

POSITRON—ATOM BOUND STATES AND INTERACTIONS

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Some recent progress in theoretical investigations of the interactions of low-energy positrons with atoms is presented. The emphasis being on studies of the positronic atoms, ie. atoms that are known to form electronically stable bound states with a positron. A variety of computational methods, configuration interaction, a hybrid configuration-interaction-Kohn, and hyperspherical close-coupling methods have been used to investigate a variety of phenomena. These include the structure of positron-atom bound states, elastic positron-atom scattering, in-flight annihilation and positronium formation during positron-atom scattering.

1. Introduction

The interactions of low-energy positrons with atoms provides a host of problems for both experimentalists and theorists alike ¹. Even for one of the most fundamental problems in positron physics, whether a positron can form an electronically stable bound state with a neutral atom, the first universally accepted calculation of positron binding to a neutral atom (lithium) was only performed in 1997 ^{2,3}.

This paper reviews some of our theoretical progress in understanding low-energy positron-atom physics post-2002 when two of the present au-

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thors published a review ⁴ of the known positronic atoms ($e^+\text{He}(^3S_e)$, $e^+\text{Li}$, $e^+\text{Be}$, $e^+\text{Mg}$, $e^+\text{Ca}$, $e^+\text{Cu}$, $e^+\text{Zn}$, $e^+\text{Sr}$, $e^+\text{Ag}$ and $e^+\text{Cd}$). A ‘positronic atom’ has still not been demonstrated experimentally, but this research is partly motivated by the concurrent experimental progress due to the “Surko” positron trap, which is able to produce pulsed cold positron beams with Energies < 500 meV and widths < 25 meV ¹.

A number of computational methods have been applied to study positronic atoms ⁴, such as stochastic variational methods (SVM) ⁵, many-body perturbation theory ^{6,7,8}, and quantum Monte-Carlo ⁹ methods. The configuration-interaction (CI) method has become one of the more successful approaches, despite its particular challenges, and we report here on some improved CI calculations of the structures of various positronic atoms ^{10,11}. We also report on studies of positron-atom annihilation using a hybrid CI-Kohn variational scattering method ^{12,13}. Finally, we discuss the results of multi-channel hyperspherical close-coupling (HSCC) calculations for positron scattering from sodium in the low-energy range ¹⁴.

2. CI calculations of positron-atom interactions

The presence of localised electron-positron pairing means that all positron-atom calculations are extremely demanding. The LS -coupled CI wavefunction looks like

$$\Psi_{LS} = \sum_{I=1}^{N_{CI}} c_I \phi_\alpha(\mathbf{r}_0) \phi_\beta(\mathbf{r}_1) \dots \phi_\omega(\mathbf{r}_N), \quad (1)$$

where \mathbf{r}_0 is the positron, and $\mathbf{r}_{>0}$ are the electron/s co-ordinates. Antisymmetry for the electron orbitals and the Clebsch-Gordan coefficients are both implied. The fundamental problem facing CI methods is that, when expanding a wavefunction with single-particle orbitals, viz.

$$\phi_i(\mathbf{r}) = P_{i,\ell_i}(r) Y_{\ell_i,m_i}(\hat{\mathbf{r}}), \quad (2)$$

to accurately represent the CI wavefunction requires the inclusion of a large number of radial functions and partial-waves. Predominantly Laguerre type orbitals (LTOs) are employed to ensure radial basis orthogonality.

The CI calculations are performed in the frozen-core approximation, where the valence-frozen core electron interactions are treated exactly. This is based on Hartree-Fock core orbitals with additional core polarisation potentials; a $V_{p1}(r_i)$ is semi-empirically tuned to reproduce the $1e^-$ spectrum, and a di-electronic term $V_{p2}(\mathbf{r}_i, \mathbf{r}_j)$ is also included. The CI method requires

the diagonalisation of large matrices, towards 10,000 for e^+/e^- systems, and towards 500,000 for the sparse matrices of the $e^+/2e^-$ systems. These procedures are covered in detail elsewhere¹⁵.

