

Excited, bound and resonant positron-atom systems

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Abstract. Calculations have demonstrated that eleven neutral atoms can bind positrons, while many more can bind positronium. This is a short review of recent progress made in understanding some of the underlying mechanisms. The emphasis here being on configuration interaction calculations with excited state configurations. These have demonstrated the existence of a $^2\text{P}^\circ$ excited state of $e^+\text{Ca}$, which consists predominantly of a positronium cluster orbiting the Ca^+ ion in the $L = 1$ partial wave. Preliminary results are presented of excited state positron binding to a model alkali atom, where the excited $^1\text{P}^\circ$ states are stable over a limited region. Implications for the unnatural parity, $^{2,4}\text{S}^\circ$, states of PsH , LiPs , NaPs and KPs are also discussed. The $e^+\text{Mg}$, $e^+\text{Cu}$, $e^+\text{Zn}$ and $e^+\text{Cd}$ systems show a lack of a $^2\text{P}^\circ$ excited state, each instead possessing a low-energy p -wave shape resonance of varying strength.

1. Introduction

Whilst a ‘positronic atom’ remains to be observed experimentally, calculations over the past decade, or so, have conclusively demonstrated that a wide-range of atomic systems can bind to positrons. This article highlights the progress made in our understanding of some of the underlying mechanisms involved since a review was published by the present authors in 2002 [1]. The emphasis here is on the insights gained from a series of large-scale configuration interaction (CI) and stochastic variational method (SVM) calculations that have been applied to various bound state systems and their scattering brethren with excited state configurations.

Preliminary results are presented of excited state positron binding to a model alkali atom. The ground $^1\text{P}^\circ$ states are shown to be stable over a limited range of ionisation potentials, while the excited $^1\text{S}^\circ$ and the ground $^1\text{P}^\circ$ states appear to be unstable. These calculations were motivated, in part, by the Surko group measurements of positron binding energies in molecules which show extraordinary agreement with the atomic trend for the ground state $^1\text{S}^\circ$ model alkali atom [2]. The precise measurements have enabled the development of an empirical model that predicts ground state energies [3], and have guided a simple computational model that predicts the emergence of the second bound state with a node along the molecular axis at around the same energies as the experiment [4, 2].

2. Positron-atom binding mechanisms

The heuristic model for positron binding to atoms is simply based on the ionisation potential of the atom [5]. This dictates to what extent the positron can draw the electron outwards, thereby

polarising the atom. A positron-atom wavefunction can be schematically represented as [6, 7, 8]

$$\Psi = c_0 \Phi(\text{Atom})\phi_{e^+}(\mathbf{r}_p) + c_1 \Omega(\text{Atom}^+)\omega_{\text{Ps}}(\mathbf{R}_{\text{Ps}}) + c_2 \Xi(\text{Atom}^{2+})\xi_{\text{Ps}^-}(\mathbf{R}_{\text{Ps}^-}) + \dots \quad (1)$$

where the three components shown here represent a positron orbiting a polarised atom at a distance \mathbf{r}_p , a polarised positronium (Ps) cluster orbiting the residual atomic ion at \mathbf{R}_{Ps} , and even a polarised positronium ion (Ps^-) cluster orbiting the atomic ion at \mathbf{R}_{Ps^-} .

For the systems so far known to bind, being the group I/IB and group II/IIB atoms, only one or two electrons are active. The current best estimates of positron-atom binding energies are summarised in Figure 1. Shown in the figure is the result of a $^1\text{S}^e$ model positronic alkali atom, where an additional local potential acts on the valence electron only [5]. This provides a tuning-knob that changes the ionisation potential of the atom. This is discussed further shortly.

