The stability and structure of the (m^{Z+},e^-,e^-,e^+) system

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The stability and structure of the (m^{Z+},e^-,e^-,e^+) system is studied as a function of the mass of the m^{Z+} particle and for $Z=1$, 2, 3, and 10. The $Z=1$ system can be regarded as an analog of the *A*Ps system (where *A* is a group I or IB atom of the periodic table) and was found to be stable for all values of m^+. This is supportive of the idea that all the group I and IB atoms can bind Ps. The (m^{2+},e^-,e^-,e^+) system is stable for all $m^{2+}/m_e \leqslant 0.68$ and evolves into a configuration best described as (m^{2+},Ps^-) when $m^{2+}/m_e \to 0$. The (m^{3+},e^-,e^-,e^+) system was stable for a mass range given by $m^{3+}/m_e \leqslant 0.066\,32$, which suggests that positrons could form Feshbach resonances in collisions with positive ions which are isolectronic with the group II and IIB columns of the periodic table. The (m^{3+},e^-,e^-,e^+) system has the unusual property that it has a mass range where it becomes more compact while its binding energy simultaneously decreases. The (m^{10+},e^-,e^-,e^+) system is also stable at $m^{10+}/m_e = 0.002\,54$, which implies stability for all mass ratios less than 0.002 54. In total, the calculations suggest that the (m^{Z+},e^-,e^-,e^+) system is stable whenever the $m^{Z+}+\mathrm{Ps}^-$ or $(m^{Z+},e^-)+\mathrm{Ps}$ breakups represent the lowest energy dissociation channel. As part of the analysis some improved estimates of the properties of the KPs ground state are reported.

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I. INTRODUCTION

The calculation of the structure and stability of Coulombic three-body systems with arbitrary masses is a topic with a long history [1]. The initial calculation of the helium atom ionization potential by Hylleraas [2] was important since it confirmed the correctness of the new wave mechanics. Even more interesting, the existence of the H^- ion, so important in astrophysics, was predicted by explicit calculation [3,4]. The stability of the positronium negative ion Ps^- was also demonstrated by explicit calculation [5]. (Note that, since systems containing positrons can decay by electron-positron annihilation, we use the term stability to refer only to the ability to form bound states that are stable against the various electronic dissociation channels.) There have been many other investigations into Coulomb three-body systems [6–13]. The Coulombic four-body system has also been the subject of investigation, with Ps_2 and HPs attracting some attention in recent years [14,15].

One area of ongoing research is the study of the stability of various three- and four-particle systems for constituents with different masses [1,16,17]. This work is important to the understanding of the stability conditions since the structures are known to depend crucially on the mass of the particles. For example, the structures of (p,e^-,e^-), (p,p,e^-), and (e^+,e^+,e^-) are completely different. Only recently has the usefulness of these types of calculations in determining the ability of positrons to bind to atoms and atomic ions been fully appreciated [18,19]. Many years ago it was shown by computational investigations that the (p,e^-,e^+) system is stable only when the mass of m^+ exceeds $2.20m_e$ [20–25]. Those calculations demonstrated conclusively that it was not possible to bind a positron to atomic hydrogen. While this is an important result, it cannot be usefully applied to deduce information about positron binding other atoms in the periodic table. However, another three-body system (m^+,e^-,e^-) does yield information about the ability of positrons to bind to one-electron atoms. This system was found to be stable for $0.697\,78 \leqslant m^+/m_e \leqslant 1.6343$ [18]. The mass limits correspond to stability for energy values of the (m^+,e^-) subsystem satisfying $0.205\,498 \leqslant E(m^+,e^-) \leqslant 0.310\,196$ (energies in hartree). These energy limits roughly correspond to the ionization potentials of neutral atoms that are known to bind a positron. The (m^+,e^-,e^+) system can be regarded as an analog of a typical positronic atom with a single valence electron, and its structure as a function of $E(m^+,e^-)$ was seen to be reminiscent of the structure of known positronic atoms as a function of the parent atom ionization potential [18].

Similarly, the $(m^{Z+},2e^-,e^+)$ system can be regarded as an analog of a number of positron-atom (ion) systems (the notation $(m^{Z+},2e^-,e^+)$, is used to represent the (m^{Z+},e^-,e^-,e^+) complex). For $Z=1$, the $(m^+,2e^-,e^+)$ system can be regarded as an analog of the *A*Ps system where *A* corresponds to an alkali-metal or group IB atom. When $Z=2$, one obtains the $(m^{2+},2e^-,e^+)$ system which can be regarded as an analog of e^+A where *A* corresponds to a divalent group II or IIB atom of the periodic table. Finally, the $(m^{3+},2e^-,e^+)$ system with $Z=3$ is related to the e^+A^+ system where A^+ is a member of the group II or IIB isoelectronic series.

In the present work, the stability and structure of the $(m^{Z+},2e^-,e^+)$ system is studied using the stochastic variational method [26–30]. It is seen that the $(m^+,2e^-,e^+)$ system is stable for all values of m^+, while the $(m^{2+},2e^-,e^+)$ system was already known to be stable for all $m^{2+}/m_e \leqslant 0.68$ [31]. The positively charged $(m^{3+},2e^-,e^+)$ complex also has a region of stability; this occurs when $m^{2+}/m_e \leqslant 0.066\,32$, and the system evolves into a configuration best described as $m^{3+}+\mathrm{Ps}^-$ as $m^{3+}/m_e \to 0$. All equations and results are re-

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TABLE I. The $(m^{Z+},2e^-,e^+)$ system dissociation products and energies for different ranges of the $X_m=m^{Z+}/m_e$ mass ratio. The fourth column gives stability conditions for the given dissociation channel as determined by explicit calculations.

