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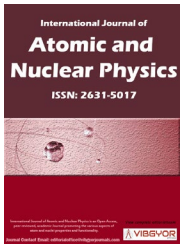
Excitation of the 2^1S, 2^1P and n = 3, 4, 5 (n^1P) of Helium by Positron Impact



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Abstract

We report cross-sections for excitations of 21S, and 21P state of helium atom by positron impact using the scaled Born positron (SBP) approach. Particular attention is paid to the n^1P (n = 3, 4, 5) states which for the first time, integral cross sections are investigated using the SBP method. The possibility of using the SBP approach to estimate the contribution of open channels effects is discussed. An investigation on the determination of Z_{eff} classical (Z_{eff} = Z) in the context of SBP method illustrate the good convergence characteristics of the procedure.

Keywords

Born, Positron, Scaling

PACS: 34.80.Dp

Introduction

Positron-atom scattering has been an important area of research in the last years. For astrophysicists, the knowledge of elastic, ionization and inelastic cross sections would be very welcome as a important information about the interstellar medium [1]. Important area using positron as incident particle is the scans of the human brain in high-resolution positron emission of radiation by positron annihilation [1]. Also well known that material science researchers would like to have a better notion about electronic excitation using positron as incident particle (models to identify vacancies) [1,2]. Also a series of experiments involving positron impact with targets in general has been done recently [2] so that the theoretical calculations are extremely important for a adequate comparison. A suitable theoretical method should be capable of dealing with several important aspects of the positron-target scattering, i.e., electronic excitation, polarization of the target, ionization, multichannel effects, and positronium (Ps) formation. Some important theoretical works in the field of positron-atom collision was made by Chaudhuri, et al. [3] using the close-coupling approximation (CC), Reeth and Humberston [4] using the Kohn variational method (KVM), Singh, et al. [5] using optical-model potential, and several others studies can be obtained in the literature [6-8]. Specifically the positron-He atom scattering represent a good test for several theoretical developments, the helium atom as a stable target, has been the workhorse for many of the recent advances in low energy positron physics (see Refs. [8,9]).

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The motivation of this work is to study the inelastic positron-helium scattering to He atom for the 2^1S, and 2^1P states using the SBP approach. We report also cross sections for the n^1P (n = 3, 4, and 5) states and we include a preliminary study on the open channels (estimative) to see the effect these channels on the inelastic scattering of helium (2^1P state).

The first Born approximation (FBA) is traditionally used as a first study on cross sections of atoms and molecules by electron or positron impact as incident particle. First calculations of positron-He scattering have been performed by Massey and Mousa using the FBA [10]. They used only the ground state for He and positronium (Ps) formation and obtained reasonable cross sections. Another extensive and important study based on the Born approximation was presented also by Joachain [11]. From the FBA studies it became clear that more sophisticate approaches to the problem were required. In particular the SBP approach has as point start the FBA and we will see that the SBP approach is able to describe positron-atom scattering (subsequent papers using the SBP approach show equally good results for H_2 [12], and C_6H_6 [13] targets).

In Sec.2 we will identify the SBP method for investigated the 2^1S (2^1P) state and in particular the n^1P states (n = 3, 4, 5) of He atom by positron impact. In Sec.3 computational procedures and results are discussed. Conclusions are presented in Sec.4.

Theory

The FBA is used here as the starting point, i.e., the plane wave is the correct function at infinity for an positron-atom scattering. The scaling method proposed here applies only to integrated excitation cross sections, not to angular distributions. In a generic form the FBA can be written as

$$\sigma_{\mathrm{Born}} = \left[\left(4\pi a_o{}^2 \mathrm{R}\right)/\mathrm{E}\right] f_{\mathrm{FBA}} \qquad (1)$$

The scaling Born positron (SBP) approach replaces the E (energy) that appears in the denominator of Eq. (1) by $E + E_{exc} + E_{Ps}$ and Eq. (1) is rewritten as

$$\sigma_{\mathrm{SBP}} = \left(f_{\mathrm{accur}}/f_{\mathrm{Born}}\right).f\left(\mathrm{E}\right).\sigma_{\mathrm{Born}} \qquad (2)$$

Where

$$f\left(\mathrm{E}\right) = \left[\left(\frac{E}{E+\left(Eps+Eex\right)}\right)\right] \qquad (3)$$

