Positron attachment to the He doubly excited states

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The projection method is used to demonstrate the existence of positron attachment to three doubly excited states of helium. The $e^+\text{He}(2s^2 \, 1S^o)$, $e^+\text{He}(3s^2 \, 1S^o)$, and the $e^+\text{He}(2s2p \, 3P^o)$ states have binding energies of 0.447 eV, 0.256 eV and 0.486 eV respectively. These energies were computed with the stochastic variational method and the configuration interaction method. These states will exist as resonances in the $e^+\text{He}$ continuum and the $e^+\text{He}(2s^2 \, 1S^o)$ state could be detectable in the $e^+\text{He}$ collision spectrum. The existence of a series of $e^+\text{He}(ns^2 \, 1S^o)$ resonances associated with the $\text{He}(ns^o)$ double Rydberg series is also predicted and an explicit calculation demonstrating the existence of the $e^+\text{He}(3s^2 \, 1S^o)$ state is reported.

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In this paper the ability of a positron to attach itself to the doubly excited states of helium is demonstrated by explicit calculation using the same projection operator approach that was originally used in some of the earliest calculations of the helium doubly excited spectrum [1,2]. Besides the intrinsic interest in such exotic Coulomb systems, the result provides a pathway to providing experimental confirmation that positrons can be attached to electrically neutral atoms to form bound states.

It is now widely accepted that positrons can form bound states with a variety of atoms [3,4]. While the evidence for positron binding is very strong, it is mainly derived from calculation. Binding energies range from 0.0129 eV in the case of $e^+\text{Na}$ [5] to 0.50 eV for the $e^+\text{Ca}$ ground state [6].

There is solid experimental evidence that positrons can form bound states with a variety of molecules. The energy resolved positron annihilation cross sections for a number of molecules (e.g. $\text{C}_3\text{H}_8$, $\text{C}_6\text{H}_{14}$) show features that have been identified as Feshbach resonances formed by the trapping of positrons to the vibrationally excited states [7]. Positron binding to vibrationally excited states of molecules is thought to be the mechanism responsible for the large positron annihilation rates observed for many molecules in gas phase positron annihilation spectroscopy experiments [8].

While the experimental evidence of positron binding to molecules is good, there is no experimental evidence that could be construed as demonstrating the existence of positron-atom bound states. One possible signature would be the existence of resonant structures associated with atomic excited states in the positron scattering spectrum. Years of experimentation, however, have revealed little evidence for the existence of resonant states in positron-atom scattering spectra [9,10,11].

A number of schemes have been put forward to demonstrate the existence of positron-atom bound states [12-14]. The most recent proposal suggested that positron scattering experiments be performed on open shell transition-metal atoms having polarizabilities and ionization energies conducive to binding positrons [15]. Open shell systems are recommended since such systems would have low-lying excited states that could also bind a positron. Positron binding to these low-lying excited states would result in Feshbach resonances appearing in the low-energy annihilation cross section. However, the transition-metal atoms most likely to bind a positron represent difficult propositions for experimentation.

The present paper demonstrates that three of the doubly excited states of helium, namely the $\text{He}(2s^2 \, 1S^o)$, $\text{He}(3s^2 \, 1S^o)$ and $\text{He}(2s2p \, 3P^o)$ states can attach a positron with attachment energies exceeding 0.250 eV. The $e^+\text{He}(2s^2 \, 1S^o)$ and $e^+\text{He}(3s^2 \, 1S^o)$ states should manifest themselves as broad resonances in the $e^+\text{He}$ continuum. A positron cannot excite the $\text{He}(2s2p \, 3P^o)$ state from the $\text{He}(1s^2 \, 1S^o)$ ground state since there is no exchange interaction between the positron and electrons. These states can be regarded as the analogues of the triply excited negative ion resonances which are present in the electron-helium spectrum at 57 - 61 eV incident energy [16,17,18].

