

# **51 Positron Collisions**

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# **Contents**



### **Abstract**

The positron is the antiparticle of the electron, having the same mass but opposite charge. Positrons undergo collisions with atomic and molecular systems in much the same way as electrons do. Thus, the standard scattering theory for electrons can also be applied to positron scatter-

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ing. However, there are a number of important differences from electron scattering, which we outline below.

Since the positron is a distinct particle from the atomic electrons, it cannot undergo an exchange process with the bound electrons during a collision, as is possible with electrons. Thus, the nonlocal exchange terms that arise in the description of electron scattering are not present for positrons. This leads to a simplification of the scattering equations from those for electrons. However, there are scattering channels available with positron scattering that do not exist with electrons. These are dealt with in Sect. [51.1.](#page-0-0)

Historically, beams of low-energy positrons were difficult to obtain and, consequently, there is considerably less experimental data available for positrons than for electrons. This was particularly true for quantities that required large incident positron fluxes, such as differential scattering cross sections and coincidence parameters. The recent development of cold trap-based positron beams with high resolution and high brightness by the San Diego group [\[1\]](#page-8-1) has enabled significant progress in experimental positron scattering, which is discussed in Sect. [51.3.](#page-4-0)

Throughout this chapter we will employ atomic units unless otherwise noted.

#### **Keywords**

positron differential  $\cdot$  elastic  $\cdot$  excitation  $\cdot$  ionization  $\cdot$  $positionium formation \cdot total cross sections$ 

# <span id="page-0-0"></span>**51.1 Scattering Channels**

Positrons colliding with atomic and molecular systems have the same scattering channels available as for electrons, viz., elastic, excitation, ionization, and for molecules, dissociation. However, two channels exist for positrons that do not exist for electrons, viz., positronium formation and annihilation.

#### <span id="page-1-0"></span>**51.1.1 Positronium Formation**

Positronium, a bound state of an electron–positron pair (Chap. [28\)](http://dx.doi.org/10.1007/978-3-030-73893-8_28), can be formed during the collision of a positron with an atomic or molecular target. The positronium *atom* (Ps) can escape to infinity leaving the target in an ionized state with a positive charge of 1. Thus, this process can be difficult to distinguish experimentally from direct ionization, where both the incident positron and the ionized electron are asymptotically free particles. The positronium atom can exist in its ground state or in any one of an infinite number of excited states after the collision. These states form two series; a singlet series  $(S = 0)$  referred to as parapositronium (*p*-Ps) and a triplet series  $(S = 1)$  referred to as orthopositronium (*o*-Ps). The level structure of both these series is, to order  $\alpha^2$ , where  $\alpha$  is the fine-structure constant, identical to that of hydrogen, but with each level having half the energy of the corresponding hydrogenic state.

Positronium formation is a rearrangement channel, and thus, is a two-center problem. Because positronium is a light particle, having a reduced mass one-half that of an electron, the semiclassical type of approximations used in ion–atom collisions (Chap. [53\)](http://dx.doi.org/10.1007/978-3-030-73893-8_53) are not applicable here. We will discuss various theoretical approaches to this process in Sect. [51.2](#page-2-0) and give references to experimental results in Sect. [51.3.](#page-4-0)

Positronium formation in the ground state has a threshold that is 1/4 of a Hartree (6:80285 eV) below the ionization threshold of the target. This means that it is normally the lowest inelastic channel in positron scattering from neutral atoms. For atoms with a small ionization potential, such as the alkalis, this channel is always open. The energy range between the positronium threshold and the first excited state of the atom is known as the Ore gap. In this range, positronium formation is the only possible inelastic process.

### <span id="page-1-1"></span>**51.1.2 Annihilation**

Annihilation is a process in which an electron–positron pair is converted into two or more photons. It can occur either directly with a bound atomic electron or after positronium formation has taken place. The direct annihilation cross section for a positron of momentum  $k$  colliding with an atomic or molecular target can be written as [\[2\]](#page-8-2)

$$
\sigma_{\rm a} = \frac{\alpha^3 Z_{\rm eff}}{k} \left( \pi a_0^2 \right) , \qquad (51.1)
$$

where  $Z_{\text{eff}}$  can be thought of as the effective number of electrons in the target with which the positron can annihilate. If  $\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, \mathbf{x})$  is the wave function for the system of a positron, with coordinate  $x$ , colliding with an  $N$ -electron target, then

$$
Z_{\text{eff}} = \sum_{i=1}^{N} \int \! \mathrm{d} \, \mathbf{r}_1 \mathrm{d} \, \mathbf{r}_2 \dots \mathrm{d} \, \mathbf{r}_N \, \big| \Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N; \mathbf{r}_i) \big|^2 \,. \tag{51.2}
$$

