alpha_0}{1 + \frac{2\alpha_0|eB|}{\pi k^2} e^{-\frac{k^2}{2|eB|}}} \quad (2)$$

Where α represents the fine-structure constant, a dimensionless fundamental physical constant in quantum electrodynamics (QED). It characterizes the strength of electromagnetic interactions between charged particles. α_0 represent the fine-structure constant in the absence of a magnetic field ($B=0$). e represent for the elementary charge, B represent the magnitude of the magnetic field. k represent to the wave vector and k^2 represents the square of the wave vector.

Now using the wave function ψ_{1s} in (1) and integration with dt with the involvement of δ -function and putting value of (2) assuming $r = \frac{1}{\sqrt{\omega}}$, we get.

$$\sigma_{1s}(\omega) = \frac{2Z^2}{3\omega} \left(\frac{\alpha_0}{1 + \frac{2\alpha_0|eB|}{\pi k^2} e^{-\frac{k^2}{2|eB|}}} \right) \left(\frac{Z}{a_0} \right)^3 e^{-\frac{2Z}{a_0\sqrt{\omega}}} \quad (3)$$

Now using the wave function ψ_{2s} in (1) and integration with dt with the involvement of δ -function we get.

$$\sigma_{2s}(\omega) = \frac{Z^2}{3\omega} \left(\frac{Z}{a_0} \right)^3 \left(\frac{\alpha_0}{1 + \frac{2\alpha_0|eB|}{\pi k^2} e^{-\frac{k^2}{2|eB|}}} \right) \left(1 - \frac{Z}{2a_0\sqrt{\omega}} \right)^2 e^{-\frac{Z}{a_0\sqrt{\omega}}} \quad (4)$$

Now using the wave function ψ_{3s} in (1) and integration with dt with the involvement of δ -function we get.

$$\sigma_{3s}(\omega) = \frac{8Z^2}{81\omega} \left(\frac{Z}{a_0} \right)^3 \left(\frac{\alpha_0}{1 + \frac{2\alpha_0|eB|}{\pi k^2} e^{-\frac{k^2}{2|eB|}}} \right) \left(1 - \frac{2Z}{3a_0\sqrt{\omega}} + \frac{2Z^2}{27a_0^2\omega} \right)^2 e^{-\frac{2Z}{3a_0\sqrt{\omega}}} \quad (5)$$

On taking ratio of (3) and (4) we get,

$$\sigma_{2s} = \frac{1}{2} \left[\left(1 - \frac{Z}{2a_0\sqrt{\omega}} \right)^2 e^{\frac{Z}{a_0\sqrt{\omega}}} \right] \sigma_{1s} \quad (6)$$

This equation (6) shows photo ionization cross section of 2s is $\frac{1}{2} \left[\left(1 - \frac{Z}{2a_0\sqrt{\omega}} \right)^2 e^{\frac{Z}{a_0\sqrt{\omega}}} \right]$ times to than of 1s.

$\left(1 - \frac{Z}{2a_0\sqrt{\omega}}\right)^2$ this term accounts for the screening effect due to the presence of the electron in the 1s state. It represents the reduction in the effective charge felt by the electron in the 2s state due to the shielding effect of the 1s electron. $e^{\frac{Z}{a_0\sqrt{\omega}}}$ this term introduces an exponential factor that accounts for the Coulomb interaction between the electron in the 2s state and the nucleus. It represents the probability amplitude for the electron to be found at a particular distance from the nucleus. $\frac{\sigma_{1s}}{2} \left[\left(1 - \frac{Z}{2a_0\sqrt{\omega}}\right)^2 e^{\frac{Z}{a_0\sqrt{\omega}}} \right]$ this overall expression is multiplied by $\frac{\sigma_{1s}}{2}$, which indicates that the transition from 2s to 1s is governed by a probability factor that is half as likely as the transition from 1s to 2s. The provided expression describes the photoabsorption cross section for a transition from the 2s state to the 1s state in a hydrogen-like atom. It takes into account the atomic number, Bohr radius, incident photon frequency, and the probabilities associated with different states. This expression is a fundamental component in understanding the absorption of photons by electrons in different energy states of the atom. Similarly taking ratio form (5) and (4) we get,

$$\sigma_{3s} = \frac{8}{81} \left[\left(1 - \frac{2Z}{3a_0\sqrt{\omega}} + \frac{2Z^2}{27a_0^2\omega}\right)^2 e^{-\frac{4Z}{3a_0\sqrt{\omega}}} \right] \sigma_{1s} \quad (7)$$

