Expectation values of the e^+He($^3S^e$) system

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Close to converged energies and expectation values for e^+He($^3S^e$) are computed using a ground state wave function consisting of 1500 explicitly correlated Gaussians. The best estimate of the e^+He($^3S^e$) energy was −2.250 595 08 hartree, which has a binding energy of 0.000 595 08 hartree against dissociation into Ps+He$^+$. The 2γ annihilation rate for the spin doublet state was 5.713×10^9 s^{-1}. The estimated annihilation rate with the core He$^+$ electron was 2.506×10^6 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 demonstarted 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 $^3S^e$) [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^+He($^3S^e$) 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^+He($^3S^e$) 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^+He($^3S^e$) 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^+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^+He($^3S^e$) [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 ortho-positronium-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 ∞.

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 5.9163×10^{-4} hartree [1] was only improved by 0.0345×10^{-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 1.38×10^{-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 1.0×10^{-6} hartree.

There are two possible total spin multiplicities for the e^+He($^3S^e$) state. The positron can be coupled to the electron spin-triplet pair to give a doublet $^2S^e$ or a quartet $^4S^e$ state. The states are degenerate if one ignores the hyperfine interactions. Despite being degenerate, the $^2S^e$ and $^4S^e$ states have totally different annihilation properties and the 2γ annihilation process does not occur for the $^4S^e$ state.

TABLE I. Behavior of some $e^+\mathrm{He}(^3S^e)$ expectation values for a sequence of ECG type variational calculations of increasing size. The He nucleus is assumed to have infinite mass. The binding energy with respect to dissociation into $\mathrm{Ps}+\mathrm{He}^+$ is denoted by ε while Γ_c is the annihilation rate with the "core" electron. All quantities are given in atomic units with the exception of the 2γ annihilation rates which are in units of 10^9 s^{-1}.

N	$\langle V\rangle/\langle T\rangle+2$	$\langle r_{\mathrm{He}^{2+}e^+}\rangle$	$\langle r^2_{\mathrm{He}^{2+}e^-}\rangle$	$\langle r_{e^+e^-}\rangle$	$\langle r_{e^-e^-}\rangle$	$\langle\delta(\mathrm{He}^{2+}-e^+)\rangle$	Γ_c	Γ_d	ε
500	1.29×10^{-6}	15.7736	174.623	9.4733	15.3615	8.3226×10^{-7}	0.002 4601	5.687 16	0.000 591 63
650	5.64×10^{-7}	15.7648	174.268	9.4690	15.3525	7.4534×10^{-7}	0.002 5013	5.699 02	0.000 592 43
800	9.57×10^{-7}	15.7544	173.828	9.4638	15.3421	7.7074×10^{-7}	0.002 4882	5.699 95	0.000 594 30
900	3.50×10^{-7}	15.7930	175.641	9.4831	15.3810	7.8074×10^{-7}	0.002 4787	5.705 98	0.000 594 70
1000	5.97×10^{-8}	15.8044	176.258	9.4887	15.3923	7.4573×10^{-7}	0.002 4973	5.707 92	0.000 594 88
1200	6.40×10^{-8}	15.8047	176.300	9.4888	15.3926	7.3999×10^{-7}	0.002 4972	5.711 88	0.000 594 99
1500	1.38×10^{-8}	15.8056	176.360	9.4894	15.3936	7.0900×10^{-7}	0.002 5065	5.712 78	0.000 595 08
600[a]	3.23×10^{-6}	15.7496	173.535	9.4612	15.3377	9.7023×10^{-7}		7.5207	0.000 5937

[a]See Ref. [4].