While this formula can be naively derived by assuming that the positron can only annihilate with an electron if it is at the identical location, it actually follows from a quantum electrodynamical treatment of the process [\[3\]](#page-8-3). If the wave function  $\Psi$  is approximated by the product of the undistorted target wave function times a positron scattering function  $F(x)$ , then

$$
Z_{\rm eff} = \int d\boldsymbol{r} \,\rho(\boldsymbol{r}) \big| F(\boldsymbol{r}) \big|^2 \,, \tag{51.3}
$$

where  $\rho$  is the electron number density of the target. Thus, in the Born approximation, where  $F$  is taken as a plane wave,  $Z_{\text{eff}}$  simply becomes the total number of electrons  $Z$  in the target. However, a pronounced enhancement of the annihilation rate in the vicinity of the Ps formation threshold due to virtual Ps formation was predicted [\[4,](#page-8-4) [5\]](#page-8-5). Subsequently, the Born approximation was shown to be grossly inadequate by the San Diego group, who found annihilation rates  $(Z_{\text{eff}})$  at room temperature that are an order of magnitude larger for some atoms and even up to five orders of magnitude larger in large hydrocarbon molecules. Furthermore, there is evidence that only the outer shell of electrons takes part in the annihilation process. Two mechanisms have been proposed in order to explain these large values for  $Z_{\text{eff}}$ . One involves the enhancement of the direct annihilation process below the Ps formation threshold due to the attractive nature of the positron–electron interaction, which increases the overlap of positron and electron densities in the atom or molecule. The second mechanism is referred to as resonant annihilation, which occurs after the positron has been captured into a Feshbach resonance, where the positron is bound to a vibrationally excited molecule. A summary of the above results can be found in the review article by *Gribakin* et al. [\[6\]](#page-8-6).

When a positron annihilates with an atomic electron, the most likely result is two 511 keV photons, if the positron– electron pair are in a singlet spin state (parapositronium). In the center-of-mass frame of the pair, the photons are emitted in opposite directions to conserve momentum. However, in the laboratory frame, the bound electron has a momentum distribution which is reflected in the photon directions not being exactly 180 degrees apart. This slight angular deviation, called the angular correlation, can be measured and gives information about the momentum distribution of the bound electrons. This quantity is given by [\[3\]](#page-8-3)

$$
S(q) = \sum_{i=1}^{N} \int \mathrm{d}r_1 \dots \mathrm{d}r_{i-1} \, \mathrm{d}r_{i+1} \dots \mathrm{d}r_N \qquad (51.4)
$$

$$
\times \int \mathrm{d}r_i \, \mathrm{d}x \, \mathrm{e}^{\mathrm{i}q \cdot x} \left| \Psi(r_1, r_2, \dots, r_N; x) \, \delta(r_i - x) \right|^2,
$$

where  $q$  is the resultant momentum of the annihilating pair. In evaluating this quantity, the positron is assumed to be thermalized in the gas before undergoing annihilation. Experimentally, only one component of  $q$  is measured, so that  $S(q)$  is integrated over the other two components of the momentum to obtain the measured quantity. The spin triplet component of an electron–positron pair (orthopositronium) can only decay with the emission of three or more photons that do not have well-defined energies. This is a much less probable process than the two-photon decay from the singlet component.

### <span id="page-2-0"></span>**51.2 Theoretical Methods**

The basic theoretical approaches to the calculation of positron scattering from atoms and molecules were originally developed for electron scattering and later applied to the positron case. Thus, we emphasize here only the differences that arise between the electron and positron cases, both in the theoretical formulations, and in later sections, in the nature of the results.

The lowest-order interaction between a free positron and an atomic or molecular target is the repulsive static potential of the target

$$
V_{\rm s} = \langle \psi_0 | V | \psi_0 \rangle \,, \tag{51.5}
$$

where  $\psi_0$  is the unperturbed target wave function, and V is the electrostatic interaction potential between the positron and the target. Since this interaction has the opposite sign from that for electron scattering, the static potential also has the opposite sign in these two cases. On the other hand, the next higher-order of interaction is polarization, which arises from the distortion of the atom by the incident particle. If we represent this distortion of the target to first order by the wave function  $\psi_1$ , as in the polarized-orbital approximation, for example, then the polarization interaction can be represented by the potential

$$
V_{\rm p} = \langle \psi_0 | V | \psi_1 \rangle. \tag{51.6}
$$

This potential is attractive for both positron and electron scattering and has an asymptotic form with leading term  $-\alpha_d/2r^4$ , where  $\alpha_d$  is the static dipole polarizability (Sect. [24.2.3\)](http://dx.doi.org/10.1007/978-3-030-73893-8_24) of the target. Thus, the static and polarization potentials for positron scattering from ground state systems are of opposite sign and tend to cancel one another. This leads to very different behavior from the electron case where they are of the same sign. In particular, the elastic scattering cross sections for positron scattering from an atom are much smaller than for electron scattering, and the phase shifts (Sect. [49.1.1\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49) have very different magnitudes and dependencies on energy. This is illustrated for the case of scattering from helium in Fig. [51.1,](#page-2-1) where the results of the highly ac-

