

LETTER TO THE EDITOR

Positron binding to calcium, a configuration interaction study

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Abstract. The configuration interaction (CI) method is applied to the study of the positron–calcium system. A large basis CI investigation shows that positronic calcium, $e^+\text{Ca}$, is stable with a binding energy of 0.220 eV and an annihilation rate of $0.64 \times 10^9 \text{ s}^{-1}$. The stability of $e^+\text{Ca}$ suggests that the heavier group II elements could also bind a positron, and positron binding to strontium can be regarded as highly likely. The possibility of experimental detection is discussed.

The recent discovery that the alkaline atoms, calcium, strontium and barium, could form a stable negative ion has been one of the most interesting recent results in the field of negative ion physics. Both theoretical and experimental evidence for the existence of the $\text{Ca}^- 4s^2 4p$ ground state were first presented in 1987 [1, 2]. This result stimulated a lot of theoretical activity and it was quickly shown that both strontium and barium could also form stable negative ions [3–6]. In this letter, it is demonstrated that positronic calcium is electronically stable and therefore that calcium can bind a positron as well as an electron. This letter is part of a series investigating the physics of positron–atom binding and thereby revealing aspects about the nature of positron–atom interactions that have been hitherto inaccessible.

The first rigorous evidence that a positron could be bound to a neutral atom was presented in 1997 and 1998 when two independent calculations demonstrated that positronic lithium was stable with a binding energy of about 60 meV [7, 8]. Since that time, additional calculations have shown that positrons can bind to beryllium, metastable helium ($\text{He}(^3\text{S}^e)$), sodium, magnesium, copper, silver, zinc and cadmium [9–19]. While the calculations of the systems heavier than beryllium did not give rigorous evidence of binding, the predictions of binding were rigorous with respect to the underlying model Hamiltonians. Most of these calculations of positron binding to neutral atoms were performed with the stochastic variational method (SVM) or a related method [9, 20–22].

While the SVM and its fixed core variant (FCSVM) have been successful in predicting positron or positronium (Ps) binding to a number of atoms, the calculations have become increasingly tedious as the size of the atom has increased. Calculations on $e^+\text{Zn}$ [16] and KPs [23] each took almost a year of continuous computation on a variety of DEC ALPHA machines, and even then the binding energies had only converged to an accuracy of 25% (or worse). An initial attempt to use the FCSVM to demonstrate positron binding to calcium was abandoned when a pilot calculation failed to show indications of binding. Although this pilot calculation could not be taken as establishing a failure to bind, it was clear that it could take months of computation to establish whether binding was possible or not. Under such circumstances, investigations on the possible existence of $e^+\text{Ca}$ using the FCSVM were halted until a more efficient method of establishing binding was developed.

One of the problems with establishing positron binding to calcium lies in the fact that the ionization potential of calcium is 6.1132 eV [24] and thus the lowest energy dissociation threshold is the $\text{Ca}^+(4s) + \text{Ps}(1s)$ threshold. The positron affinity to calcium must therefore exceed $|E(\text{Ps}) - E(\text{Ca}^+)| = 6.80285 - 6.1132 = 0.6896$ eV for a positron to bind to calcium. Because of this, the condition for positron binding to calcium is more stringent than the condition for positron binding to those group II and IIB elements with an ionization potential exceeding 6.80 eV.

In this letter, the configuration interaction (CI) method [25] is applied to the problem of positron–calcium binding. The CI method is one of the most widely used methods for performing atomic structure calculations. Recent calculations on positronic copper have shown that the CI method can be used to establish positron binding to atoms [17], and in the case of the extensive calculations of Dzuba *et al* [18] can give a reasonably precise estimate of the model Hamiltonian binding energy. The CI method has also recently been used to establish positron binding to cadmium and positronium binding to copper [19], although in these cases the binding energies were far from converged.