E_{ps} is the positronium energy, E_{exc} is the excitation energy, E is the energy incident of positron particle, f_{accur} is an accurate dipole value from experiments or from accurate wavefunctions, and f_{Born} is the dipole value from first Born approximation (FBA). As observed in Eq. (3), E is increased by a constant ($E_{Ps} + E_{ex}$) and this modification has some consequences practical to the performance of the SBP method [9,12,13]. The constant is related with energy of the incident positron in the field of the nucleus and the bound electrons of the target and the Eq. (3) can be seen as the scaling factor to represent the correlation between the positron and electrons of the target. It may be mentioned that cross sections obtained using the FBA are identical for electron and positron as projectiles but the f(E) factor identify the incident positron. The positronium (Ps) energy used in the eq. (3) is written as

$$E_{ps} = B - 6.8\ eV \qquad (4)$$

Where B is the binding energy of the electron of target represent the positron particle. The f(E) factor reduces the FBA at low energies while keeping the validity of the Born approximation at high energies and the SBP approach has the effect of correcting the FBA. When dealing with dipole transitions the long-range character of the dipolar coupling requires a larger number of partial waves and because of it, higher partial waves are not well described for several sophisticates *ab initio* methods (furthermore can add considerably to the computational effort [4)]. This consideration is especially important, i.e., in the practical such an effort can be avoided if above a certain angular momentum the remaining partial waves, which are weakly scattered, are obtained from a weak collision theory such as the FBA**.** As we will see, in principle, the SBP approach can generate cross sections reliably and quickly when compared with sophisticates methods and experimental data. The SBP approach can provide realistic excitation cross sections for many targets, which are not only difficult to measure but also cannot easily be calculated with existing theories. The propose of the present work consist in the study of two cases; first, as cited before, cross sections for the excitation of the 2^1S, and 2^1P state of He atom using the SBP approach. The results are important to note that, from the point of view of the theoretical formulation, the SBP method offers results very similar with sophisticate theories. Second, investigate as the open channel

can interfere on the cross sections. A study using open channels represent a effort manageable and with the problem in mind, let us define an alternative mechanism, i.e., "pseudo coupling" and we will verify as this procedure alternative can produces similarity or difference with sophisticates methods. In the Eq. (3) we define the term

$$E_{ex} \rightarrow \sum_{n}^{\infty} \text{¿¿}_{ex} \Big)_{n}$$

and Eq. (2) can be rewritten as

$$\sigma_{SBP} = \left(f_{accur}/f_{Born}\right).\left[E \Big/ \left(E + E_{ps} + \sum_{n}^{\infty} \text{¿¿}_{ex}\right)_{n}\right].\sigma_{Born} \quad (6)$$

It is important to point out that in the Eq. (5) the $\sum_{n}^{\infty} \text{¿¿}_{ex}\Big)_{n}$ term can be constructed for "*n* states" and the influence of open channel on the compared 2^1P state can be observed (this type of indirect study is not common but can be opportune). Evidently, in this context we will see that results using Eq. (5) are not refined (multichannel coupling represent a flux competition among all possible electronic transitions, positronium formation, including ionization, with all being due to the positron impact) more can be extremely relevant when compared with sophisticate methods and experimental data.

Computational Procedures and Results

Excitation to the 2^1S, and n^1P states

We have used Hartree-Fock calculations to represent the ground state of the target with the same basis set used (Cartesian Gaussian) in Ref. [14]. With this basis set we have obtained a excitation energy of 19.48 eV for 2^1S, and 21.21 eV for 2^1P state. The n^1P states (n = 3, 4, 5) are listed in Table 1. The positronium energy (E_{ps}) is 6.1 eV.

In Figure 1 we show the SBP integral cross section for the $1^1S \rightarrow 2^1S$ electronic transition compared with the FBA only. As observed the SBP approach not only reduces the cross sections magnitude at low energies, but also shifts the peak to a higher "E" vality of the FBA intact. As expected the SBP converge to the FBA at high energies.

