

# Study Radial and Momentum Space Properties and Compton Profile of Excited He Metastable Atoms

S. D. Jhala

Department of Physics, M G Science Institute, Ahmedabad, Gujarat, India

## ABSTRACT

Excited metastable atoms like H (2S), He (2<sup>1</sup>S) and He (2<sup>3</sup>S) are examined in terms of various radial and momentum space properties and also the Compton profile J(Q). Quantitative differences as compared to their ground state counterparts are also discussed here. The physical significance of this study is also indicated. The obtained results for metastable atoms also lead us towards the scaling law Radius × ionization energy = Constant.

**Keywords:** Radial charge density, momentum space properties and Compton profile

## I. INTRODUCTION

Atoms, molecules and ions in excited state metastable states are known to possess remarkable different properties compared to their normal counterparts. (e.g. Barsden & Jochain) [1], Christophorou [2], Jacka et al [3]. The metastable H (2S) atoms for example, possesses a large lifetime and a large electric polarizability. We expect that various radial and momentum space properties as well as the Compton profile J(Q) of such atoms would also be different from those of the ground state species. These properties have been investigated in this present paper for three well known metastable atoms, viz. H(2S), He(2<sup>1</sup>S) and He(2<sup>3</sup>S), with reference to the ground state He(1<sup>1</sup>S). This work also gives information of their charge density  $\rho(r)$ , the diamagnetic susceptibility  $\chi$ , momentum density  $\gamma(p)$  and the momentum moments  $\langle p \rangle^\alpha$  with  $\alpha = -1$  and  $+2$ . For normal atoms, theoretical data of all these properties are available in literature by Patil [4], Angulo[5], Sharma & Tripathi [6], Biggs et al [7] and others. Study of all these properties for these metastable atoms are little difficult experimentally. With very hardly available data on the properties of

these metastable states of He, here quantitative study is discussed. Throughout atomic units are used here.

## II. THEORETICAL MODELS AND METHODS

The wave function of the 2S – Hydrogen atom is well defined. For the two other systems like He(2<sup>3</sup>S) and He(2<sup>1</sup>S) we have employed the accurate variational wave function, as given by Bransden & Jochain [1]. If  $r_1$  and  $r_2$  are the co-ordinates of the atomic electrons in he, then the wave function of the (2<sup>3</sup>S) state is,

$$\Psi(r_1, r_2) = N_t [ u(r_1)v(r_2) - u(r_2)v(r_1) ] \quad (1)$$

Where,  $N_t$  = Normalization constant and ,

$$u(r) = (Z_i^3/\pi)^{1/2} \cdot e^{-Z_i r} \quad (2.a)$$

$$V(r) = (Z_0^3/8\pi)^{1/2} (1 - (Z_0 r/2)) e^{-(Z_0 r/2)} \quad (2.b)$$

Here the recent values of the variational parameters quoted by Vucic et al [8] are used i.e.

$$Z_i = 1.994 \quad \text{and} \quad Z_0 = 1.551 \quad (3)$$

The wave function of the (2<sup>1</sup>S) state is,

$$\Psi_s(r_1, r_2) = N_s [ u(r_1)v(r_2) + u(r_2)v(r_1) ] \quad (4)$$

The individual electron orbitals are,

$$u(r) = (M/\sqrt{4\pi})e^{-2r} \tag{5.a}$$

$$v(r)=(N/\sqrt{4\pi})(e^{-(\tau_1 r)}-e^{-(\tau_2 r)}) \tag{5.b}$$

having parameter [8] , M = 5.656854, N = 0.619280,  $\tau_1 = 0.865$  and  $\tau_2 = 0.432784$ .

The ground state He is accurately described by a parametric HF wave function given by Bransden & Jochain [1].