Dissociation products	Threshold energy	$X_m=m^{Z+}/m_e$ mass limits	Stable?
		$Z=1$	
$(m^+,e^-)+\mathrm{Ps}$	$-X_m/2(1+X_m)-0.25$	$X_m>0.02460$	Stable for all X_m
$m^++\mathrm{Ps}^-$	-0.26200507	$X_m<0.02460$	Stable for all X_m
		$Z=2$	
$(m^{2+},2e^-)+e^+$	$E(m^{2+},2e^-)$	$X_m>0.2907$	Stable for $X_m\leqslant 0.68$
$(m^{2+},e^-)+\mathrm{Ps}$	$-2X_m/(1+X_m)-0.25$	$0.006039<X_m<0.2907$	Stable for all X_m
$m^{2+}+\mathrm{Ps}^-$	-0.26200507	$X_m<0.006039$	Stable for all X_m
		$Z=3$	
$(m^{3+},2e^-)+e^+$	$E(m^{3+},2e^-)$	$X_m>0.05966$	Stable for $X_m\leqslant 0.06632$
$(m^{3+},e^-)+\mathrm{Ps}$	$-9X_m/2(1+X_m)-0.25$	$0.002675<X_m<0.05966$	Stable for all X_m
$m^{3+}+\mathrm{Ps}^-$	-0.26200507	$X_m<0.002675$	Stable for all X_m
		$Z=10$	
$(m^{10+},2e^-)e^+$	$E(m^{10+},2e^-)$	$X_m>0.002540$	Stable for $X_m\leqslant 0.002541$
$(m^{10+},e^-)+\mathrm{Ps}$	$-50X_m/(1+X_m)-0.25$	$0.0002402<X_m<0.002540$	Stable for all X_m
$m^{10+}+\mathrm{Ps}^-$	-0.26200507	$X_m<0.0002402$	Stable for all X_m

ported in atomic units with the exception of the electron-positron annihilation rate which is given in SI units.

II. RESULTS OF CALCULATIONS

All calculations reported in this work used the stochastic variational method (SVM). Since this method and its application to positron binding systems have been thoroughly described in a series of articles [19,26–30] only the briefest description is given here. The SVM expands the wave function in a linear combination of explicitly correlated Gaussians (ECGs). Such basis functions have the property that the matrix elements of the Hamiltonian are relatively quick and easy to evaluate. Therefore, the energy of the wave function can be rapidly optimized by performing a random (stochastic) search over the exponential parameters that define the basis. The method has been tested on a number of many-body problems in different areas of physics and it has been proved to be both accurate and reliable [28,30].

The $(m^{Z+},2e^-,e^+)$ system has a number of different fragmentation modes. The lowest energy dissociation modes as a function of $X_m=m^{Z+}/m_e$ (note that the notation $X_m=m^{Z+}/m_e$ is adopted in this manuscript) are listed in Table I.

A. $Z=1$

Explicit calculations have shown that a number of atoms with a single valence electron can bind positronium. The first example was HPs (with $m^+\rightarrow\infty$), which was first shown to be stable in 1951 [32] and was indirectly observed experimentally in 1992 [33]). The HPs atom has been exhaustively studied in recent years [14,15]. The system with $m^+=m_e$ is the positronium molecule Ps_2, which has also been known to be stable for a long time [34].

It is worth noting that it has been conjectured that the $(M_1^+,M_2^+,m_3^-,m_4^-)$ system is stable provided two of the like charges have the same mass [35]. The present investigation on the $(m^+,2e^-,e^+)$ system is testing part of this conjecture.

Ab initio and model potential calculations have shown that Ps can bind to a number of group I and IB atoms. The stability of LiPs was rigorously established with an *ab initio* calculation [36], and the current best estimate of the binding energy is about 0.0123 hartree [37]. The stability of the heavier alkali-metal atom compounds, NaPs and KPs have also been demonstrated with the fixed core variant of the SVM [26,37,38]. Finally, the configuration interaction method has demonstrated the stability of CuPs [39]. These positive results cannot directly be used to determine whether other alkali atoms can bind Ps. For example, e^+Li and e^+Na are known to be stable, but K, Rb, and Cs are not expected to bind a positron.

For the present set of calculations a basis containing 350 ECGs was used. Table II gives the energies, annihilation rates, and other expectation values for a variety of X_m values. The values for calculations with $m^+=m_e$ (Ps_2) and $m^+\rightarrow\infty$ (HPs) are taken from the close to exact calculations of Usukura *et al.* [40]. Table II also gives expectation values for LiPs, NaPs, KPs, and Ps^-.

A basis of dimension 350 can predict the binding energies of the $(m^+,2e^-,e^+)$ system at an accuracy level of better than 0.1%. For example, the energy of HPs was $-0.789\,186$ hartree, giving a binding energy of $0.039\,186$ hartree. This binding energy agrees to within 0.1% with the much larger (basis dimension 1600) calculation of Usukura *et al.* [40], which gave a binding energy of $0.039\,197$ hartree. The annihilation rate, depending as it does on short-range electron-positron correlations, is accurate to only about 1%. A basis with 350 ECGS gives an HPs annihilation rate of $2.447\times10^9\ \mathrm{s}^{-1}$. This is 1% smaller than the

TABLE II. Properties of the family of systems consisting of $(m^+,2e^-,e^+)$ and another positive singly charged object. The basis size is denoted by N. All quantities are given in atomic units with the exception of the annihilation rate which is in units of 10^9 s^{-1}. The magnitude of the binding energy against dissociation into the lowest energy fragmentation channel is given by $|\varepsilon|$. The effective values of X_m for LiPs, NaPs, KPs, and CuPs were derived from the neutral atom ionization energies as described in the text. The δ-function expectation value is given for the sum over all electrons. The properties of Ps^- are shown for the sake of comparison. The notation a^{-b} represents $a\times10^{-b}$.