Two different annihilation rates for the 2γ process are given in Tables I and II. The first is for the doublet state and denoted by Γ_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

$$\Gamma_d = T_a\langle\Psi|\sum_{i=1}^{2} O^S_{ip}\delta(\mathbf{r}_i-\mathbf{r}_p)|\Psi\rangle \tag{1}$$

$$= T_a\sum_{i=1}^{2}\langle\delta(\mathbf{r}_i-\mathbf{r}_p)\rangle_S, \tag{2}$$

[3,18,19], where the sum is over the electron coordinates Eqs. (1) and (2) and $p=3$ is the positron coordinate, the δ function expectation is evaluated in a_0^3, and Γ_d is given numerically in s^{-1}. The constant $T_a=4\pi r_e^2 c=2.018\,788\times10^{11}$ to lowest order in quantum electrodynamics. The operator O^S_{ip} 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 $\mathrm{He}^+(1s)$ state as

$$\Lambda_{1s} = T_a\int d^3r_2\left|\int d^3r_1\ \phi^*_{1s}(\mathbf{r}_1)\hat{O}^s_N\Psi(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_2)\right|^2 \tag{3}$$

[3], Since the two electrons in $e^+\mathrm{He}(^3S^e)$ are spatially separated with radial expectations of $\approx0.75a_0$ and $\approx15.4a_0$, it is possible to regard annihilation events with these two electrons as physically distinct. One can identify Λ_{1s} as the annihilation rate with the loosely bound valence electron, hence

$$\Gamma_c = \Gamma_d - \Lambda_{1s} \tag{4}$$

is the core annihilation rate. The core annihilation rate of $\Gamma_c=2.5065\times10^6$ s^{-1} is about 2200 times smaller than the valence annihilation rate.

The largest calculation gaves $\Gamma_d=5.713\times10^9$ s^{-1}. Although no variational principle applies, the steady increase in Γ_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 $^2S^e$ annihilation rate given by Frolov [4] was 7.5207×10^9 s^{-1}. This estimate is too large by a factor that seems to

TABLE II. Properties of the $e^+\mathrm{He}(^3S^e)$ ground state. Data are given an infinite He 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 denoted T_+ and T_-. The core $\mathrm{He}^+(1s)$ electron was not included in the evaluation of the FCSVM expectation values with the exception of ε and Γ_c.

Property	Present SVM	FCSVM
N	1500	463
$\langle V\rangle/\langle T\rangle+2$	1.38×10^{-8}	—
E	−2.250 595 08	−0.250 5863
ε	0.000 595 08	0.000 5863
$\langle T_-\rangle$	1.065 1974	0.130 507
$\langle T_+\rangle$	0.120 2004	0.120 234
$\langle r_{\mathrm{He}^{2+}e^-}\rangle$	8.057 58	15.4524
$\langle r_{\mathrm{He}^{2+}e^+}\rangle$	15.805 61	15.8902
$\langle r_{e^-e^-}\rangle$	15.393 57	—
$\langle r_{e^+e^-}\rangle$	9.489 36	3.148 72
$\langle 1/r_{\mathrm{He}^{2+}e^-}\rangle$	1.052 5352	0.104 720
$\langle 1/r_{\mathrm{He}^{2+}e^+}\rangle$	0.091 1392	0.090 7740
$\langle 1/r_{e^-e^-}\rangle$	0.102 9083	—
$\langle 1/r_{e^+e^-}\rangle$	0.288 1180	0.485 193
$\langle r^2_{\mathrm{He}^{2+}e^-}\rangle$	176.360	356.266
$\langle r^2_{\mathrm{He}^{2+}e^+}\rangle$	359.518	363.781
$\langle r^2_{e^-e^-}\rangle$	726.547	—
$\langle r^2_{e^+e^-}\rangle$	186.906	13.5235
$\langle\delta(\mathrm{He}^{2+}-e^-)\rangle$	1.274 64	0.004 2882
$\langle\delta(\mathrm{He}^{2+}-e^+)\rangle$	7.0900×10^{-7}	$7.726\,38\times10^{-7}$
$\langle\delta(e^+-e^-)\rangle$	0.018 8654	0.037 6481
Γ_d	5.712 78	5.7013
Γ_c	0.002 5065	0.001 0454

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 $^2S^e$ state is "unstable and rapidly decays by the Auger transition to the ground $1\,^1S(L=0)$ 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 statement seems to be based on the premise that $^2S^e$ state is a linear combination of e^+He($^3S^e$) and e^+He($^1S^e$) states. This is not the case since the electron-positron Coulomb interaction does not allow exchange interactions and therefore cannot change the total spin of the two electrons and thereby permit a quick decay to the helium singlet ground state. The positron annihilation channels dominate the decay of the e^+He($^3S^e$)$^2S^e$ state.

