Expectation values of the $e^+\text{He}^3(3S)$ system

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Close to converged energies and expectation values for $e^+\text{He}^3(3S)$ are computed using a ground state wave function consisting of 1500 explicitly correlated Gaussians. The best estimate of the $e^+\text{He}^3(3S)$ energy was $-2.250\,595\,08$ hartree, which has a binding energy of $0.000\,5916$ hartree against dissociation into Ps+He$^+$. The $2\gamma$ annihilation rate for the spin doublet state was $5.713 \times 10^9\,s^{-1}$. The estimated annihilation rate with the core He$^+$ electron was $2.506 \times 10^8\,s^{-1}$. The derived enhancement factor for annihilation with the He$^+(1s)$ core was $2.29$, just over 10% smaller than the enhancement factor derived from analyses of annihilation during $e^+$-He$^+$ scattering. The diffuse nature of the wave function, with well separated He$^+$ and Ps subsystems, is demonstrated to be on the threshold of satisfying the formal criteria that define a quantum halo state.

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I. INTRODUCTION

In 1998 it was shown that a positron could bind itself to the lowest triplet state of neutral helium, i.e., He$(2\,3S)$ [1,2] with a binding energy of $0.000\,5916$ hartree against dissociation into Ps+He$^+$. Subsequently the best estimate of the binding energy was improved to $0.000\,5924$ hartree [3] and then to $0.000\,5937$ hartree [4]. These two latter calculations were aimed at elucidating detailed knowledge about the positron annihilation process. The structure of the $e^+\text{He}^3(3S)$ state has been identified as a positronium (Ps) atom weakly bound to a He$^+(1s)$ ion.

In this work, a wave function of the $e^+\text{He}^3(3S)$ state giving an energy converged to an accuracy of about $10^{-7}$ hartree was obtained with the stochastic variational method (SVM). In addition, other ground state expectation values are computed. There are a number of reasons why this is interesting. First, since the $e^+\text{He}^3(3S)$ system has only four active particles it is possible to generate a close to converged binding energy. Next, there are a number of other atoms that can bind a positron [5]. Fully ab initio calculations are not possible for systems such as e$^+\text{Na}$ with 13 active particles, so recourse has been made to the fixed core stochastic variational method (FCSVM) [5–7]. The positronic bound state of triplet helium is an obvious system with which to validate the approximations and assumptions of the FCSVM. Finally, examination of previous work shows that the enhancement factor for the positron annihilating with the core He$^+(1s)$ electron in $e^+\text{He}^3(3S)$ [3,8] and the enhancement factor for positron annihilation with He$^+(1s)$ in a positron-He$^+$ collision [9] are almost the same (the enhancement factor can be defined as the factor that the annihilation rate calculated as a simple product of the electron and positron densities needs to be increased in order to agree with the exact annihilation rate). This raises the possibility that enhancement factors for positron-atom annihilation could be the same as enhancement factors for pickoff annihilation during orthopositronium-atom interactions. This could then allow the cross correlation of positron scattering data with positronium scattering data. A better understanding of the positron annihilation rate in strong Coulomb fields and with core electrons is also a topic of relevance to the field of positron annihilation spectroscopy [10–15].

II. RESULTS OF THE CALCULATION

The SVM used for this work has been described in a number of papers [7,16,17] and only the briefest description is given here. The SVM uses a wave function written as 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 [7,17].

The present set of calculations used the 650 ECG basis of [3] as a starting point. This basis was enlarged to 800, 900, 1000, 1200, and 1500 ECGs with each sized basis subjected to an extensive optimization before being used as the starting point to further enlarge the basis. All the optimizations of the ECG basis were done with the He mass set to $\infty$.

