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The effect of virtual positronium formation on positron–atom scattering

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Abstract. A new method is proposed to calculate the contribution of virtual Ps-formation to elastic positron–atom scattering. The calculations were performed using the many-body perturbation theory approach. It is shown that for the scattering of positrons by hydrogen and helium atoms, the virtual Ps-formation contribution is about 30% and 20% of the total correlation potential, respectively. Good agreement was obtained with the results of precise variational calculations and with experimental data.

In this paper a new method is proposed to calculate the contribution of virtual positronium (Ps) formation to elastic positron–atom scattering, within the many-body perturbation theory approach. The interaction of the projectile with the target is described by the non-local energy-dependent correlation potential. It is shown that for the scattering of positrons by hydrogen and helium atoms, the virtual Ps-formation contribution is about 30% and 20% of the total correlation potential, respectively. There is good agreement with the results of precise variational calculations and experimental data. The application of the method to positron scattering from many-electron atoms is straightforward.

The interaction of low-energy positrons with atoms is characterized by large correlation effects. These correlations were successfully treated in variational calculations for hydrogen (Schwartz 1961, Bhatia *et al* 1971, 1974, Register and Poe 1975) producing nearly exact results for the s-, p- and d-wave phaseshifts. For heavier atoms a number of different methods have been used. Among these are, the polarized-orbital approximation (McEachran *et al* 1977), the close-coupling approximation (Basu *et al* 1990) and the many-body theory (Amusia *et al* 1982, Dzuba *et al* 1993). Though in some cases a good agreement with experimental data has been achieved, a general question as to the effect of Ps-formation on positron–atom scattering below the Ps-formation threshold remains. The many-body approach is an excellent tool for studying the contribution of the various physical mechanisms in positron–atom scattering and for investigating the difference between positron–atom and electron–atom scattering.

The scattering problem is effectively reduced, by the many-body approach, to a single-particle equation with a non-local energy-dependent correlation potential $\Sigma_E(\boldsymbol{r}, \boldsymbol{r}')$, that describes the interaction of the projectile with the many-electron target. If the Hartree–Fock approximation is used as the zero-order approximation, the matrix elements of the correlation potential, $\langle f|\Sigma_E|i\rangle$, may be represented by the diagrammatic expansion in figure 1.

As is well known, the most important diagrams in electron–atom scattering are the second-order diagrams (figures 1(a) and 1(f)) and the higher-order corrections which

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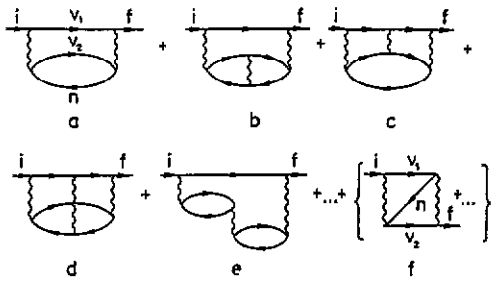

Figure 1. Diagrammatic expansion for the matrix element of the correlation potential $\langle f|\Sigma_E|i\rangle$. The upper line in parts (a)–(e) corresponds to the projectile (electron or positron). The exchange diagrams in brackets are present only for electron–atom scattering.

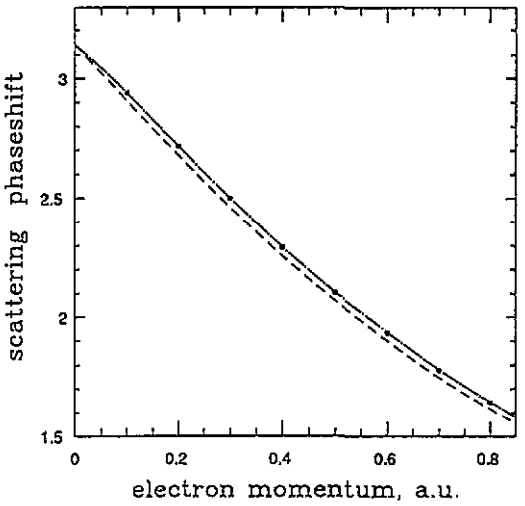

Figure 2. Phase shifts for electron–hydrogen s-wave triplet scattering. (- - - -), Hartree–Fock approximation; (— · —), with the polarization potential taken into account; (•), variational calculations of Schwartz (1961).