Now, this wave function can be employed to calculate the charge density  $\rho(r)$  as a function of the one electron variable as per by Parr & Young [9]. Thus, for the (2<sup>3</sup>S) state the charge density is,

$$\rho(r) = 2N_i[u^2(r)+v^2(r) - 2I_{ov}u(r)v(r)] \tag{6}$$

Where;  $I_{ov}$  is the overlap integral of the 1s and 2s orbitals of eqns. (2 a) and ( 2 a ) respectively. The charge density of the (2<sup>1</sup>S) state is

$$\rho(r) = 2N_s[u^2(r) + v^2(r) + 2I'_{ov}u(r)v(r)] \tag{7}$$

Further, we can calculate the expectation vale  $\langle r^2 \rangle$  from the  $\rho(r)$  and the diamagnetic susceptibility  $\chi$  from the  $\langle r^2 \rangle$  as follows

$$\langle r^2 \rangle = 4 \pi \int \rho(r) r^4 dr \text{ and } \chi = (1/6)\langle r^2 \rangle \tag{8}$$

**\*Momentum space properties and Compton profile :**

The momentum density  $\Upsilon(p)$  is defined through the fourier transform  $\bar{\Psi}(p_1, p_2)$  of this spatial wave functions given above [5]. The momentum density oh He (2<sup>3</sup>S) can be represented as,

$$\Upsilon(p) = 2N_i[U^2(p)+V^2(p)-2I_pU(p)V(p)] \tag{9}$$

Where U and V are the momentum transform of the orbital eqns (2.a) and (2.b) respectively, and  $I_p$  is the overlap integral of U and V . Also we have for (2<sup>1</sup>S) state,

$$\Upsilon(p)= 2N_s[ U^2(p) + V^2(p) + 2I'_pU(p)V(p)] \tag{10}$$

Where, U & V now correspond to the momentum fourier transform of eqns. ( 5.a) and (5.b) and  $I'_p$  is the appropriate overlap integral.

Let us consider the various momentum expectation value which can be defined from momentum density  $\Upsilon(p)$  as follows,

$$\langle p^\alpha \rangle = \int p^\alpha \Upsilon(\vec{p}) d\vec{p} = 4\pi \int_0^\infty p^{\alpha+2} \Upsilon(p) dp \tag{11}$$

Here  $\langle p^\alpha \rangle$ , for different values of  $\alpha$  are known to have relevant physical meaning. E.g.  $\langle p^{-1} \rangle$  is twice the height of the peak of the Compton profile,  $\langle p^0 \rangle$  is the no. Of electrons of the atomic system and  $\langle p^2 \rangle$  is twice the kinetic energy of atomic electron.

In the impulse approximation, the atomic Compton profile  $J_{nl}(Q)$  of the electron is given by [7],

$$J_{nl}(Q) = \frac{1}{2} \int_Q^\infty |\chi_{nl}(p)|^2 p dp \tag{12}$$

Where,  $\chi_{nl}$  is the momentum Fourier transform of the spatial wave function of the atomic electron.

easy way to comply with the conference paper formatting requirements is to use this document as a template and simply type your text into it.

**III. RESULTS AND DISCUSSION [Page Style ]**

All All the properties defined in section: 2 are explicitly calculated foe H(2S), He(1<sup>1</sup>S) , He(2<sup>1</sup>S) and He(2<sup>3</sup>S)atoms. The integral involved here are obtained analytically or numerically.

**Table 1.** Radial properties of the atoms (in a.u.)

Atom	R orb	$\langle r^2 \rangle$	$\rho(0)$	Susceptibil ity $\chi$
He(1 <sup>1</sup> S)	0.6	1.19	3.6	0.2
H(2S)	5.25	42	0.04	7
He(2 <sup>1</sup> S)	4.50	33.7	2.60	5.62
He(2 <sup>3</sup> S)	3.50	20.7	2.58	3.45

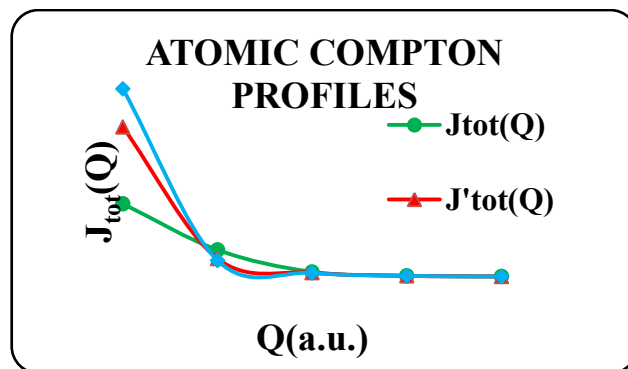
**Table 2.** Momentum space properties of metastable atoms

Atom	$\Upsilon(0)$	$\langle p^{-1} \rangle$	$\langle p^2 \rangle$
H(2S)	25.9	5.42	2.25
He(2 <sup>1</sup> S)	19.5	5.4	4.3
He(2 <sup>3</sup> S)	7.7	4.4	4.4

