Elastic scattering of intermediate-energy positrons and electrons by alkali atoms

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In this paper we present the total elastic scattering cross section for collisions of intermediate energy (500–1000 eV) positrons and electrons by alkali atoms (Li, Na, K, Rb). Calculations are done by using the first Born approximation with polarization plus static interaction. The static interaction is obtained by using a Hartree–Fock–Slater type wave function for the target atom and the polarization interaction is modeled by using a pseudopotential.


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1. Introduction

Intermediate energy collisions of positrons and electrons with atoms are of current interest. In particular, measurements of total scattering cross sections for collisions of positrons and electrons with rare gas atoms have been made recently (see, for example, Kauppila et al. (1) and papers cited therein). Estimates of cross sections for elastic collisions of intermediate energy positrons and electrons with alkali atoms, which are reported in the present work, are of special interest because of the similarity between single valence alkali atoms and the hydrogen atom. There are no measurements for positron–alkali atom cross sections in any energy range. However, some theoretical calculations are available for very low energy elastic collisions (2–5) and positronium formation in alkali atoms (6–7).

For alkali atoms, the ionization energy is smaller than 6.8 eV, the binding energy of positronium, and hence positronium can be formed even for zero energy positrons. In case of electron–atom collisions, on the other hand, a possibility of electron exchange exists. In our calculations the Born approximation is used and no account of rearrangement or inelastic processes is taken.

2. Static and polarization potentials

In the collisions of positrons and electrons with atoms two interactions play an important role. At low energies the target atom is distorted by the projectile and the dominant interaction is the polarization interaction. The amount of polarization of the target atom depends on the magnitude of the projectile charge and the polarization interaction is attractive for both the electron and the positron. At high energies, on the other hand, the projectile spends such a little time in the vicinity of the target atom that the target hardly has any opportunity to get distorted and the overall interaction is dominated by the static Coulomb field of the target atom. The static interaction depends on the sign of the projectile charge and it is attractive for electrons and repulsive for positrons.

Consider a neutral target with Z electrons interacting with a projectile of charge e, e is +1 for a positron and −1 for an electron. The positions of the Z bound electrons with respect to the target nucleus are indicated by \( r_1, r_2, \ldots r_Z \) and that of the projectile by \( r_p \). The static potential experienced by the projectile due to the target atom is

\[
V_a(r_p) = \epsilon e^2 \left\langle \Psi \left| \frac{Z}{r_p} \sum_{i=1}^{Z} \frac{1}{|r_i - r_p|} \right| \Psi \right\rangle
\]

where \( \Psi(r_1, r_2, \ldots r_Z) \) is the ground state target wave function. In our calculations, we took this wave function as the Hartree–Fock function in the form of a Slater determinant,

\[
\Psi(r_1, \ldots r_Z) = (Z!)^{-1/2} \phi_1(r_1) \ldots \phi_Z(r_Z)
\]

where \( \phi_i \) are one-electron spin–orbitals. Using the orthogonality of these orbitals, we can write

\[
V_a(r_p) = \frac{Z e^2}{r_p} \sum_{i=1}^{Z} \frac{1}{|r_i - r_p|} \phi_i(r_i)^2 d \mathbf{r}
\]

In general, the amplitude for scattering of a projectile by a potential \( V(r) \) in the Born approximation is given by

\[
f(\hat{k}, \hat{k}_p) = -\frac{m}{2\pi\hbar^2} \int dr \exp\left(ik \cdot r\right) V(r) \times \exp\left(-ik_p \cdot r\right)
\]
where \( k_f \) and \( k_i \) are the initial and the final relative momenta of the projectile. For elastic collisions, \( |k_f| = |k_i| = k \). The potential \( V(r) \) in the above equation is not the exact interaction between the projectile and the target atom. This potential \( V(r) \) is obtained by averaging over the positions of all the target electrons so that in the first Born approximation the scattering of the projectile is from a fixed center of force. Defining the momentum transfer \( q = k_f - k_i \), the scattering amplitude due to the static potential is

\[
\begin{align*}
\left[4a\right] f_d(q) &= -\frac{m}{2\pi\hbar^2} \int dr \, e^{iq \cdot r} V_o(r) \\
&= -\frac{2e}{a_0 q^2} \left[Z - F(q)\right]
\end{align*}
\]

where

\[
\begin{align*}
\left[4b\right] F(q) &= \sum_{j=1}^{Z} \int dr \, e^{iq \cdot r} |\phi_j(r)|^2
\end{align*}
\]
is the form factor of the target atom.