represent the correlations within the excited atom (figures 1(b) and 1(e)), (see e.g. Kelly 1968, Amusia and Cherepkov 1975, Chernysheva *et al* 1988). It has been shown that these higher-order corrections can essentially be taken into account within the second-order diagrams (figures 1 (a) and 1(f)) by calculating the wavefunction of the excited electron (ν_2) in the field of a hole (n) (Amusia and Cherepkov 1975). Physically these second-order and higher-order correction diagrams describe the polarization of the target atom by the projectile. Accordingly, the correlation potential resulting from these diagrams (figure 1(a), (e), (b), etc, i.e. diagrams containing only two interactions of the projectile with the target, and exchange terms), $\Sigma_E^{\rm pol}$, will be referred to hereafter as the polarization potential. At large distances it has the well known asymptotic behaviour, $\Sigma_E^{\rm pol}(r, r') \simeq -(\alpha/2r^4)\delta(r - r')$, where α is the dipole polarizability. The high accuracy of this approximation for the electron–atom scattering is illustrated in figure 2 where we present the s-wave phaseshifts for electron–hydrogen triplet scattering. The calculated phaseshifts (δ) were obtained using the technique of Amusia and Cherepkov (1975) and Amusia *et al* (1982) as $\delta = \delta^{\rm HF} + \Delta\delta$, where $\delta^{\rm HF}$ is the phaseshift due to the static Hartree–Fock potential of the target, and $\Delta\delta$

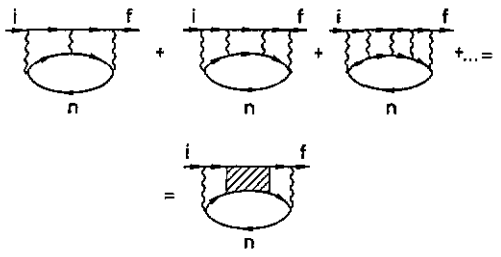

Figure 3. Correlation potantial diagrams corresponding to Ps-formation. The upper line describes the positron. The rectangle on the right-hand side represents the propagation of the electron–positron pair.

is the additional phaseshift due to the polarization potential. A comparison with the results of the variational calculations by Schwartz (1961), shows that $\Delta\delta$ agrees with $\delta^{\mathrm{var}} - \delta^{\mathrm{HF}}$ to an overall accuracy of about 3%.

When the same approximation for Σ (without the exchange diagrams) is used to calculate the positron–hydrogen s-wave phaseshifts, there is a large discrepancy between the polarization-potential results and variational calculations (see figure 4). This suggests that there is a physical process other than polarization that is important in the interaction of a slow positron with an atom. We believe that the physical process that is occurring is virtual Ps-formation, the importance of which has been demonstrated in, e.g., Amusia *et al* (1976), Basu *et al* (1989) and Dzuba *et al* (1993). Indeed, during the scattering process the positron may virtually form a Ps atom with an atomic electron. This process is represented diagrammatically by the series in figure 3. The correlation potential that results from the sum of this series (Σ_E^{Ps}) will be referred to as the Ps-formation potential.

In the case of electron–atom scattering the series in figure 3 is sign-alternating and hence each successive term partially cancels the previous term, giving a small total. In the case of positron–atom scattering all the terms in the series are negative and the whole ladder series representing the Ps-formation potential plays an important part in the scattering process.

Since a Ps bound state exists in an electron–positron system, the system is non-perturbative and therefore it is not possible to directly sum the series. In order to avoid this problem we have represented the entire series by the diagram shown in figure 3, where the shaded rectangle describes the propagation of the electron–positron pair. In the present paper we adopt the following approximation to calculate the Ps-formation potential:

$$\langle f|\Sigma_E^{\mathrm{Ps}}|i\rangle = \sum_n \int \frac{\langle fn|V|\tilde{\Psi}_{1s,K}\rangle\langle\tilde{\Psi}_{1s,K}|V|ni\rangle}{E+\varepsilon_n-(E_{1s}+K^2/2M)+\mathrm{i}\delta}\,\frac{\mathrm{d}^3K}{(2\pi)^3} \qquad (1)$$

where $V = -1/|r-r_1|$ is the electron–positron Coulomb interaction, $\Psi_{1s,K}$ is the wavefunction of the Ps atom in the ground state, moving with momentum K, $E_{1s}+K^2/2M$ is the energy of this state, M is the mass of the Ps atom, n is the hole state and ε_n is its energy. The tilde above $\Psi_{1s,K}$ indicates that this wavefunction is orthogonal to the single electron states of the atomic ground state. This is necessary since the shaded block in the RHS of the diagramatic equation in figure 3 is constructed from the excited electron states. When the energy of the projectile increases beyond the Ps-formation threshold, (1) acquires an imaginary part which for $f = i$ is proportional to the square of the Ps-formation amplitude $\langle\tilde{\Psi}_{1s,K}|V|ni\rangle$.

