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CALCULATIONS OF TOTAL IONIZATION CROSS SECTION FOR NOBLE GASES

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We have computed total ionization cross section (TICS) for noble gases by impact of electron and positron using truncated coupled state Born approximation (TCSBA). High quality Hartree-Fock Slater orbitals are used to model the target wave function. We have already computed some ionization results [1, 2] for noble gas series by impact of electron and positron as well, but in this paper, we are presenting for Neon, Argon, Krypton and Xenon. We have compared TICS results with other available theoretical results as well as experimental data. It is observed that full orthogonalization of target wave function significantly improves present results and provides better agreement with experimental data for the noble gas series. Our present results are found in excellent agreement with other calculations. However, some discrepancies suggested that more theoretical as well as experimental work is required in future to improve the data.

KEY WORDS: Cross Section, Ionization, Noble gases.

Introduction

The study of collision processes gave new ideas about internal structure of atom. The ionization of noble gas atoms by impact of charged particles continuously attracts a deep interest in collision physics for several reasons. Also the collision processes have the paramount importance for understanding various branches of science and advanced technology. The collision of electron (positron) with noble gases, play a dynamic role in many fields, *e.g*. in the initiation of plasma from neutral gases and medical field etc. On the account of various uses, we can say that noble gases are very fruitful for human life. Due to characteristic properties, noble atoms are used in lighting, photography and high powered gas lasers. On the practical side, reliable knowledge of ionization cross section for above processes is very important for applications in plasma and discharge physics. In recent years, much progress has been made in the theoretical as well as experimental treatment ionization processes.

TOTAL IONIZATION CROSS SECTION FOR NEON

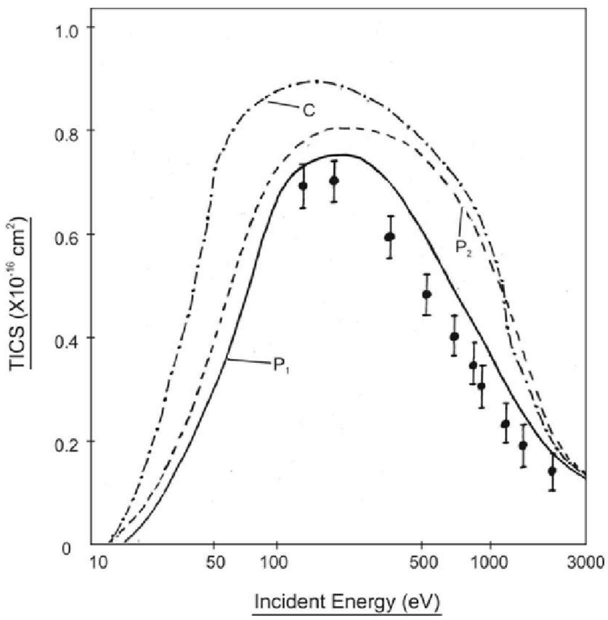

Figure (1)	:	**Total Ionization Cross Section for Neon.**
————————	:	Present results (P_1) for electron
— — — — — — —	:	Present results (P_2) for positron
— • — • —	:	(C) Chang and Altick [13]
(experimental point with error bar)	:	Experimental results of Sorokin *et al* [14]

Most of the theoretical work on positron impact ionization of atoms is based on the distorted wave formalism. Using this approximation Moxom *et al* [3] and Kara *et al* [4] measured the cross sections for Krypton by impact of positron. Ballance *et al* [5] studied about electron impact ionization cross section for Neon atom using *R*-matrix with pseudo states (RMPS) method. Marler *et al* [6] studied positron impact ionization cross section for inert gases by using a qualitatively different method. McEachran and Stauffer [7] have been investigated positron impact ionization cross section by applying relativistic complex optical – potential method. Bartlett and Stelbovics [8] have measured the total ionization cross section of Xenon by impact of electrons having energy from threshold to 3 KeV and compared their data with Born calculations using high-quality Hartree- Fock Slater orbitals. Pindzola *et al* [9] have reported the configuration average distorted wave calculations for electron impact ionization of Xenon. Recently, using continuum distorted wave and first Born approximation, Montanari and Miraglia [10] reported total ionization cross sections of Neon, Argon, Krypton and Xenon by impact of positron.

