Journal of Atomic, Molecular, Condensate & Nano Physics
Vol. 1, No. 2, pp. 45–63, 2014
ISSN 2349-2716 (online); 2349-6088 (print)
Published by RGN Publications

http://www.rgnpublications.com

Positron Interactions with Atoms and Ions

Research Article

A. K. Bhatia

NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771, USA
Anand.K.Bhatia@nasa.gov

Abstract. A number of processes are possible in the interactions of positrons with atoms and ions. These are scattering from various targets, formation and annihilation of positronium atoms, bound states, and resonances. Calculations of these processes, using different methods, are described. Scattering of positronium atoms from various targets is discussed. Positronium beams can be produced by the photodetachment of negative positronium ions. Calculations of cross sections by two different methods are indicated.

Keywords. Positron Interactions; Atoms; Ions

PACS. 34.80Uv; 36.10Dr

Received: July 30, 2014 **Accepted:** August 21, 2014

Copyright © 2014 A. K. Bhatia. *This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.*

1. Introduction

Dirac, in 1928, combining the ideas of quantum mechanics and the ideas of relativity invented the well-known relativistic wave equation. In his formulation, he predicted an antiparticle of the electron of spin $\hbar/2$. He thought that this particle must be a proton. Dirac [1] published his interpretation in a paper '*A theory of electrons and protons*'. It was shown later by the mathematician Hermann Weyl (see [2]) that the Dirac theory was completely symmetric between negative and positive particles and the positive particle must have the same mass as that of the electron. In his J. Robert Oppenheimer Memorial Prize Acceptance Speech, Dirac [2] notes that 'Blackett was really the first person to obtain hard evidence for the existence of a positron but he was afraid to publish it. He wanted confirmation, he was really over cautious'. Positron, produced by the collision of cosmic rays in a cloud chamber, was detected experimentally by Anderson [3] in 1932. His paper was published in Physical Review in 1933. The concept of the positron and its detection were the important discoveries of the 20th century.

2. Why Positron Physics is Interesting?

It is a particle, just like an electron. It has a positive charge while the electron has a negative charge. For this reason positron can form a positronium atom and positron annihilation with an electron can take place. This replaces in the calculations exchange in the case of two electrons and there are no nonlocal exchange terms in the equations for the scattering of positrons from atoms. This can be a tool for understanding of practical systems:

(i) Angular-correlation experiments to probe the Fermi surfaces of solids.
(ii) PET scans of the human brain. This is now commonly used these days.
(iii) Observation of annihilation of 511 keV line from the center of the galaxy (Bussard et al. [4]).

3. Calculations and Results for Various Processes

The simplest system to work on is the positron-hydrogen scattering. Such a system could have bound states and resonances just as in the case of electrons. Also, there is no need to invoke the Pauli principle because these are distinct particles. The positron is an antiparticle of the electron. But we find that the absence of exchange does not make matters simple. During their encounter, the two particles could be in a virtual positronium state or could annihilate giving a 511 keV line.

The low-energy non-relativistic Hamiltonian is of the same form as in the electron-hydrogen case, except for two changes of signs. This ‘minor’ difference has several implications.

$$H = -\nabla_1^2 - \nabla_2^2 + V, \tag{1}$$

where

$$V = \frac{2Z}{r_1} - \frac{2Z}{r_2} - \frac{2}{r_{12}}, \tag{2}$$

$$r_{12} = |\vec{r}_1 - \vec{r}_2|. \tag{3}$$

We are using Rydberg units. In the above potential V, r_1 is the coordinate of the incident positron and r_2 is the electron coordinate. These distances are measured from the position of the nucleus of charge Z, assumed fixed. The positron feels a repulsive potential as it penetrates the atom while the electron always feels an attraction.

Our aim is to calculate phase shifts for the scattering of a positron at low energies from the hydrogen atom. Knowing the phase shifts, we can calculate the cross section σ for the scattering:

$$\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2(\delta_l), \tag{4}$$

where k^2 is the energy of the incident positron and l is the partial wave.

We write the wave function in the static approximation as given below:

$$\Psi(\vec{r}_1,\vec{r}_2) = \phi(\vec{r}_2)u(\vec{r}_1), \tag{5}$$

where u is the scattering function and ϕ is the target function which is given by

$$\phi(r) = \sqrt{\frac{Z^3}{\pi}}\exp(-Zr) \quad \text{and} \quad u(\boldsymbol{r}) = (u(r)/r)Y_{l0}(\Omega). \tag{6}$$

In this approximation the resulting potential is repulsive. The simplest approximation given above in Eq. (5) for the elastic scattering is called the static approximation. Notice, in this case there is no exchange as for two electrons.

For $Z = 1$ and $l = 0$, and for the incident positron momentum $\boldsymbol{k}$ we get the scattering equation for $u(r_1)$ given below

$$\left[\frac{d^2}{dr_1^2} - 2\exp(-2r_1)\left(1+\frac{1}{r_1}\right) + k^2\right]u(r_1) = 0. \tag{7}$$

Solution of this equation gives phase shifts which are negative. The scattering function is given by

$$u(r_1) = A\sin(kr_1 + \delta) \quad r_1 \text{ tending to infinity} \tag{8}$$

For large values of r_1, the amplitude A can be taken independent of the distance

$$\frac{du(r_1)}{dr_1} = u'(r_1) = Ak\cos(kr_1 + \delta) \tag{9}$$

where δ is the phase shift. It is easy to calculate the phase shift in this case. From these two equations, we get

$$A = \sqrt{u(r_1)^2 + (du(r_1)/dr_1)^2} \tag{10}$$

and

$$\delta = \tan^{-1}[u/u'] - kr_1. \tag{11}$$

This method can be easily generalized to the higher values of the angular momentum but then one has to use Bessel functions of order l.

There are other methods which have been discussed by F. Calogero in his book '*Variable Phase Approach in Potential Scattering*'.

It is well known that there is a polarization potential $\frac{\alpha}{r_1^4}$ which is attractive both for electrons and positrons, where α is the polarizability and it is $4.5a_0^3$ for the hydrogen atom. Adding this potential to the equation (7), we find that the two potentials tend to cancel each other in the case of the positrons. This gives some improved results but they are still not very satisfactory.