To take into account the effect of the polarization of the target atom, we have to resort to a pseudopotential since the short range behavior of the polarization interaction is not known. As mentioned earlier, in the first Born approximation the projectile is scattered from a fixed scattering center and hence the use of a model polarization potential that has correct limiting behavior at \( r = 0 \) and at \( r \to \infty \) is justified. At long range the polarization potential \( V_{pol} \) should behave as \(-\frac{1}{2} \alpha e^2/r^4 \) where \( \alpha \) is the static dipole polarizability of the target atom and this potential should vanish at \( r = 0 \). This suggests the functional form of the polarization potential to be

\[
\begin{align*}
\left[5\right] V_{pol} &= -\frac{1}{2} \alpha e^2 e^2 r^2/(\sqrt{r^2 + d^2})^3
\end{align*}
\]

where \( d \) is a variable parameter whose exact nature will be discussed later. With this choice of the potential, the polarization component of the scattering amplitude obtained by substituting from \([5]\) into \([3b]\) is

\[
\begin{align*}
\left[6\right] f_{pol}(q) &= \frac{\alpha e^2}{q a_0} \int_0^\infty dr \, \frac{r^3 \sin (qr)}{(r^2 + d^2)^3} \\
&= \frac{\pi}{16} \frac{\alpha e^2}{q a_0} (3 - qd) \exp(-qd)
\end{align*}
\]

Note that for central potentials, the elastic scattering amplitude depends only on the magnitude of the momentum transfer \( q \) which is related to the scattering angle \( \theta \) by \( q^2 = 2k^2 (1 - \cos \theta) \). The total scattering amplitude is simply the sum of the two amplitudes, \( f(q) = f_d(q) + f_{pol}(q) \). The total elastic scattering cross section is given by

\[
\begin{align*}
\sigma_{el}(k) &= 2\pi \int_0^\infty |f(q)|^2 \sin \theta \, dq \\
&= 2(k a_0)^{-2} \int_0^\infty |f(q)|^2 q \, dq (\pi a_0^2)
\end{align*}
\]

3. Results

In the calculation of the elastic scattering amplitude using the static potential, one obtains the form factor of the target atom \([4b]\) as a bonus. Previous studies \([8]\) have shown that the form factor and hence the elastic scattering amplitude are not very sensitive to the effects of electron correlation. This fact was also verified in our preliminary calculations of form factors of the helium atom where it is almost trivial to take electron correlations into account. Accurate form factors for various atoms have been tabulated in standard reference tables \([9]\) and their calculation for alkali atoms provided checks on our present work. The ground state wave functions of various alkali atoms are the Hartree–Fock functions as listed by Clementi and Roetti \([10]\).

For our model polarization potential, two quantities were needed – the polarization \( \alpha \) and the parameter \( d \). The static dipole polarizabilities of Li, Na, K, and Rb, in units of \( a_0 \), are 161,97, 163,32, 278,72, and 294,24, respectively \([11]\). The polarization potential \([5]\) exhibits a minimum at \( r = d/\sqrt{2} \) and is, therefore, most attractive there. The parameter \( d \) is, then, roughly of the order of the size of the atom. In all calculations, \( d \) was taken to be twice the radius of the principal maximum of the charge density of the outermost atomic orbital. For the ground states of all the atoms these radii have been calculated using self-consistent Dirac–Slater wave functions \([12]\). For Li, Na, K, and Rb, therefore, the \( d \) parameters, in units of \( a_0 \), are 5,994, 6,474, 8,172, and 8,644, respectively.