There are two reasons for neglecting the internal excitations of the Ps atom in (1). Firstly, the 1s state provides the smallest energy denominator. Secondly, the amplitude

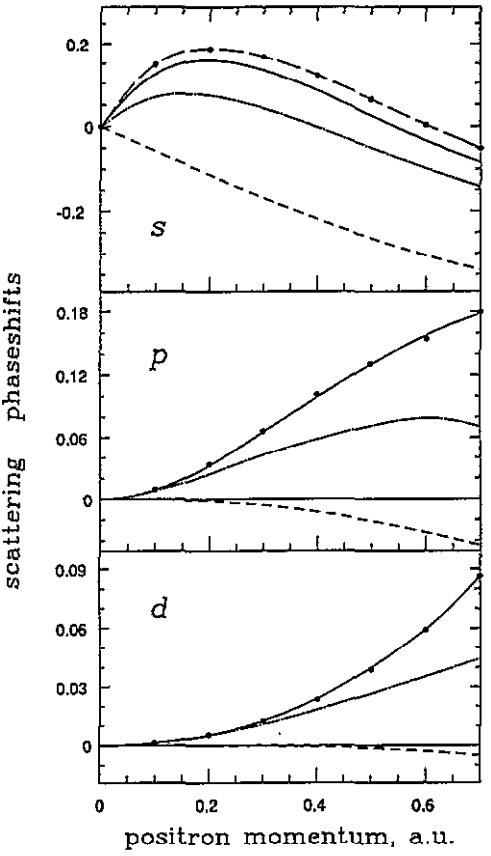

Figure 4. Phase shifts for positron–hydrogen scattering in s-, p- and d-waves. (- - - -), static (Hartree) approximation; (— · —), with the polarization potential taken into account; (——), same as the preceding line with the Ps-formation contribution added; (•), variational calculations by Bhatia *et al* (1971) (s-wave), (1974) (p-wave), Register and Poe (1975) (d-wave). For the sake of clarity the variational results for the s-wave are connected by the broken curve.

of Ps-formation in the 1s state is considerably larger than that for Ps-formation in an excited state. The reason for this is that the probability of the re-arrangement process (Ps-formation) decreases exponentially with increasing positron–atom distance. Therefore one may conjecture that the Ps-formation amplitude is proportional to the wavefunction of the Ps atom at small distances. If this is true then the amplitude of Ps-formation in excited states is suppressed, e.g. for the 2s state, by a factor of $1/2\sqrt{2}$ (or $\frac{1}{8}$, if we consider the amplitude squared as in (1)).

Since the electron–positron pair in the intermediate state in the RHS of figure 3 does not interact with the atom, we may represent its wavefunction in the following way:

$$\Psi_{1s,K}(r, r_1) = \varphi_{1s}(r - r_1)\, e^{iK\cdot R} \tag{2}$$

where $\varphi_{1s}(r - r_1) = 1/\sqrt{8\pi}\, e^{-|r-r_1|/2}$ is the hydrogen-like wavefunction of a Ps atom in the ground state, and $R = \frac{1}{2}(r + r_1)$ gives the position of the centre of mass of the Ps atom. The orthogonalization of $\Psi_{1s,K}$ to the electron states, n, occupied in the ground state

of the atom is achieved as follows:

$$|\tilde{\Psi}_{1s,K}\rangle = \left(1 - \sum_n |n\rangle\langle n|\right)|\Psi_{1s,K}\rangle\,. \tag{3}$$

As is known the Ps atom has zero charge density and therefore there is no static interaction between the ground-state Ps atom and the ionic residue. Therefore, the use of the plane wave to approximate the centre of mass motion of the Ps atom is consistent with the neglect of the excited states of the Ps atom.

In the case of hydrogen the matrix element $\langle\tilde{\Psi}_{1s,K}|V|ni\rangle$ (n is the hydrogen 1s state, $\psi_{1s}(r_1)$) is given by

$$\langle\tilde{\Psi}_{1s,K}|V|ni\rangle = \int\int \varphi_{1s}(r - r_1)\,e^{iK\cdot R}\left[-\frac{1}{|r - r_1|} - V_{1s}(r)\right]\psi_{1s}(r_1)\varphi_i(r)\,dr\,dr_1 \tag{4}$$

where $V_{1s}(r) = -\int |\psi_{1s}(r_1)|^2/|r - r_1|\,dr_1$ is the electrostatic potential of the 1s electron in the hydrogen atom. Equation (4) coincides with the one obtained using re-arrangement collision theory for the Ps(1s)-formation in positron–hydrogen collisions (Massey and Mohr 1954), if one uses the prior form of the interaction, and given the initial positron state, $\varphi_i(r)$ is calculated in the static field of the hydrogen atom.

The identity of $\langle\tilde{\Psi}_{1s,K}|V|ni\rangle$ with the the expression for the Ps-formation amplitude obtained from the theory of rearrangement collisions, holds for many-electron atoms as well, though the matrix elements have a more complicated form.

