Positron attachment to the $He(ns^2 {}^{1}S^e)$ states

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Calculations based on the projection method and using explicitly correlated Gaussians are used to confirm the existence of positron attachment to two doubly excited states of helium. The $e^+\text{He}(2s^2 \ ^1S^e)$ and $e^+\text{He}(3s^2 \ ^1S^e)$ states have binding energies of 0.449 and 0.286 eV. These estimates of the resonance energies are nearer to the variational limit than previous calculations. These states will exist as resonances in the e^+ -He scattering continuum, and complex rotation calculations have been used to estimate their widths.

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I. INTRODUCTION

The ability of a positron to attach itself to the doubly excited states of helium has recently been demonstrated by explicit calculations [1]. These calculations were performed using the same projection operator approach that was originally applied in some of the earliest calculations of the helium doubly excited spectrum [2,3]. The results identified a possible pathway for experimental confirmation that positrons can be attached to electrically neutral atoms to form bound states.

There exists a substantial amount of calculational evidence that positrons can form bound states with a variety of atoms [4–6]. Binding energies range from 0.0129 eV in the case of e^+ Na [7] to about 0.50 eV for the e^+ Ca ground state [8]. However, there is no experimental evidence that could be construed as unambiguously demonstrating the existence of positron-atom bound states despite the numerous experiments providing evidence of positron binding to molecules [9].

One possible signature for positron-atom binding would be the existence of resonant structures associated with atomic excited states in the positron scattering spectrum. Many years of experiment, however, have provided no hard evidence regarding the existence of resonant states in positron-atom scattering spectra [5,10,11]. A number of schemes have been put forward to demonstrate the existence of positron-atom bound states [12–16]. None of these schemes have resulted in experiments.

The present article uses the stochastic variational method (SVM) [4,17,18] to provide improved information about the positron attachment resonances associated with the He($2s^2$ ¹S^e) and He($3s^2$ ¹S^e) doubly excited states. The structures of these resonances are initially analyzed using bound-state methods by using projection operators that prevent decay into an autoionizing continuum [2,3]. The complex rotation (CR) method is then used to estimate the widths of both resonances. [19].

The $e^+\text{He}(2s^2 \ ^1S^e)$ and $e^+\text{He}(3s^2 \ ^1S^e)$ structures may manifest themselves as resonances in the e^+ + He continuum. An initial search for the $e^+\text{He}(2s^2 \ ^1S^e)$ resonance in a positronhelium scattering experiment was not successful [20]. The present improved estimates of the positions and widths of these resonances might aid any future experimental effort.

II. METHODOLOGY

A. Stochastic variational method using the QHQ ansatz

The SVM [4,17,18], in conjunction with the projection operator formalism was used to determine the wave functions of the resonance states. The SVM diagonalizes the Hamiltonian in a basis of explicitly correlated Gaussians (ECGs). The nonlinear parameters of the ECG basis are optimized by a trial and error process. Such a process is possible since the matrix elements of the Hamiltonian in an ECG basis are computed easily and quickly. The dimensions of the SVM expansion for the e^{+} He($2s^{2}$ $^{1}S^{e}$) and e^{+} He($3s^{2}$ $^{1}S^{e}$) states were 1000 and 1300 ECGs, respectively.

The projection method [2,3] provides an easy to implement method for the identification of resonances and determination of their positions. In this method, the target electrons are not allowed to occupy those low-lying states that could result in the autoionization of the system. Such a calculation is often referred to as a QHQ calculation, with the Q symbolizing the action of a projection operator. One example of the application of the projection method was an investigation of the He⁻ resonances associated with the He doubly excited states [24].