In Figure 2 we show again the SBP integral cross section for the $1^1S \rightarrow 2^1S$ electronic transition compared with the convergent close-coupling (CCC) method [15] (with and without ionization and Ps formation). The CCC method [15] is an able method and the target states are obtained in the square-integrable orthogonal Laguerre basis. As observed in Figure 2 the SBP approach exhibit a similar shape with the CCC method [15] but with significantly different in magnitude at low energies. The obvious difference between the methods is mainly due to the different treatments, i.e., the SBP approach

Table 1: Excitation energy for n^1P states (n = 3, 4, 5).

He(state)	E_{exc} (eV)
31P	23.08
41P	23.74
51P	24.04

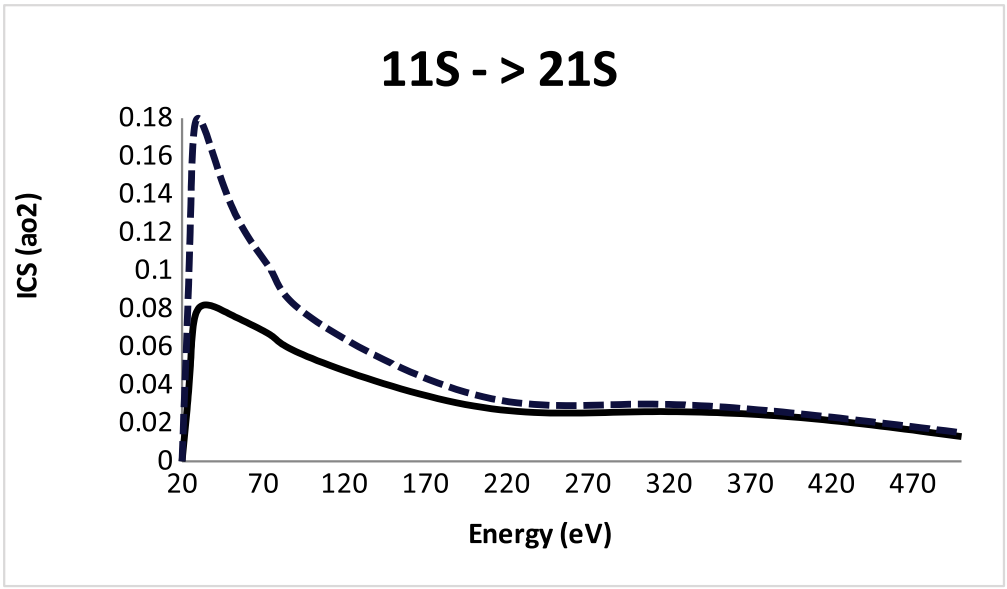

Figure 1: Integral cross section (ICS) for 1^1S-2^1S excitation of He atom by positron impact. Solid line, SBP approach; Dashed line, FBA.

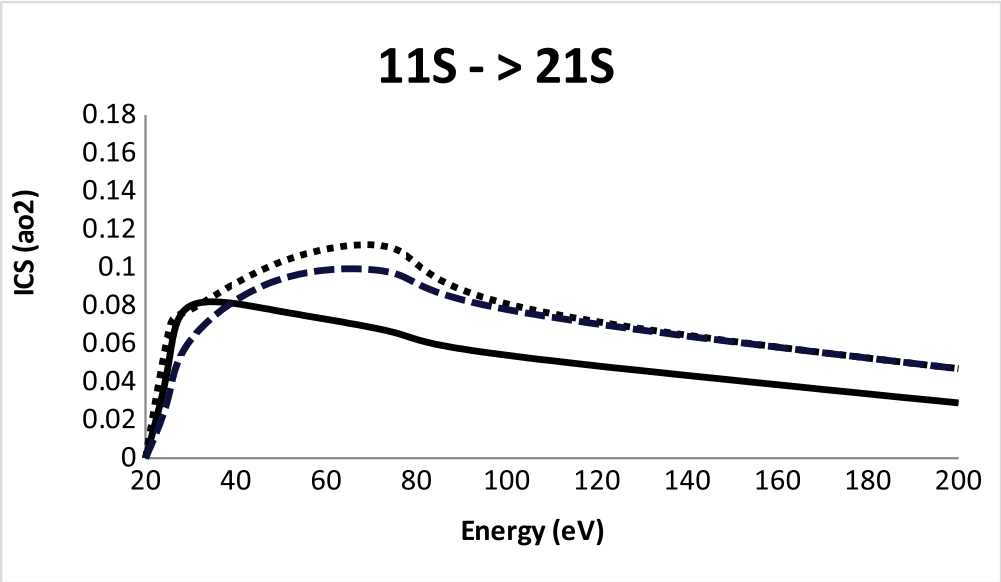

Figure 2: Integral cross section (ICS) for 1^1S-2^1S excitation of He atom by positron impact. Solid line, SBP approach; Dashed line, CCC method (without ionization and Ps formation) [15]; Dot line, CCC method (with ionization and Ps formation) [15].

