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Low-energy positronium scattering from noble-gas atoms

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Synopsis van der Waals C_6 coefficients are calculated *ab initio* for positronium interactions with noble-gas atoms using the random-phase approximation with exchange (RPAE). These are scaled slightly to create our best predictions. Comparisons are made with existing configuration interaction and semi-empirical data.

Compared with electron-atom and positron-atom scattering, positronium (Ps)-atom scattering is difficult to treat theoretically, chiefly because both scattering objects have an internal structure [1].

Here we are concerned with low-energy Ps scattering from noble-gas atoms. We plan to study this problem by confining the electron-positron pair in a spherical cavity with a noble-gas atom at the centre. Finding the energy eigenvalues will enable the phase shifts (and hence all information about the scattering process) to be determined.

At low energies, the long-range interaction between the Ps atom and the noble-gas atom plays an important role in the scattering [2]. It is attractive and behaves asymptotically as

$$U(R) \simeq \frac{C_6}{R^6}, \qquad (1)$$

where R is the distance between the two centres of mass and C_6 is the van der Waals coefficient for the pair of atoms. It is important to have accurate values of these C_6 coefficients because, e.g., they appear in the effective range expansion for the $l \geq 2$ phase shifts [3], and hence play a vital role in scattering cross sections.

As the first step toward including the long-range van der Waals interaction between the noble-gas and Ps atoms, we have performed *ab initio* calculations of the Ps–noble-gas C_6 coefficients in the random-phase approximation with exchange (RPAE) [4]. Mitroy and Bromley have previously calculated the C_6 coefficients for Ps–noble-gas interactions using the configuration interaction method for Ps-He and a semi-empirical method for the other pairs [5].

We began by calculating dynamic dipole polarizabilities α for both atoms over a range of imaginary frequencies. Then the C_6 coefficients were calculated by evaluating the integral

$$C_6 = \frac{3}{\pi}\int_0^\infty \alpha_{\rm Ps}(\mathrm{i}\omega)\alpha_X(\mathrm{i}\omega)\,\mathrm{d}\omega \qquad (2)$$

numerically, where X represents the noble-gas atom.

Table 1 shows our best predictions of C_6 for the Ps–noble-gas pairs alongside the previous calculations by Mitroy and Bromley. Our best predictions were obtained by multiplying each *ab initio* value of C_6 by the ratio between the experimental and RPAE values of the static polarizability of the noble-gas atom. The maximum deviation from Mitroy and Bromley's values is 3%. We expect our values to be the most accurate data available for the C_6 coefficients for Ps–noble-gas scattering.

Table 1. C_6 values for Ps–noble gas pairs (in a.u.).

Pair	Present	Ref. [5]
Ps-He	13.45	13.37
Ps-Ne	26.69	26.74
Ps-Ar	99.00	98.50
Ps-Kr	147.4	144.1
Ps-Xe	228.2	221.6

We intend to use these data to develop an accurate theoretical description of low-energy Ps–noble-gas-atom collision processes.

References

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