The first good calculation was carried out by Schwartz [5].

If we picture an electron incident on the hydrogen atom we find that the two electrons tend to stay on either side of the nucleus because of the repulsion between them. But in the case of positron scattering on the hydrogen atom, the positron and electron tend to arrange themselves on the same side of the nucleus, with the result that the correlations between them become very important. These correlations can be represented by the coordinate r_{12}. Moreover, there is always the possibility of virtual positronium formation which has the wave function depending on this coordinate. Schwartz [5] used the Kohn variational principle with a correlated wave function of Hylleraas type, but without this coordinate in the exponential part of the wave function:

$$\Phi(r_1,r_2,r_{12}) = \exp(-\delta r_1 - \gamma r_2)\Sigma_{l,m,n} C_{lmn} r_1^l r_2^m r_{12}^n. \tag{12}$$

The summation is over integers l, m and n and δ and γ are the nonlinear parameters, which can be varied to get the best results.

Schwartz [5] calculated **S**-wave phase shifts for e^+-H elastic scattering. But his calculation suffered from singularities. In spite of this, he could obtain fairly accurate results.

His results have no bound principle for $k > 0$. That is, only the scattering length has a bound principle. This can be shown by the Kohn variational principle.

A much better calculation has been carried out by Bhatia et al. [6] which did not suffer from the above-mentioned singularities. They calculated phase shifts below the positronium pickup threshold in e^+-H elastic scattering.

They used a generalized Hylleraas-type wave function, that is, they also had r_{12} in the exponential part of the wave function, and they used the projection operator formalism of Feshbach [7]. The closed channel wave function is given by

$$\Phi(r_1,r_2,r_{12}) = \exp(-\delta r_1 - \gamma r_2 - \alpha r_{12})\Sigma C_{lmn} r_1^l r_2^m r_{12}^n, \tag{13}$$

where, the additional nonlinear parameter is α. The total wave function is given by

$$\Psi(\vec{r}_1,\vec{r}_2) = u(\vec{r}_1)\phi(r_2) + \Phi(r_1,r_2,r_{12}). \tag{14}$$

They constructed the optical potential using the projection operators $\boldsymbol{P}$ and $\boldsymbol{Q}$. The projection operator $\boldsymbol{P}$ projects onto the ground state, while $\boldsymbol{Q} = \mathbf{1} - \boldsymbol{P}$ projects out of this state. Also, these operators have properties

$$P^2 = P \text{ and } Q^2 = Q \qquad \text{(Idempotent)}, \tag{15}$$

$$PQ = 0 \qquad \text{(Orthogonal)}, \tag{16}$$

$$P + Q = 1 \qquad \text{(Completeness)}. \tag{17}$$

Now the differential equation for the scattering function is given by

$$\left[\left(\frac{d^2}{dr_1^2} - 2\exp(-2r_1)\left(1+\frac{1}{r_1}\right) + k^2\right)u(r_1) - \sum_{\lambda}^{N} \frac{V_\lambda(r_1)\langle V_\lambda u\rangle}{DE_\lambda}\right] = 0, \tag{18}$$

where $DE_\lambda = E - \varepsilon_\lambda$, ε_λ are the eigenvalues of the QHQ problem and $E = -1 + k^2$. The last term in the above equation is called the optical potential.

We will not go into details here except to mention that the optical potential can be shown to be negative definite, which means that it is always attractive. Furthermore, the calculated phase shifts can be shown to have a rigorous lower bound to the exact phase shifts. That is the calculated phase shifts are approaching the exact phase shifts from below and the exact phase shifts can be higher than the calculated phase shifts. Therefore, their results satisfy a rigorous bound principle. Bhatia et al. [6] solved Eq. (18) for various combinations of the nonlinear parameters with increasing number of terms in the generalized Hylleraas wave function. We show in Table I for $k = 0.1$, 0.6 and 0.7 how the phase shifts increase as the number of terms is increased in the optical potential. As the number of terms is increased, the optical potential becomes more negative. This table also shows that for $N = 0$, just the static approximation given in Eq. (7), gives negative phase shifts, as stated earlier. Also, it is clear that the phase shifts have a lower bound and they will increase further if the number of terms N in the closed channel wave function, Eq. (13), is increased.

Table I. Phase shifts with respect to the number of terms

$k\backslash N$	0	4	10	20	35	56	84
0.1	−0.0580	0.12416	0.14158	0.14553	0.14756	0.14777	0.14788
0.6	−0.3042	−0.0262	−0.0025	−0.0001	0.00226	0.00281	0.00301
0.7	−0.3400	−0.0796	−0.0059	−0.0563	−0.0534	−0.0526	−0.0524

The scattering length is defined as

$$\lim_{k\to 0} k\cot\delta = -1/a\,. \tag{19}$$

This equation shows that when the phase shifts have lower bounds, the scattering length a has an upper bound. To prove these rigorous bounds, we need to study the Kohn variational principle.

To illustrate the calculation of the scattering length, let us write the scattering equation in a simple form for large values of r such that all the short-range potentials do not contribute in the scattering equation

$$u'' + (\alpha/r^4)u = 0,\ \ u(r) = r - a + C_1/r + C_2/r^2 + C_3/r^3,\ \ u'' = 2C_1/r^3 + 6C_2/r^4 + 12C_3/r^5\,. \tag{20}$$

Therefore,

$$2C_1/r^3 + 6C_2/r^4 + 12C_3/r^5 + (\alpha/r^4)[r - a + C_1/r + C_2/r^2 + C_3/r^3] = 0\,. \tag{21}$$

Knowing $u(r)$ beyond the range of the short-range potentials and then equating the various powers of r, we get

$$u = r + a[-1 + \alpha/(6r^2)] - \alpha/(2r) + \alpha^2/(24r^3)\,. \tag{22}$$

For any value $u(r)$ at large r, we can determine the scattering length a. By having more coefficients for $u(r)$ in Eq. (20), we can improve the accuracy of the functions u to determine the scattering length.