The Hamiltonian for the N = 2 electron and one positron system is

$$H = -\sum_{i=1}^{N+1} \frac{\nabla_i^2}{2} - \sum_{i=1}^{N} \frac{2}{r_i} + \frac{2}{r_{N+1}} + \sum_{i (1)$$

The projection of the unwanted states was accomplished by adding an orthogonalizing pseudoprojector (OPP) [1,4,18,25, 26] to the Hamiltonian. In the case of a calculation of the doubly excited states with n = 2 the purpose of the OPP would be to exclude the He⁺(1s) state from being occupied. The OPP operator would be

$$\lambda \hat{P} = \lambda \sum_{i} |1s\rangle \langle 1s|, \qquad (2)$$

where the sum is over electron coordinates. Choosing λ as a large positive number results in a ground-state wave function which has a very small overlap with the He⁺(1s) state. The expectation value of \hat{P} is always positive and is smallest when the overlap with the He⁺(1s) state is smallest. The minimization of the energy that is inherent to any variational

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TABLE I. Comparisons of the energies (in a.u.) of some He doubly excited states. All energies are given with respect to the He²⁺ thresholds. Four sets of helium energies are given. One set, E_{CR} , was taken as the real part of the energy from complex rotation calculations. The three other sets are taken from QHQ Feshbach projection calculations.

State		$E_{ m QHQ}$			
	E_{CR}	$E_{ m Hylleraas}$	$E_{ m CI}$	$E_{\rm SVM}$	
He $(2s^2 \ ^1S^e)$	-0.777 818 [21]	-0.778774 [2]	-0.778 781 [1]	-0.778 786	
$\frac{\text{He}(3s^2 \ ^1S^e)}{}$	-0.353 54 [22]	-0.354 48 [23]	-0.354 562 [1]	-0.354 570	

calculation acts to minimize the expectation value of the $\lambda \hat{P}$ operator.

The 1s state was expanded as a linear combination of 12 Gaussians. The OPP operator was modified for calculations of the doubly excited He($3s^2$) state. In this case, Gaussian expansions of the 2s and 2p states were added to the projector. The 2p state was expanded as a linear combination of eight Gaussians. The energies of the 1s, 2s, and 2p projectors were $-1.999\,996\,1$, $-0.499\,923\,7$, and $-0.499\,999\,32\,a.u.$, respectively. The parameter λ was set to 1×10^5 a.u. for the present calculations.

III. CALCULATION RESULTS

A. The helium doubly excited states

The energetics of positron binding depend on the ionization energies of the parent atom. When the ionization energy of the parent atom is larger than the positronium binding energy, i.e., -0.250 hartree, the threshold for binding is simply governed by the energy of the parent atom; i.e., the lowest-energy dissociation channel is the $e^+ + A$ channel where A represents the atomic ground state. When the ionization energy of the parent atom is smaller than the positronium binding energy, the threshold for binding is simply the positron binding energy added to the energy of the parent atom with one electron removed; i.e., the lowest-energy dissociation channel is the Ps + A^+ channel where A^+ is the ground state of the positive ion. More detailed discussions of the energetics of positron binding are available [4,5].

Table I compares the SVM QHQ energies of some helium doubly excited states with earlier calculations. Both the configuration interaction (CI) [1] and SVM $\text{He}(2s^2 \ ^1S^e)$ energies lie about 10^{-5} a.u. below the earlier Hylleraas calculation [2].

It is not surprising that the present calculations are more variationally complete since the Hylleraas calculation was done more than 40 years ago. The SVM energy of -0.778786 a.u. was the lowest energy and was obtained with a basis of dimension 150. Further optimization of the energy was not possible since linear dependence problems result in the calculation becoming numerically unstable with respect to further enlargement of the ECG basis. The projection method energies, E_{QHQ} , of the He($2s^2 \, {}^{1}S^e$) state in Table I differ from that determined by the more dynamically complete complex rotation method by less than 0.001 a.u.

The SVM energy of the He $(3s^2 \ ^1S^e)$ state was -0.354570 a.u. This is less than 10^{-5} a.u. below the CI energy of -0.354562 a.u. Both calculations are compatible with an earlier QHQ calculation carried out with a Hylleraas basis [23].