The CI-Kohn method is a natural extension of the CI method¹², requiring the addition of long-range Bessel and Neumann orbitals which are orthogonalised against the short-range CI basis. The CI-Kohn method, in the end, requires solving a large set of linear equations. Table 1 shows the convergence of the s -wave phase shifts and annihilation parameter, $Z_{\text{eff}}(k)$ from a series of CI-Kohn calculations of low-energy positron-hydrogen scattering at $k = 0.4 a_0^{-1}$ with the inclusion of orbitals up to a maximum angular momentum J , and including a minimum of 25 LTOs per ℓ .

Table 1. Results of CI-Kohn calculations of low-energy elastic e^+ -H scattering $k = 0.4 a_0^{-1} \approx 2.2$ eV. The s -wave phase shifts $\langle \delta_0 \rangle$ and annihilation parameter $\langle Z_{\text{eff}}^0 \rangle$ are given for a series of calculations J .

J	N_{CI}	$\langle \delta_0 \rangle$	$\langle Z_{\text{eff}}^0 \rangle$	J	N_{CI}	$\langle \delta_0 \rangle$	$\langle Z_{\text{eff}}^0 \rangle$
0	1010	-0.19921	0.453	10	8786	0.11660	2.699
1	2954	-0.01003	1.017	11	9411	0.11730	2.749
2	3786	0.05338	1.465	12	10036	0.11781	2.792
3	4411	0.08173	1.796	Variational ^{16,17}		0.1201	3.327

The convergence of both the phase shifts and Z_{eff} is currently being examined in detail elsewhere¹⁰ for both CI and CI-Kohn calculations. The slow-convergence with J in Table 1 towards the variational limit is typical of partial-wave expansions, and is seen to be quite severe for even simple systems (e^+ -H scattering).

There are a variety of extrapolation methods to estimate the partial-wave increments to any expectation value ΔX^J where $J > J_{\text{max}}$ ^{18,10}. Some of these methods follow Gribakin and Ludlow¹⁹ who used perturbation theory to show that the asymptotic forms scale as $\Delta X^J \propto (J + \frac{1}{2})^{-p}$, where for energy $p_E = 4$ and annihilation rates scale even slower ($p_Z = 2$). For a given CI calculation, the asymptotic region is not reached, and alternate methods are required. One of the best methods¹⁸, labelled in Figure 1, is based on the two-term form:

$$\Delta Z_{\text{eff}}^J = \frac{A_Z}{(J + \frac{1}{2})^2} + \frac{B_Z}{(J + \frac{1}{2})^3}. \quad (3)$$

the results of this and four other methods are shown in Figure 1. Reliable estimates can be obtained of positron-atom systems using large-scale CI calculations when combined with careful extrapolation.

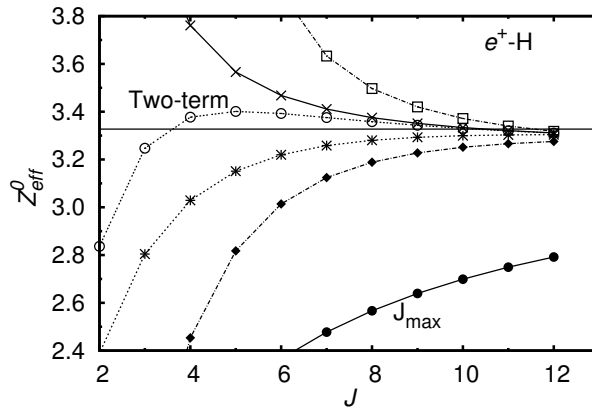


Figure 1. Five different CI extrapolation methods of extrapolating the positron-hydrogen scattering Z_{eff} data of Table 1. The explicit CI calculations are marked as J_{max} . The method marked as two-term corresponds to Eqn.3.

