Nonrelativistic variational calculations of the positronium molecule and the positronium hydride

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Highly accurate ground-state nonrelativistic variational calculations of Ps_2, ^1HPs, and $^\infty HPs$ are reported. The calculations have been performed using 5000 explicitly correlated Gaussian basis functions and yielded the lowest variational energy upper bounds for these systems to date. The relative accuracies of the energies obtained are of the order of 4×10^{-10} a.u. for Ps_2 and 2×10^{-9} a.u. for HP. Several expectation values have also been computed for each system, as well as electron-positron annihilation rates.

Since the theoretical prediction of their stability [1,2], the positronium molecule and the positronium hydride have been subject to numerous theoretical studies (see, for example, Refs. [3–16], and references therein). The interest in these systems has increased in the last decade due to rapidly growing computer capabilities that have allowed treatment of four-particle and even larger quantum systems with high accuracy and due to the experimental observations of several positronic systems including HPs [17]. The positronium hydride and, especially, the positronium molecule are important systems among four-particle systems with Coulombic interactions. They are of great interest in astrophysical applications and in solid-state physics. Thus, very accurate solutions of the Schrödinger equation for the stationary bound states of these systems and predictions of expectation values related to measurable quantities are desirable. It should be noted that obtaining precise binding energies with many converged significant figures in the calculations is not only of purely technical interest. Very well converged calculations are often needed to obtain adequate precision in determining expectation values of some operators related to quantities other than the total energy of the system. Those expectation values may converge much slower than the total energy. This happens because the weight assigned by the operators to certain regions of the phase space may be large in comparison to the significance of these regions to the total energy. An example of such an operator is the Dirac delta function dependent on an interparticle distance. When Gaussian basis functions are used in the calculation, the expectation value of this operator is often significantly underestimated or overestimated. In such a situation the Dirac delta function may be determined several orders of magnitude less precisely than the total energy. However, the needed accuracy of the expectation values of the delta function may, in some cases, be quite high in order to yield adequately accurate values of such quantities as transition properties that depend on differences between expectation values of the delta function calculated for different states. Operators, whose expectation values converge slowly such as those of the delta function, also appear in the expressions for relativistic corrections and in *n*-photon decay rates. In this work we have attempted to perform calculations that yield not only very accurate total energies and wave functions but also can be used to evaluate expectation values of different operators with a very high precision.

The lowest variational energy upper bound to date for the Ps_2 ground state, according to our knowledge, remains that from the work of Usukura *et al.* [9], where the value of −0.516 003 789 058 a.u. was reported. In that calculation the authors used 1600 explicitly correlated Gaussians (ECGs). For $^\infty HPs$ (an infinitely heavy mass of the proton was assumed), the lowest energy of −0.789 196 740 a.u. was computed in Ref. [16] using 1800 ECG functions. In the case of the finite hydrogen mass (^1HPs) the lowest energy value was obtained by the present authors [18] and it was −0.788 870 706 6 a.u. In that work we used 3200 explicitly correlated Gaussian functions with premultipliers in the form of even powers of the distance between the proton and the positron.

In the calculations reported here we have used simple ECG functions (without premultipliers) in the following form:

$$\phi_k = \exp[-\mathbf{r}'(A_k \otimes I_3)\mathbf{r}] = \exp[-\mathbf{r}'(L_k L_k' \otimes I_3)\mathbf{r}]. \quad (1)$$

In the above expression, $\mathbf{r}$ is a nine-component vector,

$$\mathbf{r} = \begin{bmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \\ \mathbf{r}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{R}_2 - \mathbf{R}_1 \\ \mathbf{R}_3 - \mathbf{R}_1 \\ \mathbf{R}_4 - \mathbf{R}_1 \end{bmatrix}, \quad (2)$$

where the $\mathbf{R}_i$'s are the original Cartesian coordinates of the particles in the laboratory coordinate system. A_k is a symmetric, positive definite 3×3 matrix of exponential parameters that are unique for each basis function, $\otimes$ stands for the Kronecker product, and the prime is used to denote a matrix or a vector transposition. Explicitly correlated Gaussian functions (1) can also be written in a more conventional way;

$$\phi_k = \exp[-\beta_{12,k}R_{12}^2 - \beta_{13,k}R_{13}^2 - \beta_{14,k}R_{14}^2 - \beta_{23,k}R_{23}^2 - \beta_{24,k}R_{24}^2 - \beta_{34,k}R_{34}^2], \quad (3)$$

where parameters $\beta_{ij,k}$ are related to the elements of matrices A_k and L_k in Eq. (1).