The main problem in applying the CI method to a positron binding system is a consequence of the attractive electron–positron interaction. The electron–positron correlations are so strong that for some systems (e.g. $e^+\text{Na}$) it is best to regard the electron and positron as coalescing into something approximating a positronium cluster, i.e. a superposition of states representing weakly bound positronium. The accurate representation of a Ps cluster with single particle orbitals centered on the nucleus requires the inclusion of terms with quite high angular momenta. For example, orbitals with $L = 10$ were included in the still far from converged calculations on $e^+\text{Cu}$ [17]. In spite of these problems, the CI method can be a useful tool in establishing positron binding since usefully accurate (if not converged) calculations can be done in a reasonable amount of computer time. Once binding has been established, the expenditure of the additional effort associated with the potentially more accurate FCSVM methods becomes justified.

The CI method is one of the standard approaches for computing atomic structures, so only a brief description needs to be given here. The atomic wavefunction is taken to be a linear combination of states created by coupling atomic states with single particle positron states using the usual Clebsch–Gordan coupling coefficients:

$$|\Psi; LS\rangle = \sum_{i,j} c_{i,j} \langle L_i M_i \ell_j m_j | LM_L \rangle \langle S_i M_{S_i} \frac{1}{2} \mu_j | SM_S \rangle \Phi_i(\text{Atom}; L_i S_i) \phi_j(\mathbf{r}_0). \quad (1)$$

In this expression $\Phi_i(\text{Atom}; L_i S_i)$ is an antisymmetric atomic wavefunction with good L and S quantum numbers. The function $\phi_j(\mathbf{r}_0)$ is a single positron orbital. The positron orbitals and the electron orbitals that make up the wavefunction are written as a product of a radial function and a spherical harmonic, namely

$$\phi(\mathbf{r}) = P(r)Y_{lm}(\hat{\mathbf{r}}). \quad (2)$$

The Hamiltonian for an atom consisting of N_e valence electrons and a positron was

$$H = \sum_{i=1}^{N_e} -\frac{1}{2}\nabla_i^2 - \frac{1}{2}\nabla_0^2 + \sum_{i=1}^{N_e} (V_{\text{dir}}(\mathbf{r}_i) + V_{\text{exc}}(\mathbf{r}_i) + V_{p1}(\mathbf{r}_i)) - V_{\text{dir}}(\mathbf{r}_0) \\ + V_{p1}(\mathbf{r}_0) + \sum_{i<j}^{N_e} \frac{1}{r_{ij}} - \sum_{i=1}^{N_e} \frac{1}{r_{i0}} - \sum_{i<j}^{N_e} V_{p2}(\mathbf{r}_i, \mathbf{r}_j) + \sum_{i=1}^{N_e} V_{p2}(\mathbf{r}_i, \mathbf{r}_0). \quad (3)$$

In this expression, the \mathbf{r}_i refer to the electron coordinates while \mathbf{r}_0 refers to the positron coordinate. The direct potential (V_{dir}) representing the interaction with the core is derived from a Hartree–Fock wavefunction and is the same (although opposite in sign) for the electron

and the positron. The basis set of Koga *et al* [26, 27] was used to compute the wavefunction of the $\text{Ca}^+ 4s^2 \text{S}^e$ ground state and the resulting 1s, 2s, 3s, 2p and 3p orbitals were used to define the core direct and exchange interactions. The exchange potential (V_{exc}) between the valence electrons and the Hartree–Fock core was also computed exactly. The one-body polarization potential (V_{p1}) is a semi-empirical polarization potential derived from an analysis of the spectrum of the parent atom or ion. It has the functional form

$$V_{p1}(r) = -\frac{\alpha_d g^2(r)}{2r^4}. \quad (4)$$

The factor α_d is the static dipole polarizability of the core and $g^2(r)$ is a cutoff function designed to make the polarization potential finite at the origin. The same cutoff function has been adopted for both the positron and electrons. In this work, $g^2(r)$ was defined to be

$$g^2(r) = 1 - \exp(-r^6/\rho_l^6), \quad (5)$$

where ρ_l is an adjustable l -dependent cutoff parameter. The two-body polarization potential (V_{p2}) is defined as

$$V_{p2}(\mathbf{r}_i, \mathbf{r}_j) = \frac{\alpha_d}{r_i^3 r_j^3} (\mathbf{r}_i \cdot \mathbf{r}_j) g(r_i) g(r_j). \quad (6)$$

