Ionization of atoms by positron impact: Applications of the Scaled Born Method

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Received 17 March 2026; accepted 9 June 2026

Positron emission tomography (PET) scans can be used to investigate the pathogenesis of neurological disorders and diseases such as Alzheimer's and Parkinson's. PET scans use positrons to resolve an image of the internal biochemical process occurring inside the body, *i.e*., ionization cross sections. Knowledge of ionization cross sections for atoms is evidently crucial in PET technology. We will discuss some recent developments of the scaled Born positron (SBP) method for ionization of atoms. The SBP method was originally proposed for electronic excitations of atoms (J.L.S. Lino, $Chin.J.Phys.\mathbf{54}$ (2016)504). First Born approximation (FBA) and the atomic orbital wavefunctions have been approximated by Roothaan-Hartree-Fock, and the scattered positron and ejected electron have been approximated by a plane wave and Coulomb wave as proposed by Barlett $etal.$ (Atomic Data Tables **86** (2004) 235). It is shown that the SBP method combined with an analytical factor results in a efficient method when compared with the sophisticated and traditional binary-encounter-dipole (BED) model. Results of ionization cross sections of H, He, Ne, and C atoms using the new representation are presented to illustrate the applicability of the improved SBP method.

Keywords: Born; positron; ionization; atoms.

DOI: https://doi.org/10.31349/RevMexFis.72.060401

1. Introduction

Positron-impact ionization cross sections represent a powerful tool for biomedical research and enable the imaging of internal molecular process occurring in vivo in real time [1]. A database of ionization cross sections can be used, for example, as a starting to investigate the pathogenesis of neurological disorders and diseases such as Alzheimer's disease [1]. For example, positherapy utilizes positrons to destroy cancer cells [1] and has proven useful in treating cancers where conventional methods are less effective. Positherapy also is a safer alternative to current radiotherapy approaches due the low range of the emitted positron. In recent years, there has been increasing interest in studying biological molecules such as DNA by electrons and positrons impact ionization cross sections of atoms. It is worth mentioning that after losing sufficient energy, positrons undergo annihilation and release gamma rays which can be observed by "positron emission tomography (PET)" scans and their applicability in medicine is imperative, which justifies further studies on the topic. A series of experiments involving positron impact with several atoms has been conducted recently (see Ref.[2-4]) and evidently theoretical calculations are extremely important for an adequate comparison. Some methods, such as Born approximation [5], the distorted plane wave method [6], and the binary-encounter-Bethe (BEB) dipole model [7,8] have been used to calculate ionization cross sections by positron impact. Accurate ionization cross sections still remain an important and challenging endeavor. The scaled Born positron (SBP) method was originally proposed by Lino [9-12] for studies involving electronic excitation of atoms and molecules by positron impact. As we will demonstrate, the SBP method can be adapted for ionization cross sections of atoms (the merit of SBP method is important, *i.e*., avoid arduous mathematical equations, and computational complexity [13]). In Sec. 2 we identify the SBP method and in Sec. 3 computational procedures and results are discussed. Conclusions are presented in Sec. 4.

2. Theory

The well-known FBA was first applied to treat electron scattering at high incident energies in 1926. Since then significant effort and investment have been made carried out by several researchers involving the FBA as a suitable starting point [5]. As is well known, for sufficiently fast electrons (or positron) the cross sections for a collision with an atomic target are expected to be promising but for low and intermediate energies the FBA is not sufficient. In this article, we will show that the SBP method is appropriate for low, intermediate, and high incident positron energies. In the FBA the plane wave represents the correct function at infinity for a positron colliding with a target and also represent the simplest collision theory that uses target wave function explicitly. The FBA does not properly incorporate target distortion and resonances. We will see that the SBP method include such possibilities. The traditional FBA can be written as

$$\sigma = \left[\frac{(4\pi {a_o}^2 R)}{E}\right] f_{\rm FBA}, \tag{1}$$

where

$$f_{\rm FBA} = \left(-\frac{1}{2}\pi\right) < S_{kf}\,|\,V\,|\,S_{ki} > . \tag{2}$$