<span id="page-2-1"></span>

**Fig. 51.1** Total elastic cross sections for electron (*dashed line*) and positron (*solid line*) from helium atoms [\[8,](#page-8-7) [10,](#page-8-8) [11\]](#page-8-9). The higher-order phase shifts were calculated from effective range theory (Sect. [49.1.1\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49)

curate variational calculations for scattering by electrons and positrons are shown. There is a corresponding difference in sign between the electron and positron s-wave phase shifts for very small values of the incident momentum. In fact, the positron phase shift goes through zero, which leads to the Ramsauer minimum in the positron total cross section, as shown in Fig. [51.1.](#page-2-1) The large difference in magnitudes between the electron and positron  $s$  and  $p$ -wave phase shifts leads to the large difference in the total elastic cross sections, as shown  $[7-9]$  $[7-9]$ .

Higher-order terms in the interaction potential may also give important contributions to scattering cross sections. For a detailed discussion, see the article by *Drachman* and *Temkin* [\[12\]](#page-8-12).

A simple potential scattering calculation using the sum of the static and polarization potentials, but without the exchange terms that are present for the electron case, can be applied to elastic scattering calculations for closed shell systems (Sects. [51.3.1,](#page-4-1) [51.3.2\)](#page-4-2). The potentials defined above can also be used in a distorted-wave approximation (Chap. [49\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49), which can be applied to excitation and ionization by positron impact. Once again, the complicated exchange terms that arise in electron scattering are absent here [\[13\]](#page-8-13).

For positrons with high enough incident energies  $(\approx 1 \,\text{keV})$ , the first Born approximation will become valid (Chap. [49\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49). Since the first Born approximation is independent of the sign of the charge of the incident particles, this indicates that as the incident energy increases, the corresponding cross sections for electron and positron scattering will eventually merge. From flux conservation arguments, this means that the positronium formation cross section will rapidly decrease as the incident energy increases. In fact, from experimental measurements, the total cross sections (summed over all possible channels) for electron and positron scattering appear to merge at a much lower energy than the cross sections for individual channels [\[14\]](#page-8-14). More elaborate calculations for high energy scattering have been carried out in the eikonal-Born series [\[15\]](#page-8-15) (Chap. [49\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49). These approximations allow for both polarization and absorption (i.e., inelastic processes) and yield good agreement with elastic experimental measurements of differential cross sections at energies above 100 eV. A detailed analysis [\[9,](#page-8-11) [15\]](#page-8-15) of the various contributions to the scattering indicates that absorption effects due to the various open inelastic channels play a much more important role here than for electron scattering.

A more elaborate treatment of positron scattering is based on the close-coupling approximation (Chap. [49\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49), where the wave function for the total system of positron plus target is expanded using a basis set comprised of the wave functions of the target. Once again, there are no exchange terms involving the positron and, in principle, a complete expansion including the continuum states of the target would include the possibility of positronium formation. However, such an expansion is not practicable if one wants to calculate explicit cross sections for positronium formation. Even in cases where such cross sections are not required, the considerable effect that the positronium formation channels can have on the other scattering cross sections is best included by a close-coupling expansion that includes terms representing positronium states plus the residual target ion. There is a problem of double counting of states in such an expansion but, in practice, this does not appear to be a problem if the number of states in the expansion is not large. Also, in many cases, additional pseudo states have to be included in the expansion in order to correctly represent the long-range polarization interaction.

A close-coupling expansion including positronium states is a two-center problem, i.e., it includes the centers of mass of both the target and the positronium states. This means that one is faced with a problem of considerable computational complexity [\[16–](#page-8-16)[21\]](#page-8-17).

Another way to take into account the effects of open inelastic channels without the complications of a full closecoupling approach is to use optical potentials. These are often based on a close-coupling formalism [\[9,](#page-8-11) [22\]](#page-8-18) and lead to a complex potential, the real part of which represents distortions of the target (such as polarization), while the imaginary part allows for absorption (i.e., flux into open channels not explicitly represented). Such an approach was developed by *Chen* et al. [\[23\]](#page-8-19) and applied to the noble gases [\[24\]](#page-8-20). Recently, a simple approach based upon an optical potential model, yielded good results for the positronium formation cross section in the noble gases [\[25\]](#page-8-21).

*Bray* and *Stelbovics* [\[26\]](#page-8-22) applied the convergent closecoupling (CCC) method to the scattering of positrons from atoms. This method includes contributions from the continuum states of the target and sufficient terms in the expansion are included to ensure numerical convergence. Positronium states have been included via psuedostates for positron scattering with helium [\[27\]](#page-8-23). A single-center adiabatic-nuclei version has been used for positron scattering with molecular hydrogen [\[28\]](#page-8-24).

