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POSITRON IMPACT IONIZATION OF INERT GAS ATOM

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We have computed ionization cross section (ICS) of Krypton by impact of positron using close coupling approximation method. High quality Hartree-Fock Slater orbitals are used to model the target wave function. We have already computed the ionization results [1, 2] for inert gas atoms (Ne, Ar, Kr, and Xe) by electron as well as positron impact, but in this paper, we are presenting for Krypton atom only. We have compared our ICS 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.

Keywords : Position, Ionization, Inert gas atom, close coupling.

INTRODUCTION

The birth of collision physics gave the new ideas about internal structure of atoms. Positron impact ionization of inert gases continues to attract a deep interest in collision physics for several reasons. The study of positron impact ionization of Krypton atom is an essential aspect of atomic physics because it provides complete knowledge of atomic structure and scattering process. In fact, the collision processes have the paramount importance for understanding various branches of science and advanced technology. The collision of positron with Krypton plays a dynamic role in many fields, *e.g.* in the initiation of plasma from neutral gas and medical field etc. Due to characteristics properties of Krypton, it is used in lighting, photography and high powered gas lasers. On the practical side, the reliable knowledge of ionization cross sections 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 of positron impact ionization process. The convergent close coupled (CCC) methodology of Bray and Stelbovics [3] has provided the best correlation of scattering theory with experimental results. The close coupling approximation is the successful non-perturbative approach which is also used to computational treatment of ionization process.

Most of the theoretical work on positron impact ionization of atoms is based on the distorted wave formalism. Using this approximation, Moxom *et al* [4] and Kara *et al* [5] have measured the cross sections for Krypton by impact of positron. Marler *et al* [6] have studied about positron impact ionization cross sections for inert gases by using a qualitatively different method. By applying relativistic complex optical-potential method, McEachran and Stauffer [7] have investigated positron impact ionization cross sections. Recently, we [8] have presented our calculated cross section results of ionization of Krypton by impact of positron (electron).

THEORY

We consider positron scattering by an inert gas containing *N* electron and with nuclear charge Z (=*N*). Denoting the position vector of the positron (i^{th} electron) relative to the atomic nucleus by $r_p(r_i)$ the Hamiltonian *H*, for this system may be written as

$$H = -\frac{1}{4}\nabla_R^2 + H_{P_s}(t) + H_A(r_1, \ldots\ldots\ldots, r_N) + V(r_p, r_0, r_1, \ldots\ldots\ldots\ldots, r_N) \qquad \text{---- (1)}$$

where $t = r_p - r_1$, $i = 0, 1, 2, \ldots\ldots., N$

H_{P_s} is the electron Hamiltonian,

$$H_{P_s}(t) = -\nabla_t^2 - \frac{1}{t}$$

H_A is the atomic Hamiltonian

$$H_A(r_1, \ldots\ldots\ldots, r_N) = \sum\nolimits_{t=1}^{N} \left(-\frac{1}{2}\nabla_i^2 - \frac{z}{r_1} + \sum\nolimits_{j<i}^{N} \frac{1}{|r_i - r_j|} \right) \qquad \text{---- (2)}$$

And *V* is the interaction between the electron and the atom,

$$V(r_p, r_0, r_1, \ldots\ldots., r_N) = \left(\frac{Z}{r_p} - \sum_{t=1}^{N} \frac{1}{|r_p - r_i|} \right) - \left(\frac{Z}{r_p} - \sum_{t=1}^{N} \frac{1}{|r_0 - r_i|} \right)$$

In writing equation (1), we adopted a partition in which the zeroth electron (r_0) is combined with the positron to form electron and the remaining electrons are left with the atoms.

In the frozen target approximation, we expand the collisional wave function for the system ψ, as

$$\psi = A \sum\nolimits_a G_a(R_0) \phi_a(t_0)\, \chi(S_0)\, \psi_0\, (x_1 \ldots\ldots\ldots\ldots, x_N) \qquad \ldots (3)$$

Here *A* is the electron antisymmetrization operator, the sum is over electron states ϕ_a, ψ_0 is the (normalized) ground state of the frozen atomic target and $\chi(S_i)$ is the spin function for the i^{th} electron ($= \alpha$ or β in the usual notation). The function G_α specifies the motion of the electron centre of mass when it is in the state ϕ_α. Under the Hamiltonian (1) the total electronic spin and the positron spin are separately conserved, for this reason the positron spin need not be explicitly mentioned.