One motivation for the present investigation was the realization that the doubly excited states of helium have energetics very similar to those of the Mg atom. This binds a positron with a binding energy of 0.465 eV [19], and also supports a prominent $p$-wave shape resonance in the elastic scattering channel at 0.096 eV incident energy [19,20]. Table 1 compares energies of the doubly excited states of helium with the Mg($3f, 3f'$) states. The binding energy of the Mg$^+$(3s) ground state is −0.55254
The CI method was first applied to the calculation of the He doubly excited states. The basis included 49 LTOs for \( \ell = 0 \), and 50 LTOs for the other \( \ell \)'s. The largest \( \ell \) value used in these calculations was \( \ell = 8 \). The CI energies are given in Table I and were extrapolated to the \( \ell = \infty \) limit using a procedure described shortly. They agree with the \( E_{QHQ} \) energies to within \( 10^{-5} \) a.u.

\[
H = -\sum_{i=1}^{N+1} \frac{\nabla^2}{2} - \sum_{i=1}^{N} \frac{2}{r_i} + \frac{2}{r_{N+1}} + \sum_{i<j} \frac{1}{|r_i - r_j|} - \sum_{i=1}^{N} \frac{1}{|r_{N+1} - r_i|}, \tag{1}
\]

is then diagonalized in a large single particle basis of Laguerre type orbitals (LTOs).

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**TABLE II:** Calculated energies of some $e^+\text{He}$ states. The CI calculations are also given with a $J \to \infty$ correction as discussed in the text. The binding energies are denoted by $\varepsilon$.

| State          | Method | $J$ | $(E)_J$ (a.u.) | $\varepsilon$ (a.u.) | $\varepsilon$ (eV) |
|----------------|--------|-----|----------------|-----------------------|--------------------|
| $e^+\text{He}(2s^2 \ 1S^e)$ | CI     | 12  | -0.793557     | 0.014756              | 0.4015             |
|                | CI     | $\infty$ | -0.795058    | 0.016277              | 0.4429             |
|                | SVM    |     | -0.795190     | 0.016409              | 0.4465             |
| $e^+\text{He}(2s2p \ 3P^e)$ | CI     | 9   | -0.776306     | 0.014814              | 0.4031             |
|                | CI     | $\infty$ | -0.779362    | 0.017869              | 0.4863             |
|                | CI     | 12  | -0.468860     |                       |                    |

It has been shown that successive increments, $\Delta E_J$, of the binding energy is much larger than that of the $\text{He}(1s)$ state wave function which has a very small overlap with the $\text{He}^+(1s)$ state. The parameter $\lambda$ was set to $10^6$ a.u. for the present calculations. The $1s$ state was expanded as a linear combination of 12 gaussians. The SVM energy of the $\text{He}(2s^2)$ state was $-0.778766$ a.u., i.e. $5 \times 10^{-6}$ a.u. below the CI energy. The dimension of the largest SVM calculation of the $e^+\text{He}(2s^2)$ state was 900 ECGs. The SVM binding energy of the positron to the $\text{He}(2s^2)$ state given in Table II was 0.016409 a.u. Examination of the convergence pattern suggests that the SVM energy is within $2 \times 10^{-4}$ a.u. of the variational limit. The SVM and CI binding energies for this state are in excellent agreement when the respective uncertainties arising from finite size basis sets are taken into consideration.

The $e^+\text{He}(2s^2 \ 1S^e)$ system is also likely to support a $2\text{Po}$ shape resonance just above the $\text{He}(2s^2 \ 1S^e)$ threshold. This is based on the similarity of the $\text{He}$ and $\text{Mg}$ polarizabilities and the positron attachment energies in the $2\text{S}$ channel. The $e^+\text{Mg}^2\text{Po}$ shape resonance was located at 0.00351 a.u. above the elastic scattering threshold and had a width of 0.00396 a.u. [24].

It is likely that there will be an infinite series of resonances associated with the set of $\text{He}(ns^2)$ doubly excited states. An investigation of the $(m^2+, 2e^-, e^+)$ system revealed that this system remains bound when the mass $m^{2+} \to 0$ [41]. Decreasing the $m^{2+}$ mass weakens the effective strength of the $m^{2+}-e^-$ interaction and provides an analogue of the $\text{He}^+\text{ns}(e^-)$ interaction. A first test was performed by a CI investigation of the $e^+\text{He}(3\ell,3\ell')$ systems. In this case the single particle basis was orthogonalized to the $\text{He}^+(1s, 2s, 2p)$ states. The CI energy of the $\text{He}(3s^2)$ state is $-0.354562$ a.u. Since the removal energy of the electron with respect to the $\text{He}^+(3\ell)$ threshold, $-0.132340$ a.u., is less than the positronium ground state energy of $-0.25$ a.u., the threshold for attaching a positron to the $\text{He}(3s^2)$ state is at $-0.472222$ a.u.

The CI calculation for the $e^+\text{He}(3s^2)$ state gave an energy of $-0.481643$ a.u. The binding energy of this state is 0.009420 a.u. The stability of this system provides strong evidence for an infinite number of $e^+\text{He}(ns^2)$ type resonances. It is likely that the rich resonance structures of the PsH system [42] will be replicated for positron interactions with the doubly excited helium atoms.