Property	HPs [40]	CuPs[a] [53]	Ps_2 [40]	LiPs	NaPs	$X_m=0.60$	KPs	$X_m=0.10$	$X_m=0.02$	Ps^- [43]
X_m	∞	1.314	1.0	0.656	0.607	0.60	0.469	0.10	0.020	
N	1600		1600	900	960	350	1080	350	350	
$\langle V\rangle/\langle T\rangle+2$	3^{-7}		3.0^{-10}			1.4^{-5}		3.8^{-5}	4.0^{-6}	
I	0.50	0.28394	0.250	0.19816	0.18839	0.18750	0.15896	0.045455		
E	−0.789197	−0.5483	−0.516004	−0.460456	−0.446810	−0.451931	−0.414066	−0.307961	−0.271875	−0.262005
$\|\varepsilon\|$	0.039197	0.01433	0.016004	0.012341	0.008419	0.014431	0.005104	0.012506	0.009870	0.012005
$\langle r_{m^+e^-}\rangle$	2.312	4.09	4.487	5.112	5.731	5.522	6.592	17.12	76.15	
$\langle r_{m^+e^+}\rangle$	3.662	5.52	6.033	6.393	7.287	6.999	8.006	17.64	76.18	
$\langle r_{e^-e^-}\rangle$	3.575		6.033	6.791	7.691	6.735	8.215	8.324	8.537	8.549
$\langle r_{e^+e^-}\rangle$	3.480		4.487	4.825	5.279	4.773	5.514	5.398	5.484	5.490
$\langle\delta(\mathbf{r}_{e^-}-\mathbf{r}_{e^+})\rangle$	0.02446		0.02212	0.02130	0.02081	0.02165	0.02010	0.02075	0.02057	0.02073
$\Gamma_{2\gamma}$[b]	2.469[c]	~2	2.232[c]	2.156	2.086	2.185	2.029	2.094	2.078	2.093

[a]About 30% of the binding energy for CuPs comes from an extrapolation. The overall uncertainty due to the extrapolation is about ±10%.
[b]The annihilation rates for LiPs, NaPs, and KPs contain a contribution from the core.
[c]The annihilation rates for HPs and Ps_2 calculated from Eq. (5) are slightly different from those reported in [40]. The rate for Ps_2 is the rate per positron.

annihilation rate of the largest calculation of Usukura *et al.* [40]. During the course of very many SVM calculations we have noticed that the annihilation rate tends to asymptote to its converged value from below. This is probably related to the incorrect functional form of the ECG basis functions at the coalescence points. A general assessment would be that the annihilation rate has a systematic tendency to be about 1% too small, with additional fluctuations of about 1% due to the stochastic method used to generate the basis at each X_m. The radial expectation values for the present calculation, such as the mean electron-m_x^+ distance of $2.311a_0$ or the mean positron-m_x^+ distance of $3.661a_0$, are quite well converged and agree with the Usukura *et al.* calculation to an accuracy of about ±1 in the fourth significant digit. Another measure of accuracy is the virial theorem expectation value $\langle V\rangle/\langle T\rangle$. This is equal to exactly −2 for the exact wave function. The largest deviation from the exact value for the entire X_m range was 3.8×10^{-5}.

This $(m^+,2e^-,e^+)$ system has two classes of dissociation thresholds, depending on the mass of the m^+ particle, which are listed in Table I. When $X_m<0.024\,60$ the $m^+ + Ps^-$ configuration is the lowest energy dissociation threshold and at

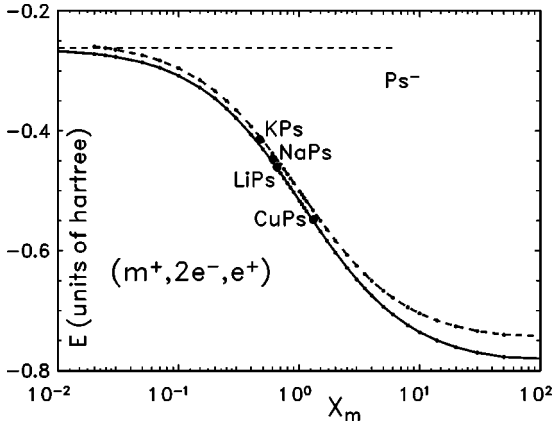

FIG. 1. Energy of the $(m^+,2e^-,e^+)$ system as a function of the X_m mass ratio (solid curve). The energy of the $(m^+,e^-)+Ps$ dissociation threshold is shown as the dashed line. The points for LiPs, NaPs, KPs, and CuPs were plotted using an equivalent mass defined by Eq. (6).

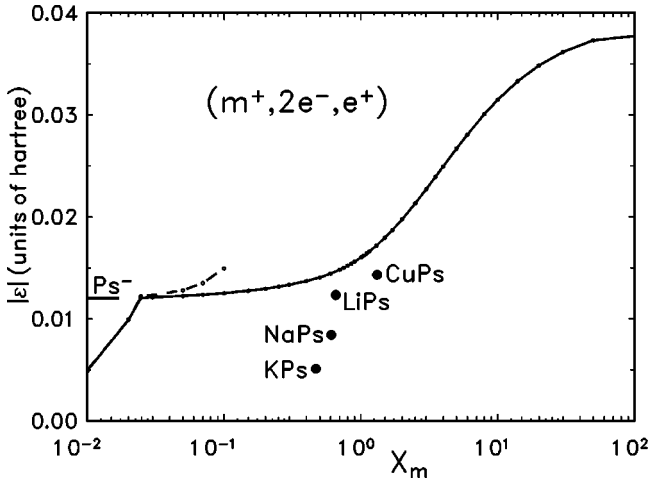

FIG. 2. The binding energy of the $(m^+,2e^-,e^+)$ system as a function of the X_m mass ratio (solid curve). The dashed line gives the binding energy for the (m^+,Ps^-) model as defined by Eqs. (2) and (3). The points for LiPs, NaPs, KPs, and CuPs were plotted using an equivalent mass defined by Eq. (6). The binding energy for the Ps^- ground state is denoted by the horizontal line on the left axis.