Table I lists a number of expectation values obtained from this sequence of calculations with an increasingly larger ECG basis. The original binding energy of $5.9163 \times 10^{-4}$ hartree [1] was only improved by $0.0345 \times 10^{-4}$ hartree when the ECG basis dimension was enlarged from 500 to 1500. Although the search strategy used in the original calculation was primitive when compared with later strategies, it did succeed in obtaining a good energy as there were only three active particles in the system.

The expectation value for the virial theorem $\langle V \rangle/\langle T \rangle$ provides an estimate of the wave function accuracy. When the interparticle interaction $V$ consists solely of Coulomb interactions this expectation value should be $-2$ exactly. The difference of the 1500 ECG wave function from $-2.0$ was only $1.38 \times 10^{-8}$. Examination of the convergence pattern of the energy and the virial theorem for the successively larger calculations suggests that the energy should be accurate to a precision better than $1.0 \times 10^{-6}$ hartree.

There are two possible total spin multiplicities for the $e^+\text{He}^3(3S)$ state. The positron can be coupled to the electron spin-triplet pair to give a doublet $^3S$ or a quartet $^5S$ state. The states are degenerate if one ignores the hyperfine interactions. Despite being degenerate, the $^5S$ and $^3S$ states have totally different annihilation properties and the $2\gamma$ annihilation process does not occur in the $^3S$ state.
Two different annihilation rates for the $2\gamma$ process are given in Tables I and II. The first is for the doublet state and denoted by $\Gamma_d$. It is proportional to the probability of finding an electron and a positron at the same position in a spin singlet state according to

$$\Gamma_d = T_a \langle \sum_{i=p}^2 O_{ip}^S \delta(r_i - r_p) | \Psi \rangle$$

(1)

$$= T_a \sum_{i=p}^2 \langle \delta(r_i - r_p) \rangle S, \quad (2)$$

[3,18,19], where the sum is over the electron coordinates Eqs. (1) and (2) and $p=3$ is the positron coordinate, the $\delta$ function expectation is evaluated in $a^3_{dp}$ and $\Gamma_d$ is given numerically in s$^{-1}$. The constant $T_a=4\pi r_e^2 c=2.01878 \times 10^{11}$ to lowest order in quantum electrodynamics. The operator $O_{ip}^S$ is a spin projection operator to select spin singlet states for the $ip$ electron-positron pair. Details of the spin operator analysis are in the Appendix.

In addition it is also possible to identify a core annihilation rate. One can define the annihilation rate leaving the residual ion in a He$^+(1s)$ state as

$$\Lambda_{1s} = T_a \int d^3r_2 \int d^3r_1 \phi_{1s}(r_1) \hat{O}_{1s}^V | \Psi(r_1,r_2) |^2$$

(3)

[3]. Since the two electrons in e$^+\text{He}^3(S')$ are spatially separated with radial expectations of $=0.154 d_0$ it is possible to regard annihilation events with these two electrons as physically distinct. One can identify $\Lambda_{1s}$ as the annihilation rate with the loosely bound valence electron, hence

$$\Gamma_c = \Gamma_d - \Lambda_{1s} \quad (4)$$

is the core annihilation rate. The core annihilation rate of $\Gamma_c=2.5065 \times 10^9$ s$^{-1}$ is about 2200 times smaller than the valence annihilation rate.

The largest calculation gives $\Gamma_d=5.713 \times 10^9$ s$^{-1}$. Although no variational principle applies, the steady increase in $\Gamma_d$ as the basis size was enlarged is quite common in calculations with ECG basis sets. This increase with increasing basis size occurs because ECGs do not have the correct asymptotics at the e$^+e^-$ coalescence point [7,17,20,21]. The $\frac{3}{2}S'$ annihilation rate given by Frolov [4] was $7.5207 \times 10^9$ s$^{-1}$. This estimate is too large by a factor that seems to

<table>
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<tr>
<th>$N$</th>
<th>$\langle V \rangle / \langle T \rangle + 2$</th>
<th>$\langle r_{He^2-e^+} \rangle$</th>
<th>$\langle r_{He^2-e^+}^2 \rangle$</th>
<th>$\langle r_{e^-} \rangle$</th>
<th>$\langle r_{e^-}^2 \rangle$</th>
<th>$\langle (\delta N^{He^2-e^+}) \rangle$</th>
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<td>7.5207</td>
<td>0.0005937</td>
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</table>

$\frac{\text{See Ref. [4]}}{}$
be $4/3$ as Frolov incorrectly evaluated the matrix elements of the spin-projection operator.