THEORY

In the case of the electron (positron) impact ionization of a target atomic orbital, the truncated coupled state Born approximation is given by

TOTAL IONIZATION CROSS SECTION FOR ARGON

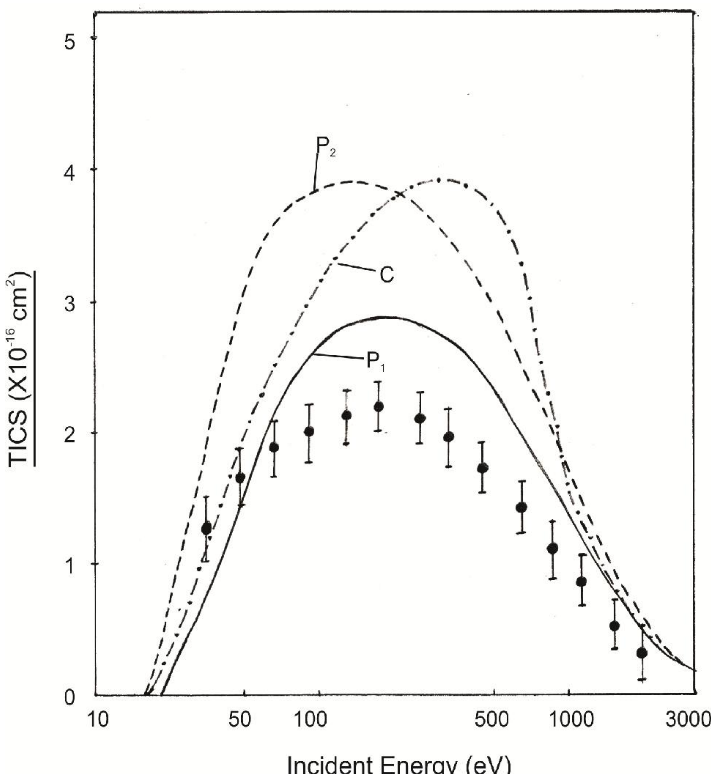

Figure (2) : **Total Ionization Cross Section for Argon.**

——————— : Present results (P_1) for electron

— — — — — : Present results (P_2) for positron

— • — • — : (C) Chang and Altick [13]

Experimental results (dots with error bars) : Experimental results of McCallionin *et al* [15]

$$d\sigma = \frac{4k'K^2}{kq^4} \left|(e^{-iq.r})_{nlm\,K}\right|^2 d\Omega\, d\Omega_K dK \qquad \text{... (1)}$$

where σ is the ionization cross section, $d\Omega$ and $d\Omega_K$ are elements of solid angle about the scattered and ejected electrons respectively. n, l and m are the usual orbital, angular and magnetic quantum numbers, k is the incident electron (positron) momentum (directed along the positive z axis), k' is the scattered electron momentum, K is the ejected electron momentum and $q = k - k'$ is momentum transfer.

The matrix element is given by

$$(e^{-iq.r})_{nlm\,\boldsymbol{K}} = \int \psi_{\boldsymbol{K}}^{(-)^*} e^{-iq.r}\, \phi_{nlm} d^3r \qquad \text{... (2)}$$

where ϕ_{nlm} is the target orbital wave function and $\psi_{\boldsymbol{K}}^{(-)}$ is the ejected electron wave function. To evaluate equation (1), all momenta must be expressed in terms of the known variables and the integration variables [1].