In order to calculate the Ps-formation potential Σ_E^{Ps} (equation (1)), the φ_{1s} and the plane wave (centre-of-mass) wavefunctions of the Ps atom, and the Coulomb interaction were expanded in terms of spherical harmonics with respect to the origin ($r = 0$ and $r_1 = 0$). After the integration over the angular variables Σ_E^{Ps} is reduced to a seven-fold sum over the angular momenta involving the radial integrals times the products of $3j$-symbols. The radial integration and the integration over the absolute values of K were performed numerically.

The total correlation potential is then found by adding the Ps-formation potential to the polarization potential. For hydrogen the latter was obtained by direct summation over the intermediate states of figure 1(a), with the electron wavefunctions ν_2 calculated in the field of the nucleus and including both discrete and continuous s, p and d excitations (the exact polarizability of hydrogen $\alpha = 4.5$ was reproduced within an accuracy of a few per cent). The phaseshifts for hydrogen were calculated using the FORTRAN version (Gul'tsev and Gribakin 1991) of the codes described in Amusia and Chernysheva (1983). For helium the polarization potential $\Sigma_E^{pol}(r, r')$ including both the electron–hole interactions and screening within the atom, was calculated using the Feynman technique as per Dzuba *et al* (1989, 1991) (its long-range behaviour corresponded to $\alpha = 1.26$ which is 91% of the actual polarizability of helium (Weast 1988)). The phaseshifts were obtained from the asymptotic behaviour of the radial wavefunction.

The s-, p- and d-wave phaseshifts for positron–hydrogen scattering are shown in figure 4. The contribution from the Ps-formation potential is large for all partial waves. The agreement with the variational calculations for the p and d-wave phaseshifts is very good, whereas the s-wave phaseshifts are slightly underestimated.

The neglect of the Ps atom excitations means that both the virtual formation of the Ps atom in an excited state and the polarization of the Ps atom by the ionic field are ignored in our calculation. As there is actually an attractive potential due to the polarization of the Ps atom by the ionic residue, the plane-wave approximation underestimates the Ps centre-of-mass wavefunction at small distances. This causes the underestimate in Σ_E^{Ps} and hence in the phaseshifts. This effect is noticeable in the s-wave scattering but is much smaller in

higher partial waves. The plane-wave approximation is much more accurate for the latter due to the presence of the repulsive centrifugal potential for the Ps centre-of-mass motion.

On the other hand the role of Ps excitations can be checked by the results of the close-coupling approximation calculations of Mitroy (1993) and Sarkar *et al* (1993). They found that when the $n = 2$ excited states of the Ps atom were included the s-wave, phaseshifts increased by about 0.02 in the range $k = 0.1 - 0.7$. Note that this value is roughly equal to the difference between the variational phaseshifts and that of our calculation (see figure 4). The close-coupling calculations also show that the role of the Ps excitations is much smaller in the p-wave phaseshifts.

The positron–helium total cross sections are shown in figure 5. Here also there is a large contribution from the Ps-formation potential which produces good agreement with experimental results, as well as with the variational calculations presented in Humberston (1978). The slight deviations observed may be attributed to the use of the plane-wave approximation of the centre-of-mass motion of the Ps atom.

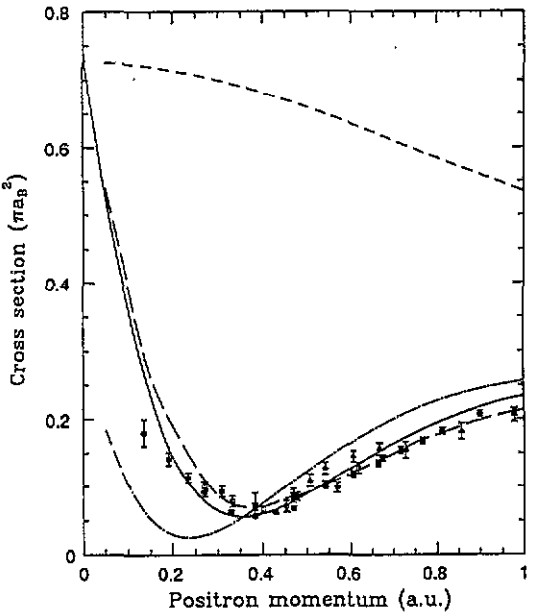

Figure 5. Scattering cross sections for positron–helium scattering. Calculation: (- - - -), static (Hartree) approximation; (— · —), with the polarization potential taken into account; (——), same as the preceding line with the Ps-formation contribution added; (– – –), variational calculations presented in Humberston (1978). Experiments: (•), Stein *et al* (1978); (△), Canter *et al* (1972); (□), Sinapius *et al* (1980).

It has been shown (Dzuba *et al* 1993) that the positron–atom annihilation rates are highly sensitive to the magnitude of the correlation potential. We believe that the approximation proposed in this paper enables one to accurately calculate the Ps-formation contribution to positron scattering by many-electron atoms, as well as to the corresponding annihilation rates.

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