3. CI calculations of positron-atom bound states

The positronic atom system which has had the most number of estimates computed for its binding energy is $e^+\text{Mg}$, some of which are seen in Table 2. The extrapolated CI results are in good agreement with the older fixed-core SVM results. New calculations of the alkaline-earth metal positronic atoms

Table 2. Results of various calculations of $e^+\text{Mg}$.

Method	ε (hartree)	$\langle r_e \rangle$ (a_0)	$\langle r_p \rangle$ (a_0)	Γ_v (10^9 sec^{-1})
CI $J = 12$	0.01542	3.405	7.040	0.6127
CI $J = \infty$	0.01667	3.443	6.957	0.9267
FCSVM ⁴	0.01561	3.437	7.018	0.943
DMC ⁹	0.0168(14)	—	—	—
MBPT ⁶	0.0362	—	—	—

are underway ¹¹ with parallelised code allowing for an order of magnitude more configurations than our previous calculations ²⁰.

Interim results of positron binding to the alkaline-earth metal atoms Ca and Sr ¹¹ are shown here graphically in Figure 2 alongside the present best estimates of the known positronic atom binding energies. Figure 3 shows the known positronic atom annihilation rates. The dotted lines are from calculations of positron binding to a model alkali atom ⁴.

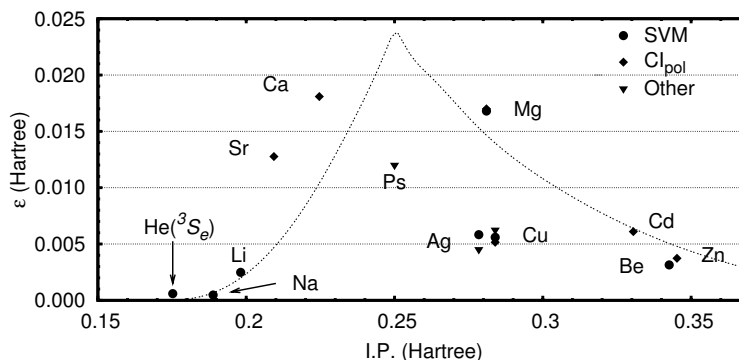


Figure 2. Positronic atom binding energies against dissociation as a function of the atomic ionisation potential.

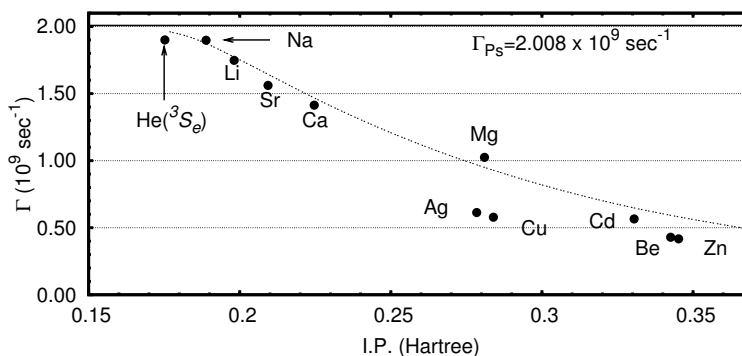


Figure 3. Spin-averaged annihilation rates Γ_v as a function of ionisation potential.

4. CI calculations of positron-atom annihilation

The CI-Kohn method was implemented to investigate low-energy *elastic* positron scattering from the one-electron atoms, H and Cu ¹², and the one-electron ions, He⁺, Li²⁺, B⁴⁺ and F⁸⁺ ¹³. The crucial parameter obtained from the CI-Kohn wavefunctions is the annihilation parameter, $Z_{\text{eff}}(k)$, at energies below the first inelastic threshold.

The threshold behaviour of e^+ -Cu scattering was of primary interest to show that the presence of a bound state does not imply a massive Z_{eff} . The CI-Kohn method found $Z_{\text{eff}} = 73$ at threshold, and the behaviour with k is shown in Figure 4. A secondary consideration was that for some systems; the noble gases, alkanes, and F/Cl/Br substituted alkanes, a semi-

empirical scaling exists²¹. This scaling implies a huge Z_{eff} for the Group II metal vapours, which is not the case for Cu. Figure 4 also shows a p -wave interaction on the verge of forming a shape resonance, resulting in a p -wave Z_{eff}^1 that can exceed that of the s -wave.