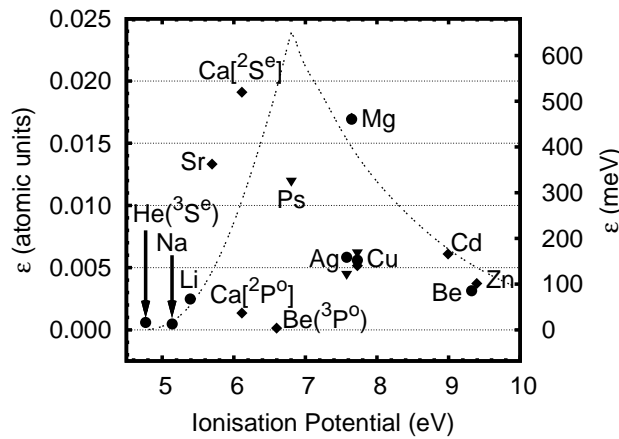


Figure 1. Theoretical e^+ -atom binding energies versus the parent atomic ionisation energy [1]. The \bullet were computed with the SVM, the \blacklozenge are CI_{pol} -based, the \blacktriangle are other calculations. The total $2S+1L\pi$ symmetries are implicit: the one- e^- atoms are $^1\text{S}^e$, the two- e^- atoms are of $^2\text{S}^e$. The (...) indicate the excited parent state symmetry, the [...] are the overall symmetry. The line is a model $^1\text{S}^e$ e^+ -alkali atom system [5].

Each positronic atom wavefunction generally consists of a significant Ps-fraction when the ionisation potential lies to the left of the Ps atom energy $E_{\text{Ps}} = 6.8$ eV. The computational representation of either a localised Ps cluster (or a significant component of Ps^-) in a wavefunction is computationally demanding [1]. In the extreme case of CI calculations of the $^1\text{S}^e$ $e^+\text{Li}$ system, which has only one active electron, orbitals with angular momentum of up to $\ell = 30$ were required to demonstrate binding [9].

3. Excited state positron-atom binding mechanisms

Despite the computational challenges, the existence of a $^2\text{P}^o$ excited state of $e^+\text{Ca}$ has been demonstrated. The structure consists predominantly of a Ps cluster orbiting the residual Ca^+ ion in the $L = 1$ partial wave [10]. This raises the possibility of detecting the formation of positronic bound states by an optical ($^2\text{P}^o \rightarrow ^2\text{S}^e$) transition between the $e^+\text{Ca}$ states [11]. There is also the possibility of performing a far more challenging experiment using a low-energy Ps-beam scattering off Ca where $E_{\text{Ps}} > 5.619$ eV produces charge transfer [10].

A large set of model CI calculations were undertaken to examine the systematics of excited states with $L = 1$. The Hamiltonian was chosen to be identical to that used previously for an investigation of positron binding to a model (one-electron) alkali atom [5], so only a brief summary of the technical details is given here. Firstly, the singly-charged atomic ionic core was based on the $1s^2 2s^2 2p^6$ orbitals taken from a Hartree-Fock calculation of neutral sodium. The exact core-valence exchange operator was replaced by a local exchange potential, tuned to reproduce the low-lying neutral sodium spectrum. Finally, an additional potential of the

form $V_{\text{model}}(r) = d_1 r \exp(-\frac{3}{2}r)$ is added where $d_1 \in [0.2, -5.6]$ a.u., giving ionisation energies $I.P. \in [4.8, 13.0]$ eV, and neutral atom dipole polarisabilities, $\alpha_d \in [209, 23.5] a_0^3$.

The present CI calculations were performed with a minimum of 25 single-electron and 25 single-positron Laguerre-type orbitals for each partial wave [12]. The same sets of orbitals were then LS -coupled together such that the overall symmetry of the electron-positron wavefunction was either $^1S^e$, or $^1P^o$. Due to computational limitations, L_{max} was chosen to be 15 for $^1S^e$ while $L_{\text{max}} = 9$ was chosen for $^1P^o$.

Figure 2 shows the binding energy of the ground state of the $^1S^e$ symmetry (the upper three curves), and the first-excited state in the $^1P^o$ symmetry (the lower two curves). The top-most curve is the set of previous fixed-core SVM (FCSVM) calculations [6], which provided close to converged $^1S^e$ values. The present CI calculations, denoted by the dashed-dot L_{max} curves, are seen to consistently lie below those values, particularly for the lower ionisation potentials. This is the region where the wavefunction is dominated by Ps, and the CI expansion is very slowly convergent with respect to L_{max} [13, 9]. The final two dotted curves in Figure 2, marked by $L = \infty$, are the results of performing a sequence of three smaller CI calculations with $L_{\text{max}} - 1$, $L_{\text{max}} - 2$, and $L_{\text{max}} - 3$, and then using known convergence patterns to extrapolate to the $L = \infty$ limit [14]. The resulting $L = \infty$ CI $^1S^e$ binding energies are significantly improved by this procedure, and visually are as good as the SVM for $I.P. > 6.0$ eV.

