Scattering of low-energy electrons and positrons by atomic beryllium: Ramsauer–Townsend effect

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Abstract
Total cross sections for the scattering of low-energy electrons and positrons by atomic beryllium in the energy range below the first inelastic thresholds are calculated. A Ramsauer–Townsend minimum is seen in the electron scattering cross sections, while no such effect is found in the case of positron scattering. A minimum total cross section of 0.016 $a_0^2$ at 0.0029 eV is observed for the electron case. In the limit of zero energy, the cross sections yield a scattering length of $-0.61 a_0$ for electron and $+13.8 a_0$ for positron scattering.

Keywords: electron scattering, beryllium, Ramsauer–Townsend effect, positron scattering

In their pioneering work, Ramsauer and Kollath (1930) and Townsend and Bailey (1922) independently discovered a very pronounced minimum in the cross sections for the scattering of electrons by rare gas atoms. This Ramsauer–Townsend (RT) effect has now been observed in the scattering of both electrons and positrons by various rare gas atoms (Kauppila and Stein 1989), by several hydrocarbon molecules (McCorkle et al 1978) and in atom–atom scattering (Feltgen et al 1973). The RT minimum appears in the cross sections only when long-range polarization of the target (atom or molecule) by the slow incident projectile (electron or positron) is taken into account along with the static interaction representing the unperturbed average static electric field of the target.

In the present work we have calculated total cross sections for the scattering of low-energy electrons and positrons by atomic beryllium. So far, no experimental results on the measurements of cross sections for the scattering of electrons or positrons by beryllium are available. However, a few calculations have been carried out for the scattering of both electrons and positrons by beryllium. For electron-beryllium scattering, Fursa and Bray (1997) calculated the total cross sections from 10 to 1000 eV using the convergent close-coupling method. Using the method of R-matrix with pseudo-states, Bartschat et al (1997) calculated the elastic scattering cross sections for electron impact in the energy range from 2 to 100 eV. For positron scattering, Szmytkowski (1993) calculated the elastic scattering cross sections, using the polarized orbital approximation, for positron energies below 100 eV. Also, for positron impact, Bromley et al (1998) used model potentials to calculate the integrated elastic cross sections for positron energies below 10 eV.

We have obtained, for the first time, an RT minimum in the total cross sections for the scattering of electrons by a light alkaline-earth element, namely, beryllium. On the other hand, scattering of low-energy positrons by beryllium does not exhibit any RT effect.

The interaction potential between the projectile (electron or positron) and beryllium target atom is represented by a real function, free of adjustable parameters, consisting of the sum of the static potential, $V_{st}$, the energy-dependent correlation-polarization potential, $V_{cp}$, and, for the case of electron scattering only, the exchange potential, $V_{ex}$. In what follows, we use atomic units unless stated otherwise. The static potential is determined by the radial part of the electron density of beryllium, $\rho(r)$, and is given by

$$V_{st} = \frac{Ze}{r} - 4\pi\rho \int \frac{\rho(r')}{r_0} r'^2 dr', \quad (1)$$

where $r_0$ is the larger of $r$ and $r'$. The electron density was calculated using the Hartree–Fock wave functions of
Clementi and Roetti (1974). Here $q$ is $-1$ for electron scattering and $+1$ for positron scattering making the static interaction attractive for electrons and repulsive for positrons. The correlation-polarization potential $V_{cp}$ is energy-dependent (Seaton and Steenman-Clark 1977) and attractive for both electron and positron scattering. The form used here is

$$V_{cp}(k, r) = -\frac{\alpha_d r^2 + \alpha_q - k^2/Z}{2(r^2 + d^2)^{3/2}}. \quad (2)$$

where $Z (= 4)$ is the atomic number, and $\alpha_d (= 37.8 \text{ a.u.})$ and $\alpha_q (= 304 \text{ a.u.})$ are the static dipole and quadrupole polarizabilities of the target (McDaniel 1989). In general, for any atom the values of the energy-dependent nonadjustable parameter $d$ are obtained by setting the right-hand side of (2) equal to the correlation energy at a radial distance $r = R_{\text{orb}}$ (1.965 a.u. for beryllium) corresponding to the density peak of the outermost occupied orbital of the target atom. Additional details of the various parts of the interaction potential are discussed in Reid and Wadehra (1994). The correlation energy is taken from the work of Perdew and Zunger (1981) and of Jain (1990) for the cases of electron and positron scattering, respectively. Finally, we used the exchange interaction of Riley and Truhlar (1975) which we have found to be a computationally fast and reliable interaction for calculations of other target atoms including rare gas atoms (Reid and Wadehra 1994).

Using these parts of the projectile-beryllium interaction in the radial Schrödinger equation, we have calculated various phase shifts as a function of projectile energy ($E = \hbar^2 k^2/2m$). We do this numerically using an adaptive step-size Burlisch–Stoer method, based on Press et al. (1996), with an initial step-size on the order of $10^{-10} a_0$. It was necessary to integrate out to a distance equal to at least the deBroglie wavelength of the incident particle to get stable results. The phase shifts, $\delta_\ell(k)$, are used to calculate partial wave cross sections which are added together to obtain the total cross sections, $\sigma(k)$, below the lowest inelastic thresholds. The expansion of the total cross section in terms of partial cross sections is

$$\sigma(k) = 4\pi \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_\ell. \quad (3)$$

For the energy range studied here no more than the first 8 partial waves ($\ell = 0 \ldots 7$) were needed to provide fully converged cross sections.