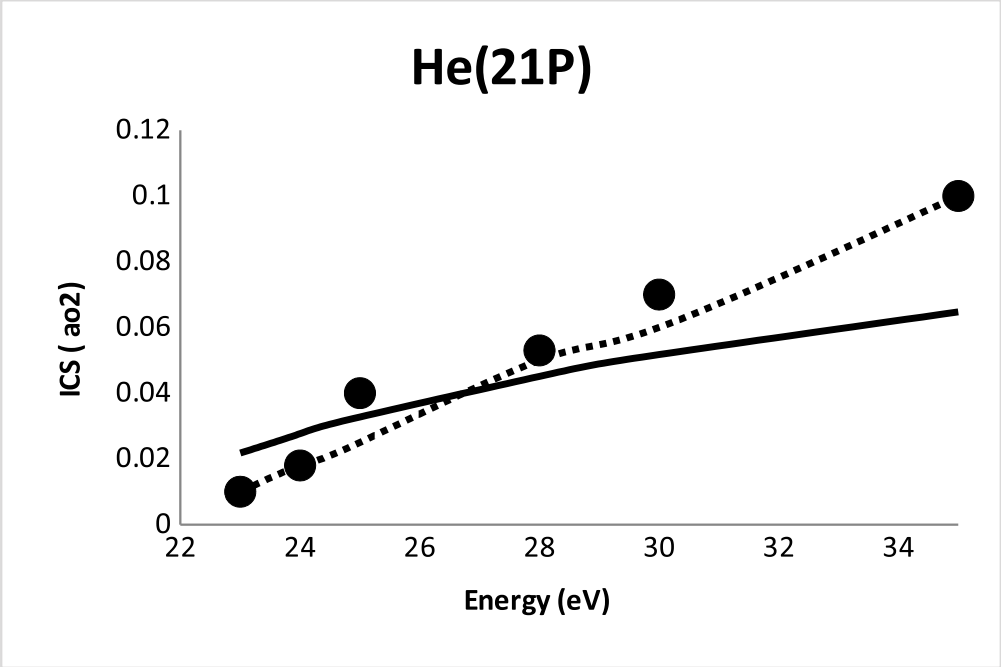

Figure 3: Integral cross section (ICS) for 1^1S-2^1P excitation of He atom by positron impact. Solid line, SBP approach; Dot line, CCC method (with ionization and Ps formation) [15]; Black circle, experimental data [15].

not include ionization and Ps-formation. Although ionization and Ps-formation channels are expected to play an important role in this energy region our cross sections are very similar with CCC method [15]. At high energies the SBP approach and CCC method [15] exhibit a good level of agreement. This agree is very important, i.e., the CCC method [15], as cited before is able to perform calculations for positron-atom scattering but the method [15] can be considerably enlarge the computational effort. This same computational effort is obviously not found in the SBP approach.

In Figure 3 we show the SBP integral cross section for the $1^1S \rightarrow 2^1P$ electronic transition compared with the convergent close-coupling (CCC) method (with ionization and Ps formation)

[15] and experimental data [15]. As observed in Figure 3 again the SBP approach exhibits a similar shape with the CCC method [15]. It is obvious that the largest effect of ionization and Ps-formation channels occurs at lower energies and the cross sections using SBP approach are in principle valid at low energies.

In Figure 4 we show the SBP integral cross section for the $1^1S \rightarrow 2^1P$ electronic transition compared now with the DWA (electronic excitation only) [16] at intermediate and high energies. In Figure 4 a good agree between the SBP approach and the DWA [16] can be observed at intermediate and high energies and this is evidently encouraging.

