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Structure of the LiPs and e^+Be systems

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Abstract. Close to converged energies and wave functions for the positron binding systems, LiPs and e^+Be are computed using the stochastic variational method. Binding energies and annihilation rates from both *ab-initio* and fixed core calculations are determined and found to be in agreement. The *ab-initio* binding energy of e^+Be was 0.00316 Hartree while that for LiPs was 0.01237 Hartree.

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Key words: positron, positronium, stochastic variation method, atomic structure, positronic atom

1 Introduction

The LiPs and e^+Be systems are two examples of exotic positron binding systems. These systems have four electrons and one positron and are amenable to calculations using the stochastic variational method (SVM) [1–4]. Both of these systems were determined to be electronically stable in 1998 [3,5].

Since that time the structure of these two systems have been investigated by a variety of methods. Further demonstrations of the stability of the e^+Be system were made using the configuration interaction (CI) [6,7] and the quantum monte carlo (QMC) method [8,9]. The CI calculation was made using a fixed core model and the best SVM calculation so far reported was that performed with the fixed core stochastic variational method (FCSVM) [3,7,10,11]. The stability of the LiPs system has so far been established using the QMC [8] and SVM methods. Both the fixed core and fully *ab-initio* variants of the SVM have been applied to the calculation of the LiPs ground state [3,5,10,12].

The present work uses the *ab-initio* SVM to generate close to converged energies for the e^+Be and LiPs systems. The new wave function and binding energy for the e^+Be system represents a substantial improvement over any previous *ab-initio* calculation. The new binding energy for this system is almost a factor of two larger than the previous

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SVM value [3]. The new binding energy for LiPs is about 2% larger than the earlier SVM binding energy for this system. The new SVM binding energies are in agreement with earlier FCSVM estimates of the binding energies [10, 11].

2 Method and results

The SVM has been described in a number of articles [2, 3, 13] and 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 Hamiltonian matrix elements that can be computed very quickly and the energy is optimized by performing a trial and error search over the exponential parameters that define the basis. The SVM has been used to solve a number of many-body problems in different areas of physics [2, 3]. The largest basis set used in the present calculations comprised 2200 ECGs. Once the wave function has been obtained, other expectation values such as the electron-positron annihilation rate, and mean inter-particle distances are easily obtained [3].

The FCSVM [3] uses a $1s^2$ frozen core to reduce the number of active particles from five to three. The core is taken from a Hartree-Fock calculation and direct and exchange integrals between the valence and core particles are done exactly. Semi-empirical core polarization potentials are used to represent the relaxation of the core due to the motion of the valence particles. An orthogonalizing pseudo-potential was used to enforce Pauli blocking between the valence and core electrons. The strength parameter, of the pseudo-potential was set to 10^5 Hartree. The present FCSVM calculation for LiPs was a slight improvement (the numbers of ECGS was increased from 900 to 1000) over a previous calculation [10]. The basis for the e^+Be calculation is essentially the same as that used in an investigation of whether this state could be considered as a quantum halo state [11].

Table 1 tracks the energies of the LiPs and e^+Be systems as a function of the dimension of the ECG basis. The final energy for LiPs, -7.7404316 Hartree is compatible with a previous estimate of the expected variational limit [10]. The nuclear mass was set to infinity for all the calculations reported in Table 1. This is also true for all the expectation values given in Table 2. The binding energies were computed using an Li energy of -7.4780603 Hartee [14,15] and a Be energy of -14.667356 Hartee [16]. Expectation values computed with the FCSVM are also given in Table 2.

Table 1: Convergence of the energy of the LiPs and e^+Be systems as a function of basis set size.