B. The e^+ He($2s^2$) doubly excited state

The dimension of the largest SVM calculation of the e^+ He(2 s^2) state was 1000 ECGs. Some expectation values, including the annihilation rate, are given in Table II. The e^+ binding energy is determined by reference to the He(2 s^2) energy of -0.778786 a.u. The SVM binding energy of the positron to the He(2 s^2) state given in Table II was 0.016517 a.u. This was computed with an OPP parameter of $\lambda = 1 \times 10^5$ a.u. This represents an improvement in the binding energy of 0.00009 a.u. over the previously reported SVM binding energy of 0.016272 a.u. [1]. A CI calculation gave a binding energy of 0.016272 a.u. [1]. As with most variational calculations the binding energy is an underestimate of the exact binding energy failed due to linear dependence problems [18]. The SVM and CI binding energies for this state

TABLE II. Results of QHQ calculations for the e^+ He states. The three-body energy of the state is given in a.u.. The two thresholds for binding are -0.778786 and $-\frac{2}{9} - \frac{1}{4} = -0.472222 \bar{2}$ a.u., and ε_J gives the binding energy (in a.u. and eV) against dissociation. The mean electron-nucleus distance $\langle r_p \rangle$ and the mean positron-nucleus distance $\langle r_p \rangle$ are given in units of a_0 . The $\langle \Gamma \rangle$ column gives the spin-averaged annihilation rate (in units of 10^9 s^{-1}).

Calculation	E	$\langle r_e \rangle$	$\langle r_p \rangle$	$\langle \Gamma \rangle$	ε_J (a.u.)	$\varepsilon_J \; (\mathrm{eV})$
			e^+ He $(2s^2 \ ^1S^e)$			
CI [1]	-0.795058		· · · ·		0.016272	0.4428
SVM [1]	-0.795210				0.016424	0.4469
SVM present	-0.795303	3.630	6.904	1.1150	0.016 517	0.449 5
			e^{+} He(3 s^{2} ¹ S^{e})			
CI [1]	-0.481643		. ,		0.009 421	0.2564
SVM present	-0.482726	8.074	9.336	2.1893	0.010 504	0.2858

are in agreement when the respective uncertainties arising from finite-size basis sets are taken into consideration.

The spin-averaged annihilation rate of 1.115×10^9 s⁻¹ is approximately half that of a free-space spin-averaged positronium atom (which has $\langle \Gamma \rangle = 2.008 \times 10^9$ s⁻¹ [27]). This implies that the wave function is an almost equal mixture of two configurations [5]. One configuration consists of a positron orbiting the polarized He(2s²) atom, while the other can be described as a polarized positronium atom orbiting the He⁺(2s) cation.

C. Similarities between the $e^+Mg(3s^2)$ and $e^+He(2s^2)$ states

The structure of the $e^+\text{He}(2s^2 \ ^1S^e)$ state is very similar to that of the $e^+\text{Mg}(3s^2 \ ^1S^e)$ state. The $e^+\text{He}(2s^2 \ ^1S^e)$ binding energy of 0.01652 a.u. is only 4% smaller than the binding energy of the positron to the Mg(3s²) ground state, namely, 0.01704 a.u. [28]. Next, the annihilation rates are similar. The $e^+\text{He}(2s^2)$ annihilation rate of $1.115 \times 10^9 \ s^{-1}$ is about 10% larger than the latest SVM $e^+\text{Mg}(3s^2)$ annihilation rate of $1.014 \times 10^9 \ s^{-1}$ [8]. This is about half the annihilation rate of the spin-averaged ground state of a positronium. The mean positron radius $\langle r_p \rangle$ of 6.923 a_0 for $e^+\text{Mg}(3s^2)$ [8] is within 1% of the mean positron radius for $e^+\text{He}(2s^2)$, namely, 6.904 a_0 .

The reason for the similarity lies in the structures of the $He(2s^2)$ and $Mg(3s^2)$ parent atoms, which are also very similar. The binding energy of the $Mg^+(3s)$ ground state is -0.55254 a.u. [29], while the $He^+(2s)$ binding energy is -0.50 a.u. The binding energy of the $Mg(3s^2)$ ground state with respect to the $Mg^+(3s)$ threshold is -0.2810 a.u., while the binding energy of the $He(2s^2)$ resonance with respect to the $He^+(2s)$ state is -0.2778 a.u. [21]. The radial expectation value $\langle r_e \rangle$ is 3.276 a_0 for the $He(2s^2)$ state and 3.164 a_0 for the $Mg(3s^2)$ state. The respective dipole polarizabilities are 76.2 a_0^3 for the $He(2s^2)$ state [1] and 71.3 a_0^3 for the $Mg(3s^2)$ state [27].