the very smallest values of $X_m = m^+/m_e$, the system evolves into a $m^+ + \mathrm{Ps}^-$ configuration. The two fragments must bind to each other since they are oppositely charged. The condition $m^+ = 0.024\,60 m_e$ was determined by the requirement that the binding energy of the (m^+, e^-) subsystem is the same as the binding energy of the Ps^- ion. The dissociation products are $\mathrm{Ps} + (m^+, e^-)$ when $X_m > 0.024\,60$.

The total energy of the $(m^+, 2e^-, e^+)$ system is shown as a function of X_m in Fig. 1 while the binding energy system as defined by Table I is shown in Fig. 2. It is clear that the system is bound for all values of m^+. The smallest m^+ for which a calculation was explicitly done was $X_m = 0.020$. This lies just below the 0.024 60 mass ratio for the transition to the $m^+ + \mathrm{Ps}^-$ dissociation threshold and can be used to infer stability for the $X_m \to 0$ limit.

At the lower limit for X_m the system is expected to evolve into an $m^+ + \mathrm{Ps}^-$ configuration. The interparticle mean distance of the $(0.05 m_e^+, e^-)$ ground state is $73 a_0$. At such distances, the field of the m^+ particle should not have a large influence upon the ability of the electron to bind positronium or affect the structure of the resulting Ps^- cluster.

The binding energy and other expectation values at the smallest value of X_m considered, 0.020, support this model. Regarding the Ps^- system as a point particle leads to a mean m^+-Ps^- distance given by

$$\langle R_{Ps^- \text{-} m^+} \rangle \approx 1.5 \frac{(3 + X_m)}{3 X_m}. \tag{1}$$

The actual distance at $X_m = 0.020$ is $76.2 a_0$ while the distance predicted by Eq. (1) is $75.5 a_0$. Examination of the electron-electron and electron-positron distances $\langle r_{e^- e^-} \rangle$ and $\langle r_{e^- e^+} \rangle$ also demonstrates that the two electrons and the positron are coalescing into Ps^- at small X_m. From Table II it is seen that these expectation values at $X_m = 0.020$ are within 0.2% of those of the Ps^- ground state.

An approximate expression for the binding energy against dissociation for the (Ps^-, m^{Z+}) configuration is

$$\varepsilon \approx \begin{cases} \dfrac{3Z^2 X_m}{2(3 + X_m)}, & X_m < X_{crit}, \quad (2) \\ \dfrac{3Z^2 X_m}{2(3 + X_m)} + 0.262\,005\,07 - \dfrac{Z^2 X_m}{2(1 + X_m)} - 0.250, & X_m > X_{crit}, \quad (3) \end{cases}$$

where X_{crit} is determined by the solution of the equation

$$\frac{3Z^2 X_m}{2(3 + X_m)} = 0.012\,005\,07. \tag{4}$$

The critical value of X_m is 0.024 60 for $Z = 1$. The justification for an expression of this type has been presented previously [31]. For X_m less than 0.002 460 the binding energy is estimated to be that of a negatively charged ion of mass $3m_e$ binding the m^+ particle. For $X_m > 0.024\,60$, the internal energy of Ps^- is added to that of the $(3m_e^-, m^+)$ system and then the energies of the Ps and (e^-, m^+) dissociation fragments are subtracted to give the binding energy. This model predicts a binding energy of 0.009 934 hartree at $X_m = 0.020$. The actual energy coming from the explicit calculation was 0.009 870 hartree.

It is useful to estimate the electron-positron pair annihilation rate since this can be used to give insight into the structure of the system. The spin-averaged 2γ annihilation rate is proportional to the probability of finding an electron and a positron at the same position in a spin singlet state. If the different spin states are averaged, the annihilation rate can be written as

$$\Gamma_{2\gamma} = 2\pi r_e^2 c \langle \Psi | \sum_i \delta(\mathbf{r}_i - \mathbf{r}_p) | \Psi \rangle = 1.009\,39 \times 10^{11} \sum_i \langle \delta(\mathbf{r}_i - \mathbf{r}_p) \rangle \tag{5}$$

[15,41,42], where the sum is over the electron coordinates and $\Gamma_{2\gamma}$ is given numerically in s^{-1}.

Figure 3 shows the spin-averaged annihilation rate as a function of X_m. One property of the finite dimension ECG basis expansions is that there is a tendency for the computed annihilation rate to slightly underestimate the exact annihilation rate. Also shown in Fig. 3 are accurate estimates of the annihilation rate for HPs and Ps^- as taken from Table II. The annihilation rate approaches that of Ps^- as $X_m \to 0$. The computed annihilation rate of $2.078 \times 10^9\ \mathrm{s}^{-1}$ at $X_m = 0.020$ is slightly smaller than the Ps^- lifetime of $2.093 \times 10^9\ \mathrm{s}^{-1}$ [43]; but the difference between the two rates is smaller than the uncertainty associated with using a basis of finite dimension.