The 3γ process is the dominant annihilation channel for the quartet $^4S^e$ 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

$$\Gamma_{3\gamma}(e^+\mathrm{He}\ ^4S^e) \approx \frac{4\Gamma_{3\gamma}(^3\mathrm{Ps})}{3\Gamma_{2\gamma}(^1\mathrm{Ps})}\Gamma_{2\gamma}(e^+\ \mathrm{He}^2S^e) \tag{5}$$

Using the best estimates from Table II and $\Gamma_{2\gamma}(^1\mathrm{Ps}) = 8.0325\times10^9\ \mathrm{s}^{-1}$, $\Gamma_{3\gamma}(^3\mathrm{Ps}) = 7.2112\times10^6\ \mathrm{s}^{-1}$, gives $\Gamma_{3\gamma}(e^+\mathrm{He}\ ^4S^e) = 6.838\times10^6\ \mathrm{s}^{-1}$.

The coalescence matrix element, $\langle\delta(\mathrm{He}^{2+}-e^-)\rangle$, 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, Γ_c varied most as the basis dimension was increased. But the increase in Γ_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 ECGs was included in the basis primarily to given 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($^3S^e$) 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

$$\begin{aligned}\varepsilon(e^+\mathrm{He}^3) &= 2.250\,228\,47 - 2.249\,636\,16\\ &= 0.000\,592\,31\ \text{hartree}\end{aligned} \tag{6}$$

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

TABLE III. The annihilation rate (in units of $10^9\ \mathrm{s}^{-1}$) for annihilation with the He$^+(1s)$ core electron computed using Eqs. (9) and (4). The ratio of these two values is identified as the enhancement factor. The enhancement factor for the FCSVM calculation was taken to be 0.0025602/0.0010454.

Calculation/Basis	Eq. (9)	Eq. (4)	G
SVM/500	0.001 0978	0.002 4601	2.241
SVM/650	0.001 0978	0.002 5013	2.278
SVM/800	0.001 0976	0.002 4882	2.267
SVM/900	0.001 0968	0.002 4787	2.260
SVM/1000	0.001 0966	0.002 4973	2.277
SVM/1200	0.001 0966	0.002 4972	2.277
SVM/1500	0.001 0966	0.002 5065	2.286
FCSVM/463	0.001 0454	—	2.397
e^+-He$^+$ scattering[a]	—	—	2.52
e^+-He$^+$ scattering[b]	—	—	2.56

[a]See Ref. [9].
[b]See Ref. [24].

$$\begin{aligned}\varepsilon(e^+\ \mathrm{He}^4) &= 2.250\,318\,82 - 2.249\,725\,85\\ &= 0.000\,592\,97\ \text{hartree}.\end{aligned} \tag{7}$$

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,

$$\Gamma = U_S T_a G \int d^3r\ \rho_{e^+}(\mathbf{r})\rho_{e^-}(\mathbf{r}), \tag{8}$$

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 $^2S^e$ core annihilation rate with the He$^+(1s)$ orbital can therefore be written as

$$\Gamma = \frac{3T_aG}{4}\int d^3r\ \rho_{e^+}(\mathbf{r})\rho_{1s}(\mathbf{r}), \tag{9}$$

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

$$\rho_{e^+}(\mathbf{r}) = \int d^3r_1 \int d^3r_2 \Psi(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r})\Psi^*(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}). \tag{10}$$

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^+-He^+ scattering was 2.52 [9]. This enhancement factor was tuned at $k \approx 1.0 a_0^{-1}$ and there was a 14% variation in G from $k=0.25 a_0^{-1}$ to $k=1.50 a_0^{-1}$. 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 $Z_{\rm eff}$ using an equation similar to Eq. (9), and finally identifying G as the ratio of the exact $Z_{\rm eff}$ to the approximate $Z_{\rm eff}$. This procedure yielded $G=2.56$ [24].