The variational method (Chap. [49\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49) uses an analytic form of trial wave function to represent the total system. The parameters of this analytic function are determined as part of the method. Given a trial wave function with sufficient flexibility and a large enough number of parameters, essentially exact results can be obtained in the elastic energy range and the Ore gap. Because the complexity of the trial function increases as the square of the number of electrons in the target, only positron scattering from hydrogen, helium and lithium, and the hydrogen molecule have been treated by this method to date [\[10,](#page-8-8) [29,](#page-8-25) [30\]](#page-8-26).

Many-body theory has been applied to positron scattering from the noble gases below the positronium formation threshold. Of particular importance is the ability of manybody theory to account for positron–atom and electron– positron correlations, which have a large influence on both the scattering dynamics and the annihilation rate. Many-body theory has produced very good agreement with the most recent experimental results for elastic differential scattering [\[31\]](#page-8-27).

In the case of direct ionization, there appears to be quite distinct threshold behavior of the cross sections for electron and positron collisions. For electrons, the Wannier threshold law (Sect.  $56.3.1$ ) has an exponent of 1.127, while a similar analysis for positrons [\[32\]](#page-8-28) yields an exponent of 2:651. However, the existence of the positronium formation channel leaves in question whether this analysis will give the dominant term at the threshold. For a fuller discussion, see [\[33\]](#page-8-29) and references therein. An experimental investigation of the threshold ionization of helium [\[34\]](#page-8-30) obtained a value 2:2. This was followed by a theoretical investigation that considered anharmonic corrections to the Wannier threshold law to explain the experimental results [\[35\]](#page-8-31). A recent measurement within 2 eV of the ionization threshold obtained a value of 1:1 [\[36\]](#page-8-32).

There has been an investigation [\[37\]](#page-8-33) of the behavior of the elastic cross sections at the positronium formation threshold, which predicts the occurrence of a Wigner cusp for the noble gases using R-matrix methods. A comprehensive set of measurements using a high-resolution trap-based beams of the elastic scattering cross section about the positronium formation threshold revealed a family of Wigner cusps in the noble gases [\[38\]](#page-8-34). Subsequent measurements of the elastic scattering cross section about the positronium formation threshold in molecules that are isoelectronic with helium and neon, and did not show a Wigner cusp [\[39\]](#page-8-35).

# <span id="page-4-1"></span><span id="page-4-0"></span>**51.3 Particular Applications**

### **51.3.1 Atomic Hydrogen**

Because of the difficulty of taking measurements in atomic hydrogen, the available experimental data has so far been restricted to total cross sections, as well as to total ionization and positronium formation cross sections. Essentially exact variational calculations have been carried out in the elastic energy regime and the Ore gap [\[10\]](#page-8-8). These calculations are used to benchmark many-body theory [\[40\]](#page-8-36).

Ionization cross sections have been measured by both the Bielefeld and London groups ([\[41,](#page-8-37) [42\]](#page-8-38) and references therein) and have been calculated in a number of approximations [\[24,](#page-8-20) [26,](#page-8-22) [43](#page-8-39)[–45\]](#page-8-40). However, disagreements between the experimental measurements mean that there is at present no reliable way of assessing the various theoretical approximations used. More elaborate calculations with asymptotically correct wave functions have been used to determine triple differential cross sections for ionization [\[46,](#page-8-41) [47\]](#page-8-42). However, the task of integrating these to produce total cross sections is a formidable one.

The total positron–hydrogen cross section has also been measured by the Detroit group [\[48\]](#page-8-43) and is in quite good agreement with calculations based upon the coupledpseudostate [\[45\]](#page-8-40) and the convergent close-coupling [\[49\]](#page-8-44) methods, except at very low energies where the experimental uncertainties are the greatest.

In order to determine reliable positronium formation cross sections, the explicit positronium states have to be included. Several such calculations have been carried out [\[17–](#page-8-45)[20\]](#page-8-46). These indicate the necessity of explicitly including positronium formation channels in the expansion of the total wave function in order to obtain accurate results, even for elastic scattering. The most recent calculations [\[45,](#page-8-40) [49,](#page-8-44) [50\]](#page-8-47) are in quite good agreement with various experiments [\[41,](#page-8-37) [51\]](#page-8-48) over the majority of the energy range.

As is the case for electron scattering, positron cross sections exhibit resonances (Sect. [49.1.3\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49). These have been extensively studied by *Ho* [\[52\]](#page-8-49), who used variational and complex rotation methods.