Results obtained by Bhatia et al. [6] for 84 terms in the Hylleraas wave function, along with the results of Schwartz [5] are shown in Table II.

Table II. S-wave e^+-H phase shifts

k	Bhatia et al. [6]	Schwartz [5]	Houston and Drachman [11]
0.1	0.1483	0.151	0.149
0.2	0.1877	0.188	0.189
0.3	0.1677	0.168	0.169
0.4	0.1201	0.120	0.123
0.5	0.0624	0.062	0.065
0.6	0.0039	0.007	0.008
0.7	−0.0512	−0.054	−0.049

We see that the results obtained by Schwartz [5] are quite good but they differ from the results of Bhatia et al. [6] at $k = 0.1$, 0.6 and 0.7.

Up to now these results have stood the test of time and have provided a benchmark for future calculations.

A similar calculation for P-wave has been carried out for e^+-H elastic scattering by Bhatia et al. [8]. This calculation is more complicated than the S-wave calculation. We will not go into details here but simply give their results in Table II, along with another calculation by Armstead [9]. The results of Bhatia et al. [8] are very accurate and we see the agreement with the results of Armstead [9] is very good.

Table III. P-wave e^+-H phase shifts

k	Bhatia et al. [8]	Armstead [9]
0.1	0.0094	0.009
0.2	0.0338	0.033
0.3	0.0665	0.064
0.4	0.1016	0.102
0.5	0.1309	0.132
0.6	0.1547	0.156
0.7	0.1799	0.178

In the above calculations, phase shifts are calculated using the expression

$$\lim u(r) = \sin(kr_1 - l\pi/2 + \delta) \quad r_1 \text{ tending to infinity} \tag{23}$$

Where l is the partial wave and δ is the phase shift. For S-waves $l = 0$ and for P-waves $l = 1$.

For higher partial waves, the Born approximation can be used. Wadehra [10] has given the expression

$$\tan(\delta_l) = \frac{\pi k^2}{(2l-1)(2l+1)(2l+3)}\left(\alpha + \frac{3\alpha_2 k^2}{(2l-3)(2l+5)}\right), \tag{24}$$

where α_2 is the quadrupole polarizability of the hydrogen atom and its value is $15.0\mathrm{a}_0^5$. We give phase shifts in Table IV, calculated from the above expression for $l = 2$ to 7 for $k = 0.1$, 0.2 and 0.3, as an illustration. These results are independent of charge of the incident particle. Therefore, they are the same for electrons and positrons. The phase shifts decrease as the angular momentum increases.

Table IV. Positron-hydrogen atom scattering phase shifts for higher partial waves

l	$K = 0.1$	$k = 0.2$	$k = 0.3$
2	0.00135	0.005625	0.013329
3	0.00045	0.001817	0.004149
4	0.000204	0.000821	0.001861
5	0.000110	0.000441	0.000997
6	0.000066	0.000264	0.000597
7	0.000043	0.000171	0.000385

I will discuss a simple method which gave fairly accurate results. This is called the Harris method. The calculations were carried out by Houston and Drachman [11]. In this method, the total wave function is written as

$$\left.\begin{aligned}\Psi_T &= \psi_1 + \tan\delta_T \psi_2 + \Phi(r_1, r_2, r_{12}),\\ \psi_1 &= (kr_1)^{-1}\sin(kr_1)\phi(r_2),\\ \psi_2 &= (kr_1)^{-1}\cos(kr_1)(1-\exp(-\varepsilon r_1))\phi(r_2).\end{aligned}\right\} \tag{25}$$

The last term is finite for r_1 tending to zero for any small value of ε. They calculate eigenvalues of the Hamiltonian, using the correlation wave function Φ. Let us call them λ_β where $\beta = 1, 2, \ldots, N$ for N terms in the closed channel function Φ. Projection of Φ_β onto the function ψ_T is given by

$$\langle \Phi_\beta | H - E | \Psi_T \rangle = 0. \tag{26}$$

If $E = -1 + k^2$ is chosen as $E = \lambda_\beta$, then it follows that

$$\tan\delta_T = -\langle \Phi_\beta | H - \lambda_\beta | \Psi_1 \rangle / \langle \Phi_\beta | H - \lambda_\beta | \Psi_2 \rangle. \tag{27}$$

From this equation, phase shifts can be determined easily because all the quantities are known. By suitable choice of nonlinear parameters in Φ, the closed channel wave function, we can get the desired values of k at which phase shifts are desired. The phase shifts obtained by Houston and Drachman [11] are also shown in Table II. We see that that their results are fairly accurate. They also calculated the scattering length for which they obtained $a = -2.10278a_0$ which is, not only in agreement with Schwartz's value $-2.10a_0$ [5], but it is an improvement over his result.

Positron scattering calculations by atomic hydrogen at intermediate energies have been carried out by Higgins, Burke and Walters [12]. They used the R-matrix formulation and calculated cross sections for $\boldsymbol{S}$, $\boldsymbol{P}$, $\boldsymbol{D}$ and $\boldsymbol{F}$ waves.

They have also calculated phase shifts at low energies for $\boldsymbol{S}$, $\boldsymbol{P}$, $\boldsymbol{D}$ and $\boldsymbol{F}$ waves. Their low energy results for $\boldsymbol{S}$ and $\boldsymbol{P}$ waves agree very well with those given in Tables II and III.

Kernoghan et al. [13] have calculated cross sections for positronium-formation, excitation and ionization of hydrogen atoms for positrons in the energy range 30 to 100 eV incident on atomic hydrogen. This is a 33-state close-coupling calculation. Their results, shown in Table V, agree very well with the measurements carried out by Zhou et al. [14]. The experimental results of ref. [14] are taken from ref. [13].