1. Comparisons with LiPs, NaPs, KPs, and CuPs

The stability of the $(m^+, 2e^-, e^+)$ system for all possible values of X_m has implications for the binding of Ps to the other alkali-metal and group IB atoms in the periodic table. First, we make the assumption that the (m^+, e^-) system with the same binding energy as a group I or IB atom can be regarded as an analog of that atom. The equivalent mass M^+

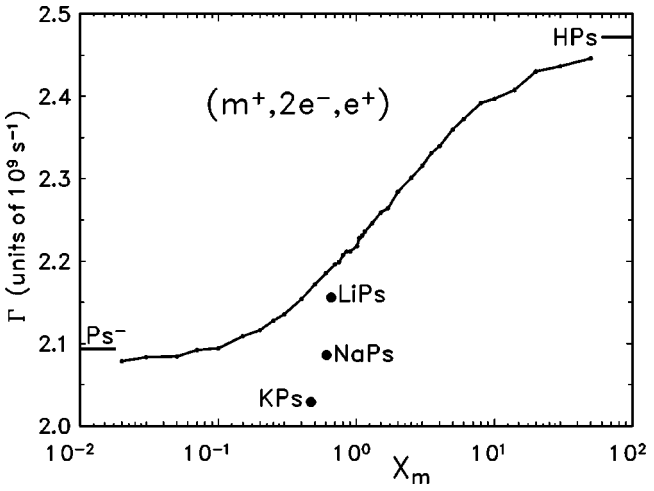

FIG. 3. The annihilation rate (in units of 10^9 s^{-1}) of the $(m^+,2e^-,e^+)$ system as a function of X_m. The annihilation rates for the Ps^- and HPs systems are denoted by the horizontal lines on the left and right axes, respectively. The points for LiPs, NaPs, and KPs were plotted using an equivalent mass defined by Eq. (6). The small fluctuations in the curve occur because the basis for each X_m is different and was generated using a stochastic search (the annihilation rate for CuPs was not plotted since its uncertainty is quite large).

for an alkali-metal or group IB atom is defined by the equation

$$\varepsilon_A = \frac{M^+ m_e}{2(M^+ + m_e)}, \tag{6}$$

where the ionization potential of the neutral atomic parent is denoted by ε_A. The equivalent masses for Cu, Li, Na, and K were $1.314m_e$, $0.656m_e$, $0.607m_e$, and $0.469m_e$, respectively. This suggests that the structures of the *A*Ps complexes should be more like Ps_2 than HPs, and this is supported by the data in Table II. The *A*Ps annihilation rate and interparticle expectation values are all closer to those of Ps_2 than HPs.

It is apparent from Table II and Figs. 1–3 that the behavior of the *A*Ps expectation values as a function of their equivalent mass is consistent with the X_m variation of the properties of the $(m^+,2e^-,e^+)$ ground state. For example, the binding energy of the *A*Ps system increases with M^+ just as the $(m^+,2e^-,e^+)$ energy increases with X_m. Similarly, the annihilation rate of the *A*Ps system increases with M^+ as the $(m^+,2e^-,e^+)$ rate increases with X_m. The expectation values of the interparticle distances listed in Table II, e.g., $\langle r_{e^-e^-}\rangle$, for the *A*Ps and $(m^+,2e^-,e^+)$ also show similar trends as M^+ or X_m increases or decreases.

The analogy between the *A*Ps and $(m^+,2e^-,e^+)$ systems is not exact; for example, the *A*Ps systems have annihilation rates that are smaller by about 5%. The *A*Ps binding energies shown in Fig. 2 are also smaller than those of $(m^+,2e^-,e^+)$; it is likely that this is due to the increased magnitude of the repulsive interaction when the positron penetrates the core. It is also worth noting that the convergence of the binding energy of KPs could be significantly improved.

The present calculations suggest that one should expect Feshbach resonances associated with H(2*s*), Li(3*s*), and Na(4*s*) and excitations in Ps+*A* scattering systems. (There have been a number of studies of such resonances in the Ps+H scattering system [14,44–47].) The dynamics that supports Ps binding to (m^+,e^-) irrespective of the parent system binding energy certainly applies to these excited states. The weak binding of the electron to the alkali-metal core for excited states means that the Coulomb field of the core cannot disrupt the binding of Ps to this electron to form a Ps^- cluster.

On the basis of the present data it is possible to assert with some confidence that the heavier group I and IB atoms Ag and Au would bind positronium. Silver has almost the same ionization energy as copper so one would expect that it would therefore have a similar Ps binding energy. It is worth noting in passing that the binding energies of positronic copper and positron silver e^+Cu and e^+Ag are about the same size [48]. Gold has a larger ionization energy than either silver or copper, and hence would likely bind Ps more strongly.

Making a similar prediction about the heavier alkali-metal atoms Rb and Cs is not quite so clear cut. The stability of $(m^+,2e^-,e^+)$ for all X_m is certainly supportive of the idea of Ps binding. However, Fig. 2 shows the energies of NaPs and KPs lying considerably below the ε vs X_m curve. So the issue needing resolution is whether stronger repulsion of the positron by the alkali-metal core can prevent Ps binding. While the absolute proof will come from an explicit calculation, a very good indication can come from a model calculation with a more realistic potential. What we have done is use Na as a model alkali-metal atom [49]. A model Hamiltonian, with an additional short range potential to adjust the strength of the interaction between the core and valence electron, was diagonalized in the 960-term ECG basis used to describe the NaPs ground state. A model atom with the same ionization potential as Rb had a Ps binding energy of 0.0045 hartree, while the Ps binding energy for model Cs was 0.0038 hartree. The ability of the model to make realistic predictions was checked by doing a model calculation with the Hamiltonian tuned to the potassium ionization energy. It gave a Ps binding energy of 0.0050 hartree which agrees quite well with that of the full KPs calculation.

2. Structure of KPs

As part of the current exercise an improved description of the KPs ground state was obtained. This entailed the enlargement of the ECG basis from 980 to 1080 ECG basis functions and some further optimization. In every other respect the details of the calculation are the same as those reported earlier, and the reader is referred to an earlier work [38].