The choice of matrix A_k in the Cholesky-factored form, $L_k L_k'$, is convenient from a computational standpoint since this leads to no restrictions on the values of the elements of L_k. Such restrictions would have to be imposed if the elements of the A_k matrices are used as the variational parameters since, as mentioned, A_k's have to be positive definite. More details describing the approach used here and those

TABLE I. Energy convergence for Ps_2, ^1HPs, and $^\infty HPs$. All values are in a.u.

Basis size	Ps_2	^1HPs	$^\infty HPs$
500	−0.516 003 770 835	−0.788 870 158 930	−0.789 196 187 887
1000	−0.516 003 787 849	−0.788 870 646 568	−0.789 196 705 369
2000	−0.516 003 789 829	−0.788 870 702 212	−0.789 196 757 758
3000	−0.516 003 790 168	−0.788 870 707 806	−0.789 196 762 859
4000	−0.516 003 790 332	−0.788 870 709 600	−0.789 196 764 467
5000	−0.516 003 790 416	−0.788 870 710 444	−0.789 196 765 251

concerning the separation of the center-of-mass motion and evaluation of matrix elements with functions (1), etc., and those describing the computational procedures involved can be found in Refs. [19–21].

Before being used in the calculations, the basis functions (1) have to be transformed by symmetry operators to account for the permutational symmetry within each group of identical particles in the system. In the present calculations particles 3 and 4 were electrons, particle 2 was a positron, and particle 1 was either a proton (in HPs) or a positron (in Ps_2). The proper symmetrization of the basis functions was achieved by applying to each basis function the $(1+\hat{P}_{34})$ projection operator in the case of HPs and the $(1+\hat{P}_{13}\hat{P}_{24})(1+\hat{P}_{12})(1+\hat{P}_{34})$ projection operator in the case of Ps_2. Here $\hat{P}_{ij}$ stands for the permutation of particles i and j. The result of applying the $\hat{P}_{ij}$ operators to basis functions (1) is equivalent to certain transformations of matrices A_k. There is an additional symmetry operator that needs to be applied to the basis functions for the Ps_2 system that reflects the charge conjugation symmetry between the two electrons and the two positrons. This operator is $(1+\hat{P}_{13}\hat{P}_{24})$ and it involves a permutation of the first electron with the first positron and a simultaneous permutation of the second electron with the second positron. A comprehensive analysis of the symmetry of the positronium molecule is given in Refs. [5,22].

In our calculations we used 5000 basis functions for each system. The basis set generation was carried out in two stages. In the first step we generated a small basis set of 100 functions and performed full optimization of all nonlinear parameters, i.e., all elements of the L_k matrix, for each of the 100 basis functions. In this step we used the minimization procedure based on the analytical gradient of the energy calculated with respect to the L_k parameters. Next the basis was enlarged to its final size of 5000 by incrementally adding 10–20 new functions to the basis set using a random selection of nonlinear parameters and optimizing one function at a time. After adding 10–20 functions the whole basis was re-optimized with the one-function-at-a-time approach. In this approach we also used the analytical gradient of the energy with respect to the exponential parameters. The formulas for the analytical gradient and remarks on its numerical implementation can be found in Refs. [19–21].