TOTAL IONIZATION CROSS SECTION FOR KRYPTON

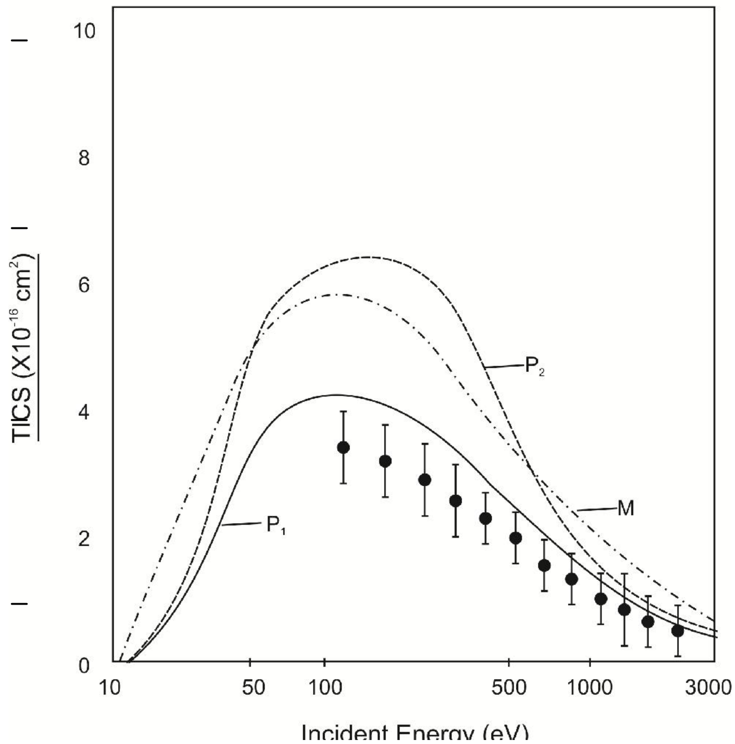

Figure (3)	:	**Total Ionization Cross Section for Krypton.**
————————	:	Present results (P_1) for electron
— — — — — — —	:	Present results (P_2) for positron
—— • —— • ——	:	**(M)** Moores [16]
	:	Experimental results of Sorokin *et al* [17]

Using equation (1), the differential cross section is given as

$$\frac{d\sigma}{d\Omega} = \frac{4k'K^2}{kq^4} \left|(e^{-i\boldsymbol{q}.\boldsymbol{r}})_{nlm\,K}\right|^2 d\Omega_K dK \qquad \text{... (3)}$$

and the total ionization cross section (TICS) of an atom is the sum for the ionization of each of the occupied orbital,

$$\sigma = \sum_{nlm} \frac{N_{nl}\sigma_{nlm}}{2l+1} \qquad \text{... (4)}$$

where N_{nl} is the number of electrons in the said orbital and the electrons are equally shared amongst the stable *m* quantum states.

The incident and ejected electrons are identical particles, so allowance has been made in equation (1) for particle exchange. To compensate for this emission, the upper integration limit of the *K* momentum integration is taken to be $\sqrt{(k^2/2 - E_0)}$, which is the momentum of an electron ejected with half of the maximum possible energy. Further, the Born approximation always yields better results, when the effects of exchange are to reduce the cross section [11].