# <span id="page-4-2"></span>**51.3.2 Noble Gases**

Because the noble gases are convenient experimental targets, a good deal of effort has gone into calculations for these targets, particularly for elastic scattering, ionization, and Ps formation. In the purely elastic energy range, i.e., for energies below the positronium formation threshold, the simple potential scattering approach using the static and polarization potentials defined above yields quite good results. Since the long-range behavior of the sum of the potentials is attractive, the scattering phase shifts for positrons must be positive for sufficiently low energies. However, as its incident energy increases, the positron probes the repulsive inner part of the potential, and the phase shifts become negative. This behavior leads to the well-known Ramsauer minimum in the integral elastic cross sections (Chap. [49\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49). The Ramsauer minimum has been observed in helium and neon ([\[53,](#page-8-50) [54\]](#page-8-51) and references therein). In the case of argon, no minimum is observed given a sufficiently high-quality beam [\[55\]](#page-8-52). In general, this differs from electron scattering, where some low-energy phase shifts can be negative (modulo  $\pi$ ) because of the existence of bound orbitals of the same symmetry.

Another difference between positron and electron scattering is exhibited by the differential cross sections (Chap. [49\)](http://dx.doi.org/10.1007/978-3-030-73893-8_49). For electrons, the shape of the cross section is determined by a few dominant phase shifts, whereas for positrons, many phase shifts contribute to the final shape [\[56\]](#page-8-53). Because of this behavior, the differential cross sections for positron scattering have much less overall structure than for electron scattering. However, the differential cross sections for positrons for many of the noble gases have a single minimum at relatively small angles, both below and above the first inelastic channel [\[57,](#page-8-54) [58\]](#page-8-55). The earlier results have been reviewed by *Kauppila* et al. [\[59\]](#page-8-56). At intermediate energies, the simple potential scattering approximation is no longer sufficient, and the inelastic channels have to be taken into account via, for example, the use of an optical potential [\[9,](#page-8-11) [15,](#page-8-15) [23,](#page-8-19) [60\]](#page-8-57) or convergent close-coupling method  $([61]$  $([61]$  and references therein). Furthermore, in the inelastic scattering regime, the existence of open channels has a much more marked effect on the shape of the differential cross sections for positron scattering than that for electrons [\[57\]](#page-8-54).

Absolute elastic differential cross sections were measured for argon, krypton, and xenon at low energies using a magnetized beam of cold positrons [\[58,](#page-8-55) [61,](#page-8-58) [62\]](#page-8-59). Magnetized beam measurements generally do not distinguish between forward and backward scattered positrons (or electrons). In this case, the reported elastic cross section is folded about 90 degrees. As with electrostatic beams, a portion of the angular scatter is indistinguishable from the incident beam, which plays an important role in the comparison of experiment and theory [\[55\]](#page-8-52). These results are in general agreement with a variety of different theoretical predictions [\[63](#page-8-60)[–65\]](#page-8-61). A method that allows the scattering phase shifts to be extracted from the folded elastic differential scattering cross section was developed recently [\[66\]](#page-8-62).

There is relatively little experimental data for the excitation of the noble gases. Some experimental work has been carried out for the lighter noble gases, helium, neon, and argon ([\[67\]](#page-8-63) and references therein), and there is satisfactory agreement between these measurements and closecoupling [\[68\]](#page-8-64), as well as distorted-wave [\[69\]](#page-8-65) calculations.

The first state-resolved absolute excitation cross sections for the  $4s[1/2]_1^{\circ}$  and  $4s[3/2]_1^{\circ}$  states of argon and the 6s  $[3/2]_1^0$  state of xenon have been measured by the San Diego group [\[6,](#page-8-6) [70\]](#page-8-66). Relativistic distorted-wave calculations are in satisfactory agreement with the experiment for ar-gon [\[71\]](#page-8-67) but less so for xenon [\[72\]](#page-8-68). Excitation of the  $n = 2$ states of helium was measured by the ANU group [\[73\]](#page-8-69). Convergent close-coupling calculations are in good agreement for both the 2<sup>1</sup>S and 2<sup>1</sup>P states [\[27\]](#page-8-23).

The total ionization and positronium cross sections have been measured extensively for all of the noble gases. In general, there is good agreement amongst the various experiments for the ionization cross section but much less so for the positronium formation cross section, with a recent exception [\[25\]](#page-8-21). A summary of the experimental work on the ionization and positronium cross sections for neon, argon, krypton, and xenon can be found in the article by *Marler* et al. ([\[74\]](#page-9-0) and references therein). A summary of the corresponding theoretical work can be found in [\[24,](#page-8-20) [25\]](#page-8-21).

Both double and triple-differential ionization cross sections have been measured for helium [\[75\]](#page-9-1) and argon [\[76,](#page-9-2) [77\]](#page-9-3). Distorted wave Born (DWBA) and three-continuum approximation (3C model) have also been applied to these systems ([\[78,](#page-9-4) [79\]](#page-9-5) and references therein).

The formation of excited-state positronium has been measured for positron scattering from helium, argon, and xenon and has been compared to a number of theoretical results [\[80\]](#page-9-6).