For the atomic ground state, we use the Hartree-Fock wave functions of Clementi and Roetti [9]. The antisymmetrization implied in (3) is easily carried out explicitly,

$$\psi = \sum_{\alpha'} G_{\alpha'}(R_0)\, \phi_{\alpha'}(t_0)\, \chi(S_0)\, \psi_0(x_1, \ldots\ldots\ldots\ldots, x_N)$$

$$-\sum_{i=1}^{N} G_{\alpha'}(R_i)\,\phi_{a'}\,(t_i)\,\chi\,(S_i)\,\psi_0\,(x_1, ..., x_i - 1, x_0, x_i + 1, ..., x_N) \quad ....(4)$$

To obtain coupled equations for the G_a, we substitute (4) into the Schrodinger equation and project with $\phi_\alpha\,(t_0)\,\chi\,(S_0)\,\psi_0\,(x_1, ..., x_N)$, this gives

$$\Sigma_{\alpha'}\,[\phi_\alpha(t_0)\,\chi\,(S_0)\,\psi_0\,(x_1, ..., x_N)\,|\,H - E\,|\,G_{a'}(R_0)\phi_{a'}(t_0)\chi(S_0)\psi_0(x_1, ..., x_N)]$$

$$-N[\phi_0(t_0)\chi(S_0)\psi_0(x_1, ..., x_N)\,|\,H - E\,|\,G_{a'}(R_1)\phi_{a'}(t_0)\chi(S_0)\psi_0(x_1, ..., x_N)] \quad ---- (5)$$

where, we have used the fact that $\psi_0(H)$ is antisymmetric (symmetric) under interchange of the x_1. In (5), E is the total energy. Assuming that the electron is incident with momentum P_0 in the state ϕ_0.

$$E = \frac{P_0^{\,2}}{4} + E_0 + \varepsilon_0$$

We take ε_0 to be the average (Hartree-Fock) energy of the state ψ_0,

i.e. $\varepsilon_0 = (\psi_0\,|\,H\,|\,\psi_0)$. Using (1) and the value of ψ_0, (5) becomes

$$(V_{R_0}^2 + P_a^2)\,G_a(R_0) = 4\sum_{a'} U_{aa'}\,(R_0)\,G_{a'}\,(R_0) - 4\sum_{a} \int L_{aa'}(R_0, R_1)\,G_{a'}\,(R_1)\,dR_1 \quad ...\ (6)$$

where $\quad P_a^2 = P_0^2 + 4(E_0 - E_a)$.

Solving the coupled equation (6) subjected to the boundary condition

$$G_a(R_0) \xrightarrow{R_0 \to \infty} e^{i\vec{P_0}.\vec{R_0}} S_{a0} + g(R_0)\frac{e^{(i\vec{P_0}.\vec{R_0})}}{R_0}$$

yields the scattering amplitude *g*, the ionization cross section (ICS) of an inert atom is obtained as follows

$$\sigma = \int \frac{P_a}{P_0}\,|\,g\,|^2\,d\Omega \quad ---- (7)$$

RESULTS AND DISCUSSION

Figure [1] shows ionization cross section for Krypton by positron impact at mid energy using close coupling approximation. In this figure, we have also shown two theoretical results *C* & *M* of Chang and Altick [10] and Moores [11] based upon distorted wave calculations respectively. The only experimental data available by Sorokin *et al* [12] has also been plotted. We have observed that our results (*P*) show a good agreement with experimental results. However, the other theoretical results provide higher cross section and did not produce experimental results. Also the trend of all results after 200 eV impact energy is similar. Below this energy more experimental data is required.