N	LiPs	e^+Be
1200	-7.7403655	
1400	-7.7404001	-14.670391
1600	-7.7404101	-14.670451
1800	-7.7404206	-14.670487
2000	-7.7404236	-14.670507
2200	-7.7404316	-14.670519
QMC [8]	$-7.7396(1)$	$-14.6688(4)$

Table 2: Properties of the LiPs and e^+Be ground states. All calculations assume an infinite nuclear mass. All quantities are given in atomic units with the exception of the annihilation rates which are in units of 10^9 s^{-1}. The positron and electron kinetic energy operators are written as T_+ and T_-. FCSVM expectation values involving electrons only take the two valence electrons into account. The core annihilation rate, $\Gamma_{\rm core}$ includes the enhancement factors mentioned in the text.

Property	LiPs		e^+Be	
	SVM	FCSVM	SVM	FCSVM
N	2200	1000	2200	1023
E	-7.7404316		-14.670519	
ε	0.012371	0.012365	0.003163	0.003181
$\langle V\rangle/\langle T\rangle + 2$	8.1×10^{-6}		2.7×10^{-6}	
$\langle T_-\rangle$	7.608486	0.342936	14.642093	1.031135
$\langle T_+\rangle$	0.132008	0.132026	0.028457	0.028295
$\langle r_{N^+e^-}\rangle$	2.8499	5.1203	1.5355	2.6538
$\langle r_{N^+e^+}\rangle$	6.4219	6.4087	9.9105	10.0479
$\langle r_{e^-e^-}\rangle$	4.7280	6.8072	2.6057	4.2137
$\langle r_{e^+e^-}\rangle$	5.6455	4.8334	9.8683	9.9612
$\langle 1/r_{N^+e^-}\rangle$	0.460251	0.268610	2.101123	0.521230
$\langle 1/r_{N^+e^+}\rangle$	1.476719	0.185742	0.141844	0.141383
$\langle 1/r_{e^-e^-}\rangle$	0.460251	0.187496	0.722927	0.280075
$\langle 1/r_{e^+e^-}\rangle$	0.269723	0.353768	0.157020	0.171513
$\langle\delta(N^+-e^-)\rangle$	3.456	0.08455	8.816	0.5283
$\langle\delta(N^+-e^+)\rangle$	8.576×10^{-6}	1.429×10^{-5}	2.520×10^{-6}	5.574×10^{-6}
$\langle\delta(e^--e^-)\rangle$	0.09112	3.199×10^{-4}	0.2679	1.446×10^{-3}
$\Gamma_{\rm total}$	2.1707	2.1709	0.4313	0.4243
$\Gamma_{\rm core}$		0.0138		0.0032

The agreement between the SVM and FCSVM binding energies listed in Table 2 is good. There is less than 1% difference between the SVM and FCSVM binding energies for LiPs. The binding energy is defined as the energy required to remove Ps from the Li atom. Both the SVM and FCSVM binding energies are close to their respective variational limits. The previous best estimate of the LiPs energy, -7.740208 Hartree, computed with a basis set of dimension 860 [10], had a binding energy that is only 0.000224 Hartree smaller than the present binding energy. Further enlargement of the basis would be expected to lead to increases in the binding energy of the order of 10^{-5} Hartree.

An earlier SVM determination of the energy for e^+Be was -14.669042 Hartree [3]. The SVM binding energy of 0.001686 Hartree was only about 50% of the size of the binding energies obtained with the FCSVM, 0.003180 Hartree [11] and a fixed core CI calculation, namely 0.003169 Hartree [7, 11]. The present SVM binding energy is 0.003163 Hartree. The FCSVM and SVM energies for the binding of a positron to the Be atom are now within 1% of each other. It has been noticed during the course of calculations that the e^+Be energy converged more slowly than the LiPs energy. The anticipated increase in the *ab-initio* SVM binding energy as the basis goes to completeness is most likely less than 10^{-4} Hartree. That the FCSVM binding energy is 1.8×10^{-5} Hartree larger than the SVM binding energy is a reflection of the slower convergence of the SVM energy for this five-body system.