The SBP method represent an improved version of FBA and as observed in Eq. (1) the SBP method replaces the E (energy) that appears in the denominator of Eq. (1), by $E + (E_{\rm exc} + E_{\rm Ps})$ and the Eq. (1) turning Eq. (1) into

$$\sigma_{\rm SBP} = \left(\frac{f_{\rm acc}}{f_{\rm Born}}\right) \cdot f(E)\sigma_{\rm Born}, \tag{3}$$

where

$$f(E) = \frac{E}{(E + E_{\rm Ps} + E_{\rm ex})}. \tag{4}$$

It is important to mention that the SBP method has important aspects that can be highlighted. First, E_{Ps} is the positronium energy of the target and is used only when the incident particle is a positron which is not identical to the target electrons. Second, E_{exc} is the excitation energy, f_{accur} is an accurate dipole value from experiments or from accurate wavefunctions, and f_{Born} is the dipole value from the FBA (these parameters are not of adjustable and this is very important in a mathematical development). Third, the constant $(E_{\rm Ps} + E_{\rm exc})$ has also some pratical consequences to the performance of the SBP method, *i.e.*, the constant is related with energy of the incident positron in the field of the nucleus and the bound electrons of the target (also can be seen as the scaling factor to represent the correlation between the positron and electrons of the target). Finally, the "scaling factor" here proposed suggests a similarity with polarization effects (Lino has shown many examples [9-12] in which the SBP method for dipole-allowed excitation into very reliable cross sections when compared with sophisticates methods). The Coulombic attraction between positrons and electrons makes an enormous difference from the always repulsive interaction between electrons. The SBP method does not incorporate real positronium formation, but it explicitly considers virtual positronium formation, *i.e.*,

$$E_{Ps} = B - 6.8 \text{ eV}, \tag{5}$$

where B is the binding energy of the electron of target. As observed, the $f(E)$ factor reduces the FBA at low energies while keeping the validity of the Born approximation at high energies [5]. Studies using the SBP method for electronic excitation of the targets by positron impact are conclusively satisfactory [9] and the method is not computationally intensive. The FBA is calculated from the sum of the partial ionization cross sections of each occupied orbital,

$$\sigma = \frac{\sum(N_{\rm nlm}\sigma_{\rm nlm})}{(2l+1)}, \tag{6}$$

where nlm orbital and it is assumed that electrons are equally shared among the available m quantum states. Mathematically the FBA for ionization may be expressed as

$$[e^{-iqr}]_{\rm nml} = \int \psi^* e^{-{\rm iqr}}\phi_{\rm nml} d^3r, \tag{7}$$

where $\varphi_{\rm nlm}$ is the target orbital wave function with the usual nlm labels for orbital, angular momentum and magnetic quantum numbers, respectively, and ψ is a Coulomb wave used to model the ejected electron. There are no arbitrary parameters or fitting constants. The SBP method does not provide differential cross sections in energy loss or angle of scattering, and no positronium formation was considered. The total ionization cross sections for the target atom is the sum over all accupied orbitals, *i.e.*, $\sigma_{\rm total} = \sigma_\sigma(1s+2s+2p+...)$.

For ionization cross sections the Eq. (3) can be written as

$$\sigma_{\rm SBP} = \left(\frac{f_{\rm acc}}{f_{\rm Born}}\right) \cdot f(E)\sigma_{\rm Born}, \tag{8}$$

where

$$f(E) = \frac{E}{(E + E_{\rm Ps})}. \tag{9}$$

3. Results and discussion

We have investigated ionization cross sections by positron impact of H, He, Ne, and C atom. In Table I, we show the data for ionization energy (B) and positronium formation energy (E_{Ps}). In Table II, we shows results for all atoms (ionization cross sections by positron impact) using the SBP method.

TABLE I. Ionization and positronium energies.

Atom	B(eV)	E_{Ps}(eV)
H	13.6	6.8
He	24.50	17.70
Ne	21.56	14.76
C	11.26	4.40

TABLE II. Ionization cross sections for H, He, Ne, and C atom by positron impact using the SBP method (10^{-16} cm^2).