The convergence of the energies of the positronium molecule and the positronium hydride (for both finite and infinite proton masses) with respect to the number of the basis functions is shown in Table I. The proton-electron mass ratio used in the calculations of ^1HPs was 1836.152 672 61. For all three systems we obtained the energy values that are the lowest energy upper bounds to date. Moreover, upon comparing the energies computed with different numbers of basis functions with the corresponding values taken from the works of Usukura *et al.* [9], Mitroy [16], and from our own work [18], one can notice that somewhat better energy convergence is achieved in the present calculations. This resulted from more thorough optimization of the exponential parameters performed in this work.

In order to determine the accuracy of the present calculations we examined the energy convergence patterns presented in Table I. Simple extrapolations gave us the values of 4×10^{-10} and 2×10^{-9} for the relative errors in the energies obtained with 5000 basis functions for Ps_2 and HPs, respectively. The better convergence of the Ps_2 energy results from the higher permutational symmetry of this system. This makes the number of the terms resulting from the symmetry

TABLE II. Expectation values for Ps_2 obtained with different basis sets. All quantities are in a.u.

Basis size	$\langle r_{e^+e^+} \rangle$	$\langle r_{e^+e^-} \rangle$	$\langle r_{e^+e^+}^2 \rangle$	$\langle r_{e^+e^-}^2 \rangle$	$\langle \delta_{e^+e^+} \rangle$	$\langle \delta_{e^+e^-} \rangle$	$\langle \delta_{e^+e^+e^-} \rangle$	$\langle \delta_{e^+e^+e^-e^-} \rangle$
500	6.033 208 400	4.487 153 726	46.374 810 41	29.112 670 56	$6.267 782 \times 10^{-4}$	$2.210 623 \times 10^{-2}$	$9.160 34 \times 10^{-5}$	4.5819×10^{-6}
1000	6.033 210 193	4.487 154 574	46.374 874 78	29.112 702 41	$6.260 488 \times 10^{-4}$	$2.211 608 \times 10^{-2}$	$9.136 30 \times 10^{-5}$	4.5765×10^{-6}
2000	6.033 210 239	4.487 154 592	46.374 877 81	29.112 703 93	$6.259 317 \times 10^{-4}$	$2.211 671 \times 10^{-2}$	$9.117 39 \times 10^{-5}$	4.5706×10^{-6}
3000	6.033 210 196	4.487 154 570	46.374 876 60	29.112 703 37	$6.257 999 \times 10^{-4}$	$2.211 691 \times 10^{-2}$	$9.109 89 \times 10^{-5}$	4.5172×10^{-6}
4000	6.033 210 225	4.487 154 583	46.374 877 82	29.112 703 97	$6.257 993 \times 10^{-4}$	$2.211 775 \times 10^{-2}$	$9.112 41 \times 10^{-5}$	4.5481×10^{-6}
5000	6.033 210 257	4.487 154 599	46.374 879 10	29.112 704 61	$6.257 980 \times 10^{-4}$	$2.211 775 \times 10^{-2}$	$9.109 67 \times 10^{-5}$	4.5536×10^{-6}

TABLE III. Expectation values for ^{1}HPs obtained with different basis sets. All quantities are in a.u.