Table V. Total cross sections (πa_0^2) for positrons incident on hydrogen atoms

Enegy (eV)	Experiment	Theory
30	4.47±0.15	4.68
50	3.51±0.14	3.41
75	2.63±0.15	2.64
100	2.21±0.13	2.13

As we move to targets with several electrons, then there are no simple expressions for the target wave functions which can be used in the calculations. Houston and Drachman [11] carried out the scattering calculations by choosing different approximations of wave functions for the helium atom. They chose the one which gave them the best polarizability of the helium atom ($\alpha = 1.376a_0^3$). The wave function is given by

$$\varphi(r) = \exp(-zr) + c\exp(-2zr), \tag{28}$$

$$\Phi(r_1, r_2) = \varphi(r_1)\phi(r_2), \tag{29}$$

where $z = 1.4558$ and $c = 0.6$. Φ is the wave function of the helium atom.

Their results for $\boldsymbol{S}$-wave are shown in Table VI.

Using the Kohn variational principle, Humberston and Campeanu [15] have calculated $\boldsymbol{P}$-wave phase shifts. Their results are also shown in Table VI.

Phase shifts for the higher partial waves can be calculated by using the expression given above in Eq. (24).

Using the Kohn variational principle in the R-matrix code, Stein and Sternlicht [16] have also calculated phase shifts. Their results agree with the above results.

Kauppila et al. [17] have measured total cross sections for the scattering for positron-He and electron-He at various energies. They find that the two cross sections are very close to each other at high energies. At high energies, only the static interaction remains. Therefore, according to the first Born approximation, total cross sections for e^+-He and e^--He should be the same. This is borne out from the results of the measurements shown in Table VII.

Table VI. S- and P-wave positron-helium phase shifts obtained by Houston and Drachman [11], and Humberston and Campeanu [15], respectively

K	S-wave phase shifts [11]	P-wave phase shifts [15]
0.1	0.035	0.003
0.2	0.049	0.010
0.3	0.039	0.019
0.4	0.020	0.030
0.5	−0.003	0.041
0.6	−0.034	0.048
0.7	−0.069	0.054
0.8	−0.106	0.058
0.9	−0.143	0.061
1.0	−0.177	0.061
1.1	−0.211	

Table VII. Measured total cross sections (πa_0^2) for positron and electron scattering from He atoms measured by Kauppila et al. [17]

Energy (eV)	e^+-He	e^--He
50	1.27	1.97
100	1.16	1.26
150	0.967	0.987
200	0.796	0.812
300	0.614	0.621
500	0.437	0.434
600	0.371	0.381

4. Annihilation Parameter, Z_{eff}

Annihilation of positrons and electrons was mentioned in the beginning. This gives rise to a 511 keV line which has been seen in the Galactic center and also in solar flares. The partial cross section for annihilation of an incoming positron and an atomic electron with the emission of two gamma rays is given by

$$\sigma_a = Z_{\text{eff}} \alpha^3 k^{-1} (\pi a_0^2), \tag{30}$$

where α is the fine-structure constant and a_0 is the Bohr radius. It approaches Z, the charge of the nucleus when the positron is represented by a free particle, as indicated by Ferrell [18]. The general expression given by Ferrell is

$$Z_{\text{eff}} = \int\int d\vec{r}_1 d\vec{r}_2 |\Psi(\vec{r}_1,\vec{r}_2)|^2 \delta(\vec{r}_1,\vec{r}_2), \tag{31}$$

Bhatia et al. [19] have calculated Z_{eff} for $l = 0$ and 1, because they already had calculated the wave functions very accurately for these two partial waves. For higher partial waves they have given a formula from which this quantity can be calculated:

$$Z_{\text{eff}}(l>1) = 4\int drr^2 \exp(-2r)(1-j_0^2-3j_1^2), \tag{32}$$

$$Z_{\text{eff}}(l>1) = \frac{k^2}{1+k^2} + \frac{6}{k^2}\left(\frac{1}{k^2}\ln(1+k^2) - \frac{1+0.5k^2}{1+k^2}\right). \tag{33}$$

Their results are given in Table VIII. Drachman [20] has also calculated Z_{eff} for positron-hydrogen. His results are also given in Table VIII.

Table VIII. Z_{eff} for positron-H scattering

k	$Z_{\text{eff}}(0)$	$Z_{\text{eff}}(0)$ (ref. [20])	$Z_{\text{eff}}(1)$	Z_{eff} (> 1)	Z_{eff} (total)
0.1	7.363	7.5	0.022	<0.001	7.385
0.2	5.538	5.7	0.090	0.001	5.629
0.3	4.184	4.3	0.187	0.004	4.375
0.4	3.327	3.3	0.294	0.010	3.631
0.5	2.730	2.7	0.390	0.022	3.142
0.6	2.279	2.3	0.464	0.039	2.782
0.7	1.950	...	0.528	0.063	2.541

It is noticed that Z_{eff} decreases as the incident momentum increases. Bhatia et al. [19] compared their results for $l=0$ with those obtained by Humberston and Wallace [21]. The agreement is good, although it improves with increasing k.

There are no calculations of Z_{eff} from $2s$ and $2p$ levels of the hydrogen atom.

Up to now no experiments have been carried out for the scattering of positrons from the excited state of the hydrogen atom. For this reason, there has not been much incentive to study the scattering from the excited states and therefore no calculations of Z_{eff} from the excited states are available.

Calculation of Z_{eff} in helium has been carried out by Drachman [20]. Here Dirac rate corresponds to 2. These calculations were improved considerably by Humberston and Reeth [22] who calculated $Z_{\text{eff}} = 3.88 \pm 0.01$ at a low energy which agreed with the experimental result 3.94 ± 0.02 of Coleman et al. [23]. Humberston and Reeth [22] find that Z_{eff} decreases at first and then at some incident positron energy it starts increasing becoming very large at the threshold of the positronium formation.

Laricchia and Wilkins [24] indicated that at higher positron energies Z_{eff} is given by

$$Z_{\text{eff}} \propto |E - E_{\text{thr}}|^{-1}, \tag{34}$$

where E is the energy of the positron, $E_{\text{thr}} = I - |E_{1s}|$ and I is the ionization potential of the atom. The above expression indicates that Z_{eff} becomes infinite when $\boldsymbol{E}$ approaches the threshold. It was shown by Garbakin and Ludlow [25] that the correct dependence should be given by

$$Z_{\text{eff}} \propto |E_{\text{thr}} - E|^{-1/2}. \tag{35}$$

In this relation, E_{thr} must include the life time of positronium and then Z_{eff} is finite. This relation gives Z_{eff} which is continuous across the threshold. This relation was further confirmed by Igarashi, Kimamura and Shimamura [26].

