J. At. Mol. Sci.
doi: 10.4208/jams.071510.072110a

Vol. **1**, No. 4, pp. 275-279
November 2010

Structure of the LiPs and e^+Be systems

J. Mitroy *

ARC Centre for Anti-matter Matter Studies and School of Engineering, Charles Darwin University, Darwin NT 0909, Australia

Received 15 July 2010; Accepted (in revised version) 21 July 2010
Published online 2 August 2010

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.

PACS: 36.10.Dr, 36.10.-k, 31.15.ac, 82.30.Gg

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

*Corresponding author. *Email address:* jxm107@rsphysse.anu.edu.au (J. Mitroy)

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]	$-7.7396(1)$	$-14.6688(4)$