In the recent work of Frolov [4], it is stated that the $3S$ state is “unstable and rapidly decays by the Auger transition to the ground $1S(L=0)$ state of the helium atom. . .The preliminary evaluations indicate that the Auger transition rate in this case is quite comparable with the and even larger than the two-photon annihilation rate”. This sensitivity is due to the fact that the positron amplitude is sensitive to the increase in basis size than any other quantity.

The 3γ process is the dominant annihilation channel for the quartet $4S$ state. The 3γ rate can be estimated from the ratio of 3γ to 2γ decay rates in positronium using the method of Ferrante [22]. For the quartet state, one has

$$\Gamma_{3\gamma}(e^+He^+4S) = \frac{4G_{3\gamma}^*(3Ps)}{3G_{2\gamma}^*(3Ps)} \Gamma_{2\gamma}(e^+He^+2S)$$  (5)

Using the best estimates from Table II and $G_{2\gamma}^*(3Ps) = 8.0325 \times 10^8$ s$^{-1}$, $\Gamma_{2\gamma}^*(3Ps) = 7.2112 \times 10^6$ s$^{-1}$, gives $\Gamma_{3\gamma}(e^+He^+4S) = 6.838 \times 10^6$ s$^{-1}$.

The coalescence matrix element, $\langle \delta(He^{2+} - e^-) \rangle$, was more sensitive to the increase in basis size than any other quantity. This sensitivity is due to the fact that the positron amplitude at the nucleus is very small and the ECG functional form is not the natural choice to describe the behavior of the relative wave function for two strongly repelling particles. With respect to the more physically interesting observables, the core rate, $\Gamma_c$ varied most as the basis dimension was increased. But the increase in $\Gamma_c$ was only 2% when the basis was increased from 500 to 1500.

A comprehensive set of expectation values, taken from the 1500 ECG wave function are listed in Table II. The FCSVM expectation values were computed with the 463 ECG wave function used in [23]. A large number of ECIGs was included in the basis primarily to give a good description of the wave function in the large r region. The differences with previously calculated expectation values [3] are small.

The positron kinetic energy is 0.120 hartree. This is slightly smaller than the kinetic energy of the positron in the Ps ground state, namely 0.125 hartree. The assertion by Frolov that the “positron moves as an almost free particle” would therefore seem to be untenable.

The energies of the different mass variants of $e^+He^+(3S)$ were computed by rediagonalizing the Hamiltonian with the 1500 ECG basis but with $m_{He^3}$ set to 5495.86 $m_e$ and $m_{He^4}$ set to 7294.30 $m_e$. The binding energy of $e^+He^3$ was

$$\epsilon(e^+He^3) = 2.250 \ 228 \ 47 - 2.249 \ 636 \ 16 = 0.000 \ 592 \ 31 \ \text{hartree}$$  (6)

while the binding energy of $e^+He^4$ was

$$\epsilon(e^+He^4) = 2.250 \ 318 \ 82 - 2.249 \ 725 \ 85 = 0.000 \ 592 \ 97 \ \text{hartree}.$$  (7)

A. The enhancement factor for core annihilation

The annihilation rate can also be approximately computed from the overlap between the positron density and electron density.