5. Bound State of Positron-Hydrogen

There have been attempts to find the existence of the bound state of positron-hydrogen system. Most of the calculations found that the positron does not bind with hydrogen atoms. This was shown conclusively by Aronson, Kleinman and Spruch [27]. Rotenberg and Stein [28] concluded that if the mass of the positron is $2.2m_e$, then positron does bind with hydrogen atoms. But then it is not the antiparticle of the electron.

Mitroy et al. [29], using configuration type wave functions or correlated Gaussian functions, have shown that a positron binds to various atoms. They find that the polarization potential is an essential part of the Hamiltonian. The binding energy with various atoms is shown in Table IX.

Table IX. Binding energy (Ry) of positron with various atoms

He(^{3}S)	Li	Be	Na	Mg	Ca
0.0011848	0.004954	0.006294	0.000946	0.031224	0.03300
Sr	Cu	Ag	Cd		
0.0201	0.011194	0.011664	0.01220		

Binding energy with a Ca atom is the maximum and with Na the least. In the case of e^+Li and e^+Na, the systems can be described as Ps orbiting a charge Li$^+$ and Na$^+$, respectively. System like e^+Be consists of a positron orbiting a polarized Be atom. These systems decay with lifetime of 10^{-9} sec due to the annihilation of the electron with the positron.

Dzuba et al. [30, 31], combining a configuration-interaction treatment of the valence electron and positron, with many-body perturbation description of their interaction with atomic core, find the binding energies with copper, silver and gold atoms are 170, 200, 220 meV, respectively. Their method is a relativistic method. Their results agree very well with those of Mitroy et al. [29].

Gribakin, Young and Surko [32] have shown from the measurements that positrons bind to many molecular species. For low-energy positrons, Z_{eff} is very large and depends on the size of the molecule. For alkane $C_{12}H_{26}$ it is 9800000 and for aromatic $C_{10}H_8$ it is 1240000.

6. Resonances

Autoionization states are resonances caused by scattering of an electron or positron impinging on a target ion or atom. In the case of electrons in a target or ion, they can also be produced by photoabsorption as well as by heavy-particle collisions. Resonances have been studied in great details as a result of experimental and theoretical developments together with the advent of high speed computers. The resonances we are interested in are called doubly-excited-states or Feshbach resonances. They are doubly-excited states because the electron in the lower state is at the same time raised to the higher level. They are called Feshbach resonances because they have been studied in great detail by the use of Feshbach-projection operator formalism [7]. The resonance states decay after a while. Therefore, they have a finite life time and we need to calculate widths of these resonances.

Experimentally, they appear in the form of a discrete spectrum which is embedded in the continuum. If they are formed by the absorption of photons then they show up as a line in the absorption spectra.

Resonances in the electron-atom system are ubiquitous, and it has not been very difficult to calculate them. But in the case of positron-hydrogen scattering, it has not been easy. The first successful prediction of an S-wave resonance was made by Doolen, Nuttal and Wherry [33]. They used a sparse-matrix technique for large basis sets in the complex-coordinate rotation method. In this method, the radial coordinates are transformed by an angle θ:

$$r \to re^{i\theta}. \tag{36}$$

The transformed Hamiltonian is now given by

$$H = Te^{-2i\theta} + Ve^{-i\theta}. \tag{37}$$

Their wave function is given by

$$\Phi = \exp(-a(r_1 + r_2))L_l^{(0)}(u)L_m^{(0)}(v)L_n^{(0)}(w), \tag{38}$$

with $u = a(r_2 + r_{12} - r_1)$, $v = a(r_1 + r_{12} - r_2)$ and $w = 2a(r_1 + r_2 - r_{12})$. Here $L_l^{(0)}$ is a Laguerre polynomial and a is a positive nonlinear parameter.

They found one resonance below the excitation threshold and above the positronium pickup threshold. The complex energy is given by

$$E(\text{resonance}) = \text{Re}(E) + i\,\text{Im}(E) = \text{Re}(E) - i\Gamma/2. \tag{39}$$

In this method, Im(E) is plotted versus Re(E) and one looks for stationary paths as the angle θ is increased for various nonlinear parameters in the wave function, as discussed by Ho [34]. The results of Doolen et al. [33] are shown in Table X.

Table X. Position and width of the resonance

Number of terms	Re(E)	$\Gamma/2 = -\text{Im}(E)$
286	−0.2573744	0.0000676
364	−0.2573733	0.0000674
455	−0.2573745	0.0000671
560	−0.2573740	0.0000677
680	−0.2573741	0.0000677

They conclude that the resonance is at $E = -0.257374 - 0.000067i$ within an error of no more than 10^{-6} in each part.

A more extensive calculation to predict resonances below the higher thresholds has been carried out by Varga, Mitroy, Mezei and Kruppa [35]. Their results are shown in Table XI.

It used to be thought that there cannot be resonances in positron-He$^+$ system because of the repulsive potential between the incident particle and the target. Bhatia and Drachman [36] showed the existence of several resonances by using the stabilization method. This generated some controversy for and against this prediction. Later on Ho [37] proved the correctness of our results and also calculated the width of these resonances. His results, obtained using the complex rotation method, are given in Table XII.

Table XI. Positron-hydrogen resonances below $n = 2, 3$ and 4 thresholds

Threshold	Position	$\Gamma/2$
$H\ (n=2)$	-0.257244	0.000066
	-0.250262	0.0000048
$H\ (n=3)$	-0.116094	0.000642
	-0.112006	0.0001566
$H\ (n=4)$	-0.076958	0.0000394
	-0.067714	0.0000264
	-0.064380	0.00001688

Table XII. ***S***- and ***P***-resonances in e^+-He^+ scattering

	Position	$\Gamma/2$
S-wave	-0.74099	0.12943
	-0.3712	0.0393
P-wave	-0.70869	0.17752
	-0.36956	0.04317

7. Bound States of Positronium with Atoms

Mitroy et al. [29] have calculated the binding energy of Ps with various atoms. Their results are shown in Table XIII.