There exist some measurements of  $Z_{\text{eff}}$  and angular correlation parameters for these gases [\[81\]](#page-9-7), mainly at room temperature, and calculations for them have been made in the polarized-orbital approximation [\[82\]](#page-9-8). Measurements have been made at various temperatures and are in relatively good agreement with early calculations [\[83\]](#page-9-9).

The combination of available gas-phase scattering cross sections for energies between 0 and 10 keV has been used to model a single track of a positron through argon [\[84\]](#page-9-10).

### <span id="page-5-0"></span>**51.3.3 Other Atoms**

In the case of positron scattering from the alkali atoms, the positronium formation channel is always open, and the simple potential scattering approach does not yield reliable results. The Detroit group has measured the total cross section, as well as the upper and lower bounds to the positronium formation cross section for sodium, potassium, and rubidium [\[48\]](#page-8-43). Although early close-coupling calculations of the elastic and excitation cross sections [\[85](#page-9-11)[–87\]](#page-9-12) were in surprisingly good agreement with the experimental total cross section, these calculations did not include the positronium formation channel. Subsequently, much more sophisticated calculations were carried out by the Belfast group using the

coupled-pseudo-state method, which included both eigenstates of the target, as well as positronium [\[45,](#page-8-40) [88](#page-9-13)[–90\]](#page-9-14). These calculations also showed the increasing importance of positronium formation in excited states for the alkalis: potassium, rubidium, and caesium. The overall agreement between experimental results and those from the coupledpseudo-state method are quite good for both potassium and rubidium; however, for sodium, the experimental positronium formation cross section is significantly above these theoretical calculations. A summary of the experimental work on the alkalis can be found in [\[48\]](#page-8-43), while a corresponding summary of theoretical work is given in [\[45\]](#page-8-40).

Substantial resonance features have been found in these positron–alkali atom cross sections using close-coupling calculations [\[91,](#page-9-15) [92\]](#page-9-16). More recently, various theoretical methods have been applied to the positron–lithium system ([\[93,](#page-9-17) [94\]](#page-9-18) and references therein).

The positronium formation threshold for magnesium is very low, only 0:844 eV, and hence, the elastic and positronium formation cross sections will dominate in the low-energy region. Upper and lower bounds to the Ps formation cross section in magnesium have been determined [\[48,](#page-8-43) [95\]](#page-9-19) and are in agreement with both close-coupling calculations [\[96\]](#page-9-20) and the results of many-body theory [\[97\]](#page-9-21).

### <span id="page-5-1"></span>**51.3.4 Molecular Hydrogen**

By its fundamental nature, molecular hydrogen has attracted considerable attention both experimentally and theoretically. The total elastic cross section has been measured by the Detroit group [\[51\]](#page-8-48), the London group [\[98\]](#page-9-22), and the ANU group [\[99\]](#page-9-23). There have been several theoretical calculations of this cross section by a variety of methods: Kohn variational [\[100\]](#page-9-24), R-matrix [\[101\]](#page-9-25), distributed positron model [\[102\]](#page-9-26), a Schwinger multichannel method [\[101–](#page-9-25)[103\]](#page-9-27), and convergent close-coupling calculations by the Curtin group [\[104\]](#page-9-28).

Calculations have shown the elastic cross section is strongly influenced by the positronium formation channel near the threshold. However, a recent measurement did not show any feature in the integral elastic cross section about the positronium formation threshold [\[39\]](#page-8-35).

The vibrational  $(0 \rightarrow 1)$  excitation cross section of molecular hydrogen has been measured between 0:55 and 4 eV and is in quite good agreement with theoretical calculations [\[105\]](#page-9-29) (and reference therein). The San Diego group has also measured the electronic excitation of the  $B^1\Sigma$  state from the threshold to  $30 \text{ eV}$  [\[70\]](#page-8-66). Their data are in reasonable agreement with the Schwinger multichannel calculation of *Lino* et al. [\[106\]](#page-9-30). The measured positron excitation cross section appears to be larger than that measured for electron excitation.

The ionization cross section has been determined over a wide range of energies by a number of different groups  $([107-111]$  $([107-111]$  and references therein). Since all of the above measurements are relative, they must be normalized to one another at particular energies. Theoretical calculations are in satisfactory agreement with the measurements  $(112)$  and references therein).

Electron capture to the continuum has been observed in triple-differential ionization measurements [\[113\]](#page-9-34). Reasonable agreement has been found between available experimental measurements and the distorted-wave Born approximation (with the Ward–Macek approximation; [\[79\]](#page-9-5) and references therein).

The positronium formation cross section has also been measured by a number of different groups and has been compared to the first Born approximation and a coupled-channels calculation, see [\[99\]](#page-9-23) and reference therein.

Differential elastic cross sections have been measured by the ANU group and compared to a number of calculations [\[99\]](#page-9-23). The shape of these measurements are in good agreement with the complex model potential calculation [\[114\]](#page-9-35). More recently, a single-center adiabatic-nuclei convergent close-coupling method [\[104\]](#page-9-28) showed good agreement between experiment and theory for the differential elastic cross section below the positronium formation threshold.