$$\Gamma = U_S T_S G \int d^3r \ \rho_p^*(r) \rho_e(-r),$$  (8)

where the factor of $U_S$ comes from the spin factors. The factor $G$ is the enhancement factor which incorporates the influence of short-range correlations in the annihilation rate matrix elements [8,9]. The $2S$ core annihilation rate with the He$^+(1s)$ orbital can therefore be written as

$$\Gamma = \frac{3T_S}{4} G \int d^3r \ \rho_p^*(r) \rho_{1s}(r),$$  (9)

where $\rho_{1s}(r)$ is the density of the He$^+(1s)$ orbital and

$$\rho_p^*(r) = \int d^3r_1 \int d^3r_2 \Psi(r_1, r_2; r) \Psi^* (r_1, r_2; r).$$  (10)

Table III gives core annihilation rates computed from Eqs. (4) and (9) with $G = 1$. The ratio of these two rates is used to determine the values of $G$ listed in Table III. Short-range correlations are responsible for increasing the annihilation rate by a factor of 2.29. It is reasonable to assert that $G = 2.29$ with a precision of better than 1% given its small variations for the succession of increasingly larger calculations.

The FCSVM model potential calculation of Eq. (9) is about 5% smaller than the SVM calculation. Hence, the FCSVM model potential underestimates the extent of the positron overlap with the core by 5%.
The enhancement factor derived from a semiempirical model potential analysis of $e^+\text{He}^+$ scattering was 2.52 [9]. This enhancement factor was tuned at $k = 1.00a_0^{-1}$ and there was a 14\% variation in $G$ from $k = 0.25a_0^{-1}$ to $k = 1.50a_0^{-1}$. Another estimate of the enhancement factor [24] was made by directly computing the positron density from a large Kohn variational calculation [9], then computing the annihilation parameter $Z_{\text{eff}}$ using an equation similar to Eq. (9), and finally identifying $G$ as the ratio of the exact $Z_{\text{eff}}$ to the approximate $Z_{\text{eff}}$. This procedure yielded $G = 2.56$ [24].

Therefore, the enhancement factors for direct positron annihilation with the $\text{He}^*(1s)$ state is about 10\% larger than the enhancement factor for pickoff annihilation of $^3\text{Ps}$ with $\text{He}^*(1s)$.

### III. THE $e^+\text{He}^*(3S')$ SYSTEM AS A HALO STATE

Just recently, the $e^+\text{He}^*(3S')$ system was shown to have features reminiscent of a quantum halo state [23]. Quantum halo states are a well known feature in nuclear structure physics [25–27] and are weakly bound systems of relatively large spatial extent with a large proportion of the wave function in the classically forbidden region. The ability of quantum particles to tunnel into potential barriers is a significant factor in the existence of halo states. The large separation means the wave function for an effective two-body system can be regarded as two well defined clusters. A recent quantitative definition [25,28] for a two-body halo state has two criteria:

1. there must be a large probability, $f_c$, for finding a pair of independent cluster components in the total many-body wave function and
2. a large fraction $f_h$ of the total probability density must be in the classically forbidden region of the interaction.

The critical values of $f_c$ and $f_h$ used to denote a quantum halo have been assigned to 1/2. The choice of the fractions, $f_c$ and $f_h$, is somewhat arbitrary since one sees a continuum of increasingly more pronounced halo effects as $f_c$ and $f_h$ increase in magnitude. The previous analysis of $e^+\text{He}^*(3S')$ structure was restricted to the FCSVM wave function.

Since the halo state is a diffuse state it is important to verify that the use of Gaussian type functions does not underestimate the probability densities at large $r$. The comparison of radial expectation values in Table I shows that the $\langle r^2_{\text{He}^*}\rangle$ and $\langle r^2_{\text{Ps}}\rangle$ expectation values, which are sensitive to the long range behavior of the wave function, have stabilized for the two largest calculations.