Following the work of Mitroy [28], α_d was set to $3.16 a_0^3$ while $\rho_l = 1.6516, 1.6594, 1.9324, 1.77 a_0$ respectively for $l = 0, 1, 2, 3$ orbitals (a_0 is the Bohr radius). For orbitals with $l \geq 3$, ρ_l was set to $1.77 a_0$. The cutoff parameter in the two-body polarization potential was independent of l and set to $1.75 a_0$. Since the CI calculations included orbitals with quite high angular momenta, the parameter L_{max} is used to denote the maximum angular momentum of any single orbital included in the CI calculation.

The single particle orbital bases were written as a linear combination of Slater and Laguerre basis functions. The mixed basis was used in order to minimize the linear dependence problems associated with a Slater basis. The procedure used to define the additional orbitals was twofold. First, additional single particle orbitals were added to the basis so that the set of orbitals completely spanned the space defined by the Slater-type orbital set. Then additional Laguerre-type orbitals (with the same scaling parameter, λ_α , for common L) were used to enlarge the orbital basis. A Gram–Schmidt orthogonalization of the orbital set was performed to ensure that all the electron and positron orbitals were orthonormal.

The Laguerre basis functions augmenting the Slater basis are defined by

$$\chi_\alpha(r) = N_\alpha r^{\ell+1} \exp(-\lambda_\alpha r) L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r), \quad (7)$$

where the normalization constant is

$$N_\alpha = \sqrt{\frac{(2\lambda_\alpha)^{2\ell+3} (n_\alpha - \ell - 1)!}{(\ell + n_\alpha + 1)!}}. \quad (8)$$

The function $L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r)$ is an associated Laguerre polynomial that can be defined in terms of a confluent hypergeometric function [29] as

$$L_{n_\alpha-\ell-1}^{(2\ell+2)}(2\lambda_\alpha r) = \frac{(n_\alpha + \ell + 1)!}{(n_\alpha - \ell - 1)!(2\ell + 2)!} M(-(n_\alpha - \ell - 1), 2\ell + 2, 2\lambda_\alpha r). \quad (9)$$

The Laguerre functions were not computed using the power series expression for the confluent hypergeometric function. Rather, the recursion relation

$$(n+1)L_{n+1}^\alpha(x) = (2n+\alpha+1-x)L_n^\alpha(x) + (n+\alpha)L_{n-1}^\alpha(x) \quad (10)$$

was used with $L_0^{2\ell+2}(x)$ and $L_1^{2\ell+2}(x)$ as starting values. The matrix elements for the basis were not computed analytically, instead all the orbitals were tabulated on an r -space grid and the matrix elements computed using numerical quadrature.

Various expectation values were computed to provide information about the structure of the ground state. The mean distances of the (valence) electrons and the positron from the nucleus are denoted by $\langle r_e \rangle$ and $\langle r_p \rangle$. The positronic atom will decay by electron–positron annihilation and the 2γ annihilation rate is computed to give an estimate of the lifetime (the 2γ rate also gives information about the tendency for the electron and positron to form a cluster). The annihilation rate for the 2γ decay summed over all possible final states [30–32] is

$$\begin{aligned} \Gamma &= 4\pi c\alpha^4 a_0^2 N_e \langle \Psi(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}; \mathbf{r}_0) | \hat{O}_{N_e}^s \delta(\mathbf{r}_{N_e} - \mathbf{r}_0) | \Psi(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}; \mathbf{r}_0) \rangle \\ &= 4\pi c\alpha^4 a_0^2 N_e \int d^3\tau \left| \hat{O}_{N_e}^s \Psi(\mathbf{r}_1, \dots, \mathbf{r}_{N_e}; \mathbf{r}_{N_e}) \right|^2. \end{aligned} \quad (11)$$

The symbols in front of the integral sign represent the usual quantities in atomic physics: c is the speed of light and α is the fine structure constant. The operator $\hat{O}_{N_e}^s$ is a projection operator that selects spin-zero combinations of the N_e electron and the positron. The annihilation rates with the valence (Γ_v) and core (Γ_c) electrons are given separately so the two rates should be added together to give the net annihilation rate.

