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Analytical Absorption Cross-Section for Photon by a Hydrogen 2s Atom

Boniface Otieno Ndinya* and Stephen Onyango Okeyo†

Department of Physics and Materials Science, Maseno University, Private Bag, Maseno, Kenya

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Abstract We calculate the absorption cross-section for photon by a hydrogen 2s atom using the quantum-classical approximation for the total photo cross-section of many electron atoms. With the application of the first-order term of the Baker–Hausdorff expansion, the absorption cross-section for the hydrogen 2s atom decreases to a minimum, the Cooper pair minimum, at low photon energy. Such a minimum is absent in the exact absorption cross-section for photon by a hydrogen 2s atom. We have extended the calculation for the absorption cross-section of the hydrogen 2s atom using the quantum-classical approximation for the total photo cross-section of many electron to include the second-order term of the Baker–Hausdorff expansion and observed a great reduction in the dip associated with the Cooper pair minimum at the zero crossing.

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Key words: absorption cross-section, Cooper pair minimum and Baker–Hausdorff expansion

1 Introduction

In dipole approximation the absorption cross-sections for photon by a one-electron atom with charge Ze is described by^[1–2]

$$\sigma(\omega) = \frac{2\pi\alpha}{\omega} \int_{-\infty}^{+\infty} dt \langle \Psi | D^+(0) D(t) | \Psi \rangle e^{i\omega t}, \quad (1)$$

where

$$D(t) = e^{-iH_f t} D_0 e^{iH_f t}, \quad (2a)$$

is the time-dependent dipole operator, α is the fine structure constant, and Ψ is the initial state (ground-state) wave function. The dipole operator in acceleration form is given by^[3]

$$D_0 = \frac{Z}{i\omega} \frac{1}{r^2} \cos \phi. \quad (2b)$$

The frequency ω of the photon determines the final energy E_f through $\omega = E_f - E_i$. The angular dependence in (1) is separated algebraically by inserting a complete set of spherical harmonics $\sum |lm\rangle \langle lm|$ at appropriate places, to obtain^[2]

$$\langle \Psi | D^+(0) D(t) | \Psi \rangle = \int_0^\infty dr \langle \psi | d_0^\dagger e^{-iH_i t} d_0 e^{iH_0 t} | \psi \rangle, \quad (3a)$$

where $\psi = \langle 00 | r | \Psi \rangle$ is the independent one-electron atoms spatial wave function, $e^{-iH_i t} = \langle l0 | e^{-iHt} | l0 \rangle$ with the one-electron Hamiltonian

$$H_l = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} + \frac{l(l+1)}{2r^2}, \quad (3b)$$

$$d_0 = \langle l0 | D_0 | 00 \rangle = \frac{1}{\sqrt{3}} \frac{Z}{i\omega} \frac{1}{r^2}. \quad (3c)$$

We substitute (3a) in (1), noting that the dipole operator as expressed in (3c) is proportional to the centrifugal

potential, to obtain^[2]

$$\sigma(\omega) = \frac{2\pi\alpha Z^2}{3\omega} \int_{-\infty}^{+\infty} dt \langle \psi | (H_1 - H_0) e^{-iH_1 t} \times (H_1 - H_0) e^{iH_0 t} | \psi \rangle e^{i\omega t}, \quad (4a)$$

which reduces to

$$\sigma(\omega) = \frac{2\pi\alpha Z^2}{3\omega} \int_{-\infty}^{+\infty} dt \langle \psi | e^{-iH_1 t} e^{iH_0 t} | \psi \rangle e^{i\omega t}. \quad (4b)$$

The dynamical problem to be solved involves forward propagation of the state ψ until time t on the “lower” potential surface described by the Hamiltonian H_0 , followed by backward propagation on the “upper” potential surface with Hamiltonian H_1 . Writing $H_1 - H_0 = \Delta$ the obvious approximation is the first-order term of the Baker–Hausdorff expansion

$$\langle \psi | e^{-iH_1 t} e^{iH_0 t} | \psi \rangle = \langle \psi | e^{-i(H_0 + \Delta)t} e^{iH_0 t} | \psi \rangle \approx \langle \psi | e^{-i\Delta t} | \psi \rangle. \quad (5a)$$

This amounts to neglecting all commutators between H_0 and H_1 and is therefore essentially a quantum-classical approximation for the total photo cross-section of many electron atoms.^[2]

We substitute (5a) in (4b) to obtain

$$\sigma(\omega) = \frac{2\pi\alpha Z^2}{3\omega} \int_{-\infty}^{+\infty} dt \langle \psi | e^{i(\omega - \Delta)t} | \psi \rangle. \quad (5b)$$

The initial states of the atom ψ is represented by the one-electron atoms spatial wave function

$$\psi_{1s} = 2Z_{1s}^{3/2} r e^{-Z_{1s} r}, \quad (6a)$$

$$\psi_{2s} = 2(Z_{2s}^3/8)^{1/2} r (1 - Z_{2s} r/2) e^{-Z_{2s} r/2}, \quad (6b)$$

for the hydrogen 1s and 2s orbitals with effective charges Z_{1s} and Z_{2s} respectively.

