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, i.e. 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 range from the structure of positron-atom bound states, elastic positron-atom scattering and in-flight annihilation through to positronium (Ps) 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 since 2002 when two of the present authors published a review of the known positronic atoms ($e^+\text{He}(^3\text{S}_e)$, $e^+\text{Li}$,
$e^+\text{Be}, e^+\text{Mg}, e^+\text{Ca}, e^+\text{Cu}, e^+\text{Zn}, e^+\text{Sr}, e^+\text{Ag}$ 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.

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

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

$$\Psi_{LS} = \sum_{l=1}^{N_{CI}} c_l \phi_\alpha(r_0) \phi_\beta(r_1) \ldots \phi_\omega(r_N), \quad (1)$$

where $r_0$ is the positron, and $r_{>0}$ are the electron/s co-ordinates. Anti-symmetry 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

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

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 $V_{p_1}(r_i)$ is semi-empirically tuned to reproduce the $1e^-$ spectrum, and a di-electronic term $V_{p_2}(r_i, r_j)$ 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 elsewhere \textsuperscript{15}.

The CI-Kohn method is a natural extension of the CI method \textsuperscript{12}, 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 of a series of CI-Kohn calculations of low-energy positron-hydrogen scattering at $k = 0.4 a_0^{-1} \approx 2.2$ eV with the inclusion of orbitals up to a maximum angular momentum $J$, here including a minimum of 25 LTOs per $\ell$. The annihilation parameter, $Z_{\text{eff}}(k)$ is also given.

<table>
<thead>
<tr>
<th>$J$</th>
<th>$N_{CI}$</th>
<th>$\langle \delta_0 \rangle$</th>
<th>$\langle Z_{\text{eff}} \rangle$</th>
<th>$\langle \delta_0 \rangle$</th>
<th>$\langle Z_{\text{eff}} \rangle$</th>
</tr>
</thead>
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<tr>
<td>0</td>
<td>1010</td>
<td>-0.19921</td>
<td>0.453</td>
<td>10</td>
<td>0.11660</td>
</tr>
<tr>
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<td>1.017</td>
<td>11</td>
<td>0.11730</td>
</tr>
<tr>
<td>2</td>
<td>3786</td>
<td>0.05338</td>
<td>1.465</td>
<td>12</td>
<td>0.11781</td>
</tr>
<tr>
<td>3</td>
<td>4411</td>
<td>0.08173</td>
<td>1.796</td>
<td>Variational \textsuperscript{16,17}</td>
<td>0.1201</td>
</tr>
</tbody>
</table>

The convergence of both the phase shifts and $Z_{\text{eff}}$ is currently being examined in detail elsewhere \textsuperscript{10} for both CI and CI-Kohn calculations. The slow-convergence with $J$ in Table 1 towards the $J \to \infty$ limit is typical of all partial-wave expansions of mixed positron-electron systems, and is seen to be quite severe for even simple systems ($e^+/H$ scattering).

There are a variety of methods to estimate the partial-wave increments $\Delta X^J$ where $J > J_{\text{max}}$ to any expectation value \textsuperscript{10}. Some of these extrapolation methods follow Gribakin and Ludlow \textsuperscript{18} 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 in practice, and alternate methods are required. One of the better methods, labelled in Figure 1, is based on the two-term form:

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

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 \( Z_{\text{eff}} \) data of Table 1. The explicit CI calculations are marked as \( J_{\text{max}} \). 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 are underway \(^{11}\) with parallelised code allowing for an order of magnitude more configurations than our previous calculations \(^{19}\).

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 lines are from calculations of positron binding to a model alkali atom.

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

Figure 3. Spin-averaged annihilation rates $\Gamma_\nu$ 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$^+$, Li$^{2+}$, B$^{4+}$ and F$^{8+}$. 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 $e^+\text{-Cu}$ scattering was of primary interest to show that the presence of a bound state does not imply a massive $Z_{\text{eff}}$. 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, F/Cl/Br substituted alkanes $Z_{\text{eff}}$ semi-empirically scales as $\log(Z_{\text{eff}}) \approx B |I - E_{Ps}|^{-1} + A$. This would imply a huge $Z_{\text{eff}}$ for the metal vapours, which is not the case. Figure 4, however, shows that the $p$-wave interaction is on the verge of forming shape resonance, resulting in a $p$-wave contribution that exceeds that of the $s$-wave.

![Figure 4](image.png)

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

Elastic positron-positive ion scattering was performed firstly because most of the CI-Kohn machinery was in place, but also because of suggestions to use positive ions to cool positrons. Previous calculations have looked at the phase shifts, these are the first annihilation calculations. Figure 5 shows that $Z_{\text{eff}}$ is generally negligible. In particular, for a 300K thermal swarm (ie $k \approx 0.05 \ a_0^{-1}$) $Z_{\text{eff}}^{(0)} \approx 10^{-51}$. This means that $e^+ - \text{Atom}^{n+}$ cooling schemes can ignore annihilation.
5. Ps-formation during $e^+\text{-Na}$ scattering

Our HSCC calculations were motivated by a recent experiment that measured the positronium (Ps) formation cross sections \(^{21}\) (ie. the probability of an electron undergoing charge transfer from the atom to the positron during the collision). This experiment found strong disagreement with previous close-coupling calculations \(^{22,23}\) for energies near and below 1 eV. Speculation arose in Ref. \(^{21}\) 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 agreement with previous CC calculations \(^{22,23}\) and disagreement with the experimental data below 2 eV \(^{21}\). The accurately-known Ps-Na\(^+\) scattering length \(^{24}\) is reproduced by our calculations, and hence, our low-energy results are reliable. Experiment needs to revisit the sub $E = 2$ eV region.

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 a better understanding of the nature of few-body interactions involving positrons and atoms.
Figure 6. Ps-formation cross sections during $e^+\cdot$Na scattering.

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