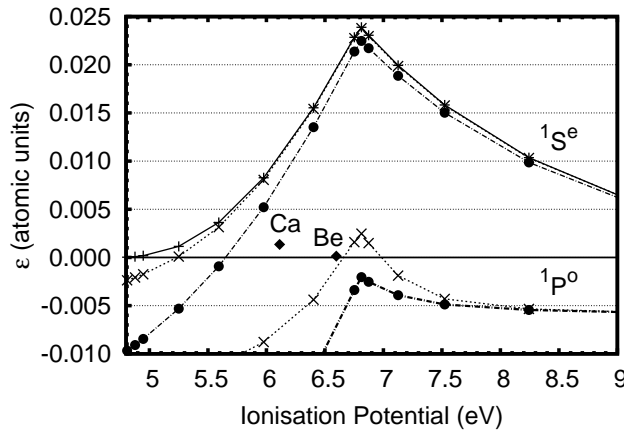


Figure 2. Binding energies of a model positronic alkali atom in the $^1S^e$ and $^1P^o$ symmetries. The (—) solid line is from FCSVM calculations of the $^1S^e$ series [5]. The two (— · —) dash-dot lines are from the CI L_{max} calculations, the two (·····) dotted lines are the $L = \infty$ extrapolated results, the two (♦) results are from CI calculations [10], as discussed in the text.

The L_{max} $^1P^o$ calculations are all unbound, although a modest enlargement of the basis should produce binding. The extrapolation procedure to $L = \infty$ shows a small region where the system is actually bound. The 'stable' ionisation potential range is likely to be a minimum, since larger CI calculations will improve the description of a Ps-cluster orbiting the Atom^+ ion. There are no equivalent $L = 1$ FCSVM calculations to compare with.

There are no actual one-electron atom energies that lie in this range, however these calculations do provide additional motivation for the existence of the known two-electron excited positronic atoms. Shown for comparison in Figure 2 are the binding energies of the two known two-electron, one positron systems [10]. These correspond to the $^2P^o$ state of $e^+\text{Ca}$, and of a positron bound to metastable ($^3P^o$) Be. Essentially, the two-electron systems with low-ionisation energies have an additional p -wave binding mechanism, as they are expected to have a significant component of Ps^- , which will always bind in all partial waves to the residual Atom^{2+} [10].

Some other states were also investigated. Firstly, the second eigenstate in the $^1S^e$ symmetry was also computed as a by-product of the calculations shown in Figure 2. None of the excited state energies indicated binding, nor did their extrapolation. For example, for the model atom with $d_1 = -1.95$, (and an $I.P. = 6.8112$ eV) the ground state has the radius of the electron

$\langle r_e \rangle = 4.29 a_0$, while the positron has $\langle r_p \rangle = 6.67 a_0$. For the first excited state $\langle r_e \rangle = 3.37 a_0$, which is roughly that of the parent model atom, while $\langle r_p \rangle = 32.5 a_0$, which is heading out towards the extent of the Laguerre-based radial basis.

The unnatural parity, $^1P^e$, state is also of fundamental interest. This is due to recent large scale CI calculations that showed the existence of a second, annihilation suppressed, unnatural parity, $^2,4S^o$, state of PsH, NaPs and KPs [15, 16]. The positron is essentially bound to the second bound states of the H^- , Na^- and K^- ions which have np^2 $^1P^e$ -type configurations [17, 18]. This has sparked some interest in other systems such as the unnatural parity resonances in e^+H [19].

The $^2,4S^o$ LiPs state, however, appears to be Borromean [16]. It is necessary to demonstrate that all of the parent $^3P^e$ states Li, e^+Li , and Ps are all themselves unstable. Firstly, both Li and Ps unnatural states are known to be unstable [18, 20]. Secondly, both CI and SVM calculations found no evidence for the stability of both Li and e^+Li unnatural states [16].