Computation of $f_h$ requires an estimate of $R_0$. The asymptotic potential for $\text{Ps}$ moving in the field of the $\text{He}^+$ ion is $V(r) \sim \alpha_e/r^2$. So the classically forbidden region is given by the condition $R_0 = \sqrt{\alpha_e(2 \times e)}$. Using $e = 0.00059508$ hartree gives $R_0 = 13.188 a_0$. Examination of the electron and positron densities as a function of $r$ gives $f_h = 0.477$, very close to the FCSVM value of $f_h = 0.478$ [23] (note, $f_h$ in [23] was underestimated by 0.004).

The cluster fraction for $e^+\text{He}^*(3S')$ decomposed into a $|\Psi_{\text{He}^*}\Psi_{\text{Ps}}\rangle$ product form is

$$f_e = \int d^3R \left| \langle \Psi_{\text{He}^*}\Psi_{\text{Ps}}|\Psi_{e^+\text{He}^*}\rangle(R) \right|^2 \quad (11)$$

where

$$\langle \Psi_{\text{He}^*}\Psi_{\text{Ps}}|\Psi_{e^+\text{He}^*}\rangle(R) = \int d^3\rho \ d^3r_1 \ \Psi_{\text{He}^*}^*(r_1) \Psi_{\text{Ps}}(\rho) \times \Psi_{e^+\text{He}^*}(r_1, \rho, R), \quad (12)$$

and $R = (r_1 + r_2)/2$ and $\rho = (r_3 - r_2)$. (Note, an ECG basis permits an easy transformation from $(r_2, r_3)$ coordinates into $(\rho, R)$ coordinates [17]). The final value obtained was $f_e = 0.975$. The cluster fraction for the FCSVM wave function was $f_e = 0.976$ [23] The Gaussian representations of the $\text{Ps}$ and $\text{He}^*$ wave functions used in Eq. (12) gave energies that were within $10^{-7}$ hartree of the exact ground state energies.

Another useful halo state parameter is the ratio $(X^2)/R_0^2$. In this expression $X^2$ is the mean square distance between the two objects making up the halo while $R_0$ denotes the critical radius at which the motion of the objects becomes classically forbidden. A halo state can be characterized by the condition $(X^2)/R_0^2 \geq 2$ [25]. The expectation $X^2$ is set to

$$X^2 = \frac{\int d^3R \left| \langle \Psi_{\text{He}^*}\Psi_{\text{Ps}}|\Psi_{e^+\text{He}^*}\rangle \right|^2}{\int d^3R \left| \langle \Psi_{\text{He}^*}\Psi_{\text{Ps}}|\Psi_{e^+\text{He}^*}\rangle \right|^2}. \quad (13)$$

This is the mean square radius of the projection of the $e^+\text{He}^*(3S')$ wave function onto a $\Psi_{\text{He}^*}\Psi_{\text{Ps}}$ product wave function. Explicit calculation with the 1500 ECG wave function gives $X^2/R_0^2 = 360.1/13.188 = 2.070$, so the $e^+\text{He}^*(3S')$ ground state just satisfies this halo state criteria. An alternate definition of $X^2$ based on the electron and positron radial expectations, e.g.,

$$X^2 = \langle r^2_e \rangle/2 + \langle r^2_c \rangle - 0.75, \quad (14)$$

would give $X^2/R_0^2 = 355.37/13.188 = 2.644$ (0.75 is $\langle r^2_c \rangle$ for $\text{He}^*$ ground state).

The analysis of the halo state properties of $e^+\text{He}^*(3S')$ using an $ab\ initio$ SVM wave function gives the same conclusion as the earlier analysis using an FCSVM wave function. The $e^+\text{He}^*(3S')$ ground state exhibits the features that characterize a halo state, although it just fails to satisfy the formal criteria of a 50\% probability of finding the particles in the classically forbidden region.

### IV. CONCLUSION

To summarize, a close to converged binding energy is reported for the $e^+\text{He}^*(3S')$ ground state. The convergence pattern and virial theorem expectation value suggests that the energy is converged to better than $10^{-6}$ hartree.