$\left(1 - \frac{2Z}{3a_0\sqrt{\omega}} + \frac{2Z^2}{27a_0^2\omega}\right)^2$ this term encapsulates the screening effect due to the presence of the electron in the 1s state. It represents the reduction in the effective charge felt by the electron in the 3s state due to the shielding effect of the 1s electron. $e^{-\frac{4Z}{3a_0\sqrt{\omega}}}$ this term introduces an exponential factor that accounts for the Coulomb interaction between the electron in the 3s state and the nucleus. It represents the probability amplitude for the electron to be found at a particular distance from the nucleus. $\frac{8}{81} \left[\left(1 - \frac{2Z}{3a_0\sqrt{\omega}} + \frac{2Z^2}{27a_0^2\omega}\right)^2 e^{-\frac{4Z}{3a_0\sqrt{\omega}}} \right] \sigma_{1s}$ the overall expression is multiplied by $\frac{8\sigma_{1s}}{81}$, indicating that the transition from 3s to 1s is governed by a probability factor that is $\frac{8}{81}$ times as likely as the transition from 1s to 3s. The provided expression describes the photoabsorption cross section for a transition from the 3s state to the 1s state in a hydrogen-like atom. It takes into account the atomic number, Bohr radius, incident photon frequency, and the probabilities associated with different states. This expression is fundamental in understanding the absorption of photons by electrons in different energy states of the atom.

Results and Discussion

The observation shows that total photoabsorption increase with increasing in change in momentum of electron in field. The increase in total photon absorption with an increasing change in momentum of an electron in a field can be attributed to a phenomenon known as resonance. Additionally, as the change in momentum of the electron increases, it becomes more likely to reach an energy level that matches the energy of the incident photon. This leads to a higher probability of photon absorption.

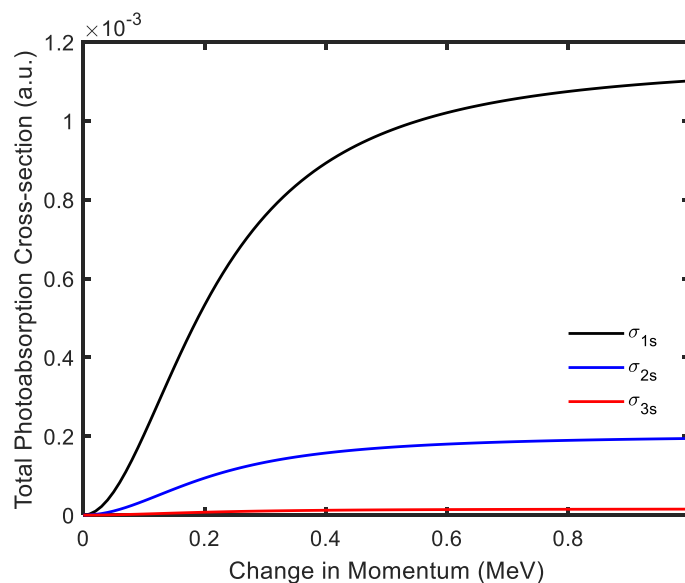


Figure 1: Change in momentum vs Photoabsorption cross section

The photoabsorption for 1s is higher than 2s and 3s, and 2s is higher than 3s with momentum. In a hydrogen atom, electrons are arranged in energy levels or shells, labeled with quantum numbers (n). The energy levels are quantized, meaning they have discrete energy values. 1s, 2s, and 3s represent different energy levels or shells. Specifically: 1s is the lowest energy level. 2s is at a higher energy level than 1s. 3s is at a still higher energy level than 2s. When it comes to photoabsorption, it's important to understand the concept of resonance. Photons will be absorbed if their energy matches the energy difference between two electronic states. In the case of hydrogen, this corresponds to transitions between energy levels. Photoabsorption for 1s is higher than 2s and 3s. This is because the energy difference between 1s and the higher energy levels (2s and 3s) is larger. Consequently, photons with higher energies are required to induce transitions from 1s to 2s or 3s. These photons are less likely to be present in the incident radiation, leading to a lower probability of absorption. 2s has higher photoabsorption than 3s with momentum. The energy gap between 2s and 3s is smaller than that between 1s and 2s or 1s and 3s. This means that photons with slightly lower energy can induce transitions between 2s and 3s. Therefore, 2s has a higher probability of photon absorption compared to 3s. The probability of photoabsorption depends on the energy differences between the electronic states. Smaller energy differences allow for absorption of a wider range of photon energies, leading to a higher probability of absorption.

