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Relativistic calculations of positron scattering from xenon (Xe) 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 xenon atom using a simple optical model potential to represent interaction between positron and target atoms. In the calculation, we employ a parameter-free model potential for the correlation polarization and absorption potential as devised for positron-atom scattering. Our calculated differential cross sections compare fairly well with the experimental results

Keywords : Relativistic calculation, positron scattering.

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1. Introduction

In recent years, positron atom scattering has been the focus of extensive study both experimentally and theoretically [1-6]. The study of the positronic system offers more sensitive test to understand atomic interactions than the electron does. In particular, the possibility of a genuine rearrangement process namely positronium formation (PS) is possible. The opening of new channels has no parallel to electron-atom scattering. 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 collisional 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^+-Xe 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 0.6–500 eV. The details can be found in our earlier paper [7].

The optical potential $V(r)$ is represented as

$$V(r) = V_R(r) + i\,V_A(r) \qquad (1)$$

Here $V_R(r)$ 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 (pQV_a) as devised by Reid and Wadehra [3] and also by Sun *et al* [10].

2. Interaction potentials

(A) Positron correlation polarization potential :

The positron correlation polarization (PCP) potential is defined as a functional derivative of the correlation energy with respect to $\rho(r)$ *i.e.*

$$V_{\text{corr}}(r) = \left[1 - \frac{1}{3} r_s \frac{d}{dr_s}\right] \varepsilon_{\text{corr}}(r_s) \tag{2}$$

with r_s as a density parameter satisfying $\frac{4}{3}\pi r_s^3 \rho(r) = 1$, where $\rho(r)$ is the target undistorted electronic density. Finally, an analytic expression is obtained (in atomic units) as :

$$V_{\text{corr}} = \begin{cases} [-1.82/\sqrt{r_s} + (0.051 \ln r_s \\ \quad - 0.115) \ln r_s + 1.167]/2; & r_s < 0.302 \\ (-0.92305 - 0.09098/r_s^2)/2; & 0.302 \le r_s \le 0.56 \\ [-8.7674 r_s (r_s + 2.5)^{-3} + (-13.51 \\ \quad + 0.9552 r_s)(r_s + 2.5)^{-2} + 2.8655 \\ \quad (r_s + 2.5)^{-1} - 0.6298]/2; & 0.56 \le r_s \le 8.0 \end{cases} \tag{3}$$

we further mention that in the limit $r_s \to \infty$ the correlation polarization should approach the correct form of the polarization *i.e.* $V_{\text{LR}} = -\alpha_0/2r^4$. Thus, depending on the location of the projectile from the target, $V_{\text{PCP}}(r)$ for e^+-atom system is taken as

$$V_{\text{PCP}}(r) = \begin{cases} V_{\text{corr}}(r), & r \le r_c \\ V_{\text{LR}}(r), & r \ge r_c \end{cases} \tag{4}$$

Here r_c is the point where the V_{corr} and V_{LR} cross each other for the first time.

(B) Positron absorption potential :

According to the quasi-free scattering approximation, the absorption potential for a projectile with local kinetic energy $E = p^2/2m$ passing through a free electron gas of density $\rho(r)$ is given by

$$V_{\text{abs}}(r, E) = -\frac{1}{2}\rho(r)\bar{\sigma}(k_F, p) v_{\text{loc}} \tag{5}$$

Here, $v_{\text{loc}} = [2(E - V_R(r))/m]^{1/2}$ is the local velocity of the projectile for $(E - V_R) \ge 0$ and $k_F = [3\pi^2\rho(r)]^{1/3}$ is the Fermi momentum. The $\bar{\sigma}(k_F, p)$, the average quasi-free binary collision cross section, is given by

$$\bar{\sigma}_b = \frac{1}{p}\int N(k_F, q) | p - q | dq \times \int \frac{d\sigma_b}{d\Omega}\left(\frac{1}{p_0^2}\delta(p_0 - p_f)\Theta(q', k_F)\right) dg \tag{6}$$