To support the conclusion that the $^1P^e$ state of e^+Li is unstable, a series of $^1P^e$ model-alkali atoms were also computed with the CI basis as above. None of these states, across the entire range of ionisation potentials, showed any sign of binding. This is best seen in the $\langle r_p \rangle \approx 29.4 a_0$ across the entire range of d_1 , while the $\langle r_e \rangle$ stays at roughly the radius of the parent atom. These results suggest that e^+Na and e^+K are also not stable in the $^1P^e$ symmetry.

4. Positron-atom scattering resonances

The e^+Mg $^2P^o$ system was used to introduce a method of quantum scattering that extracts phase shifts from pseudostate energy shifts [21], which essentially relies on the fact that a finite- L^2 basis forms a soft-box at some radius [22]. In contrast to the situation for e^+Ca , large-scale CI calculations have shown that e^+Mg has a low-lying $^2P^o$ shape resonance as opposed to a true bound state [21]. Using the pseudostate-shift method the elastic scattering cross sections were computed for e^+Mg , e^+Cu and e^+Zn [22]. These results are shown in Figure 3, along with preliminary calculations of e^+Cd . Also shown is the total cross section for e^+Mg scattering as measured by the Detroit group, which had a beam width of approximately 1 eV. Energies of sub-100 meV are accessible with present positron-beam technologies [23].

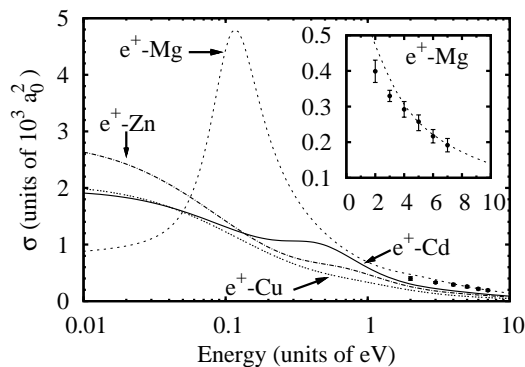


Figure 3. The elastic scattering cross section, σ (in units of $10^3 a_0^2$), for e^+Mg , e^+Cu and e^+Zn as a function of energy (in eV) [22]. Also shown are preliminary calculations of e^+Cd scattering. The experimental (total) cross section for e^+Mg scattering is also given [24].

Apart from the elastic cross section, it is straightforward with the pseudostate shift method to compute the annihilation parameter, Z_{eff} [22]. The results for e^+Mg , e^+Cu , e^+Zn and e^+Cd are shown in Figure 4, where the two weak p -wave resonances are more prominent than in the elastic cross section. The systematic variation in the Z_{eff} resonance position and width between atoms was previously predicted with scattering from a simple exploratory-model potential [25], which supports the well-known idea that a p -wave resonance makes a transition to the bound state as the potential deepens, effectively pulling it under-water.

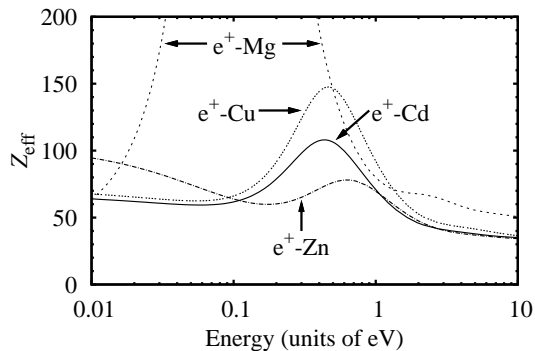


Figure 4. The positron annihilation parameter, Z_{eff} , for e^+ -Mg, e^+ -Cu and e^+ -Zn scattering as a function of energy (in eV) [22]. Also shown are preliminary calculations of e^+ -Cd scattering.

5. Conclusions

Our understanding of positron-atom and positronium-atom excited states has seen rapid progress in the last few years. The calculations presented here of a simple model-alkali atom helps to explain the positron physics involving non s -wave states. The accurate description of these excited states with CI wavefunctions is extremely challenging due to the presence of positronium. The main result is that the $^1P^o$ symmetry does admit bound states over a limited range of atoms. This, however, should be merely taken as the first estimate. CI calculations with an extrapolation of the radial basis towards a complete basis set would be more definitive [26].

Acknowledgments

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