Table XIII. Binding energy (Ry) of Ps with various atoms

H	Li	Na	K	Cu
0.077834	0.024682	0.016838	0.006550	0.007482

Cheng, Babikov and Schrader [38] has given an expression to find the binding energies of positron with various atoms. The equation is written as

$$\gamma^2 = -0.2793V_i - 0.1466\alpha + 0.0238V_i\alpha + 03646N_s + 1.6757, \tag{40}$$

where N_s is the number of valance s electrons, V_i is the ionization potential in eV and α is the polarizability of the atom in Angstrom units. They have calculated binding to a number of atoms and their results are in fair agreement with those of Mitroy et al. [29].

8. Properties of Ps⁻ and Photodetachment

The positronium negative ion, consisting of two electrons and a positron, is particle stable and decays only by e^+ and e^- annihilation into gamma rays. The singlet state with a life of 1.244×10^{-10} sec decays into two gamma rays while the triplet state with a life time of 1.4205×10^{-7} sec decays into three gamma rays. Its existence was first predicted by Mohorovicic [39] in 1934. It was shown by Wheeler [40] in 1946 by a variational calculation that two electrons and a positron have a bound state.

Bhatia and Drachman [41] calculated its ground state (^{1}S) energy by using a trial function of the Hylleraas form given in Eq. (12). They had nonlinear parameters γ and δ and $\alpha = 0$ in Eq. (12). They calculated expectation values of delta functions, and cusp conditions as well and they are given by

$$\nu_i = \langle \delta(r_i) d/dr_i \rangle / \langle \delta(r_i) \rangle, \tag{41}$$

$$\nu_{12} = \langle \delta(r_{12}) d/dr_{12} \rangle / \langle \delta(r_{12}) \rangle, \tag{42}$$

Here r_1 and r_2 are the relative distances of electrons 1 and 2 with respect to the positron, and $r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$. The nonlinear parameter γ is equal to 0.604 for all values of $\boldsymbol{N}$. The results for the binding energies, expectation values of δ functions and cusp conditions are given in Table XIV.

Table XIV. Binding energy (Ry) of 1S state of Ps$^-$, expectation values δ functions and cusp conditions

N	δ	Binding energy	$\delta(r_i)$	$\delta(r_{12})$	ν_i	ν_{12}
120	0.296	0.024009966	0.020733	0.00017190	−0.5000	0.49347
165	0.314	0.024010079	0.020773	0.00017164	−0.4999	0.49441
220	0.313	0.024010113	0.020733	0.00017150	−0.5000	0.49508

The cusp quantities test the accuracy of wave functions near points of coalescence, since $\nu_1 = \nu_2 = -1/2$ and $\nu_{12} = +1/2$ for exact solutions of the Schrödinger equation. Our solutions are seen to be quite good.

In a later calculation, Bhatia and Drachman [42] obtained binding energy of Ps$^-$ equal to 0.0240101396 Ry for 615 terms in the wave function. Bhatia and Drachman [42] also calculated the relativistic correction -6.25×10^{-6} Ry. Therefore, the nonrelativistic energy is lowered by this amount.

To a sufficient accuracy, the Ps$^-$ decay rate is

$$\begin{aligned}\Gamma &= 2\pi\alpha^4(c/a_0)[1-\alpha(17/\pi - 19\pi/12)]\langle\delta(\vec{r}_1)\rangle \\ &= 100.6174\langle\delta(r_1)\rangle \text{ nsec}^{-1}.\end{aligned} \tag{43}$$

In the above equation, the correction term proportional to α is due to the triplet lifetime and the leading correction to the singlet lifetime. Inserting the expectation value of the δ function, we obtain the decay rate $\Gamma(\text{nsec})^{-1} = 2.0861$. This is in agreement with the measured value $\Gamma = 2.09 \pm 0.09(\text{nsec})^{-1}$, obtained by Mills [43].

Mills [43] suggested that Ps$^-$ ions could be used to generate positronium (Ps) beams of controlled energy; this would involve acceleration of Ps$^-$ ions and photodetachment of one electron. Bhatia and Drachman [44] calculated the dipole transition matrix elements by two simplifications: the initial state is represented by an asymptotic form whose normalization comes from our accurate Ps$^-$ wave function and the final state is a plane wave. They find that the cross section in the length and velocity form can be written as

$$\sigma_L = \sigma_V = (1.32 \times 10^{18}\,\text{cm}^2)\frac{k^3}{(k^2+\gamma^2)^3}, \tag{44}$$

where k is the momentum of the outgoing electron and $\gamma^2 = 0.024010113$ Ry is the binding energy of Ps^-, which is given in in Table XIV.

A scattering calculation for the final state has been carried out by Ward, Humberston and McDowell [45] to calculate the photodetachment of Ps^-. The results obtained in their calculations agree very well with those of Bhatia and Drachman [44].

9. PsH

This system, called positronium hydride, consists of a positron, two electrons and a proton. The hydrogen atom has only ^{1}S bound state but no triplet states. Therefore, positronium and hydrogen atom can form a bound state with ^{1}S state only of the hydrogen atom. The most accurate value for its total energy has been obtained by Ho [46] is −1.57505 Ry. He used correlated functions of modified Hylleraas type, involving the six inter-particle coordinates. The system is stable against dissociation into Ps+H and has a binding energy 1.021 eV.

