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Elastic scattering of positron by gold atom

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Abstract. We present relativistic calculations of the differential, integrated elastic, momentum transfer total cross sections and spin polarization parameters for positrons scattered from Gold atom using a simple optical model potential to represent interaction between positron and target atoms in the energy range 2.0 – 500 eV. In the present calculation we employ a parameter-free model potential for the correlation polarization and absorption potential as devised for positron-atom scattering. The theoretical results are obtained from relativistic approach based on solving the Dirac equation using Hartree-Fock and Dirac-Fock wave functions.

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Key words: relativistic calculation, positron scattering

1 Introduction

In recent years positron-atom scattering has become a very interesting topic in both experimental and theoretical atomic collision studies [1–6]. As an alternative to electron-atom scattering, both the similarities and the differences between electrons and positrons mean that positron scattering provides a useful, and sometimes more sensitive, test of the techniques used to study the electron-scattering processes. This fact is particularly true from the standpoint of developing model interaction potentials for projectile-atom scattering. The similarities between electrons and positrons mass, magnitude of charge, and spin! Suggest that a consistent approach to devising model potentials should incorporate these quantities using similar logic for both projectiles. The differences between electrons and positrons, the sign of the charge, the possibility of positronium formation, and the fact that positron projectiles are distinguishable from the electrons of the target atom while electron projectiles are not offer important tests of how a model potential scheme handles issues such as projectile charge,

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inelastic thresholds, and correlations among projectile and target electrons. Therefore, model potentials that can reliably produce accurate scattering data for both electron- and positron-atom scattering signify an important step in our ability to perform these calculations quickly. These complications were so severe that it is only in last few years a few close-coupling types and many body calculations on lighter atoms like hydrogen, alkali and noble gas atoms have been attempted. The situation with respect to more complicated targets is less satisfactory. Besides the intrinsic importance of these methods, model potential approach and its variant also offer good opportunity to gain insight on the collision dynamics of the positron-atom scattering.

In the present paper, we use a parameter-free model optical potential to calculate the differential scattering cross section (DCS), spin polarization parameters, momentum and total cross sections. As a test case, we are presenting few results for e^+_ Au scattering. The present theory does not include the effect of Ps-formation. The relativistic Dirac equation is solved for both the elastic and total scattering of positrons from these atoms in the impact energy of 2.0 – 500.0 eV. The details can be found in our earlier paper [7].The optical potential $V(r)$ is represented as

$$V(r) = V_R(r) + iV_A(r), \tag{1}$$

where $V_R(r)$ refers to the real part of the projectile-target interaction. The use of only this part of the interaction yields pure elastic scattering. It consists of two parts: (i) Static potential V_S which is repulsive for the positron scattering and is obtained by averaging over the target wavefunction, (ii) a parameter-free correlation polarization potential (V_P). The inclusion of absorption potential $V_A(r)$ to the $V_R(r)$ in Eq. (1) gives the total scattering that includes both the elastic and inelastic scattering process, causing an absorption in a scattering beam. In most of the optical potential calculations as mentioned above, the correlation polarization potential and the absorption potential as devised for electron impact are often used for the positron case, although there is no justification for doing that. It is only recently a few attempts [3, 8] have been made to use the polarization and absorption of the target atom by positron impact in a more consistent manner. In the present study, we examine the effect of both, a true positron correlation potential (PCP) as given by Jain [9], a positron absorption potential (p Q V_a) as devised by Reid and Wadehra [3] and also by Sun *et al.* [17]. In the present paper to explore and test the further applicability of our optical potential approach we use the same method to study the elastic electron scattering from the ground state of Au atoms. The electronic configurations of their ground state are given in Table 1. In Section 2 we have briefly outlined our calculation while our results and discussions are presented in Section 3.

Table 1: Electronic configuration, term symbols, dipole polarizability, ionization potential (I.P), first excitation threshold E and crossing points (r_c) and for Au atoms.

Z (Atomic No.)	Element	Electronic configuration	Term	Polarizability (a.u)	I.P (eV)	E_{th} (eV)	Crossing point (a.u) (r_c)
79	Au	[Xe] 6s (2) 4f (14) 5d (10) 6s (1)	^{2}S	36.1	9.2255	2.4255	3.921