The binding energy of the improved KPs wave function was 0.005 104 hartree. This is about 50% larger than the previously reported binding energy of 0.003 275 hartree. The annihilation rate of the positron with the two valence electrons was 2.0173×10^9 s^{-1} while the core annihilation rate was 0.0114×10^9 s^{-1}. These annihilation rates are marginally larger than previously reported values [38].

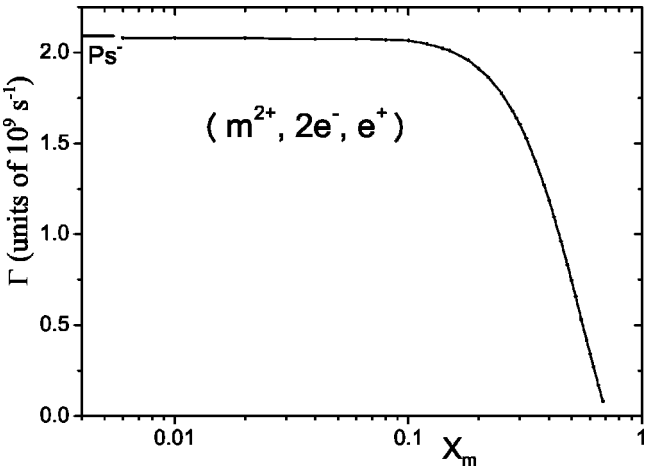

FIG. 4. The annihilation rate (in units of $10^9\ s^{-1}$) of the $(m^{2+},2e^-,e^+)$ system as a function of X_m. The annihilation rate for the Ps^- system is denoted by the horizontal line on the left axis.

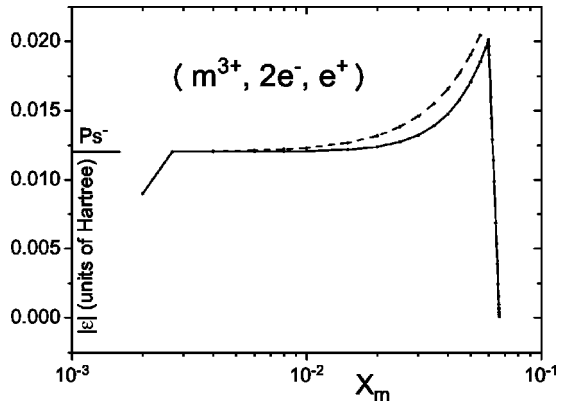

FIG. 5. The binding energy of the $(m^{3+},2e^-,e^+)$ system as a function of the X_m mass ratio (solid curve). The dashed line gives the binding energy for the (m^{3+},Ps^-) model as defined by Eqs. (2) and (3). This is practically indistinguishable from the binding energy of the explicit calculation for $X_m<0.0040$. The discontinuities in the slope indicate the boundaries between the regions with different dissociation channels. The binding energy for the Ps^- ground state is denoted by the horizontal line on the left axis.

Although it is suspected that the binding energy could increase by a further 25%, the very tedious nature of the calculations (many months of CPU time were consumed in improving the KPs wave function) means that it is desirable to report the current best estimate now and not try and drive the KPs energy and annihilation rate closer to convergence.

B. $Z=2$

The stability of the $(m^{2+},2e^-,e^+)$ system has been previously investigated with the SVM method using basis sets of dimension 400 [31] and it was shown that the system was stable for all $X_m\leqslant 0.68$. In this work the dominant influence of the (m^{2+},Ps^-) configuration at low X_m was first noted. For example, the binding energies determined from Eq. (3) agreed with the SVM binding energy to better than 5% accuracy for all $X_m<0.020$ and to better than 1% for $X_m<0.0060$ [31]. Further evidence regarding this description at small X_m is presented here.

First, the $\langle r_{e^-e^-}\rangle$ and $\langle r_{e^-e^+}\rangle$ expectation values are also consistent with the (Ps^-,m^{2+}) model. At $X_m=0.0060$, one obtains $8.543a_0$ and $5.487a_0$ respectively. These lie within 0.1% of the interparticle expectation values of the Ps^- ground states.

The annihilation rate as a function of X_m is shown in Fig. 4 and at the smallest values of X_m the annihilation appears to asymptote toward that of Ps^-. The annihilation rate is $2.082\times10^9\ s^{-1}$ at $X_m=0.0060$, which is also consistent with the idea that the system evolves into a (Ps^-,m^{2+}) configuration as $X_m\to0$. The annihilation rate decreases monotonically as X_m decreases. At the largest values of X_m (i.e., $X_m>0.2907$), the system evolves into an $(m^{2+},2e^-)$ configuration. As the e^+ becomes more weakly bound to the $(m^{2+},2e^-)$ system, it drifts further away and the annihilation rate decreases to zero.

C. $Z=3$

The $(m^{3+},2e^-,e^+)$ system can be regarded as being equivalent to a positive ion that is a member of the group II isoelectronic series. As far as we know, no calculations on this four-body system have been reported. The results reported in this section were obtained for ECG basis sets of dimension 480 or larger.

The binding energy of this system as a function of X_m is shown in Fig. 5. The system was found to be stable for all $X_m\leqslant0.066\,32$. This covers a mass range that encompasses two different dissociation regimes in their entirety and part of the third dissociation region. That the system is stable for $X_m<0.002\,675$ means it is stable whenever the $m^{3+}+Ps^-$ breakup represents the lowest energy dissociation threshold. Stability for $X_m\in[0.002\,675,0.059\,65]$ means it is stable whenever the $(m^{3+},e^-)+Ps$ breakup is the lowest energy dissociation channel. One interesting feature of Fig. 5 is its similarity in shape to the equivalent curve for the $(m^{2+},2e^-,e^+)$ system [31]. The maximum binding energy occurs at the boundary between the $(m^{2+},2e^-)+e^+$ and the $(m^{2+},e^-)+Ps$ dissociation regions. The approximate expressions of Eqs. (2) and (3) give a reliable estimate of the binding energy for $X_m<0.050$.