Here, $p(p')$ and $q(q')$ are the laboratory frame momenta of the incident positron and target electron, respectively before and after the collision. The vectors p_0 and p_f are the initial and final momenta of the positron in center-of-mass frame of the binary system. The function $N(k_F, q)$ refers to the target electron momentum distribution. The average binary collision cross section $\bar{\sigma}_b$ can be expressed as (see ref. 13)

$$\bar{\sigma}_b(k_F, p) = \frac{16\pi^2}{p^2} N(k_F) \times \begin{cases} \frac{4}{3}\frac{k_F^3}{\omega} + 4k_F + 2p \ln\left|\frac{p - k_F}{p + k_F}\right|; & p^2 - \omega \ge k_F^2 \\ \frac{4}{3}\frac{(p^2 - \omega)^{3/2}}{\omega} + 4(p^2 - \omega)^{1/2} \\ \quad + 2p \ln\left|\frac{p - \sqrt{p^2 - \omega}}{p + \sqrt{p^2 - \omega}}\right|; & k_F^2 \ge p^2 - \omega \ge 0 \end{cases} \tag{7}$$

3. Results and discussion

We are presenting our results for differential cross section (DCS) and spin-polarization parameter S. Recently Kauppila *et al* [14] have reported their measurements for absolute DCS at few selected energies (E = 5, 10 and 20 eV) in the limited angular region ($\theta \approx 30°$ to 120°). They have obtained this DCS by normalizing their relative 20 eV electron DCS values to the absolute results of Register *et al* [15]. In Figures 1(a)–1(c) we compare the present DCS with the

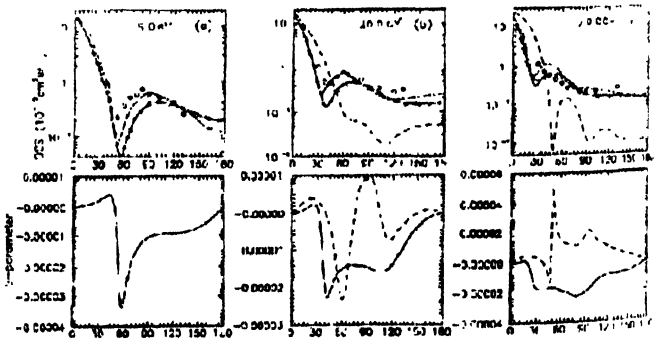

Figure 1. Differential cross section and spin polarization S parameter for e^+-Xe scattering at : (a) 5.0 eV, (b) 10.0 eV, (c) 20.0 eV. Present calculations; ——— with real potential; - - - - - with complex potential, - x - x - x - with electron absorption potential; – • – • – • – theoretical results of McEachran *et al* [16]; O O experimental results of Kauppila *et al* [14].

measured values of Kauppila *et al* [14] along with the most sophisticated calculations of non-relativistic polarized orbitals approximation of McEachran *et al* [16]. It is seen that the present DCS in SP model agree well both in shape and absolute magnitude with experiment in the forward direction at 5.0 eV and 10.0 eV but it lies below the experimental data at larger scattering angles

($\theta \geq 50°$) by a factor of three. It is also noted that the DCS structure present in data at 5.0 eV is washed out at 20.0 eV and the level of agreement between the two *i.e.* measured and calculated cross sections is good. On the other hand, calculations of McEachran *et al* [16] on the whole describe the general feature of the DCS curve better than the present calculations at each value of measured energy. One might assume that the inclusion of the relativistic effects as considered here should improve the agreement, however the present calculation hardly shows any improvement.

Further, in order to illustrate the importance of the role played by the absorption effect, on the DCS, we have also displayed the DCS in our SPa model. Our calculated DCS's with pQV_a absorption charges dramatically for $E > 5.0$ eV. The calculated angular variation exhibits deeper minima, which occur at slightly higher angles compared to the DCS in SP model employing real potentials. Furthermore, we have also computed the DCS for e^+-Xe scattering employing electron quasi-free absorption (eQV_a) with the same static and polarization interaction as used with pQV_a. This would enable us to examine the effect of eQV_a on DCS.

In the same figure we also present spin-polarization parameter (Sherman function) at the same energies. At low energies, the present phenomenological absorption potential appears not to bring any changes in the calculated values, however at higher impact energies, the results are presented in the both models SP and SPa. In all cases, S-parameter exhibits a rapid variation with scattering angles.

4. Conclusion

The scattering of positrons by xenon atom has been investigated relativistically by solving Dirac equation where the positron-target interaction has been represented by a parameter-free model polarization and absorption potential as devised for positron-atom scattering. The feature of the present calculated values of differential cross sections are broadly consistent with the experimental data. The present results also show that the relativistic effects are important with positron-atom scattering but certainly not very pronounced. The spin-polarization of the scattered positrons is hardly influenced by the spin-orbit coupling and is in accord with earlier studies.

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