Table 1 shows the radial properties like  $R_{orb}$ ,  $\langle r^2 \rangle$ , charge density at origin  $\rho(0)$  and susceptibility  $\chi$  for various atoms of present interest. Here we can note that the value of  $\langle r^2 \rangle$  is larger than the  $R_{orb}$  for an all types of atoms taken in to consideration. Also susceptibility  $\chi$  is higher in metastable He atoms compared to ground state He i.e He( 1<sup>1</sup>S). All these properties affect the bulk properties of a medium of He gas containing even a small fraction of metastable atoms. From the results we can conclude that, the ground state He(1<sup>1</sup>S) which is quite compact and relatively harder to ionize or polarize[10]. The importance of  $\rho(0)$  has been discussed by Antolin et al[11]. The three metastable atoms mentioned in Table 1 exhibits fairly large radius as well as the susceptibility. Their extended charge distributions coupled with low ionization energy and high polarizability make them more responsive to external fields. As per previous discussion (Scaling law ) product of atomic radius( $R$ ) and ionization energy ( $I$ ) remains constant. This constant is close to 0.5 a.u. for the ground state of H and He while for metastable state it is little higher and close to 0.6 a.u. Table:2 shows the momentum space properties like  $\Upsilon(0)$  at  $p=0$ ,  $\langle p^{-1} \rangle$  and  $\langle p^2 \rangle$  for an atoms of our present interest. These properties describe behaviour of charge density  $\rho(r)$  at large  $r$ .

Let consider the atomic Compton profile  $J(Q)$  which are important in calculations on inelastic photon-atom scattering. Fig:1 exhibits the Compton profile  $J(Q)$  in a.u. for our present interest atoms. Table 3 exhibits total Compton profile  $\{ J_{tot}(Q) \}$  for the atoms of our interest. From figure 1 We notice a strong

peak of the Compton profile at  $Q=0$ , for all the three metastable atoms, as against the spread out distribution in the ground state He. The behaviour at or near  $Q=0$  is dominated by the 2S electron present in metastable atoms. The large  $Q$  behaviour is due to inner electrons.



**Figure 1.** Comparison of  $J_{tot}(Q)$  for all excited metastable atoms

**Table 3.** Total Compton Profiles

Q	$J_{tot}(Q)$ for He (1 <sup>1</sup> S)	$J'_{tot}(Q)$ for He (2 <sup>3</sup> S)	$J''_{tot}(Q)$ for He (2 <sup>1</sup> S)
0	1.071	2.20	2.76
1	3.94E-01	2.66E-01	2.40E-01
2	7.16E-02	5.96E-02	5.45E-02
3	1.55E-02	1.34E-02	1.25E-02
4	4.94E-03	3.63E-03	3.42E-03
5	1.40E-03	1.18E-03	1.12E-03
6	5.38E-04	4.50E-04	4.27E-04
7	2.33E-04	1.93E-04	1.83E-04
8	1.11E-04	9.16E-05	8.68E-05
9	5.69E-05	4.66E-05	4.45E-05
10	3.12E-05	2.56E-05	2.42E-05

Figure 2 shows comparison of radial charge density  $4\pi r^2 \rho(r)$  as a function of  $r$  of He(2<sup>1</sup>S) and He(2<sup>3</sup>S). It is seen from the figures that both the graphs exhibits two peaks corresponding to the 1s and 2s orbital respectively. The large distribution for both the (2<sup>3</sup>S) and (2<sup>1</sup>S) is spread out for 2S orbital {comparatively high in (2<sup>3</sup>S)} as compared to 1s orbital. The second

peak gives the most probable distance of outer (second) electron from the nuclei of excited He. Fig:3 shows comparison of the radial momentum density  $4\pi r^2 \Upsilon(p)$  as function of momentum of He( $2^1S$ ) and He( $2^3S$ ) respectively. Like radial charge density here also we have two peaks due to the same reason but noticeable point is peaks of 2s orbital for both metastable atoms are almost spread equally i.e. almost overlapped.

All the properties discussed here would help understanding the bulk properties of the gaseous medium in which these metastable atoms exist.