The system is also stable for a small part of the energy range which has the $(m^{3+},2e^-)+e^+$ fragmentation as the lowest energy dissociation channel. The restricted mass range for positron binding is not surprising since it is not intuitively obvious how a positron can bind itself to a positive ion when the asymptotic boundary condition is broken up into $(m^{3+},2e^-)+e^+$. The energy of the parent system, i.e., $E(m^{3+},2e^-)$, is equal to $-0.552\,643\,4$ hartree at the largest X_m for binding.

The annihilation rate as a function of X_m is shown in Fig. 6. At the smallest X_m, 0.0020, the rate is $2.077\times10^9\ s^{-1}$. Once again, this is consistent with the idea that the system evolves into a (Ps^-,m^{3+}) configuration as $X_m\to0$. At $X_m=0.0020$, one obtains $8.546a_0$ and $5.488a_0$ for the $\langle r_{e^-e^-}\rangle$ and $\langle r_{e^-e^+}\rangle$ expectation values, respectively. These lie within 0.1% of the interparticle expectation values of the Ps^- ground state.

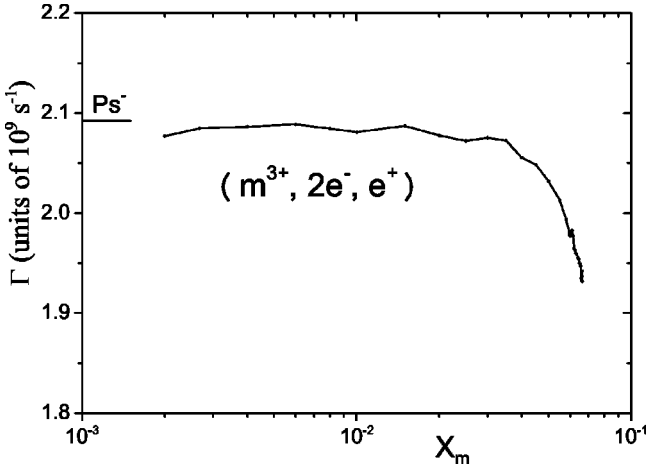

FIG. 6. The annihilation rate (in units of $10^9\ s^{-1}$) of the $(m^{3+},2e^-,e^+)$ system as a function of X_m. The annihilation rate for Ps^- is denoted by the horizontal line on the left axis.

At the larger values of X_m the annihilation rate behaves in a manner that might seem unusual. While the annihilation rate does decrease, the explicit calculations show no sign of it decreasing to zero. In effect, the annihilation rate is still quite substantial when the SVM calculations result in the system becoming unbound.

To shed further light on this behavior, the $\langle r_{m^{3+}e^-}\rangle$ and $\langle r_{m^{3+}e^+}\rangle$ expectation values have been plotted as functions of X_m in Fig. 7. The distances between the particles decrease consistently as X_m increases. For $X_m \geqslant 0.5966$ the lowest energy threshold is for $(m^{3+},2e^-)+e^+$ breakup and the binding energy of the positron to the $(m^{3+},2e^-)$ system decreases steadily as X_m increases from 0.059 66. It is somewhat counterintuitive, but the distance between the m^{3+} particle and the positron decreases while the binding energy decreases. This result was sufficiently unusual that special attention was paid to the calculations at the highest values of X_m. The basis dimension at $X_m=0.066\,30$ and $0.066\,32$ was increased to 580 and the wave function was then subjected to further optimization. At $X_m=0.06630$ the binding energy was 8.9×10^{-5} hartree and the $\langle r_{m^{3+}e^+}\rangle$ expectation was $10.4845a_0$. When X_m was increased to 0.066 32, the binding energy decreased by a factor of 3 to 3.1×10^{-5} hartree. However, the $\langle r_{m^{3+}e^+}\rangle$ expectation value actually decreased to $10.4824a_0$.

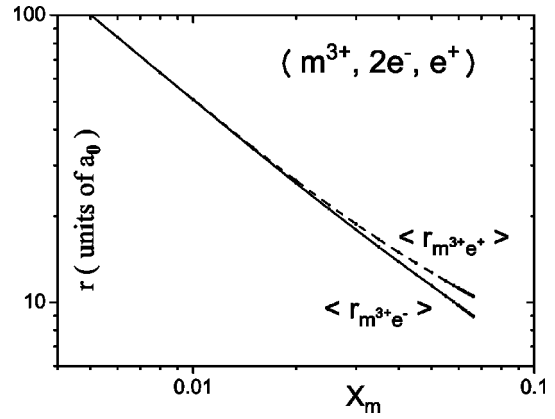

FIG. 7. The $\langle r_{m^{3+}e^-}\rangle$ and $\langle r_{m^{3+}e^+}\rangle$ expectation values (units of a_0) for the $(m^{3+},2e^-,e^+)$ system as a function of X_m.