Rotational excitation cross sections have been calculated using the Schwinger multichannel method with fixed nuclei and the adiabatic rotational approximation ([\[115\]](#page-9-36) and references therein). Recent progress in cryogenic positron traps by the San Diego group [\[116\]](#page-9-37) will enable an experimental investigation of the rotational excitation of molecular hydrogen.

#### <span id="page-6-0"></span>**51.3.5 Water**

From a biological perspective, water is fundamental, and it was recently studied experimentally and theoretically. The total scattering cross has been measured by the ANU group and compared to previous measurements and calculations ([\[117\]](#page-9-38) and references therein). The ionization cross section has been measured by the London group [\[118\]](#page-9-39). The total elastic cross section and total inelastic cross section less positronium formation have been measured by the ANU group [\[119\]](#page-9-40). These measurements were compared to R-matrix and the independent atom model (IAM) methods ([\[119\]](#page-9-40) and references therein).

Differential ionization cross sections have been measured by the London group [\[120\]](#page-9-41). Triple-differential ionization has been calculated using a second-order distorted-wave Born approximation [\[121\]](#page-9-42).

### <span id="page-6-1"></span>**51.3.6 Other Molecules**

For diatomic and triatomic molecules, most of the experimental and theoretical work has been carried out for CO,  $CO_2$ ,  $O_2$ , and  $N_2$ . Total cross sections for  $O_2$ ,  $N_2$ , and  $CO_2$ have been measured from the threshold to several hundred eV ([\[98\]](#page-9-22) and references therein). Recently, the independent atom model (IAM) was compared to measurements for  $C_2$ ,  $N_2$ , and  $O_2$  [\[122\]](#page-9-43) (and references therein). A spherical complex optical potential was used to determine the total scattering cross section for positron scattering from a number of simple molecules [\[123\]](#page-9-44).

Relative differential cross sections have been measured for CO,  $CO_2$ ,  $O_2$ ,  $N_2$ , as well as  $N_2O$ , on both sides of the positronium formation threshold [\[124\]](#page-9-45). At low energies, the gases  $N_2$ ,  $O_2$ , and CO exhibit a minimum in the DCS at small angles, as with the heavier noble gases. This minimum gradually disappears as the energy increases.

Vibrational excitation cross sections for  $CO$  and  $CO<sub>2</sub>$  have been measured [\[105\]](#page-9-29) and are in excellent agreement with the theoretical calculations of  $[125]$  for CO, and in satisfactory agreement with theory  $[126]$  for  $CO<sub>2</sub>$ . Electron excitation of the  $a^1\Pi$  and  $a'^1\Sigma$  states of N<sub>2</sub> have been measured from threshold to 20 eV [\[70\]](#page-8-66). Interestingly, the positron cross section near the threshold is approximately double that for electrons.

Impact ionization, positronium formation, and electronic excitation have been measured for  $N_2$ , CO, and  $O_2$  [\[127\]](#page-9-48). Additionally, positronium formation has been measured for  $CO<sub>2</sub>$  [\[128\]](#page-9-49).

For small polyatomic molecules, the majority of experimental and theoretical work was carried out for CH<sub>4</sub>. This includes the total cross section and quasi-elastic (summed over vibration–rotational levels) differential cross sections [\[129\]](#page-9-50). At low energies, there is a minimum in these DCS at small angles, as for the heavier noble gases which, in turn, also disappears at higher energies [\[59\]](#page-8-56). The positronium formation cross section has also been measured [\[130\]](#page-9-51).

Recently, a large number of total scattering cross section measurements of organic compounds were studied experi-mentally by the Trento group ([\[131\]](#page-9-52) and references therein). This work has been extended to purine nucleobasis and other biologically relevant molecules [\[132\]](#page-9-53) (and references therein). Additionally, a comparison of the total scattering cross section from chiral enantiomers was also made [\[133\]](#page-9-54).

Positronium formation has been measured for methanol and ethanol [\[134\]](#page-9-55). Total and elastic differential scattering, and positronium formation cross sections for a number of biologically relevant molecules have been measured by the ANU group ([\[135,](#page-9-56) [136\]](#page-9-57) and references therein). In these cases, the scattering cross sections are summed over rotational and vibrational states. Nucleobases that are solid at room temperature require a vacuum oven to produce vapor of the molecules. In these cases, relative cross sections were determined experimentally, and IAM calculations set the absolute scale at 150 eV.