D. The e^+ He(3 s^2) doubly excited state

The SVM energy of the He $(3s^{2} \, {}^{1}S^{e})$ state is -0.354570 a.u. Since the removal energy of the electron with respect to the He⁺ (3ℓ) threshold, -0.13235 a.u., is less than the positronium ground-state energy of -0.25 a.u., the threshold for attaching a positron to the He $(3s^{2} \, {}^{1}S^{e})$ state is at -0.472222 a.u., the sum of the He⁺ (3ℓ) and Ps(1s) binding energies.

The best SVM calculation with a basis dimension of 1300 ECGs gave a three-body energy of -0.482726 a.u and a binding energy of 0.010504 a.u. This energy was computed with an OPP parameter of $\lambda = 1 \times 10^5$ a.u. The SVM binding energy represents a 10% improvement over the earlier CI calculation [1].

The SVM annihilation rate of $2.188 \times 10^9 \text{ s}^{-1}$ indicates that this system possesses a well-defined Ps(1s) cluster with a structure best described as He⁺(3s) + Ps(1s). It also should contain a Ps⁻ component as expected from a study of the $(m^{2+}, 2e^-, e^+)$ system [30].

Stability of the e^+ He $(3s^2 \ ^1S^e)$ system provides supporting evidence for the existence of an infinite number of e^+ He (ns^2) type resonances. The $(m^{2+}, 2e^-, e^+)$ system is known to bind a positron as the mass $m^{2+} \rightarrow 0$ [30]. A decreasing m^{2+} mass also leads to the interaction strength between the m^{2+} and



FIG. 1. (Color online) Energies of the e^+ He($2s^2$ ${}^{1}S^e$) state computed with a succession of different ECG basis sets using three different values for the OPP parameter λ . The horizontal axis gives the $\lambda\langle P \rangle$ expectation value when the Hamiltonian with the OPP operator is diagonalized. The quality of the basis (i.e., increased dimension and more intense optimization) improves as the points for a particular λ go from right to left.

the two electrons decreasing. It provides an analog of the $He^{2+}-ns(e^{-})$ interaction as *n* increases. It is likely that the $e^{+}He$ system has a rich resonance structure in the energy region where the helium doubly excited states are located.

E. Estimation of the variational limit

Figure 1 shows the Hamiltonian expectation value for a succession of SVM wave functions at different stages of optimization. These wave functions were computed using three different values of the λ parameter in the OPP operator. Three things should happen as the basis used in the variational calculation approaches completeness. First, the energy should converge to the exact energy from above. Second, the $\lambda \langle P \rangle$ expectation value should go to zero from above. Finally, the energies of all three calculations should approach each other. These three features all seem to be occurring in Fig. 1. A visual inspection of the $\lambda = 1 \times 10^5$, 2×10^5 , and 4×10^5 curves suggests that energy reported in Table II is within 2×10^{-4} a.u. of its variational limit.

Figure 2 plots the Hamiltonian expectation value of the e^+ He($3s^2 \, {}^1S^e$) state for a succession of SVM wave functions at different stages of optimization. The Hamiltonian expectation value for this state is more sensitive to the presence of the OPP operator. This is expected since there are now three Pauliforbidden orbitals. A visual inspection suggests that the variational limit is about 0.002 a.u. lower than the best SVM energy.

IV. COMPLEX ROTATION CALCULATIONS

Complex rotation (CR) calculations were made to give estimates of the resonance widths as well as more refined estimates of the resonance positions [19,31,32]. In the CR method the Hamiltonian and wave function are transformed by making the transformation

$$\mathbf{r} \to \alpha \exp(i\Theta)\mathbf{r}.$$
 (3)



FIG. 2. (Color online) Energies of the e^+ He(3 s^2 ¹S e) state computed with a succession of different ECG basis sets using three different values for the OPP parameter λ . The horizontal axis gives the $\lambda\langle P \rangle$ expectation value when the Hamiltonian with the OPP operator is diagonalized. The quality of the basis (i.e., increased dimension and more intense optimization) improves as the points for a particular λ go from right to left.