In Figure 5 we show the SBP integral cross section for the $1^1S \rightarrow 3^1P$ electronic transition compared with the coupled-channel optical method (CCO) [16]. The two methods without Ps-formation. A good agree between the SBP approach and the CCO model [16] can be observed. The results are consistently good, giving confidences that the SBP approach is adequate when compared with the sophisticate CCO model [16].

To test the stability of the 2^1P cross section,

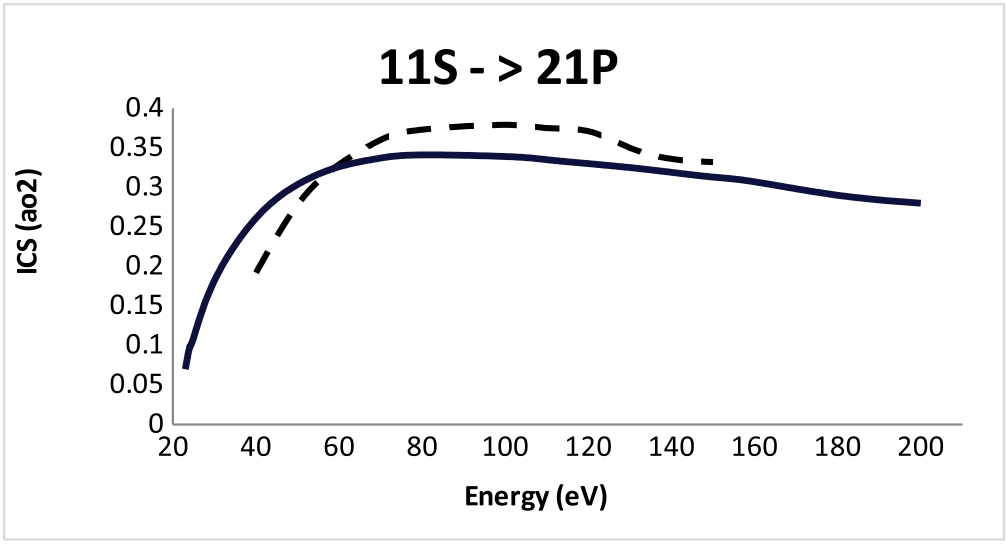

Figure 4: Integral cross section (ICS) for 1^1S-2^1P excitation of He atom by positron impact. Solid line, SBP approach; dashed line, DWA [16].

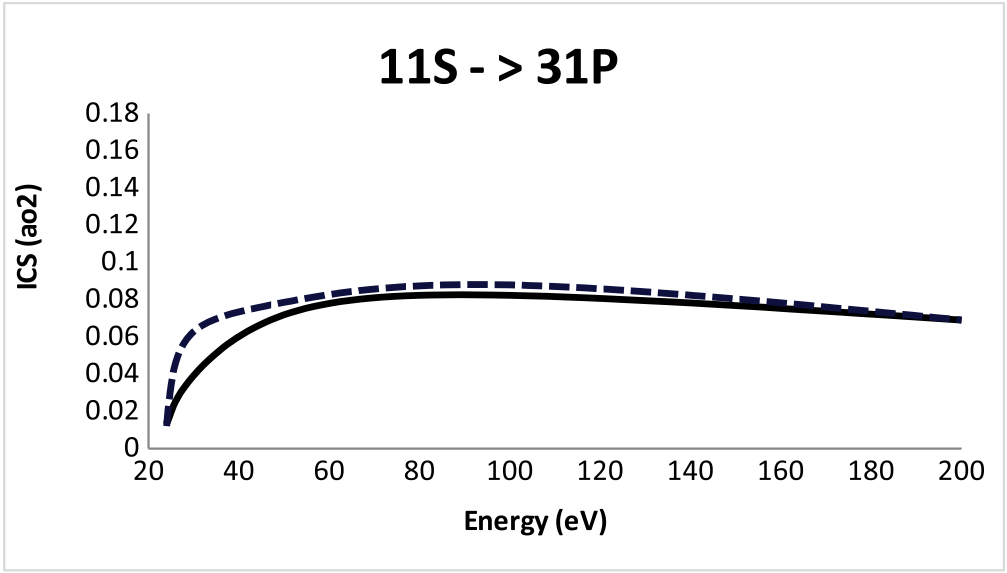

Figure 5: Integral cross section (ICS) for 1^1S-3^1P excitation of He atom by positron impact. Solid line, SBP approach; Dashed line, CCO method [17].