In the low-energy limit, the various phase shifts are small and decrease rapidly with increasing $\ell$ as $\delta_\ell(k) \sim k^{2\ell+1}$. In particular, for the s-wave ($\ell = 0$), the phase shift in the limit of zero energy behaves as, $\delta_0(k) \sim -\pi k A$, where $A$ is the scattering length. The choice of negative sign here ensures that the scattering length of a hard sphere is exactly equal to the radius of the sphere. Thus, at low energies, the contribution to the total cross section of each successively higher term in the expansion of (3) gets smaller as $\ell$ increases, with the dominant contribution coming from the s-wave. The zero-energy cross section, $\sigma(0)$, is determined completely by the scattering length since, from (3), $\sigma(0) = 4\pi A^2$. The RT minimum appears, at a sufficiently low (nonzero) projectile energy, when the s-wave phase shift passes through zero (or a multiple of $\pi$) while the contributions of higher phase shifts to the total cross section are still quite small.

In figure 1 we show the total cross sections for the scattering of electrons by beryllium as a function of incident electron energy from almost zero to the first inelastic threshold at 2.7 eV. The cross section shows clearly a minimum value of 0.016 a.u. at an incident electron energy of 0.0029 eV. In general, the contribution of the s-wave to the total cross section is expected to dominate over the contributions of higher partial waves at very low energies. However, for electron-Be scattering near the minimum the s-wave phase shift indeed becomes zero at 0.0029 eV, leading to the designation of this cross section minimum to be the RT minimum. There are limited published results for electron-beryllium cross sections in this low energy range. As a point of comparison, at an incident energy of 2 eV, our result of 270 a.u. compares favorably to the R-matrix result of Bart- schat et al. (1997) which we estimate from their figure to be in the range 250–275 a.u.

Figure 2 shows the total cross sections for the scattering of positrons by beryllium for the positron energy range below 2.5 eV, corresponding to the positronium formation threshold. However, in this case the s-wave phase shift does not pass through zero for any value of positron energy in the elastic scattering range. Absence of the RT minimum for the positron case is related to the sign of the scattering length. The lack of an RT minimum in positron-beryllium scattering has also been noted in other previous calculations (Szymkowsi 1993). Note that at very low incident energies the cross sections in both figures 1 and 2 converge to constant values. These constants give the zero energy cross sections for electron scattering ($\sigma(0)_{-e} = 4.7 \text{ a.u.}$) and for positron scattering ($\sigma(0)_{+e} = 2.39 \times 10^3 \text{ a.u.}$).

For an interaction potential that behaves asymptotically as an attractive polarization potential of the form $-\alpha_d e^2/2r^4$,
it was shown (O’Malley et al 1961, O’Malley 1963) that the energy (or \( k \))-dependence of the s-wave phase shift can be written as,

\[
\delta \pi \alpha = -A_k a k \tan(3k) \quad (4)
\]

A rearrangement of this equation leads to

\[
k \cot(\delta_0) = -\frac{1}{A} + \frac{\pi a_0}{3A^2 \alpha} k + O(k^2) \quad (5)
\]

which differs from Bethe’s effective range formula in nucleon–nucleon scattering (Joachain 1983) by having a term linear in \( k \). This modified effective range formula can be used to extract the scattering length, with correct sign and value, for both electrons and positrons scattered from Be. Figures 3 and 4 show the plots of \( k \cot(\delta_0) \) as a function of \( k \) for electrons and positrons, respectively. Extrapolation of the curves to zero energy (\( k \to 0 \)) provides the scattering length to be \(-0.61 \) a.u. for the electron-beryllium system and \(+13.8 \) a.u. for the positron-beryllium system. These scattering lengths are consistent with the zero-energy cross sections obtained above for both electron and positron scattering. For positron scattering, our value of scattering length is consistent with the value (+16 \( a_0 \)) reported by Bromley et al (1998).

Finally, we note from (4) that at sufficiently low energies the s-wave phase shift (mod \( \pi \)) can be expressed as

\[
\delta_0 \approx -A k - \frac{\pi a_0}{3a_0} \alpha \kappa^2. \quad (6)
\]

If the scattering length \( A \) is a positive number, as it is for positron-beryllium scattering, then \( \delta_0 \) will monotonically decrease and will not pass through zero. On the other hand, if \( A \) is negative, as in the electron-beryllium case, then \( \delta_0 \) will become zero for \( k \approx 3\alpha |A|/\pi a_0 \). In this case, an RT minimum will appear at projectile energy \( E_{\text{min}} \) given by

\[
E_{\text{min}} = \left( \frac{e^2}{2a_0} \right) \left( \frac{3|A| a_0^2}{\pi \alpha d} \right)^2. \quad (7)
\]

This simple relationship between the scattering length and the energy at which the RT minimum appears can be applied for electron scattering by Be. Using values of |\( A \)| and \( a_0 \) given above, we get \( E_{\text{min}} = 0.0032 \) eV, in close agreement with the location of the RT minimum at 0.0029 eV found in our calculations.

In conclusion, we have confirmed the presence of an RT minimum in the cross sections for the scattering of low-energy electrons by atomic beryllium. This minimum occurs for an incident electron energy of 0.0029 eV at which the s-wave phase shift passes through zero. For the case of low-energy positron scattering by Be, no RT minimum was found.
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