The differential cross section \( |f(q)|^2 \) consists of three terms; a purely polarization term \( |f_{pol}(q)|^2 \), a purely static term \( |f_d(q)|^2 \), and a third term \( 2 \text{Re}(f_{pol} f_d) \) which arises due to the interaction between the polarization and the static potentials. The first two terms are of the same sign for both the positron and the electron while the third term has opposite signs for positron and electron. Consequently, the total elastic cross section obtained from \([7]\) also consists of three parts. In particular, the purely polarization part of the elastic cross section is

\[
\sigma_{el, pol}(k) = \frac{9\pi^2}{128} \frac{\alpha e^2}{a_0^2} g(4kd) \pi a_0^2
\]

where

\[
g(x) = \frac{2}{x^2} \exp\left(-x\right) \left[\frac{5}{9} - 1 + \frac{2}{x} + \frac{1}{x^2}\right]
\]

Analytic expressions can also be written for the purely
TABLE 1. Total elastic cross sections (in units of \( \pi a_0^2 \)) for scattering of intermediate-energy positrons and electrons from various alkali atoms using static interaction only. The notation \( a(b) \) means \( a \times 10^b \)

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>Li</th>
<th>Na</th>
<th>K</th>
<th>Rb</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.18(−1)</td>
<td>2.65(0)</td>
<td>8.69(0)</td>
<td>1.95(+1)</td>
<td></td>
</tr>
<tr>
<td>5.16(−1)</td>
<td>2.22(0)</td>
<td>7.27(0)</td>
<td>1.63(+1)</td>
<td></td>
</tr>
<tr>
<td>4.43(−1)</td>
<td>1.91(0)</td>
<td>6.25(0)</td>
<td>1.41(+1)</td>
<td></td>
</tr>
<tr>
<td>3.88(−1)</td>
<td>1.67(0)</td>
<td>5.48(0)</td>
<td>1.24(+1)</td>
<td></td>
</tr>
<tr>
<td>3.45(−1)</td>
<td>1.49(0)</td>
<td>4.88(0)</td>
<td>1.10(+1)</td>
<td></td>
</tr>
<tr>
<td>3.10(−1)</td>
<td>1.34(0)</td>
<td>4.40(0)</td>
<td>0.94(0)</td>
<td></td>
</tr>
</tbody>
</table>

Fig. 1. Total elastic cross sections for collisions of positrons and electrons with various alkali atoms.

static part and the part of the cross section that arises due to the static polarization interaction. Instead, we present in Table 1 the purely static part of the total elastic scattering cross section for various alkali atoms at different energies. In Fig. 1 we present the total elastic cross section for collisions of positrons and electrons with alkali atoms at intermediate energies.

4. Conclusions

In this paper we have presented the total elastic cross sections for intermediate-energy collisions of positrons and electrons with alkali atoms. As far as we know, no measurements of elastic electron–alkali atom cross sections in the present energy range are available. However, a theoretical first Born calculation (13) of the total elastic cross sections for the scattering of electrons from lithium, sodium, and potassium in the present energy range is available. These total elastic cross sections compare quite well with the present results. In particular, the total cross sections, in units of \( \pi a_0^2 \), for elastic electron–lithium scattering are 0.61 and 0.39 from ref. 13 and 0.618 and 0.388 from present static interaction calculations at 500 and 800 eV, respectively. Similarly, at 500 and 1000 eV, respectively, the total elastic cross sections, in units of \( \pi a_0^2 \), for electron–sodium scattering are 2.60 and 1.33 from ref. 13 and 2.65 and 1.34 from our results, Table 1, and for electron–potassium scattering are 8.35 and 4.50 from ref. 13 our results being 8.69 and 4.40, Table 1. The agreement is quite good because of the insensitivity of the form factor to the choice of the target wave functions in the two calculations.

The cross sections presented in Table 1 are obtained by using static interaction only. The cross sections for electron and positron scattering are discernible only when both the static and the polarization interactions are included simultaneously. At very high energies when the polarization interaction becomes unimportant, the positron and electron cross sections are expected to become equal in magnitude. From Fig. 1, we note that the positron and electron cross sections have merged to within 10% for Na, K, and Rb while the merging for Li is still not very good. The trend towards merging in the energy range 500–1000 eV is so slow that it almost appears as if the ratio of the cross sections is a constant, independent of energy. This slow trend towards merging could be caused either by the large polarizability of the alkali atoms, making the polarization interaction quite significant even at high energies, or simply by the inadequacies of the polarization potential included in the present form. In the absence of any experimental information the present calculation may provide an approximate guide to elastic cross sections for scattering of positrons by alkali atoms. Also there is some evidence (6, 7) that the cross section for positronium formation in alkali atoms decreases by five or six orders of magnitudes as one goes from low-energy positrons to about 500 eV positrons. Thus if inelastic processes become unimportant at intermediate energies, the present calculations may also be used as a rough estimate for total cross sections.

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