This system can also be viewed as a positron $+H^-$ system. Then PsH must have an infinite number of bound states because of the Coulomb field between the positron and the hydrogen ion. But because of the Ps+H open channel, these states become resonances. Using a wave function in the Hartree-Fock approximation

$$\Psi_{HF} = G(x)\Phi_{H^-}(1,2). \tag{45}$$

Drachman and Houston [47] obtained the first $\boldsymbol{S}$-wave resonance parameters:

$$E_R = -1.1726 \pm 0.0007 \text{ Ry}, \tag{46}$$

$$\Gamma = (4.6 \pm 1.1) \times 10^{-3} \text{ Ry}. \tag{47}$$

The resonance parameters were also calculated by Ho [46] using the complex-rotation method. His results are given below

$$E_R = -1.205 \pm 0.001 \text{ Ry}, \tag{48}$$

$$\Gamma = (5.5 \pm 2.0) \times 10^{-3} \text{ Ry}. \tag{49}$$

The resonances have coupling with the continuum. Di Rienzi and Drachman [48] carried out a calculation for $\boldsymbol{L} = 1$ resonance where both the open and closed channels are included. Using their notation, the wave function is given by

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{x}) = F(\vec{R}_1)\varphi(\rho_1)\psi(r_2) + F(\vec{R}_2)\varphi(\rho_2)\psi(r_1) + G(\vec{x})\Phi(\vec{r}_1,\vec{r}_2). \tag{50}$$

In the above equation $\vec{r}_1$ and $\vec{r}_2$ are the position vectors of the two electrons relative to the proton taken as fixed at the origin, and $\bar{x}$ is the position vector of the positron. The center of mass of the Ps and its internal coordinates are

$$R_1 = (\bar{r}_1 + \vec{x})/2, \qquad R_2 = (\bar{r}_2 + \vec{x})/2, \tag{51}$$

$$\rho_1 = \bar{x} - \bar{r}_1, \qquad \rho_2 = \bar{x} - \bar{r}_2. \tag{52}$$

The internal coordinates of H and Ps atoms are known exactly and their wave functions are given by

$$\psi(r) = e^{(-r)}/\sqrt{\pi} \tag{53}$$

and

$$\varphi(\rho) = e^{(-\rho/2)}/\sqrt{8\pi}. \tag{54}$$

The function $F(\vec{R})$ represents Ps-H scattering. Both atoms are in unexcited states and $G(\vec{x})$ is the wave function of the positron bound to ^{1}S state of the hydrogen ion. The nonrelativistic Hamiltonian is given by

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_x^2 + 2/x + 2/r_{12} - 2/r_1 - 2/r_2 - 2/\rho_1 - 2/\rho_2. \tag{55}$$

They obtained an optical potential equation variationally for the scattering function $F(\vec{R})$ which includes exchange and the coupling between the closed and open channels. That equation with the optical potential is given below:

$$-\frac{1}{2}[\nabla^2 + k^2]F(\vec{R}) + \int d\bar{R}' K(\vec{R},\vec{R}')F(\vec{R}') + 2\sum_n \frac{V_n(\vec{R})\int d\bar{R}' V(\vec{R})F(\vec{R})}{E - E_{H^-} - \varepsilon_n} = 0, \tag{56}$$

$$E_{H^-} = -1\,\mathrm{Ry}, E_{Ps} = -1/2\,\mathrm{Ry}, \quad k^2 = 2(E - E_{Ps} - E_H) = (2E + 3)\,\mathrm{Ry}. \tag{57}$$

The exchange Kernel K and V_n have been discussed in the paper by Di Rienzi and Drachman [48].

Their calculations are rather complicated. By including $2p$ and $3p$ states of hydrogen atom, they obtained in Ry units

$$E_R = 0.3287, \quad \Gamma = 0.00060, \tag{58}$$

which compares well with the results obtained by Yan and Ho [49], and Ho and Yan [50]:

$$E_R = 0.3149, \quad \Gamma = 0.0032. \tag{59}$$

In another paper, Di Rienzi and Drachman [51] have investigated D state resonances and their results are given in Table XV.

Table XV. D states in PsH. The results are in eV

States	Energy	Γ
$E_1(3d)$	4.708	0.394
$E_1(3d + 4d)$	4.729	0.327
E_1 [49]	4.710 ± 0027	0.0925 ± 0.0054

In the above table, the first row indicates energy of the first resonance when only $3d$ state is included and the second row indicates how it changes when $3d$ and $4d$ states are included together. The last row indicates the results obtained by Yan and Ho [49].

Table XVI. Ps-H scattering cross sections (πa_0^2)

Energy(eV)	Cross section
0.068	48.3
0.272	36.2
0.612	27.3
1.088	22.4

Calculations for Ps-H scattering, using a projectile elastic close-coupling approximation, have been carried out by Ray and Ghosh [52]. They calculate $\boldsymbol{S}$-, $\boldsymbol{P}$- and $\boldsymbol{D}$-waves phase shifts. Some of their results for total cross sections are given in Table XVI.

Ray [53] has carried out calculations for Ps-Li scattering using three approximations: first Born and static-exchange approximation and two-state close-coupling approximation. The long-range dipole correlation takes into account the $2p$ state of lithium. The equations were solved in momentum space. Total elastic cross sections for the scattering in the three approximations are given in Table XVII. The results obtained in different approximations are very close to each other.

Table XVII. Total elastic cross sections (πa_0^2) for Ps-Li scattering

Energy(eV)	First born	Static-exchange	Close-coupling
30	0.258	0.259	0.265
35	0.186	0.186	0.187
40	0.136	0.135	0.135
50	0.765	0.763	0.756
70	0.298	0.298	0.295
100	0.103	0.103	0.102

She has also calculated cross sections for excitation of the lithium atoms to the $2p$ state. She finds no structure when the first Born approximation is used. However, there is a minimum at 15 eV and a maximum at 20 eV incident energies when two-state close-coupling approximation is used.

10. Conclusions

In this article, I have tried to discuss various processes involving interactions of positrons with atoms and ions. This includes scattering, bound states and resonances. It has not been possible to include the enormous work which has been carried out during the last 40 or 50 years in theory and measurements.

Acknowledgement

I would like to extend my thanks to Dr. R.J. Drachman for helpful suggestions and critical reading of the manuscript.

Competing Interests

The author declare that they have no competing interests.

Authors' Contributions

Author contributed significantly in writing this article. The author read and approved the final manuscript.