An analysis of the wave function has been used to get an estimate of the annihilation rate with the core $\text{He}^*(1s)$ electron. The enhancement factor derived from this analysis is only 10\% smaller than that derived from a model potential analysis of positron-$\text{He}^+$ scattering.

The nature of the variational theorem means other expectation values are not converged to the same degree of accuracy. The most slowly convergent quantity is the coalescence matrix element, $\langle \delta(\text{He}^* - e^+) \rangle$. Other expectation values such
as the annihilation rates should be converged to ±1% or better.

ACKNOWLEDGMENTS

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APPENDIX

There is evidently some confusion about the calculation of the annihilation rate for the $e^+He(3S)$ state of $^3S$ symmetry. Therefore, details of the calculation are given here.

The spin triplet states in the $\alpha, \beta$ notation for $+1/2$ and $-1/2$ spin projections are

$$|1\;−1\rangle = \beta(1)\beta(2),$$
$$|10\rangle = \frac{\alpha(1)\beta(2) + \beta(1)\alpha(2)}{\sqrt{2}},$$
$$|11\rangle = \alpha(1)\alpha(2).$$

This leads to the antisymmetric two-electron states

$$|\Psi; −1\rangle = [F(1,2) − F(2,1)]\beta(1)\beta(2),$$
$$|\Psi; 0\rangle = [F(1,2) − F(2,1)]\alpha(1)\beta(2) + \beta(1)\alpha(2),$$
$$|\Psi; 1\rangle = [F(1,2) − F(2,1)]\alpha(1)\alpha(2),$$

where $[F(1,2) − F(2,1)]$ is the spatial part of the antisymmetrized wave function which is normalized to 1. Using explicit values for the Clebsch-Gordan coefficients, the doublet states can be written

$$|\Psi; −\frac{1}{2}\rangle = \sqrt{\frac{3}{2}}[G(1,2,3) − G(2,1,3)]\beta(1)\beta(2)\alpha(3)$$
$$− \sqrt{\frac{3}{2}}[G(1,2,3) − G(2,1,3)]\alpha(1)\beta(2)$$
$$+ \beta(1)\alpha(2)]\beta(3),$$

where $[G(1,2,3) − G(2,1,3)]$ is the spatial part of the normalized wave function with coordinate 3 referring to the positron.

The spin projection operator $\hat{O}_S$ for a given electron-positron pair is

$$\hat{O}_S = 1 - \frac{1}{2}S^z.$$ (A9)

Table IV gives the expectation values of this operator for the different possible $\alpha, \beta$ combinations for the electron-positron pair.

The expectation value of the annihilation operator, $T_{\alpha} \Sigma_{i=1} \delta(\mathbf{r}_i − \mathbf{r}_3)\hat{O}_S$ for the $M_s = \frac{1}{2}$ state is

$$\Gamma_d = \frac{3T_{\alpha}}{4}(\langle G(1,2,3)|\delta(\mathbf{r}_1 − \mathbf{r}_3)|G(1,2,3)\rangle$$
$$+ \langle G(1,2,3)|\delta(\mathbf{r}_2 − \mathbf{r}_3)|G(1,2,3)\rangle$$
$$+ \langle G(1,2,3)|\delta(\mathbf{r}_1 − \mathbf{r}_3)|G(2,1,3)\rangle$$
$$+ \langle G(1,2,3)|\delta(\mathbf{r}_2 − \mathbf{r}_3)|G(2,1,3)\rangle).$$ (A10)

Suppose $G(1,2,3)$ is made up of a structure $\phi(1)\Phi_{3s}(2,3)$, with little overlap between the positron and $\phi(1)$. The annihilation rate would then be $\approx 6.0 \times 10^9$ s$^{-1}$ because of the 3/4 prefactor.

Table IV. Expectation values of the $\hat{O}_S$ spin projection operator with 1 = electron and 2 = positron.

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