The formalism and numerics of the CI program were initially validated by reproducing the results of a previous CI calculation of PsH by Strasburger and Chojnacki [33, 34]. Their best CI calculation gave a total energy of $-0.763\,693\,86$ Hartree. The present program with the same Gaussian basis was able to reproduce this energy to all significant figures. Being able to use a Gaussian, Slater or a Laguerre basis (or even mix the types of basis functions) is a consequence of the decision to perform all integrations using numerical quadrature.

The condition for binding is that the energy of the e^+Ca state is lower than the energy of the $Ca^+ + Ps$ dissociation channel. Given that the Ps(1s) binding energy is 0.25 Hartree, the e^+Ca

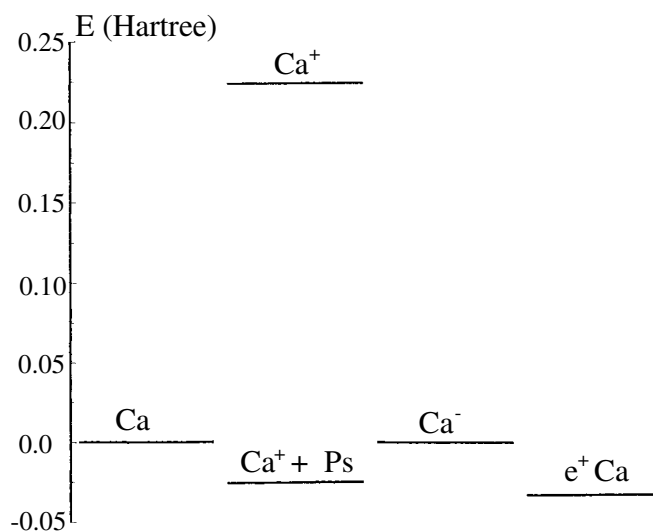


Figure 1. Energy level diagram showing the energies of Ca, Ca⁺, Ca⁻, e⁺Ca and the Ca⁺+Ps threshold. The Ca⁻ binding energy was taken to be approximately 22 meV (8.1×10^{-4} Hartree) [39].

Table 1. Results of CI calculations for e^+Ca . The total number of electron and positron orbitals up to a given L_{\max} are denoted by N_e and N_p . The energy of the positronic calcium system is denoted by $E(e^+Ca)$, with the positron binding energy in column ε . The mean (valence) electron–nucleus distance $\langle r_e \rangle$, and the mean positron–nucleus distance $\langle r_p \rangle$, are given in a_0 . The spin-averaged 2γ annihilation rates with the valence (Γ_v) and core electrons (Γ_c) are given in 10^9 s^{-1} . The energy of the neutral calcium atom with exactly the same (electron) orbital basis is in the column labelled $E(Ca)$, with the positron affinity in column PA . All energies are given in atomic units.