# <span id="page-7-0"></span>**51.4 Binding of Positrons to Atoms**

There have been many recent investigations of the possible binding of positrons to a variety atoms. As was mentioned in Sect. 48.1.2, such binding could greatly enhance the annihilation cross section and help explain the large measured values of  $Z_{\text{eff}}$  for both atoms and molecules. It has been shown theoretically that a positron will bind to a large number of one-electron and two-electron atomic systems ([\[137\]](#page-9-58) and references therein). For one-electron systems, where the ionization potential is less than 6:80285 eV, the dominant configuration is a polarized positronium (Ps) cluster moving in the field of the residual positive ion, while for twoelectron systems, with an ionization potential greater than 6:80285 eV, the dominant configuration involves a positron orbiting a polarized neutral atom [\[138\]](#page-9-59). So far, there is no experimental evidence for these positronic atoms [\[139\]](#page-9-60). However, a significant amount of theoretical work has shown that many atoms can bind a positron  $(140)$  and references therein).

Enhancement of the annihilation rate  $(Z_{\text{eff}})$  is observed in polyatomic molecules. The mechanism has been identified as vibrational Feshbach resonances mediating positron binding to molecules ([\[6\]](#page-8-6) and references therein). In the case of linear alcohols, the binding energy depends linearly upon the molecular polarizability [\[141\]](#page-9-62).

# <span id="page-7-1"></span>**51.5 Positronium Scattering**

There has been interest in positronium (Ps) scattering from atomic and molecular targets for a considerable time; see the work of *Fraser* and coworkers [\[142\]](#page-9-63) and reference therein, but only recently has this field seen much activity. This is a two-center problem with the Ps *atom* being a light particle, so semiclassical methods are not applicable. There was some theoretical work by *Drachman* and *Houston* [\[143,](#page-9-64) [144\]](#page-9-65), and recently there has been close-coupling calculations for simple target systems [\[145\]](#page-10-0). This problem has also been studied by a pseudo-potential method ([\[146\]](#page-10-1) and references therein). The long-range interactions in positron–hydrogen scattering have recently been investigated [\[147\]](#page-10-2). The London group has measured the total cross sections positronium scattering from the noble gases and small molecules  $(H_2, N_2, O_2, H_2O, CO_2,$  $SF<sub>6</sub>$ ). Unexpectedly, the total cross sections for positronium scattering have been found to be very similar to scattering by electron of the same velocity [\[148\]](#page-10-3). This has been explained in part by the polarization of the incident Ps [\[149\]](#page-10-4).

The formation of the positronium negative ion,  $Ps^-$ , has been observed [\[150\]](#page-10-5), and resonance structure has also been observed in the photodetachment of  $Ps^-$  [\[151,](#page-10-6) [152\]](#page-10-7).

The formation of molecular positronium  $(Ps<sub>2</sub>)$  has been observed [\[153\]](#page-10-8) using intense positron pulses at a metal surface. The scattering of positronium atoms by positronium atoms has been investigated theoretically [\[154,](#page-10-9) [155\]](#page-10-10) with an investigation of exciton-like nature of positronium [\[156\]](#page-10-11).

The positronium atom is a boson, and, thus, there is fundamental interest in the creation of a Bose–Einstein condensate of an antimatter–matter composite bose. A unique feature of a Ps-BEC is the possibility of stimulated annihilation or the creation of a gamma-ray laser [\[157,](#page-10-12) [158\]](#page-10-13). More detailed theoretical treatments have appeared more recently [\[159–](#page-10-14) [161\]](#page-10-15).

# <span id="page-7-2"></span>**51.6 Antihydrogen**

Positron and positronium scattering play an important role in efforts to form antihydrogen, the bound state of an antiproton and a positron. This antimatter atom is an ideal system to test CPT. In the past decade, antihydrogen has been trapped [\[162\]](#page-10-16) with the first spectroscopic measurements made recently [\[163\]](#page-10-17). In addition, the formation of an antihydrogen beam has been postulated [\[164\]](#page-10-18). Excited-state positronium has been found to be extremely useful in the formation of antihydrogen using detailed CCC calculations [\[165\]](#page-10-19).

### <span id="page-7-3"></span>**51.7 Reviews**

For a number of years, a Positron Workshop has been held as a satellite of the International Conference on the Physics of Electronic and Atomic Collisions. The Proceedings [\[166–](#page-10-20) [182\]](#page-10-21) give an excellent summary of the state of positron scattering research, both experimental and theoretical, and applications to astro and biophysics.

There are several review articles on positron scattering in gases, including the early historical development [\[183\]](#page-10-22), more comprehensive articles [\[2,](#page-8-2) [184–](#page-10-23)[186\]](#page-10-24), as well as more recent reviews [\[131,](#page-9-52) [187–](#page-10-25)[191\]](#page-10-26). There are a number of reviews of the various antihydrogen efforts [\[192](#page-10-27)[–195\]](#page-10-28) with a special issue on antihydrogen and positronium [\[196\]](#page-10-29). A review on positronium laser physics [\[197\]](#page-10-30) discusses the future for positron physics.

The book [\[198\]](#page-10-31) discusses various aspects of both experimental and theoretical positron physics.

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