Basis size	$\langle r_{p^+e^+}\rangle$	$\langle r_{p^+e^-}\rangle$	$\langle r_{e^+e^-}\rangle$	$\langle r_{e^-e^-}\rangle$	$\langle r^2_{p^+e^+}\rangle$	$\langle r^2_{p^+e^-}\rangle$	$\langle r^2_{e^+e^-}\rangle$	$\langle r^2_{e^-e^-}\rangle$	$\langle \delta_{p^+e^+}\rangle$	$\langle \delta_{p^+e^-}\rangle$	$\langle \delta_{e^+e^-}\rangle$	$\langle \delta_{e^-e^-}\rangle$	$\langle \delta_{e^+e^-e^-}\rangle$
500	3.663 475 033	2.313 145 874	3.481 162 441	3.576 992 960	16.271 716 70	7.824 557 445	15.593 287 38	15.895 478 92	$1.635\,665\times10^{-3}$	0.176 715 6	$2.442\,215\times10^{-2}$	$4.388\,081\times10^{-3}$	$3.746\,85\times10^{-4}$
1000	3.663 501 500	2.313 160 807	3.481 175 748	3.577 021 421	16.272 142 52	7.824 786 998	15.593 531 23	15.895 924 11	$1.628\,128\times10^{-3}$	0.176 949 7	$2.447\,620\times10^{-2}$	$4.367\,616\times10^{-3}$	$3.725\,53\times10^{-4}$
2000	3.663 502 576	2.313 161 416	3.481 176 079	3.577 022 692	16.272 170 05	7.824 801 361	15.593 545 38	15.895 952 43	$1.623\,934\times10^{-3}$	0.177 006 7	$2.447\,765\times10^{-2}$	$4.366\,199\times10^{-3}$	$3.693\,74\times10^{-4}$
3000	3.663 502 685	2.313 161 534	3.481 176 106	3.577 022 945	16.272 173 92	7.824 804 086	15.593 547 16	15.895 957 60	$1.623\,818\times10^{-3}$	0.177 016 9	$2.447\,774\times10^{-2}$	$4.365\,969\times10^{-3}$	$3.692\,00\times10^{-4}$
4000	3.663 502 693	2.313 161 559	3.481 176 105	3.577 023 001	16.272 174 07	7.824 804 460	15.593 547 25	15.895 958 37	$1.623\,825\times10^{-3}$	0.177 029 1	$2.447\,780\times10^{-2}$	$4.364\,226\times10^{-3}$	$3.687\,91\times10^{-4}$
5000	3.663 502 705	2.313 161 564	3.481 176 109	3.577 023 013	16.272 174 34	7.824 804 565	15.593 547 43	15.895 958 62	$1.623\,808\times10^{-3}$	0.177 029 3	$2.447\,844\times10^{-2}$	$4.363\,357\times10^{-3}$	$3.687\,79\times10^{-4}$

TABLE IV. Expectation values for $^\infty$HPs obtained with different basis sets. All quantities are in a.u.

Basis size	$\langle r_{p^+e^+}\rangle$	$\langle r_{p^+e^-}\rangle$	$\langle r_{e^+e^-}\rangle$	$\langle r_{e^-e^-}\rangle$	$\langle r^2_{p^+e^+}\rangle$	$\langle r^2_{p^+e^-}\rangle$	$\langle r^2_{e^+e^-}\rangle$	$\langle r^2_{e^-e^-}\rangle$	$\langle \delta_{p^+e^+}\rangle$	$\langle \delta_{p^+e^-}\rangle$	$\langle \delta_{e^+e^-}\rangle$	$\langle \delta_{e^-e^-}\rangle$	$\langle \delta_{e^+e^-e^-}\rangle$
500	3.661 598 605	2.311 511 288	3.480 259 880	3.574 759 980	16.254 027 48	7.812 796 965	15.583 998 02	15.874 985 46	$1.639\,838\times10^{-3}$	0.177 059 0	$2.445\,015\times10^{-2}$	$4.386\,228\times10^{-3}$	$3.748\,81\times10^{-4}$
1000	3.661 623 731	2.311 525 190	3.480 272 355	3.574 786 671	16.254 512 26	7.813 037 837	15.584 264 93	15.875 455 39	$1.629\,110\times10^{-3}$	0.177 253 6	$2.447\,607\times10^{-2}$	$4.378\,337\times10^{-3}$	$3.711\,28\times10^{-4}$
2000	3.661 624 869	2.311 525 838	3.480 272 778	3.574 787 999	16.254 535 62	7.813 049 863	15.584 277 44	15.875 478 74	$1.626\,244\times10^{-3}$	0.177 310 0	$2.448\,248\times10^{-2}$	$4.376\,174\times10^{-3}$	$3.702\,62\times10^{-4}$
3000	3.661 624 927	2.311 525 910	3.480 272 788	3.574 788 151	16.254 537 59	7.813 051 435	15.584 278 47	15.875 481 74	$1.626\,068\times10^{-3}$	0.177 325 8	$2.448\,364\times10^{-2}$	$4.375\,841\times10^{-3}$	$3.703\,51\times10^{-4}$
4000	3.661 624 946	2.311 525 915	3.480 272 792	3.574 788 163	16.254 538 09	7.813 051 538	15.584 278 69	15.875 481 90	$1.625\,320\times10^{-3}$	0.177 329 2	$2.448\,374\times10^{-2}$	$4.375\,389\times10^{-3}$	$3.698\,35\times10^{-4}$
5000	3.661 624 960	2.311 525 926	3.480 272 799	3.574 788 186	16.254 538 34	7.813 051 722	15.584 278 86	15.875 482 26	$1.625\,230\times10^{-3}$	0.177 329 5	$2.448\,406\times10^{-2}$	$4.374\,170\times10^{-3}$	$3.694\,56\times10^{-4}$