References

[1] P. A. M. Dirac, Proceedings of the Royal Society A **126**, 360 (1930).

[2] P. A. M. Dirac, in *The Development of Quantum Theory*, Gordon and Breach Science Publishers, 1971, p. 59.

[3] C. D. Anderson, Phys. Rev. **43**, 491 (1933).

[4] R. W. Bussard, R. Ramaty and R. J. Drachman, Ap. J. **228**, 928 (1979).

[5] C. Schwartz, Phys. Rev. **124**, 1468 (1961).

[6] A. K. Bhatia, Temkin, R. J. Drachman and H. Eiserike, Phys. Rev. A **3**, 1328 (1971)

[7] H. Feshbach, Ann. Phys. (N.Y.) **19**, 287 (1962).

[8] A. K. Bhatia, A. Temkin and H. Eiserike, Phys. Rev. A **9**, 219 (1974).

[9] R. L. Armstead, Phys. Rev. **171**, 91 (1968).

[10] J. M. Wadehra, J. Phys. B. **19**, L761 (1986).

[11] S. K. Houston and R. J. Drachman, Phys. Rev. A **3**, 1335 (1971).

[12] K. Higgins, P. G. Burke and H. R. J. Walters, J. Phys. B **23**, 1345 (1990).

[13] A. A. Kernoghan, D. J. R. Robinson, M. T. McAlinden and H. R. J. Walters, J. Phys. B. **29**, 2089 (1996).

[14] S. Zhou, H. Li, W. E. Kauppila, C. K. Kwan and T. S. Stein, Phys. Rev. A **55**, 361 (1997).

[15] J. W. Humberston and R. I. Campeanu, J. Phys. B.**13**, 4907 (1980).

[16] J. Stein and R. Sternlicht, Phys. Rev. A **6**, 2165 (1972).

[17] W. E. Kauppila, T. S. Stein, J. H. Smart, M. S. Debabneh, Y. K. Ho, J. P. Dawning and V. Pol, Phys. Rev. A **24**, 725 (1981).

[18] R. A. Ferrell, Rev. Mod. Phys. **28**, 308 (1956).

[19] A. K. Bhatia, R. J. Drachman and A. Temkin, Phys. Rev. A **9**, 223 (1974); **16**, 1719 (1977).

[20] R. J. Drachman, Phys. Rev. **150**, 10 (1966).

[21] J. W. Humberston and J. B. G. Wallace, J. Phys. B **5**, 1138 (1972).

[22] J. W. Humberston and P. Van. Reeth, Nucl. Instr. and Methods in Phys. Res. B **143**, 127 (1998).

[23] P. G. Coleman, T. C. Griffith, G. R. Heyland and T. L. Killeen, J. Phys. B **16**, 406 (1983).

[24] G. Laricchia and C. Wilkin, Phys. Rev. Lett. **79**, 2241 (1997).

[25] G F. Gribakin and J. Ludlow, Phys. Rev. Lett. **88**, 1632021 (2002).

[26] A. Igarashi, M. Kimura and I. Shimamura, Phys. Rev. Lett. **89**, 1232011 (2002).

[27] I. Aronson, C. Kleinman and L. Spruch, Phys. Rev. A **4**, 841 (1971).

[28] M. Rotenberg and J. Stein, Phys. Rev. **821**, 1 (1969).

[29] J. Mitroy, M. W. J. Bromley and G. G. Ryzhikh, J. Phys. B **35**, R81 (2002).

[30] V. A. Dzuba, V. V. Flambaum, G. F. Gribakin and C. Harabati, Phys. Rev. A **60**, 3641 (1999).

[31] V. A. Dzuba, V. V. Flambaum and C. Harabati, Phys. Rev. A **62**, 042504 (2000).

[32] G. F. Gribakin, J. A. Young and C. M. Surko, Rev. Mod. Phys. **82**, 2557 (2010).

[33] G. D. Doolen, J. Nuttal and C. J. Wherry, Phys. Rev. Lett. **40**, 313 (1978).

[34] Y. K. Ho, Phys. Rept, **99**, 1 (1983).

[35] K. Varga, J. Mitroy, J. Zs.Mezei and A. T. Kruppa, Phys. Rev. A **77**, 044502 (2008).

[36] A. K. Bhatia and R. J. Drachman, Phys. Rev. A **42**, 5117 (1990).

[37] Y. K. Ho, Phys. Rev. A **53**, 3165 (1996).

[38] X. Cheng, D. Babikov and D. M. Schrader, Phys. Rev. A **83**, 032504 (2011).

[39] S. Mohorovicic, Astron. Nuchr. **253**, 93 (1934).

[40] J. A. Wheeler, Ann. NY Acad. Sci. **48**, 221 (1946).

[41] A. K. Bhatia and R. J. Drachman, Phys. Rev. A **28**, 2523 (1983).

[42] A. K. Bhatia and R. J. Drachman, Nucl. Instr. and Methods in Phys. Res. B **143**, 195 (1998).

[43] A. P. Mills Jr. Phys. Rev. Lett. **46**, 717 (1981); **50**, 671 (1983).

[44] A. K. Bhatia and R. J. Drachman, Phys. Rev. A **32**, 3745 (1985).

[45] S. J. Ward, J. W. Humberston and M. R. C. McDowell, J. Phys. B **18**, L525 (1985).

[46] Y. K. Ho, Phys. Rev. A **17**, 1675 (1978).

[47] R. J. Drachman and S. K. Houston, Phys. Rev. **12**, 885 (1975).

[48] J. Di Rienzi and R. J. Drachman, Phys. Rev. A **65**, 032721 (2002).

[49] Z.-C. Yan and Y. K. Ho, J. Phys. B **31**, L877 (1998).

[50] Y. K. Ho and Z.-C, Yan, J. Phys. B **31**, L877 (1998).

[51] J. Di Rienzi and R. J. Drachman, Phys. Rev. A **66**, 054702 (2002).

[52] H. Ray and A. S. Ghosh, J. Phys. B **31**, 4427 (1998).

[53] H. Ray, J. Phys. B. **32**, 5681 (1999).