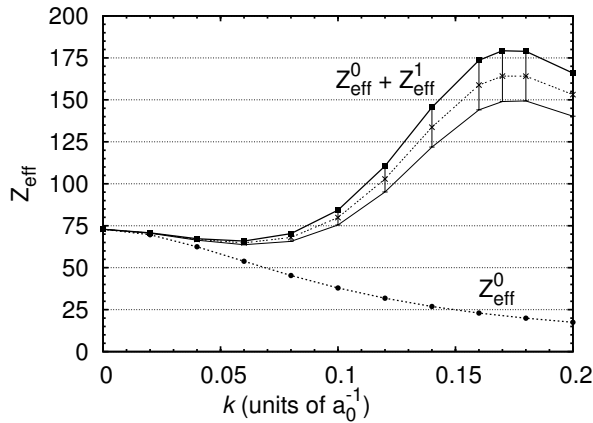


Figure 4. Annihilation parameter Z_{eff} for e^+ -Cu scattering. The p -wave contribution has a significant extrapolated component, hence three estimates are plotted.

Elastic positron-positron scattering was performed partly because of suggestions to use positive ions to cool positrons¹³. Whilst previous calculations have looked at the phase shifts, these are the first annihilation calculations. Figure 5 shows that Z_{eff} is generally negligible. In particular, for a 300K thermal e^+ swarm ($k \approx 0.05 a_0^{-1}$) with He^+ $Z_{\text{eff}}^{(0)} \approx 10^{-51}$. This means that e^+ - Atomⁿ⁺ cooling schemes can effectively ignore annihilation.

5. Ps-formation during e^+ -Na scattering

Our HSCC calculations were motivated by a recent experiment that measured the positronium (Ps) formation cross sections²² (ie. of an electron undergoing charge transfer from the atom to the positron during the collision). This experiment found strong disagreement with close-coupling (CC) calculations^{23,24} for energies near and below 1 eV. Speculation arose in Ref.²² that the calculations were not converged as sodium was later shown to be a positronic atom.

Our Ps-formation results for sodium, as shown in Figure 6, find broad

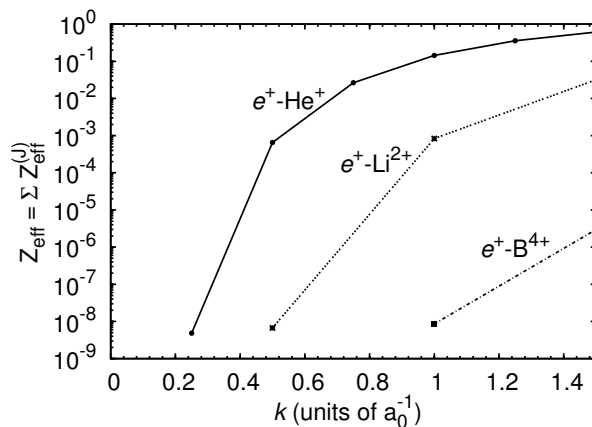


Figure 5. Annihilation parameter Z_{eff} for e^+ - Atom $^{n+}$ scattering, note that the lines are drawn through the computed data points to give the general trend.

agreement with previous CC calculations^{23,24} and disagreement with the experimental data below 2 eV²². The accurately-known Ps-Na⁺ scattering length is reproduced by our calculations, and hence, our low-energy results are reliable. Experiment needs to revisit the sub $E = 2$ eV region.