projection for each basis function four times larger than in the case of HPs (eight vs two). It should be emphasized, however, that the above-mentioned relative energy errors are only rough estimates. For this reason we do not show any extrapolated energies in Table I.

The calculations of ^{1}HPs and $^\infty$HPs have been performed independently from each other. Nonetheless, our tests showed that using the basis set generated for $^\infty$HPs in the calculation for ^{1}HPs, where only linear coefficients of the basis functions are optimized, works quite well. This is because the difference between the two systems, $^\infty$HPs and ^{1}HPs, is very small in terms of their structures and the optimization of only the linear coefficients suffices to get very good energy for ^{1}HPs with the $^\infty$HPs basis set. In fact, the calculation of ^{1}HPs with the 5000-term $^\infty$HPs basis set gave slightly lower energy than that shown in Table I. The energy was $-0.788\,870\,710\,567$ a.u. vs $-0.788\,870\,710\,444$ a.u. given in Table I. The likely reason for this is the fact that the calculations for $^\infty$HPs were slightly better converged than those for ^{1}HPs and produced a better basis set even for ^{1}HPs (growing the basis up to 5000 and optimizing the nonlinear parameters is, in some way, a trial and error process).

In Tables II–IV we present some expectation values computed with progressively larger basis sets. The expectation values of the interparticle distances and their squares for all systems show convergence that is comparable with the convergence of the total energy (they are about one order of magnitude less accurate). These values are in very good agreement with the corresponding data from works [9,16]. We also computed the expectation values of the two-particle contact densities, as well as three- and four-particle electron-positron contact densities. They can be used to make estimates of various positron-electron annihilation rates. The notation used in Tables II–IV is the following: $\langle \delta_{e^+e^-} \rangle \equiv \langle \delta(\mathbf{r}_{e^+} - \mathbf{r}_{e^-}) \rangle$, $\langle \delta_{e^+e^+e^-} \rangle \equiv \langle \delta(\mathbf{r}_{e^+} - \mathbf{r}_{e^+}) \delta(\mathbf{r}_{e^+} - \mathbf{r}_{e^-}) \rangle$, $\langle \delta_{e^+e^+e^-e^-} \rangle \equiv \langle \delta(\mathbf{r}_{e^+} - \mathbf{r}_{e^+}) \delta(\mathbf{r}_{e^+} - \mathbf{r}_{e^-}) \delta(\mathbf{r}_{e^-} - \mathbf{r}_{e^-}) \rangle$. As expected, the relative accuracy of the contact densities is significantly lower than that of the total energy. The two-particle contact densities for particles with opposite charges tend to be slightly underestimated, while the contact densities for particles with the same charge are usually overestimated. This results from the well-known deficiency of the Gaussian functions and their inability to describe the cusp behavior of the wave function. The relative accuracy drops even further for the three- and four-particle contact densities.