Rotating the coordinates into the complex plane leads to the resonant wave function being made square integrable and accessible to a basis set expansion. When the interactions are purely Coulombic, the complex scaled Hamiltonian can be written as

$$H_{\Theta} = \exp(-2i\Theta)T + \exp(-i\Theta)V_C, \qquad (4)$$

where the complex scaling parameter Θ is an arbitrary real parameter satisfying the inequality $0 < \Theta < \pi/2$. The matrix elements for *T* and *V_C* are calculated as usual. The parameter α can be varied, but in the present investigation it was set to 1. A generalized variational principle [19,32] can be applied to the complex scaled Hamiltonian. Resonant states can be identified by adjusting the Θ parameter. The complex energies of scattering states rotate in an approximately circular trajectory in the complex plane as Θ is adjusted, while resonant state energies show relatively little change as Θ changes.

The QHQ optimised basis was augmented by additional basis functions that are able to better represent the wave functions of the breakup channels [33,34]. This is best illus-



FIG. 3. Complex rotation diagram of the e^+ He $(2s^2 \ ^1S^e)$ resonance. The diagram shows the complex eigenvalue of the Hamiltonian given by Eq. (4) for values of the complex rotation angle spaced by 0.005 rad.

trated by discussion of a specific example, the e^+ He $(2s^2 \ ^1S^e)$ state, which can dissociate into the e^+ +He $(1s^2 \ ^1S^e)$ and Ps(1s) + He⁺(1s) channels.

The outer basis functions used to describe the positive energy $Ps(1s) + He^+(1s)$ breakup are designed to give a good representation of this scattering channel:

$$\Psi_{\text{out}}^{ijk} = \exp\left(-\alpha_i R^2\right) \phi_{\text{Ps}}^j(\mathbf{r}_0, \mathbf{r}_1) \phi_{\text{He}^+}^k(\mathbf{r}_2).$$
(5)

Here \mathbf{r}_0 is the positron coordinate, R is the relative distance between the Ps(1s) and He⁺ centers of mass, and \mathbf{r}_i (i > 0) are the electron coordinates. $\phi_{\text{He}^+}^j(\mathbf{r}_2)$ can be represented as a set of Gaussians (which would give an energy of $-1.999\,978$ hartree). A total of six ECGs are used to represent the $\phi_{\text{Ps}}^i(\mathbf{r}_0,\mathbf{r}_1)$ ground state (the energy of this superposition was $-0.249\,972$ hartree). The exponents, i.e., α_i , form an even tempered sequence with a constant ratio between successive terms. There were 14 terms defined by the relation $T_i = 20/1.48^i$.

The e^+ + He(1 s^2 ¹ S^e) dissociation channel basis functions were represented as

$$\Psi_{\text{out}}^{ij} = \exp\left(-\alpha_i r_0^2\right) \phi_{\text{He}}^j(\mathbf{r}_1, \mathbf{r}_2), \tag{6}$$

where \mathbf{r}_0 is the positron coordinate and \mathbf{r}_1 is the electron coordinate. There were 14 α_i Gaussians, and an approximate representation of the He ground state was constructed by multiplying together all unique combinations of the Gaussians used in the eight Gaussian representation of the He⁺ ground state.

The set of raw ECGs that would give a reasonable representation of the exit channels given by Eqs. (5) and (6) was added to the best QHQ basis representation of the e^+ He $(2s^2 \ ^1S^e)$ resonance. ECGs which had an overlap of 0.98 with any other basis function were removed from the basis. The final basis for the complex rotation calculation had a dimension of 1658 ECGs. The QHQ basis of the e^+ He $(3s^2 \ ^1S^e)$ state was similarly augmented prior to the complex rotation calculation. In this case the final basis had a dimension of 2085 ECGs.