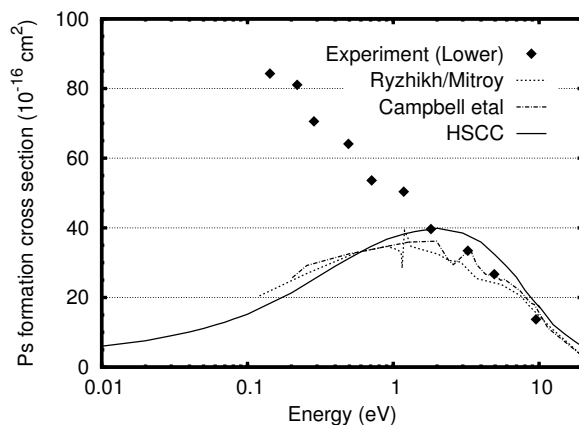


Figure 6. Ps-formation cross sections during e^+ -Na scattering.

6. Conclusions

The difficulties in computing positron-atom interactions are enough to have any sensible-minded theorist running in the other direction. We, instead, have employed a variety of methods to tackle specific problems, in the process gaining an improved understanding of the nature of the few-body interactions involving positrons and atoms.

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References

1. C. M. Surko, G. F. Gribakin, and S. J. Buckman, *J. Phys. B* **38**, R57 (2005).
2. G. G. Ryzhikh and J. Mitroy, *Phys. Rev. Lett.* **79**, 4124 (1997).
3. K. Strasburger and H. Chojnacki, *J. Chem. Phys.* **108**, 3218 (1998).
4. J. Mitroy, M. W. J. Bromley, and G. G. Ryzhikh, *J. Phys. B* **35**, R81 (2002).
5. G. G. Ryzhikh, J. Mitroy, and K. Varga, *J. Phys. B* **31**, 3965 (1998).
6. V. A. Dzuba, V. V. Flambaum, G. F. Gribakin, and W. A. King, *Phys. Rev. A* **52**, 4541 (1995).
7. V. A. Dzuba, V. V. Flambaum, G. F. Gribakin, and C. Harabati, *Phys. Rev. A* **60**, 3641 (1999).
8. G. F. Gribakin and J. Ludlow, *Phys. Rev. A* **70**, 032720 (2004).
9. M. Mella, M. Casalegno, and G. Morosi, *J. Chem. Phys.* **117**, 1450 (2002).
10. M. W. J. Bromley and J. Mitroy, in preparation.
11. M. W. J. Bromley and J. Mitroy, in preparation.
12. M. W. J. Bromley and J. Mitroy, *Phys. Rev. A* **67**, 062709 (2003).
13. S. A. Novikov, M. W. J. Bromley, and J. Mitroy, *Phys. Rev. A* **69**, 052702 (2004).
14. A. T. Le, M. W. J. Bromley, and C. D. Lin, *Phys. Rev. A* **71**, 032713 (2005).
15. M. W. J. Bromley and J. Mitroy, *Phys. Rev. A* **65**, 012505 (2002).
16. A. K. Bhatia, A. Temkin, R. J. Drachman, and H. Eiserike, *Phys. Rev. A* **3**, 1328 (1971).
17. A. K. Bhatia, R. J. Drachman, and A. Temkin, *Phys. Rev. A* **9**, 223 (1974).
18. M. W. J. Bromley and J. Mitroy, in preparation.
19. G. F. Gribakin and J. Ludlow, *J. Phys. B* **35**, 339 (2002).
20. M. W. J. Bromley and J. Mitroy, *Phys. Rev. A* **65**, 062505 (2002).
21. T. J. Murphy and C. M. Surko, *Phys. Rev. Lett.* **67**, 2954 (1991).
22. E. Surdutovich, J. M. Johnson, W. E. Kauppila, C. K. Kwan, and T. S. Stein, *Phys. Rev. A* **65**, 032713 (2002).
23. G. G. Ryzhikh and J. Mitroy, *J. Phys. B* **30**, 5545 (1997).
24. C. P. Campbell, M. T. McAlinden, A. A. Kernoghan, and H. R. J. Walters, *Nucl. Instrum. Methods Phys. Res. B* **143**, 41 (1998).