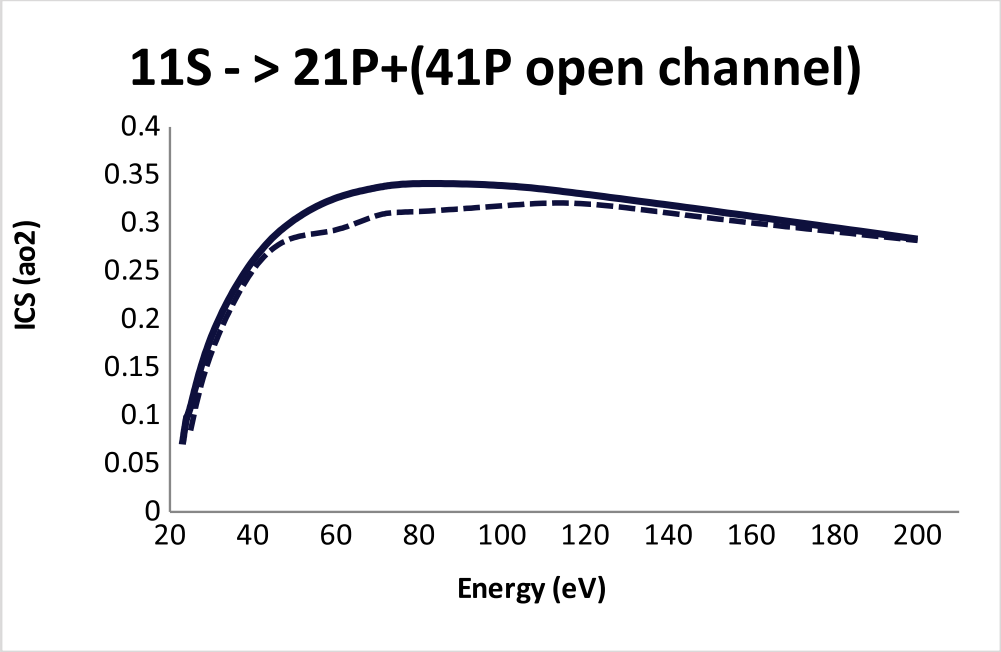

Figure 6: Integral cross section (ICS) for 1^1S-2^1P + 4^1P (open channel) excitation of He atom by positron impact using SBP approach. Solid line, 2^1P state; Dashed line, 2^1P + 4^1P (open channel).

we have performed calculations using other open channel, i.e., the influence of 4^1P as open channel on the 2^1P transition. This preliminary study represents only a indicative on the level of influence of a possible open channel. Figure 6 shows the 2^1P state with the presence of the 4^1P state as open channel (Eq. 5). As observed the presence of the 4^1P state as a open channel does not disturb the 1^1S-2^1P cross section in the SBP context. Evidently a multichannel convergence process in order to obtain reliable cross sections can be necessary.

Alternatively, the SBP approach can be used as a representation of the Z_{eff} classical "Z", i.e., when positrons annihilate on many-electron atoms, the annihilation cross sections is traditionally written as [1]

$$\sigma_a = \sigma_{2\gamma} Z_{eff} \quad (7)$$

Where

$$Z_{eff} = \int \sum_{i=1}^{z} \delta(r\text{-}r_i) \left|\psi(r_1,...,r_z,r)\right|^2 dr_1...dr_z dr \quad (8)$$

Z_{eff} is the effective number of electrons that contribute to the annihilation process, and $\psi(r_1,...,r_z,r)$ is the total wavefunction of the Z electron and one positron coordenates. If substitutes the asymptotic, plane wave function into equation (8), one obtains Z_{eff} = Z (classical). We have noted that the SBP approach can determine the Z_{eff} classical based on the Born approximation (Z_{eff} represent also an important criteria to check the quality of SBP approach using the FBA). The accuracy of the Z_{eff} Born approximation can be given by

$$Z_{eff} = \left[\left(\sigma_{Born}/\sigma_{SBP}\right)\right].Z \quad (9)$$

and in this sense the present SBP approach retains information on the Z_{eff} classical.