Besides the energy, the electron-positron annihilation rate is the most important pa-

rameter for any positron binding atom or ion. This determines the lifetime of the exotic atom once it has been formed. The annihilation rate is proportional to the probability of finding an electron and a positron at the same position in a spin singlet state according to [17–19]

$$\Gamma = 4\pi r_e^2 c \langle \Psi | \sum_i O_{ip}^S \delta(\mathbf{r}_i - \mathbf{r}_p) | \Psi \rangle \tag{1}$$

$$= 1.009394 \times 10^{11} \sum_i \langle \delta(\mathbf{r}_i - \mathbf{r}_p) \rangle_S. \tag{2}$$

The sum is over the electron coordinates, the δ-function expectation is evaluated in a_0^3, and Γ is given numerically in s^{-1}. The operator O_{ip}^S is a spin projection operator to select spin singlet states for the ip electron-positron pair. The FCSVM values of Γ were computed by adding together the annihilation rates involving both valence and core electrons. The FCSVM core annihilation rates were multiplied by enhancement factors. The enhancement factor for the LiPs $1s^2$ core was chosen to be 1.90 [20,21]. The enhancement factor for annihilation with the Be^{2+} $1s^2$ core was taken as 1.45. This value was deduced by extrapolating an assumed $1/Z$ scaling of the enhancement factors for He and Li^+ [21]. The SVM and FCSVM $\Gamma_{\rm total}$ for LiPs agree with each other to better than 1%. A larger relative difference occurs for e^+Be, but here the difference between SVM and FCSVM is still less than 2%.

The LiPs annihilation rate of 2.1707×10^9 s^{-1} is slightly larger that the spin-averaged annihilation rate of positronium, namely 2.008×10^9 s^{-1}. The structure of LiPs is best described as a positronium atom bound to a lithium atom [3, 22]. The structure of the e^+Be system is best described as a positron weakly bound to the beryllium atom ground state [3, 22]. This reveals itself in an annihilation rate of 0.4313×10^9 s^{-1} which is only 22% the size of the positronium annihilation rate. The previous SVM estimate of the e^+Be annihilation rate was 0.334×10^9 [3], significantly smaller than the present $\Gamma_{\rm total}$.

There is good agreement between the SVM and FCSVM values of the radial matrix elements $\langle r_{N^+-e^+} \rangle$ which agree to within 1%. The FCSVM matrix elements involving the electrons only include the two valence electrons in the calculation. They cannot be directly compared with the SVM expectation values due to the omission of the core electrons from the FCSVM calculation. The SVM and FCSVM expectation values of the positron kinetic energy are also in very good agreement.

The coalescence matrix elements, $\langle \delta(e^- - e^-) \rangle$ and $\langle \delta(N^+ - e^+) \rangle$ were more sensitive to the increase in basis size than any other quantity. This sensitivity is due to the fact that the wave function amplitude between two repelling particles is expected to be small at their coalescence point and the ECG functional form is not the natural choice to describe the relative wave function for two strongly repelling particles.

The expectation value for the virial theorem $\langle V \rangle / \langle T \rangle$ provides an estimate of wave function accuracy since it must be exactly -2 for any many body system composed of particles interacting by purely coulombic forces. The present SVM wave functions give values of $\langle V \rangle / \langle T \rangle$ that deviate from -2 by less than 10^{-5}.

3 Conclusions

To summarize, close to converged binding energies are reported for *ab-initio* SVM calculations of the five-body LiPs and e^+Be systems. The binding energy for LiPs is only 0.000224 Hartree greater than the previous best estimate [10]. The previous *ab-initio* calculation of the e^+Be system was large enough to establish binding, but otherwise did not give an accurate description of its structure. This latest SVM wave function represents a major improvement and the binding energy against breakup into e^++Be has been doubled. The new *ab-initio* SVM wave function gives a binding energy and expectation values that are typically within 1% of previous estimates based on fixed core calculations.

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