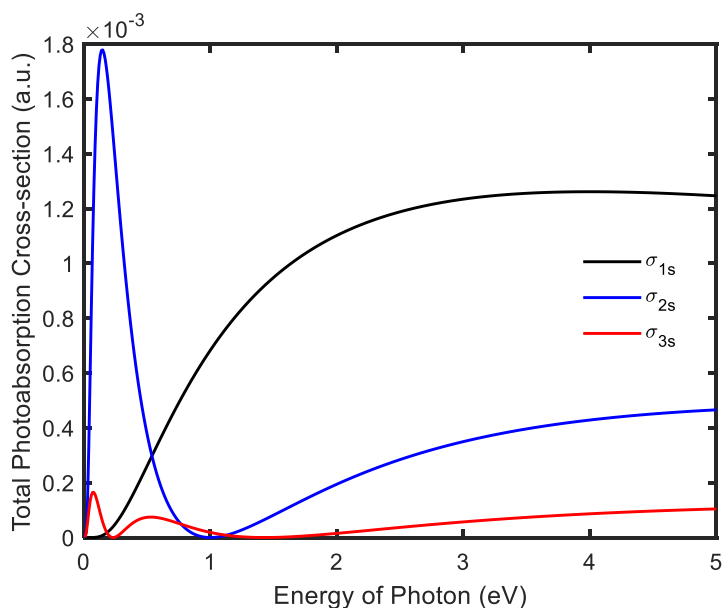


Figure 2: Energy of Photon vs Photoabsorption cross section

The behavior described in Figure 2 indicates a characteristic feature of photoabsorption spectra, particularly for atoms or molecules with discrete energy levels. Initially, the sharp increase in total photon absorption suggests the presence of absorption peaks. These peaks correspond to electronic transitions between energy levels within the system. When the energy of the incident photons closely matches the energy required for these transitions, the absorption probability is significantly higher. This is known as resonance. After this initial sharp increase, as the photon energy continues to increase (3s), the absorption probability also increases. This is because higher energy photons can induce transitions to higher energy states. These transitions may be less likely than those associated with the initial peaks, but they still contribute to the total absorption.

The ground state, denoted as 1s, represents the lowest energy level, requiring a substantial energy input to transition to higher states, like the 2s level. The 2s level, though higher in energy than 1s, is still considerably lower than states like 3s. Transitions from 2s to higher states necessitate less energy than those from 1s, resulting in a greater likelihood of absorption in the photon energy range below 0.5 eV. This accounts for the higher photoabsorption cross section observed for 2s. Conversely, the 3s state, being at an even higher energy level, demands even more energy for transitions to higher states. Consequently, at photon energies below 0.5 eV, the 2s state exhibits a higher absorption cross section as photons in this range are more likely to supply the requisite energy for a transition to a higher state, compared to transitions from 1s or 3s.

Conclusion

In conclusion, the observed increase in total photoabsorption with an increasing change in electron momentum in the field can be attributed to the phenomenon of resonance. As the electron's momentum increases, it becomes more likely to reach an energy level that matches the energy of the incident photon, resulting in a higher probability of photon absorption. The photoabsorption for the 1s state surpasses that of the 2s and 3s states, while the 2s state exhibits higher absorption than the 3s state. This disparity arises from the discrete energy levels in a hydrogen atom. Specifically, the 1s state represents the lowest energy level, requiring more

energy to transition to higher states like 2s. The transition from 2s to higher states demands less energy compared to transitions from 1s, leading to a higher absorption cross section for 2s. Characteristic features of photoabsorption spectra include an initial sharp increase in total photon absorption, indicating absorption peaks corresponding to electronic transitions. As photon energy increases (as in transitions from 3s), the absorption probability also rises. This is because higher energy photons can induce transitions to higher energy states, contributing to the overall absorption.

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