The complex trajectory for the e^+ + He($2s^2 \, {}^1S^e$) eigenvalue is shown in Fig. 3. The resonance position is defined by examining the complex trajectory and determining the point where [35]

$$\frac{\partial |E|}{\partial \Theta} \approx \text{minimum.} \tag{7}$$



FIG. 4. Complex rotation diagram of the e^+ He $(3s^2 \ ^1S^e)$ resonance. The diagram shows the complex eigenvalue of the Hamiltonian given by Eq. (4) for different values of the complex rotation angle.

For Fig. 3, this occurs at $\theta = 0.275$ rad. The position E_r and half width $\Gamma/2$ were $E_r = -0.79527$ and 0.00066 a.u., respectively. An earlier calculation with a basis of 1428 ECGs gave the position and half width as E = -0.79484 and 0.00124 a.u., respectively [1].

The complex trajectory for the e^+ He($3s^2 \, {}^1S^e$) eigenvalue is shown in Fig. 4. The dimension of the final basis for this calculation was 2085 ECGs. The position where the complex energy changed least rapidly was at $\Theta = 0.130$ rad. The resonance parameters were E = -0.48432 and $\Gamma/2 =$ 0.00539 a.u., respectively.

V. CONCLUSION

SVM calculations have confirmed the existence of two Feshbach resonances associated with the doubly excited states of helium. Improved estimates of the position and widths of the resonances have been made. Table III summarizes the results on the resonance calculations. The results that are listed in the table are those of the most complete calculations. Table III also reports collision energies with respect to the e^+ + He(1 s^2) ground state since these e^+ He resonances are potentially detectable in the e^+ + He continuum. The uncertainties in the collision energies of the resonances due to incompleteness of the ECG basis are about 6 meV for the e^+ He(2 s^2 ¹S^e) resonance and 60 meV for the e^+ He(3 s^2 ¹S^e) resonance.

The resonance widths of 36 and 294 meV are large enough to permit detection. The main question regarding detection is whether the resonances are coupled with sufficient strength to the exit channels that are most convenient for experimental detection. There has already been one attempt to detect these states in a positron-helium scattering experiment. Machacek *et al.* [20] measured the total cross section and the net positronium cross section for impact energies between 57.2 and 58.1 eV and did not see any evidence of a resonance. This experiment used a modern trap based positron beam that can achieve an energy resolution of 50 meV or better [9,36].

Reference to e^- + He scattering experiments [37–41] can be made to give an indication of the signal to noise requirements needed for detection. For example, He⁺ ions were detected in the experiment of Quéméner *et al.* [38]. The variation in the cross section for the creation of He⁺ was

TABLE III. Summary of resonance energies E_{res} (in a.u.), half widths (in a.u.), and energy relative to the helium ground state E_{coll} (in eV). CR stands for complex rotation.

State	Method	$E_{\rm res}$	Γ/2	$E_{\rm coll}$
$e^{+}\text{He}(2s^{2} {}^{1}S^{e})$ $e^{+}\text{He}(3s^{2} {}^{1}S^{e})$	SVM-CR	-0.79527	0.000 66	57.37
	SVM-CR	-0.48432	0.005 39	65.84

only 1% over the width of the He⁻ $(2s^22p)$ resonance, and the number of counts per channel exceeded 100 000 000. The statistical uncertainty in the Machacek *et al.* [20] experiment seems to be about 2% [20].

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 autoionization [39]. Another is the measurement of the optical excitation functions associated with the formation of a number of He⁻ excited states [40].

There have been many calculations of resonances occurring for positron scattering from a variety of possible atomic targets [28,42–50]. However, there has as yet been no unequivocal identification of a resonance in the experimental positron scattering spectrum of any atom [5,9]. The identified resonances are either too narrow, in the case of hydrogen or the alkalis [43,44,46,48], or located in the energy region very close to the threshold [28,42,49,51]. The present resonances are broad (when compared with others) and occur in a system that is amenable to experimentation.

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J. MITROY AND J. GRINEVICIUTE

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