Using the contact-density data obtained in the calculations with the largest basis sets, we computed the zero-, one-, two-, and three-photon annihilation rates. The two-photon annihilation rate for a system containing both electrons and positrons, which is the dominant rate for this type of system, can be computed using the following expression that involves the expectation value of the electron-positron contact density:

$$\Gamma_{2\gamma} = N_{e^+} N_{e^-} \frac{\pi \alpha^4 c}{a_0} \langle \delta_{e^+e^-} \rangle. \qquad (4)$$

Here α is the fine structure constant, a_0 is the Bohr radius, and c is the velocity of light. N_{e^+} and N_{e^-} denote the number

of positrons and electrons in the system, respectively. Taking the expectation values of $\delta_{e^+e^-}$ calculated with 5000 basis functions, one obtains the two-photon annihilation rates of $4.465\,106 \times 10^9$ s^{-1}, $2.470\,839 \times 10^9$ s^{-1}, and $2.471\,406 \times 10^9$ s^{-1} for Ps$_2$ ^{1}HPs, and $^\infty$HPs, respectively. It is possible to correct $\Gamma_{2\gamma}$ for the Coulomb and the radiative effects [23], as it was done in Ref. [24]. In order to do this, one needs to multiply the expression (4) by the factor $1 - \alpha(5 - \pi^2/4)/\pi$. The annihilation rates corrected in this way are $4.438\,838 \times 10^9$ s^{-1}, $2.456\,304 \times 10^9$ s^{-1}, and $2.456\,867 \times 10^9$ s^{-1} (again, for Ps$_2$, ^{1}HPs, and $^\infty$HPs, respectively). The above Ps$_2$ two-photon annihilation rate value differs from the one given in Ref. [24] because the authors of that work mistakenly used π^4 instead of π^2 in the expression for the correction factor.

Following the works [8,24,25] we can also evaluate the one- and three-photon annihilation rates. The corresponding expressions are

$$\Gamma_{1\gamma} = k N_{e^+} N_{e^-} \frac{32 \pi^2 \alpha^8 c}{27 a_0} \langle \delta_{e^+e^+e^-} \rangle, \qquad (5)$$

$$\Gamma_{3\gamma} = N_{e^+} N_{e^-} \frac{4(\pi^2 - 9)\alpha^5 c}{3 a_0} \langle \delta_{e^+e^-} \rangle. \qquad (6)$$

The coefficient k in Eq. (5) should be set to 1 for Ps$_2$ and to 2 for HPs because in the latter system there are two ways the electron-positron annihilation can occur and both ways have approximately equal annihilation rates [8].

The numerical values for the one- and three-photon annihilation rates obtained using the expectation values from Tables II–IV are $\Gamma_{1\gamma}(\text{Ps}_2) = 0.194\,174$ s^{-1}, $\Gamma_{1\gamma}(^1\text{HPs}) = 0.786\,058$ s^{-1}, $\Gamma_{1\gamma}(^\infty\text{HPs}) = 0.787\,501$ s^{-1}, $\Gamma_{3\gamma}(\text{Ps}_2) = 1.202\,563 \times 10^{-7}$ s^{-1}, $\Gamma_{3\gamma}(^1\text{HPs}) = 6.654\,577 \times 10^{-6}$ s^{-1}, $\Gamma_{3\gamma}(^\infty\text{HPs}) = 6.656\,103 \times 10^{-6}$ s^{-1}.

For the positronium molecule, a zero-photon annihilation process (two-photon annihilation of a e^+e^- pair followed by the internal conversion of the emitted photons) can also occur. The expression for the annihilation rate for such a process as given in Ref. [24] is

$$\Gamma_{0\gamma} = \frac{147 \sqrt{3} \pi^3 \alpha^{12} c}{2 a_0} \langle \delta_{e^+e^+e^-e^-} \rangle. \qquad (7)$$

Using the $\langle \delta_{e^+e^+e^-e^-} \rangle$ expectation value taken from Table II we get $\Gamma_{0\gamma} = 2.3220 \times 10^{-9}$ s^{-1}.

In summary, we have performed very accurate ground-state nonrelativistic calculations of the positronium molecule and the positronium hydride using explicitly correlated Gaussian functions. The computed energies set new improved variational energy upper bounds for these systems. The obtained wave functions can be used in accurate calculations of expectation values of various operators, in particular, of operators that appear in the calculations of relativistic corrections.

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