Energy(eV)	H	He	Ne	C
20	0.288	0.0008	0.0016	0.523
30	0.618	0.0378	0.087	1.117
40	0.743	0.140	0.196	1.571
50	0.779	0.230	0.287	1.821
60	0.771	0.296	0.364	1.941
70	0.746	0.342	0.429	1.991
80	0.714	0.372	0.484	1.985
90	0.681	0.391	0.528	1.958
100	0.648	0.409	0.565	1.918
150	0.515	0.424	0.660	1.660
200	0.423	0.367	0.676	1.464
250	0.359	0.351	0.660	1.276
300	0.310	0.304	0.625	1.134

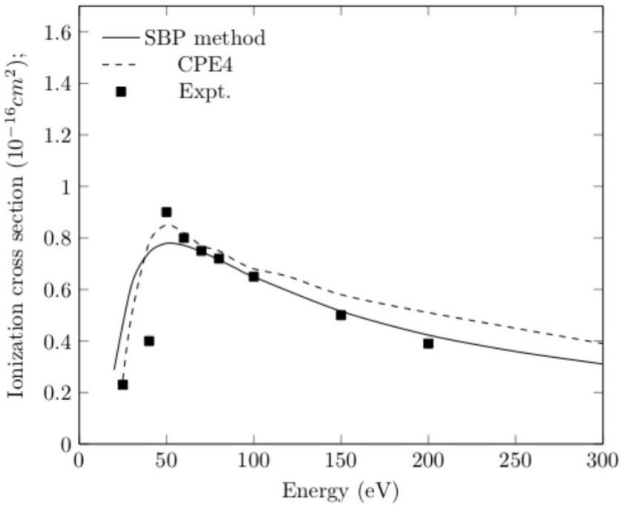


FIGURE 1. Positron-hydrogen atom ionization cross sections.

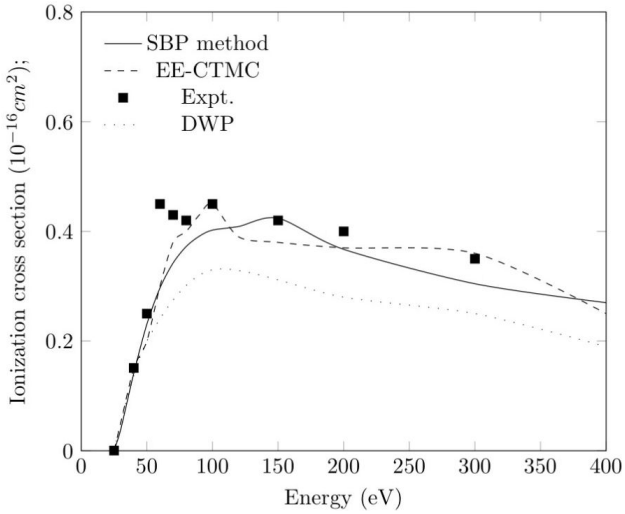


FIGURE 2. Positron-helium atom ionization cross sections.

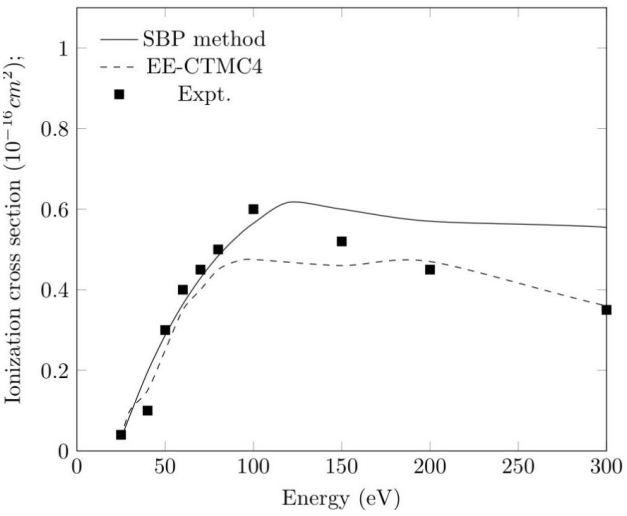


FIGURE 3. Positron-neon atom ionization cross sections.

In Fig. 1 we present positron-hydrogen atom ionization cross sections using the SBP method compared with the efficient distorted wave method (CPEA) [14], and experimental data [15]. As observed the SBP method is very similar with the CPEA [14]. The agreement with the CPEA [14] theory provides direct evidence of the accuracy of our structure model. As observed also our cross sections are in good agreement with the experimental data [14].