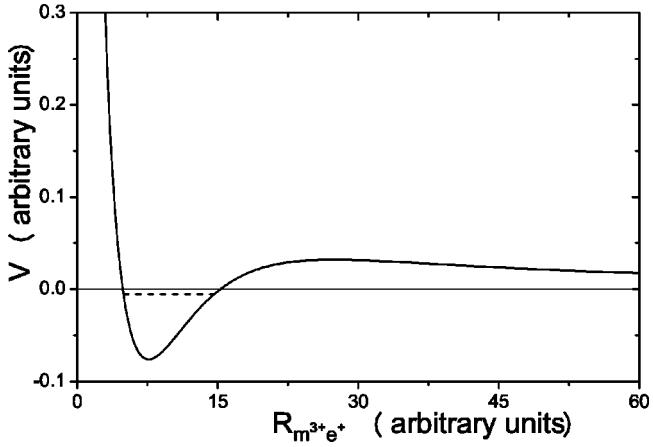

FIG. 8. A schematic diagram showing the qualitative behavior of the effective interaction potential between the $(m^{3+},2e^-)$ system and the positron as a function of $r_{m^{3+}e^+}$.

The explanation for this behavior lies in an examination of the nature of the interaction potential between the positron and the $(m^{3+},2e^-)$ system. The nature of the dominant terms in the potential can be summarized as

$$V \approx \begin{cases} \dfrac{1}{r_{m^{3+}e^+}} & \text{large distances,} \quad (7) \\ -\dfrac{\alpha_d}{2r_{m^{3+}e^+}^4} & \text{intermediate distances,} \quad (8) \\ \dfrac{3}{r_{m^{3+}e^+}} & \text{short distances,} \quad (9) \end{cases}$$

where α_d is the polarizability of the $(m^{3+},2e^-)$ system. At large distances the dominant interaction is of course the Coulomb repulsion between the positron and the $(m^{3+},2e^-)$ system. At small distances the dominant interaction is the Coulomb repulsion between the positron and the m^{3+} particle. At intermediate distances, the attractive correlation-polarization potential between the positron and the electrons is largest. The leading order term of this interaction is the adiabatic polarization potential with α_d being the static dipole polarizability of the $(m^{3+},2e^-)$ complex. A schematic diagram showing the nature of this potential is given in Fig. 8.

The important aspect of this potential is that there is a Coulomb barrier separating the well that binds the positron from the asymptotic region. So the positron will be localized in this well even as the binding energy decreases. The positron will be able to escape the well only for binding energies vanishingly close to threshold.

This provides a natural explanation for the curious behavior of $\langle r_{m^{3+}e^+}\rangle$ with increasing X_m. This expectation decreases because the $(m^{3+},2e^-)$ system becomes more compact as X_m increases. The positron will start to drift away from the $(m^{3+},2e^-)$ complex only when the binding energy gets closer to threshold (i.e., smaller than 3.1×10^{-5} hartree) than was achieved by the present set of calculations.

The present results are also compatible with the systematics of halo states that occur in nuclear systems [50]. Two-body halo states consist of a nucleon weakly bound to a residual nucleus. A large percentage (e.g., 50%) of the nucleon wave function must lie in the classically forbidden region outside the nuclear potential [50,51]. While a number of neutron halo states have been identified, it is not possible to identify a nucleus with an unambiguous proton halo. The Coulomb barrier does tend to confine a weakly bound proton to lie inside the nuclear potential well. It has been shown that three-body halo states involving a proton can be expected to have finite radial expectation values while the binding energy goes to zero [50,52].

D. $Z=10$

The stability of the $(m^{3+},2e^-,e^+)$ system for a mass range encompassing both the $m^{3+}+\mathrm{Ps}^-$ and the $(m^{3+},e^-)+\mathrm{Ps}$ dissociation thresholds suggested that stability of the $(m^{Z+},2e^-,e^+)$ system over an extended mass range may be a feature of the system general to all Z. Accordingly, the system $Z=10$ was studied.

The $m^{10+}+\mathrm{Ps}^-$ system gives the lowest dissociation threshold whenever $X_m<0.000\,240\,2$. When $X_m \in [0.000\,240\,2, 0.002\,54]$, the lowest energy threshold is that for breakup into $(m^{10+},e^-)+\mathrm{Ps}$.

An explicit SVM calculation with dimension 100 has been done for $X_m=0.002\,54$, giving a total energy of $-0.388\,849$ hartree. This corresponds to a binding energy of 0.012 170 hartree. Although the small dimension of the basis means the binding energy is an underestimate, the good agreement with Eq. (3), which gives 0.012 219 hartree, indicates that the physical picture justifying this expression is realistic. The stability at $X_m=0.002\,54$ can be used to reasonably infer stability for all $X_m<0.002\,54$.

III. SUMMARY

The structure of the $(m^{Z+},2e^-,e^+)$ system has been investigated as a function of Z and $X_m=m^{Z+}/m_e$. A universal feature of the system is its ability to form a Ps^- cluster at small X_m, thereby leading to binding whenever the m^{Z+}-e^- interaction is sufficiently weak. The system is stable for all $Z\geqslant 1$ when the $m^{Z+}+\mathrm{Ps}^-$ fragmentation gives the lowest energy dissociation threshold. Furthermore, the results of the explicit calculations for $Z\in[1,10]$ mean that it is reasonable to infer stability whenever the $(m^{Z+},e^-)+\mathrm{Ps}$ fragmentation is the lowest energy dissociation that occurs. It seems likely that the $(m^{Z+},2e^-,e^+)$ system is stable for all values of X_m such that the lowest energy dissociation channel is either the $(m^{Z+},e^-)+\mathrm{Ps}$ or the $m^{Z+}+\mathrm{Ps}^-$ fragmentation.

While the possibility of positron binding to a positively charged system is now theoretically conceivable, in practice there are no divalent ns^2 singly charged positive ions that have energetics compatible with the $(m^{3+},2e^-,e^+)$ configurations that result in positron binding. However, although a bound state would be ruled out, it is possible that Feshbach resonances associated with $n*s^2$ doubly excited states may exist. In addition, the results attest to the presence of (A^+,Ps^-) type configurations in Ps-A collisions [47]. Such configurations are likely to be most important for target atoms with small ionization potentials.

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