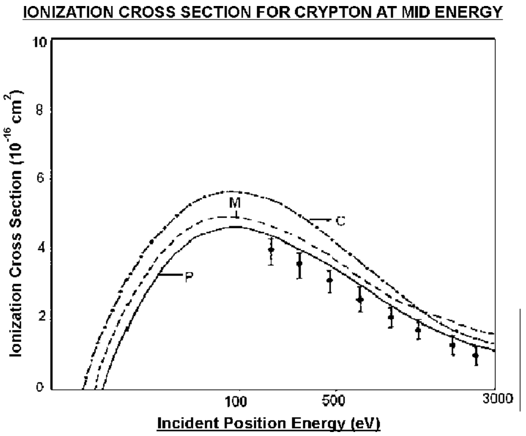

FIGURE [1] : **FIGURE CAPTIONS**

———————— : Present results (P)

— ● — ● — : Theoretical results (C) of Chang and Altick [10]

— — — — — — — : Theoretical results (M) of Moores [11]

Ɨ : Experimental results of Sorokin *et al* [12]

Figure [2] depicts the ionization cross section at higher energies. At high energies, the present calculations are in excellent agreement with experimental data. Above 1000 eV all other results show similar behaviour. Though there is still significant disagreement with experimental results, our calculations appear to be significantly better than previous quantum mechanical calculation.

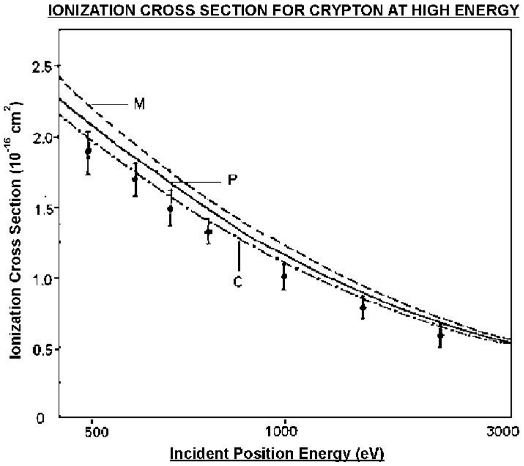

FIGURE – [2] : **FIGURE CAPTIONS**

———————— : Present results (P)

— ● — ● — : Theoretical results (C) of Chang and Altick [10]

— — — — — — — : Theoretical results (M) of Moores [11]

Ɨ : Experimental results of Sorokin *et al* [12]

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REFERENCES

1. Kumar, K. and S. Saxena, *Acta Ciencia Indica, Int. J. Phys. Sc.,* Vol. **XXXVI P**, No. **4**, 437 (2010).
2. Sharma, Kamlesh, K. and S. Saxena, Proceeding of 3rd International Conference on *Current Developments in Atomic, Molecular, Optical and Nano Physics* (**CDAMOP-2011**) held at Delhi University, Delhi, **156** (2011).
3. Bray, I. and A.T. Stelbovics, *Adv. At. Mol. Opt. Phys.,* **35,** 209 (1995).
4. Moxom, J., Ashley, P. and G. Laricchia, *Can. J. Phys.,* **74**, 367 (1996).
5. Kara, V., Paludan, K., Moxon, J., Ashley, P. and G. Laricchia, *J. Phys.* B, **30**, 3933 (1997).
6. Marler, J.P., Sullivan, J.P. and C.M. Sukro, *Phys. Rev.* A, **71**, 022701 (2005).
7. McEachran, R.P. and A.D. Stauffer, *J. Phys.* B, **43**, 215209 (2010).
8. Sharma, Kamlesh, K. and S. Saxena, Proceeding of 3rd DAE-BRNS Symposium on *Atomic, Molecular and Optical Physics*-2012 held at IISER Kolkata, **184** (2012).
9. Clementi, E. and C. Roetti, *At. Data Nucl. Data Tables,* **14,** 177 (1974).
10. Chang, D.W. and P.L. Altick, *J. Phys.* B, **29**, 2325 (1996).
11. Moores, D.L., *Nucl. Instrum. Methods, Phys. Res.* B, **179**, 316 (2001).
12. Sorokin, A.A., Shmaenok, L.A., Bobashev, S.V., Mobns, B., Richter, M. and G. Ulm, *Phys. Rev.* A, **61**, 022723 (2000).

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