*E-mail: ndinyakumbe@yahoo.com

†E-mail: onyangostiv@yahoo.com

We substitute $\psi = \psi_{1s}$ (6a) in (5b) and evaluate, the resulting time integration leads to a δ -function,^[4] fixing the radial variable to $r = \omega^{-1/2}$, to obtain the absorption cross-section for photon by a hydrogen 1s atom

$$\text{Rost } 1s = \sigma(\omega) = \frac{8\pi^2\alpha Z^2 Z_{1s}^3}{3\omega^{7/2}} e^{-2Z_{1s}/\sqrt{\omega}}. \quad (7)$$

Similarly, we substitute $\psi = \psi_{2s}$ (6b) in (5b) and evaluate, to obtain the absorption cross-section for photon by a hydrogen 2s atom

$$\text{Rost } 2s = \sigma(\omega) = \frac{8\pi^2\alpha Z^2}{3\omega^{7/2}} \frac{Z_{2s}^3}{8} \left(1 - \frac{Z_{2s}}{2\sqrt{\omega}}\right)^2 \times e^{-Z_{2s}/\sqrt{\omega}}. \quad (8)$$

In Fig. 1, taking $Z = Z_{1s} = Z_{2s} = 1$, we present the results obtained in (7) and (8) for the absorption cross-section for photon by a hydrogen 1s atom (Rost 1s) and hydrogen 2s atom (Rost 2s). We note that the absorption cross-section for hydrogen 1s atom (Rost 1s) shows perfect agreement with the exact absorption cross-section (exact 1s)^[5] and the high energy approximation using the plane wave for final state Plane wave 1s).^[3,6] However, for the hydrogen 2s atom, the calculated absorption cross-section (Rost 2s) shows a perfect agreement with the exact absorption cross-section (exact 2s)^[5] at high photon energy and poorly at low photon energy with a decrease to a minimum, Cooper pair minimum, at the zero crossing. Such a minimum is also present in the absorption cross-section for photon by a hydrogen 2s atom obtained using the high energy approximation (Plane wave 2s).^[3,6]

The present paper, extends the evaluation of (5a) to second-order term of the Baker–Hausdorff expansion to improve the absorption cross-section for photon by a hydrogen 2s atom at the zero crossing.

2 Second-Order Baker–Hausdorff Expansion

We include the second-order term of the Baker–Hausdorff expansion^[7]

$$e^{\mathbf{A}} e^{\mathbf{B}} = e^{\mathbf{A}+\mathbf{B}} e^{(1/2)[\mathbf{A}, \mathbf{B}]}, \quad (9a)$$

in Eq. (5a), to obtain

$$\begin{aligned} \langle \psi | e^{-i(H_0+\Delta)t} e^{iH_0t} | \psi \rangle \\ = \langle \psi | e^{-i\Delta t} e^{-(1/2)[H_0, \Delta]t^2} | \psi \rangle. \end{aligned} \quad (9b)$$

For hydrogen atom $Z = 1$ and $l = 0$,

$$H_0 = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr}$$

and the commutator

$$[H_0, \Delta] = -\frac{1}{r^4}. \quad (10)$$

Using the commutator relation in (10), (9b) reduces to

$$\langle \psi | e^{-i\Delta t} e^{-(1/2)[H_0, \Delta]t^2} | \psi \rangle \approx \langle \psi | e^{-i\Delta t} e^{(1/2r^4)t^2} | \psi \rangle, \quad (11)$$

which does not converge.

However, (9b) can be expressed in alternative form as

$$\langle \psi | e^{-i(H_0+\Delta)t} e^{iH_0t} | \psi \rangle$$

$$\approx \langle \psi | e^{iH_0t} e^{-i(H_0+\Delta)t} | \psi \rangle, \quad (12a)$$

as long as ψ is an eigenfunction of H_0 . Then, using equations (9a) and (10), (12a) becomes

$$\begin{aligned} \langle \psi | e^{iH_0t} e^{-i(H_0+\Delta)t} | \psi \rangle &= \langle \psi | e^{-i\Delta t} e^{(1/2)[H_0, \Delta]t^2} | \psi \rangle \\ &\approx \langle \psi | e^{-i\Delta t} e^{-(1/2r^4)t^2} | \psi \rangle, \end{aligned} \quad (12b)$$

and everything converges.

We substitute (12b) in (4b), to obtain

$$\sigma(\omega) = \frac{2\pi\alpha Z^2}{3\omega} \int_{-\infty}^{+\infty} dt \langle \psi | e^{i(\omega-\Delta)t} e^{-(1/2r^4)t^2} | \psi \rangle. \quad (13)$$

The integral over time in (13) leads to a gaussian function,^[4] resulting in the absorption cross-section for photon for many electron atoms

$$\sigma(\omega) = \frac{(2\pi)^{3/2}\alpha Z^2}{3\omega^3} \langle \psi | r^2 e^{-1/2(1-r^2\omega)^2} | \psi \rangle \quad (14)$$

that can be solved numerically. We substitute $\psi = \psi_{1s}$ and $\psi = \psi_{2s}$ in (14) and solve the resulting expression using numerical integration to obtain the absorption cross-section for photon by hydrogen 1s atom (2nd order BH 1s numerical evaluation) and hydrogen 2s atom (2nd order BH 2s numerical evaluation), as shown in Fig. 1.