L_{\max}	N_p	N_e	$E(e^+Ca)$	ε	$E(Ca)$	PA	$\langle r_e \rangle$	$\langle r_p \rangle$	Γ_v	Γ_c
0	09	12	−0.627 2587	0.059 0671	−0.637 2326	0.009 9739	4.0600	13.328	0.002 69	0.002 82
1	17	22	−0.653 9464	0.032 3794	−0.657 6532	0.003 7068	4.0740	11.326	0.019 25	0.003 78
2	24	31	−0.666 1819	0.020 1439	−0.659 5110	−0.006 6709	4.1131	8.7972	0.093 07	0.008 56
3	30	37	−0.675 3094	0.011 0164	−0.659 6534	−0.015 6560	4.1629	7.6368	0.202 13	0.012 36
4	36	43	−0.682 1375	0.004 1883	−0.659 6976	−0.022 4399	4.2078	7.1439	0.312 27	0.014 19
5	42	49	−0.686 9709	−0.000 6491	−0.659 7165	−0.027 2544	4.2445	6.9145	0.410 89	0.014 96
6	48	55	−0.690 3565	−0.004 0307	−0.659 7258	−0.030 6307	4.2731	6.7964	0.495 53	0.015 27
7	54	61	−0.692 7389	−0.006 4131	−0.659 7308	−0.033 0081	4.2951	6.7307	0.567 19	0.015 38
8	60	67	−0.694 4244	−0.008 0986	−0.659 7338	−0.034 6906	4.3115	6.6919	0.626 82	0.015 40

binding energy for a particular basis is defined as $\varepsilon = E(e^+Ca) - E(Ca^+) - 0.25$ and binding occurs when ε is negative. The calculated energy of Ca^+ in the single particle basis used for the CI calculations was $-0.436\,3258$ Hartree (in this letter all energies are given relative to the energy of the Ca^{2+} core). Therefore, the threshold for positron binding is at $-0.686\,3258$ Hartree. An energy level diagram showing the $Ca^+ + Ps$ threshold and its relative relationship with the Ca and Ca^+ energy levels is shown in figure 1.

The details of the basis and the results of the e^+Ca calculations as a function of L_{\max} are given in table 1. All of the allowed configurations that could be formed from the orbital basis were included in the CI basis. Also reported in table 1 are the results of CI calculations on the ground state of the calcium atom using exactly the same (electron) orbital basis. The calculated ionization potential of $0.223\,408$ Hartree is in good agreement with the experimental ionization potential of $0.224\,66$ Hartree. The resulting positron affinity is defined as $PA = E(e^+Ca) - E(Ca)$, with a positron affinity of $0.026\,592 = (0.250 + 0.436\,3258 - 0.659\,7338)$ Hartree needed to ensure binding. The relative position of the e^+Ca energy level is also shown in figure 1.

Formal evidence of e^+ binding to Ca was not achieved until a basis with $L_{\max} = 5$ was used. The largest calculation had $L_{\max} = 8$ and gave a positron binding energy of $-0.008\,0986$ Hartree and a (total) positron annihilation rate of $0.64 \times 10^9 \text{ s}^{-1}$. The slow convergence of the e^+Ca binding energy with L_{\max} is consistent with previous CI calculations upon positronic copper [17, 18].

It is clear from the trend of ε versus L_{\max} that the $L_{\max} = 8$ binding energy is still far from converged. However, the comparison of the FCSVM and CI calculations for the non-polarized model of e^+Cu [17] with roughly the same ionization potential suggests that a converged calculation would give a binding energy of at least -0.012 Hartree.

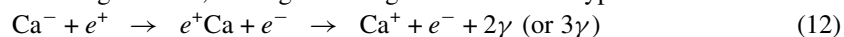
At the present time, the chief impediment to performing a larger calculation is the slow convergence of the Davidson algorithm [35] used to diagonalize the secular equations (dimension equals $33\,616$ for $L_{\max} = 8$). For reasons that at present are not entirely clear, this algorithm converges very slowly for some positron binding systems (e.g. e^+Ca , e^+Be , e^+Cd) while working quickly for others (e.g. PsH , $CuPs$) [19]. Convergence in the energy to 10^{-8} Hartree for the $L_{\max} = 8$ calculation was not achieved until over 9000 iterations were performed.