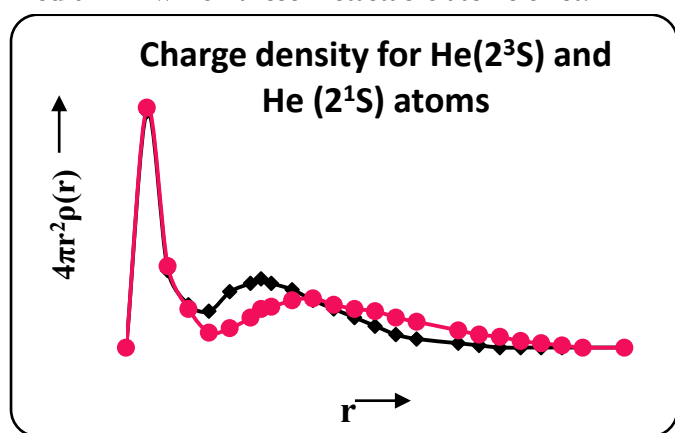


Figure 2. Comparison of Charge density for He( $2^3S$ ) and He ( $2^1S$ ) atoms

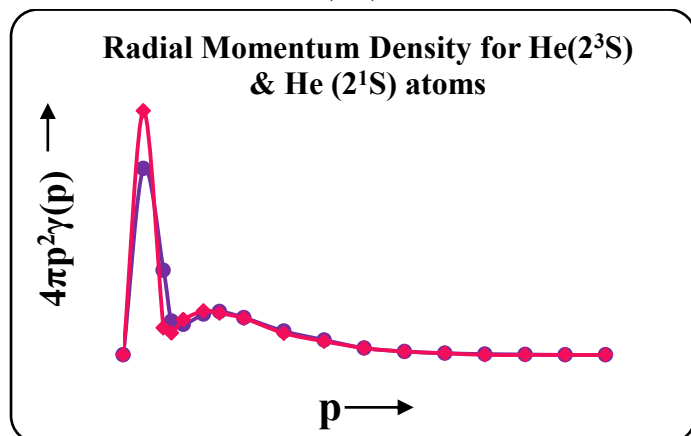


Figure 3. Comparison of Radial momentum density for He( $2^3S$ ) and He ( $2^1S$ ) atoms

#### IV. CONCLUSION

In present paper we have discussed about the different properties of ground state He and metastable state of He. Also we have compared all these properties quantitatively as well as graphically. As a result of this, behavior of all the atoms of our interest can be understood in terms of charge density, momentum density, atomic Compton profile and polarizability.

#### V. REFERENCES

- [1]. Bransden, B. (1983) & Joachain, C. J. (1983), "Physics of Atoms and Molecules", pp.278-289, Longman Publications, London.
- [2]. Christophoru, L. G. (1984); "Electron molecule interactions & their applications".
- [3]. Jacka, M., Kelly, J., Lohmann, B. & Buckmann, S. J. (1995); J. Phys.B, At. Molec. Opt. Phys. Vol 28, L361.
- [4]. Patil, S. H. (1994), J. Phys.B, At. Molec. Opt. Phys. Vol 27, pp. 1823.
- [5]. Angulo, J. C. (1976) & Williams, W. L., "Total cross sections for the scattering of low energy electrons by Helium metastable atoms" (1993), Phys. Rev. A., Vol 48, pp.5768.
- [6]. Sharma, B. S., & Tripathi, A. N.(1979), J. Phys. B., Vol 12, pp. 3107.
- [7]. Biggs, F., Mendelson, L. B. & Mann, J. B., "Hartree-Fock Compton Profile for the elements, Atomic Data and Nuclear Data Tables", Vol 16, pp.201-309.
- [8]. Vucic, S., Potvliege, R. M., & Joachain, C. J.(1989), . Phys.B, At. Molec. Opt. Phys. Vol 22, pp.3519.
- [9]. Parr, R. G. & Yang, W.(1989), "Density functional theory of atoms and molecules", Oxford press.
- [10]. Bunge, C. F., Barrientos, J. A., & Bunge, A. V.(1993), Atomic data and nuclear data tables, Vol. 53, pp.113.
- [11]. Antolin, J., Zarzo, A. & Angulo, J. C.(1993), . Phys.Rev. A., Vol 48, pp. 4149.
- [12]. Iakubov, J. T. & Khrapak, A. G.(1995), . Phys. Rev.A, Vol 51, pp.5043.