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

III. THE e^+He($^3S^e$) SYSTEM AS A HALO STATE

Just recently, the e^+He($^3S^e$) 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^+He($^3S^e$) 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 $\langle r^2_{\mathrm{He}^{2+}e^-}\rangle$ and $\langle r_{\mathrm{He}^{2+}e^+}\rangle$ 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 Ps moving in the field of the He^+ ion is $V(r) \sim \alpha_d/(2r^4)$. So the classically forbidden region is given by the condition $R_0 = \sqrt[4]{\alpha_d/(2\times\varepsilon)}$. Using $\varepsilon = 0.000\,595\,08$ 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^+He($^3S^e$) decomposed into a $|\Psi_{\mathrm{He}^+}\Psi_{\mathrm{Ps}}\rangle$ product form is

$$f_c = \int d^3R \left|\langle \Psi_{\mathrm{He}^+}\Psi_{\mathrm{Ps}} | \Psi_{e^+\mathrm{He}}\rangle(\mathbf{R})\right|^2 \tag{11}$$

where

$$\langle \Psi_{\mathrm{He}^+}\Psi_{\mathrm{Ps}} | \Psi_{e^+\mathrm{He}}\rangle(\mathbf{R}) = \int d^3\rho\ d^3r_1\ \Psi^*_{\mathrm{He}^+}(\mathbf{r}_1)\Psi^*_{\mathrm{Ps}}(\rho) \times \Psi_{e^+\mathrm{He}}(\mathbf{r}_1, \boldsymbol{\rho}, \mathbf{R}), \tag{12}$$

and $\mathbf{R}=(\mathbf{r}_3+\mathbf{r}_2)/2$ and $\boldsymbol{\rho}=(\mathbf{r}_3-\mathbf{r}_2)$. (Note, an ECG basis permits an easy transformation from $(\mathbf{r}_2,\mathbf{r}_3)$ coordinates into $(\boldsymbol{\rho},\mathbf{R})$ coordinates [17]). The final value obtained was $f_c = 0.975$. The cluster fraction for the FCSVM wave function was $f_c = 0.976$ [23] The Gaussian representations of the Ps and 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 $\langle X^2\rangle/R_0^2$. In this expression $\langle X^2\rangle$ 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 $\langle X^2\rangle/R_0^2 > 2$ [25]. The expectation $\langle X^2\rangle$ is set to

$$\langle X^2\rangle = \frac{\int d^3R R^2 \left|\langle \Psi_{\mathrm{He}^+}\Psi_{\mathrm{Ps}} | \Psi_{e^+\mathrm{He}}\rangle\right|^2}{\int d^3R \left|\langle \Psi_{\mathrm{He}^+}\Psi_{\mathrm{Ps}} | \Psi_{e^+\mathrm{He}}\rangle\right|^2}. \tag{13}$$

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

$$\langle X^2\rangle \approx \langle r^2_{e^+}\rangle/2 + \langle r^2_{e^-}\rangle - 0.75, \tag{14}$$

would give $\langle X^2\rangle/R_0^2 = 355.37/13.188^2 = 2.044$ (0.75 is $\langle r^2_{e^-}\rangle$ for He^+ ground state).

The analysis of the halo state properties of e^+He($^3S^e$) using an *ab initio* SVM wave function gives the same conclusion as the earlier analysis using an FCSVM wave function. The e^+He($^3S^e$) 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^+He($^3S^e$) 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 $He^+(1s)$ electron. The enhancement factor derived from this analysis is only 10% smaller than that derived from a model potential analysis of positron-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, $\langle \delta(\mathrm{He}^{2+} - e^+)\rangle$. Other expectation values such

as the annihilation rates should be converged to ±1% or better.