Finally, in Figure 7 we present $Z_{eff}^{(SBP)}$ for the He atom. As observed the Z_{eff} shows aspects of convergence with Z classical (Z = 2) using the 2^1S state. Figure 6 indicate that the SBP approach is significant and suggested that Eq.(8) can be used as a strategies to treat convergence characteristic of the SBP approach. The numerical data in Table 2 are obtained using the SBP approach and are listed for future reference (units a_o^2).

Conclusion

We have discussed a recently developed scaling method called scaled Born positron (SBP) for positron-He atom collision. The present paper has examined the validity of the SBP approach to calculating integral cross sections for 2^1S, and 2^1P states of He atom by positron impact. Analysis of the results indicated that the SBP is significant, with good convergence characteristics when compared with sophisticates methods at low energies. In particular the calculation for the 2^1P state using the SBP approach shown cross sections

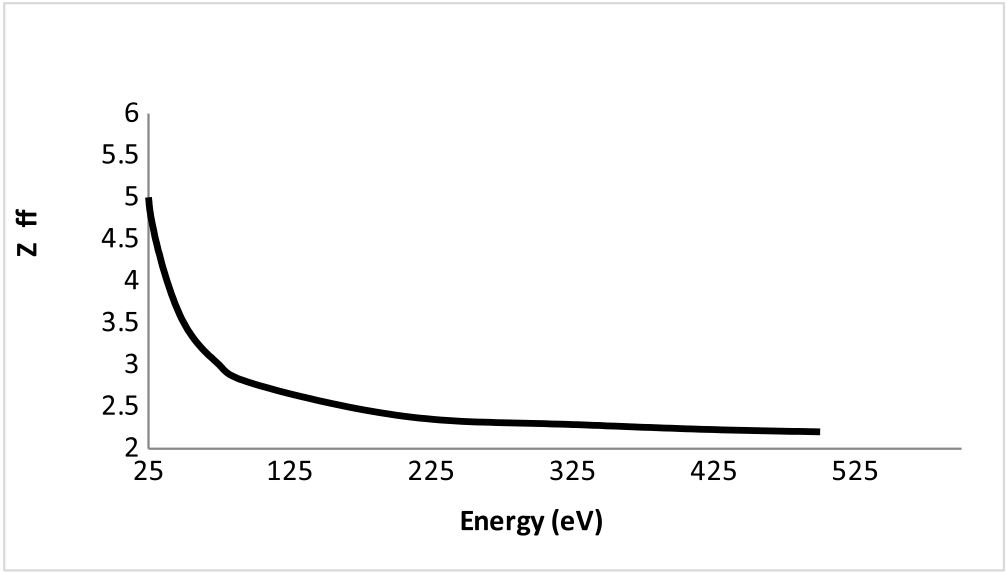

Figure 7: Z_{eff} using the SBP approach. Solid line, SBP approach.

Table 2: Electronic excitation energy and f_{accur} dipole value from accurate wavefunctions, and f_{Born} dipole value from FBA.

State	2^1P	3^1P	4^1P	5^1P
E_{exc} (eV)	21.21	23.08	23.74	24.04
f_{accur}	0.27	0.07	0.02	0.01
f_{FBA}	0.25	0.07	0.02	0.01
23	0.07682			
24	0.09789	0.01329		
25	0.11585	0.01961	0.00624	0.00268
30	0.18285	0.03921	0.01467	0.0071
40	0.26178	0.06058	0.0234	0.01153
50	0.30357	0.07181	0.028	0.01385
60	0.32603	0.07787	0.0305	0.0151
70	0.33703	0.08103	0.03187	0.01578
80	0.34142	0.08241	0.03247	0.01607
100	0.33928	0.08231	0.03248	0.01612
110	0.33546	0.0815	0.03216	0.01596
120	0.33053	0.08043	0.03171	0.01577
130	0.32507	0.07916	0.03125	0.01555
140	0.31914	0.07781	0.03075	0.0153
150	0.31307	0.07254	0.03021	0.01501
200	0.28346	0.06932	0.02742	0.01365

with great similarity with sophisticate methods and the SBP approach is economical in the sense that relatively small basis set (FBA) are capable of providing reliable cross sections with small effort computational. We also conclude that Z_{eff} classical parameter is consistently good which emphasized the importance of the SBP approach.

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