TOTAL IONIZATION CROSS SECTION FOR XENON

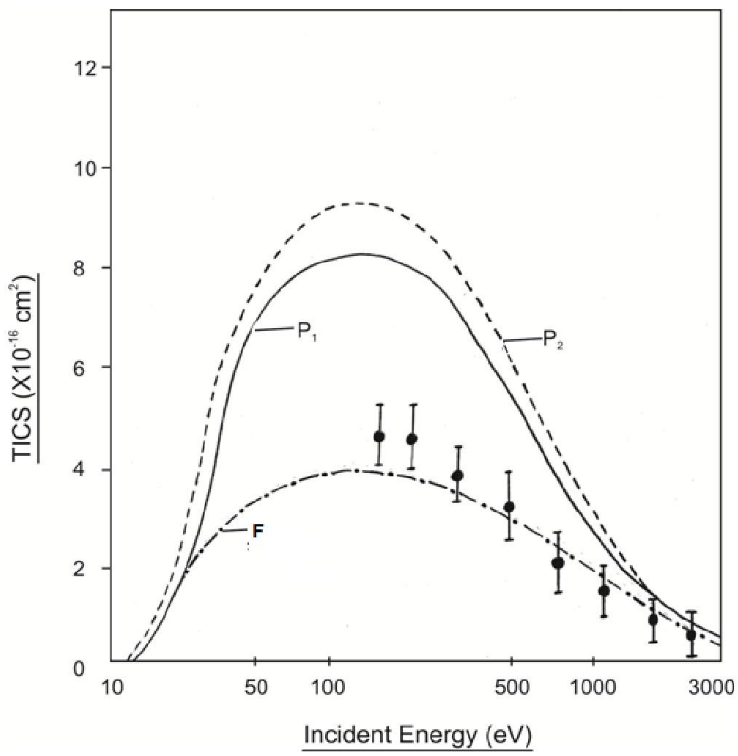

Figure (4)	**:**	**Total Ionization Cross Section for Xenon.**
———————	:	Present results (P_1) for electron
— — — — — — — —	:	Present results (P_2) for positron
—— • —— • ——	:	(F) Freund *et al* [18]
(filled circle with error bar)	:	Experimental results of Sorokin *et al* [17]

The Roothaan Hartree-Fock calculations of Clementi and Roetti [12] have been used to approximate the wave functions of occupied orbitals of the target atom. The wave function for a single atomic orbital is presented as a sum of Slater functions.

$$\phi_{nlm}(r, \theta, \phi) = \sum_{\mu} c_{\mu} A_{\mu} r^{n_{\mu}-1} e^{-\lambda_{\mu} r} Y_{lm}(\theta, \phi) \qquad \ldots (5)$$

where $Y_{lm}(\theta, \phi)$ is a spherical harmonic and

$$A_{\mu} = [(2n_{\mu})!]^{-1/2}(2\lambda_{\mu})^{n_{\mu}+1/2} \qquad \ldots (6)$$

The outgoing scattered electron is described by a plane wave and the ejected electron is modeled by the hydrogenic Coulomb wave function, which is given by

$$\psi_K^{(-)} = \frac{1}{(2\pi)^{3/2}} e^{\pi/2K} \Gamma\,(1 + i/K) e^{i\boldsymbol{K}.\boldsymbol{r}} \times F_1(-\,i/K\,, 1, -ikr - iK.r) \quad \dots (7)$$

Here Γ is the gamma function. F_1 is the confluent hyper-geometric function and K is the momentum of the ejected electron.

Results and discussion

We have computed total ionization cross section (TICS) for ionization of noble gases (*i.e*. Neon, Argon, Krypton and Xenon) by impact of electron as well as positron using truncated coupled Born approximation (TCBA) method. These computed results of electron (P_1) and positron (P_2) are compared with other available data.

Using equation (4), we have obtained TICS for electron (positron) impact ionization of noble gas series. Figure (1) represents TICS for Neon with electron (P_1) and positron (P_2) impact. The theoretical results (C) of Chang and Altick [13] are also plotted. The experimental results of Sorokin *et al* [14] are also shown in this figure. As expected the present results P1 are in good agreement with experimental data. The results of Chang and Altick give higher ionization cross section showing again no match with experimental data.

We have plotted TICS for another noble gas Argon by electron and positron impact in figure (2). Here also theoretical results (C) of Chang and Altick [13] and experimental results of McCallion *et al* [15] are also plotted for the comparison purpose. The present results P_1 give higher cross section in comparison to experimental data but with almost same trend. The other theoretical results (C) give higher cross section as compared to present results P_1 and experimental data. The TICS for Argon decreases rapidly after 1000 eV impact energy.

Figure (3) depicts present results P_1 and P_2 for total ionization cross section of Krypton. The theoretical results of Moores [16] and experimental results of Sorokin *et al* [17] are also plotted. The variation of TICS for Krypton is same as that of Argon in a good agreement with experimental data.

Figure (4) represents the variation of TICS for higher noble gas Xenon with incident energy. The experimental results of Sorokin *et al* [17] and Freund *et al* [18] are also plotted. It appears that the present theoretical results P_1 give higher cross section in comparison to experimental data. More theoretical as well as experimental results shall be required to check the accuracy of present results.

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