Reference can be made to $e^-+\text{He}$ scattering experiments to give a first order estimate on the viability of experimental detection. A number of electron scattering experiments have demonstrated electron attachment to the He doubly excited states [16, 20]. Experiments that
detection of the optical excitation of the ejected electron following auto-ionization. One example is an experiment which measured the creation of He\(^+\) varied by only 1\% over the width of the He\(^-(2s^22p)\) resonance.

Higher signal to background ratios have been achieved in e\(^-\)-He experiments that measure differential cross sections. One example is an experiment which measured the energy of the ejected electron following auto-ionization\[18\]. Another is the measurement of the optical excitation functions associated with the formation of a number of He\(^-\) excited states\[19\].

The widths of the resonances and energy resolution of current positron beams is also an important consideration. Modern trap based positron beams can achieve an energy resolution of about 20-50 meV\[20\]. An initial estimate of the widths can be made by equating the widths to those of their electron doubly excited parent states. The width of the He(2s\(^2\)) state is \(\Gamma = 0.123\) eV\[27\], the He(3s\(^2\)) state is \(\Gamma = 0.082\) eV\[22\], while the He(2s2p\(^3\)P\(^o\)) state is \(\Gamma = 0.0081\) eV\[27\]. The e\(^+\)He(ns\(^2\)) resonances should be wide enough to detect with current positron beam technology. The theoretically well-known positron-atom resonances are too narrow as in the case of hydrogen and sodium\[44, 45\], involve atoms which do not naturally exist in gaseous form\[29, 44, 45\], or require scanning over an energy range near 0.10 eV\[29\] which is difficult to achieve with existing positron beams.

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[1] A. K. Bhatia, A. Temkin, and J. F. Perkins, Phys. Rev. 153, 177 (1967).
[2] A. K. Bhatia and A. Temkin, Phys. Rev. A 11, 2018 (1975).
[3] G. G. Ryzhikh, J. Mitroy, and K. Varga, J. Phys. B 31, 3965 (1998).
[4] J. Mitroy, M. W. J. Bromley, and G. G. Ryzhikh, J. Phys. B 35, R81 (2002).
[5] D. M. Schrader, in Proceedings of the International School of Physics “Enrico Fermi”, 7-17 July 2009, edited by A. Dupasquier and A. P. Mills Jr. (Italiana di Fisica, Italy, 2010), p. 337.
[6] J. Mitroy, Phys. Rev. Lett. 94, 033402 (2005).
[7] M. W. J. Bromley and J. Mitroy, Phys. Rev. A 73, 032507 (2006).
[8] L. D. Barnes, S. J. Gilbert, and C. M. Surko, Phys. Rev. A 67, 032706 (2003).
[9] G. F. Gribakin, J. A. Young, and C. M. Surko, Rev. Mod. Phys. 82, 2557 (2010).
[10] J. P. Sullivan, S. J. Gilbert, S. J. Buckman, and C. M. Surko, J. Phys. B 34, L467 (2001).
[11] C. M. Surko, G. F. Gribakin, and S. J. Buckman, J. Phys. B 38, R57 (2005).
[12] J. Mitroy and G. G. Ryzhikh, J. Phys. B 32, L411 (1999).
[13] J. Mitroy and I. A. Ivanov, J. Phys. B 34, L121 (2001).
[14] M. W. J. Bromley and J. Mitroy, Phys. Rev. A 65, 062506 (2002).
[15] V. A. Dzuba, V. V. Flambaum, and G. F. Gribakin, Phys. Rev. Lett. 105, 203401 (2010).
[16] C. E. Kuyatt, J. A. Simpson, and S. R. Mielczarek, Phys. Rev. 138, 385 (1965).
[17] J. J. Quémener, C. Paquet, and P. Marmet, Phys. Rev. A 4, 494 (1971).
[18] P. J. Hicks, S. Cvejanovic, J. Comer, and F. H. Read, Vacuum 24, 573 (1974).
[19] P. J. M. van der Burgt, J. van Eck, and H. G. M. Heideman, J. Phys. B 19, 2015 (1986).
[20] K. W. Tranatham, M. Jacka, A. R. P. Rau, and S. J. Buckman, J. Phys. B 32, 815 (1999).
[21] Y. Ralchenko, A. Kramida, J. Reader, and NIST ASD Team, NIST Atomic Spectra Database Version 3.1.5 (2008), URL http://physics.nist.gov/asd3