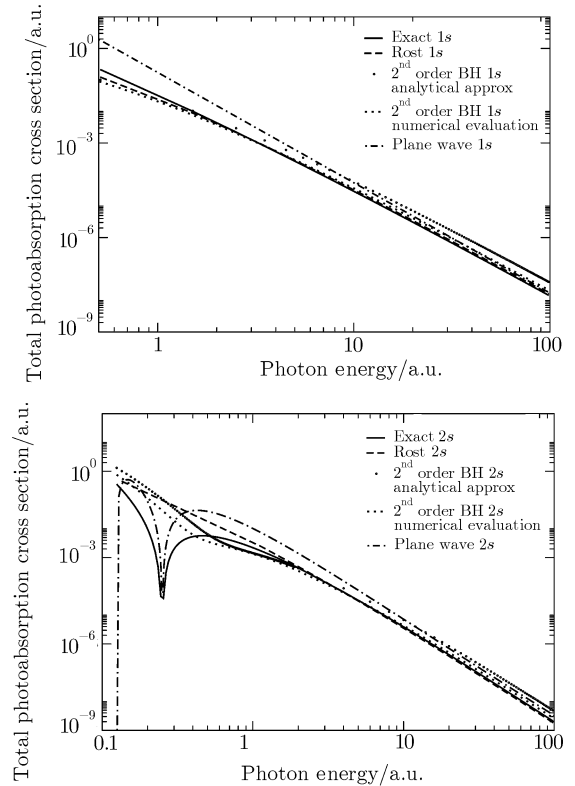


Fig. 1 The absorption cross-section for photon, to the top figure by hydrogen 1s atom and to the bottom figure by hydrogen 2s atom, compared to exact absorption cross-sections^[5] and the high energy approximation (plane waves).^[3,5]

We rewrite the term $e^{-1/2(1-r^2\omega)^2}$ in (14) as

$$e^{-1/2(1-r^2\omega)^2} \approx e^{-1/2((1-r\sqrt{\omega})(1+r\sqrt{\omega}))^2}, \quad (15a)$$

which allows us to express (14) in alternative form as

$$\sigma(\omega) = \frac{(2\pi)^{3/2} \alpha Z^2}{3\omega^3} \langle \psi | r^2 e^{-1/2((1-r\sqrt{\omega})^2 + (1+r\sqrt{\omega})^2)} | \psi \rangle. \quad (15b)$$

We note that the integral over r in (15b) with the wave function ψ extends from zero to infinity, therefore the relevant zero is one for which $r = \omega^{-1/2}$, leading to

$$\sigma(\omega) = \frac{(2\pi)^{3/2} \alpha Z^2}{3\omega^3} \langle \psi | r^2 e^{-2(1-r^2\sqrt{\omega})^2} | \psi \rangle, \quad (16)$$

that can be solved analytically. We substitute $\psi = \psi_{1s}$ and $\psi = \psi_{2s}$ in (16) and solve the resulting expression analytically to obtain the absorption cross-section for photon by hydrogen $1s$ atom (2nd order BH $1s$ analytical approx.) and hydrogen $2s$ atom (2nd order BH $2s$ analytical approx.) respectively, as shown in Fig. 1.

3 Discussion and Conclusion

We note in Fig. 1, that the application of the second-order term of the Baker–Hausdorff expansion to (4b) to obtain (14) and (16) has no effect on the absorption cross-section for photon by the hydrogen $1s$ atom (Rost $1s$). That is, the results for Rost $1s$, 2nd order BH $1s$ numerical evaluation and 2nd order BH $1s$ analytical approx are perfectly in agreement with the exact absorption cross-section exact $1s$.

However, we also note in Fig. 1, that the application of the second-order term of the Baker–Hausdorff expansion to (4b), to obtain (14) and (16), has considerably improved the absorption cross-section for photon by the hydrogen $2s$ atom around the zero crossing. These have resulted in the reduction of dip associated with the Cooper

pair minimum at low photon energy as seen in the results obtained for 2nd order BH $2s$ numerical evaluation and 2nd order BH $2s$ analytical approx. Therefore, the second-order term of the Baker–Hausdorff approximation average the absorption cross-section for photon by hydrogen $2s$ atom around the zero crossing of the $2s$ state to obtain 2nd order BH $2s$ numerical evaluation and 2nd order BH $2s$ analytical approx. which are almost comparable to the exact absorption cross-section (exact $2s$). Such an improvement cannot be achieved by the more sophisticated high energy approximation using plane waves as the final states (plane wave $2s$).

We anticipate that the inclusion of higher-order terms of the Baker–Hausdorff approximation will lead to absorption cross-section for photon by hydrogen $2s$ atom that is in perfect agreement with the exact absorption cross-sections.

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