As was noted previously [17], the accuracy of the 2γ annihilation rate is critically dependent on the value of L_{\max} and comparison with this earlier work on $e^+\text{Cu}$ suggests that the annihilation rate is a severe underestimate. It is expected that the converged annihilation rate should be approximately $1.5 \times 10^9 \text{ s}^{-1}$. This estimate is based on two independent analyses. First, the Γ vs L_{\max} table for the non(core)-polarized FSCVM model of $e^+\text{Cu}$ suggests an increase of about $0.8 \times 10^9 \text{ s}^{-1}$ [17]. Second, an analysis of positron binding to a model alkali atom demonstrated that the annihilation rate could be estimated from the ionization potential [36]. Using the calcium ionization potential of 0.224 66 Hartree as a guide would suggest a converged annihilation rate of approximately $1.4 \times 10^9 \text{ s}^{-1}$.

The present result, and previous calculations on $e^+\text{Be}$, $e^+\text{Mg}$, $e^+\text{Zn}$ and $e^+\text{Cd}$ all indicate that group II and IIB atoms attract a positron more strongly than an electron. For neutral calcium, the positron affinity of 0.034 66 Hartree exceeds the most recent estimates of the electron affinity, $6.4\text{--}9.0 \times 10^{-4}$ Hartree [37–39] by a factor of about 50. This can only be a result of a positron–atom polarization potential that is more strongly attractive than the electron–atom polarization potential. The positron–atom polarization potential is so strong that it more than counterbalances the repulsive static interaction with the rest of the atom.

The configuration interaction method has been used to investigate positron binding to calcium and to make a rigorous prediction of binding with respect to the underlying model potential. This prediction of positron binding can be regarded as realistic since the model potential employed here has previously been validated in calculations of the structure of Ca^+ [40] and Ca [28]. An earlier analysis of positron binding to a model alkali atom [36] can be used to place the existence of $e^+\text{Ca}$ into perspective. Positronic atoms with an ionization potential of less than 0.25 Hartree can be described as a positronium cluster (i.e. an electron and positron bound together in something approximating the Ps ground state) which is bound to the residual ion. For such systems, the ionization potential (i.e. the attraction of the last electron to the residual ion) seems to be the critical factor in determining whether an electronically stable positronic atom can be formed. Using the neutral Ca ionization potential of 0.224 Hartree in conjunction with figure 4 of [36] suggests that the binding energy of $e^+\text{Ca}$ should be about -0.011 Hartree. A converged calculation on $e^+\text{Ca}$ would most likely give a binding energy that was slightly larger in magnitude than this value. The calculations upon the model alkali atom predicted positron binding to atoms as long as the ionization potential exceeded 0.176 Hartree [36]. Since the heavier group II elements of the periodic table, namely Sr, Ba and Ra, all have ionization potentials larger than 0.190 Hartree, there is a strong possibility that positrons can bind to these atoms. The strontium atom, with an ionization potential of 0.209 Hartree, is the most likely of these atoms to bind a positron.

While the experimental detection of $e^+\text{Ca}$ would be difficult, it is not impossible. Since calcium has a stable negative ion, a charge exchange reaction of the type



opens the possibility of experimental detection. The use of an analogous charge exchange reaction to produce and detect positronic copper has been discussed previously [41]. Under certain kinematic conditions, the detection of positively charged copper ions, i.e. Cu^+ , can serve as a signature of the existence of $e^+\text{Cu}$ [41]. Unfortunately, the detection of Ca^+ ions would not serve as a signature of the existence of $e^+\text{Ca}$ since the positronium formation reaction leading to production of Ca^+ ions is energetically possible even at threshold. However, the detection of the electron and measurement of its energy could be used to indicate the existence of $e^+\text{Ca}$. Since the energy of $e^+\text{Ca}$ is expected to be about 1 eV below that of Ca^- , the detection of electrons with a kinetic energy 1 eV greater than that of the incident positron kinetic energy would indicate the occurrence of the charge transfer reaction and thus the formation of $e^+\text{Ca}$. Such an experiment could also be used to detect other species such as $e^+\text{Li}$ and $e^+\text{Na}$.

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