In Fig. 2 we shows positron-helium atom ionization cross sections using the SBP method compared with distorted wave plane (DWP) method [16], the sophisticate classical trajectory Monte Carlo (EE-CTMC) model (see Ref. [16]), and experimental data [16]. As observed in Fig. 2 the agreement in the shape and magnitude between the SBP method and EE-CTMC model is encouraging. This is of special relevance for the SBP method, since the EE-CTMC model demands great computational effort. From Fig. 2 can be clearly seen that the SBP method is in very good agreement with the experimental data [16]. At high energies the methods converge to the traditional FBA, validating the procedure.

Figure 3 shows positron-Ne atom ionization cross sections. Ionization of neon atom by positron impact is a fundamental process which atomic structure, positronium formation, and particle-antiparticle interactions are not fully understood in the literature. Positron scattering from neon atom is very important for the interpretation of astrophysical data [17]. Because neon is a noble gas with a high ionization potential (21.56 eV), it serves as a rigorous test for the SBP method. Fig. 3 shows our SBP method compared again with the sophisticate classical trajectory Monte Carlo (EE-CTMC4) model [17] and experimental data [17]. As observed again the theoretical results are in good agreement. The agreement between the methods are consistently good, giving confidence that the set of atomic parameters used in our SBP method are the best available set.

Finally, in Fig. 4 we show a preliminary study on the positron-carbon atom ionization cross sections. As cited before, ionization cross sections help the investigate the pathogenesis of neurological disorders and diseases such as Alzheimer's and Parkinson's. The carbon atom represent 18 % of the human body and is the major component of biomolecules such as DNA. Preliminarily, in Fig. 4 we shows ionization cross sections calculated using the SBP method compared with the BEB method for electron case only [17]. As observed, the cross sections calculated using the SBP method for positrons are in ery good agreement with those obtained using the BEB method for electrons [17]. This scenario is obviously not found for several other atoms. It is important to observe that the convergence between the cross sections using SBP method (positron) and BEB method (electron) suggests new comparative studies (for high incident positron energies, numerical convergence to the FBA is expected). The carbon atom shows signs of the presence of excitation-autoionization [17], which represents an interesting question for the future using the SBP method [19].

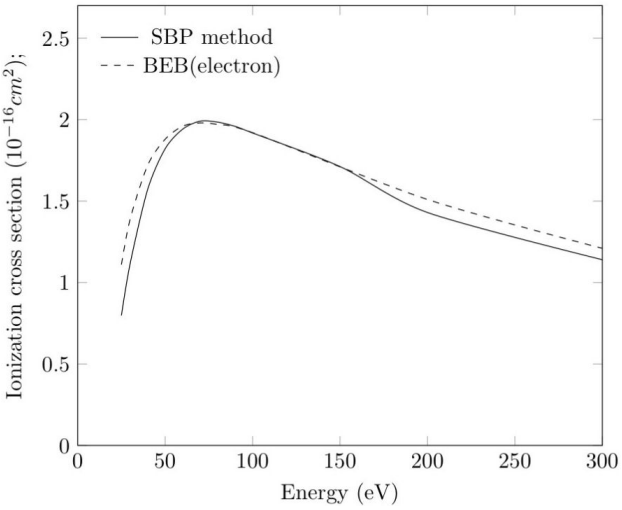


FIGURE 4. Positron-carbon atom ionization cross sections.

4. Conclusions

The scaled Born positron (SBP) method provides in conclusion good results for all the targets studied. The SBP method not diminish the value of more sophisticated methods that produce highly accurate results, though they requires orders of magnitude more computational effort than SBP cross sections. First, the SBP method will not work well on angular distribution because the scaling only change the E dependence of first Born approximation (FBA) cross sections. It is well known that the FBA cross sections do not reproduce large angle scattering well at any E, and the SBP method will not change the shape of FBA angular distributions. However, the SBP method described here will facilitate the calculation of integrated excitation, ionization, excitation-autoionization cross sections, and studies on positronium formation for targets in general, which pose difficulties to more computer-intensive theories. In conclusion the SBP method for ionization cross sections is relatively simple and efficient when compared to state-of-art ab initio theories.

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