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APPENDIX

There is evidently some confusion about the calculation of the annihilation rate for the e^+He($^3S^e$) state of $^2S^e$ symmetry. Therefore, details of the calculation are given here.

The spin triplet states in the α,β notation for $+1/2$ and $-1/2$ spin projections are

$$|1\,-1\rangle = \beta(1)\beta(2), \tag{A1}$$

$$|10\rangle = \frac{\alpha(1)\beta(2)+\beta(1)\alpha(2)}{\sqrt{2}}, \tag{A2}$$

$$|11\rangle = \alpha(1)\alpha(2). \tag{A3}$$

This leads to the antisymmetric two-electron states

$$|\Psi;-1\rangle = [F(1,2)-F(2,1)]\beta(1)\beta(2), \tag{A4}$$

$$|\Psi;0\rangle = [F(1,2)-F(2,1)]\frac{\alpha(1)\beta(2)+\beta(1)\alpha(2)}{\sqrt{2}}, \tag{A5}$$

$$|\Psi;1\rangle = [F(1,2)-F(2,1)]\alpha(1)\alpha(2), \tag{A6}$$

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

$$\begin{aligned}\left|\Psi;-\tfrac{1}{2}\right\rangle = {}& \sqrt{\tfrac{2}{3}}[G(1,2,3)-G(2,1,3)]\beta(1)\beta(2)\alpha(3)\\ & -\sqrt{\tfrac{1}{6}}[G(1,2,3)-G(2,1,3)][\alpha(1)\beta(2)\\ & +\beta(1)\alpha(2)]\beta(3)\end{aligned} \tag{A7}$$

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

	$\lvert\beta(1)\beta(2)\rangle$	$\lvert\alpha(1)\beta(2)\rangle$	$\lvert\beta(1)\alpha(2)\rangle$	$\lvert\alpha(1)\alpha(2)\rangle$
$\langle\beta(1)\beta(2)\rvert$	0	0	0	0
$\langle\alpha(1)\beta(2)\rvert$	0	$\frac{1}{2}$	$-\frac{1}{2}$	0
$\langle\beta(1)\alpha\rvert(2)$	0	$-\frac{1}{2}$	$\frac{1}{2}$	0
$\langle\alpha(1)\alpha(2)\rvert$	0	0	0	0

$$\begin{aligned}\left|\Psi;\tfrac{1}{2}\right\rangle = {}& \sqrt{\tfrac{2}{3}}[G(1,2,3)-G(2,1,3)]\alpha(1)\alpha(2)\beta(3)\\ & -\sqrt{\tfrac{1}{6}}[G(1,2,3)-G(2,1,3)][\alpha(1)\beta(2)\\ & +\beta(1)\alpha(2)]\alpha(3)\end{aligned} \tag{A8}$$

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

$$\hat{O}_S = 1-\tfrac{1}{2}S^2. \tag{A9}$$

Table IV gives the expectation values of this operator for the different possible α,β combinations for the electron-positron pair.

The expectation value of the annihilation operator, $T_a\Sigma_{i=1}^{2}\delta(\mathbf{r}_i-\mathbf{r}_3)\hat{O}_{S_{i3}}$ for the $M_s=+\frac{1}{2}$ state is

$$\begin{aligned}\Gamma_d = \frac{3T_a}{4}(&\langle G(1,2,3)|\delta(\mathbf{r}_1-\mathbf{r}_3)|G(1,2,3)\rangle\\ &+\langle G(1,2,3)|\delta(\mathbf{r}_2-\mathbf{r}_3)|G(1,2,3)\rangle\\ &+\langle G(1,2,3)|\delta(\mathbf{r}_1-\mathbf{r}_3)|G(2,1,3)\rangle\\ &+\langle G(1,2,3)|\delta(\mathbf{r}_2-\mathbf{r}_3)|G(2,1,3)\rangle).\end{aligned} \tag{A10}$$

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

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