Precise nonvariational calculation of the positronium negative ion

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The three-body Schrödinger equation is solved directly for the ground state of the positronium negative ion by using a rapidly convergent correlation function hyperspherical harmonic method, which involves no adjustable parameters. The inclusion of 169 hyperspherical functions yields the ground-state energy 0.262 004 86 a.u., which is converged to an error in the seventh significant figure. Expectation values of different functions of interparticle distances as well as the two-photon annihilation rate are calculated and compared with those obtained by variational calculations.

In the last few decades a great amount of variational work[1–7] has been done on wave functions and expectation values of the positronium negative ion $Ps^-(e^+e^-e^-)$. The binding energy of this system and its decay rate were measured recently by Mills.[8,9] In lowest order, the decay width Γ of the positronium ion is proportional to the density $\langle\delta(\mathbf{r}_{13})\rangle$ of electrons at the positron,[4,5]

$$\Gamma=2\pi\alpha^4C\langle\delta(\mathbf{r}_{13})\rangle$$
$$=100.938C\langle\delta(\mathbf{r}_{13})\rangle\ \text{nsec}^{-1}\ . \tag{1}$$

Here, $C=1+\eta$ and $\eta=\eta_1+\eta_2+\eta_3$, where η_1 accounts for radiative corrections[10] $[\eta_1=-\alpha(5/\pi-\pi/4)]$, η_2 for three-photon annihilation[11] $[\eta_2=-4\alpha(\pi/3-3/\pi)]$, and η_3 for bound-state and relativistic effects, which have not yet been calculated. The values of $\langle\delta(\mathbf{r}_{13})\rangle$, computed in previous works[4,5] are 0.020 713, 0.020 730, and 0.020 733, respectively, which correspond to the widths $2.0908C$, $2.0924C$, and $2.0928C$ nsec^{-1}. For $C=1+\eta_1+\eta_2=0.996\,824$, they correspond to 2.0842, 2.0858, and 2.0861 nsec^{-1}. The experiment[9] currently gives 2.09 ± 0.09 nsec^{-1}, which with current experimental accuracy agrees with all above-mentioned theoretical values. However, a feasible order-of-magnitude increase in the experimental precision[9] clearly demands better knowledge of the expectation values $\langle\delta(\mathbf{r}_{13})\rangle$ in order to test relativistic and radiative corrections and ground-state contributions to the decay rate.

The purpose of this work is to calculate the disputed quantities once again as well as to obtain expectation values of different functions of the interparticle distances, including the Hamiltonian, with the help of the correlation function hyperspherical harmonic method. This method was developed recently by the present authors[12–14] and is designed to provide analytically and locally correct wave functions, generally unobtainable by the variational method. The method consists of presenting a wave function ψ as a product of two factors, $\psi=\chi\phi$, where χ is chosen to account for the singular and/or clustering structure of the system. A factor ϕ is expanded into the hyperspherical harmonics and satisfies the Schrödinger equation, written in atomic units as

$$(-\tfrac{1}{2}\nabla^2+V')\phi=E\phi\ , \tag{2}$$

with the effective velocity-dependent potential V' determined[12] by the true potential V and the correlation factor χ:

$$V'=-(\nabla\ln\chi)\nabla-\frac{\tfrac{1}{2}\nabla^2\chi}{\chi}+V\ . \tag{3}$$

Here ∇ is the six-dimensional gradient. As was demonstrated in the example of the ground and excited states of the helium atom,[12–14] our method allows a very precise direct solution of the three-body Schrödinger equation. A wave function calculated by this method converges to a true solution at every point in absolute and uniform fashion, and not "on the average," as in variational approaches. That enforces similar convergence for the expectation values of different operators. Another important feature of the wave function is its correct analytic structure. The double coalescent points can be exactly taken into account in the correlation function χ, and the radial dependence of function ϕ is given analytically by the logarithmic-power-series expansions[15,16] resulting from direct solution of the Schrödinger equation. Thus the logarithmic terms, which were anticipated by Bartlett[17] and Fock,[18] are taken into account automatically and precisely. The energies and other expectation values[12–14] calculated with this wave function have an accuracy available earlier only in very elaborate variational calculations.

We use here the correlation function,

$$\chi=\exp[-\gamma(r_{13}+r_{23})-\delta r_{12}]\ , \tag{4}$$

often employed in calculations of symmetric S states of two-electron systems. The parameters γ and δ are chosen in such a way as to incorporate the most important features of the wave function. The residual wave

TABLE I. Convergence of eigenvalues (a.u.) for the ground state of the positronium negative ion for asymptotic, uncorrelated variational, variational, and uncorrelated cusp parametrizations.

(γ,δ) / K_m	Asymptotic (0.362,0)	Uncorrelated variational (0.3437,0)	Variational (0.367,−0.044)	Uncorrelated cusp (0.5,0)
0	0.192 79	0.185 15	0.211 82	0.206 69
4	0.244 03	0.241 50	0.246 81	0.246 58
8	0.252 45	0.251 38	0.253 19	0.264 85
12	0.256 12	0.255 56	0.256 30	0.261 11
16	0.258 12	0.257 73	0.258 28	0.262 07
20	0.259 33	0.259 06	0.259 44	0.262 12

function ϕ, which is expanded in hyperspherical harmonics, contains a minimum of hyperangular dependence, and therefore its hyperspherical expansion is rapidly convergent.

There are three obvious ways to choose these parameters.[12–14] They are, respectively, based on the following requirements: (i) absence of Coulomb singularities in the equation for function χ [cusp parametrization[12] $\gamma=MZ/(M+1)$, $\delta=-0.5$], (ii) minimal energy configuration (variational parametrization[19]), corresponding to the minimum of

$$E(\gamma,\delta)=\frac{\langle\chi|H|\chi\rangle}{\langle\chi|\chi\rangle}=\frac{\gamma+\delta}{8\gamma^2+5\gamma\delta+\delta^2}\times\left[2\gamma\left[\frac{M+1}{M}\gamma-2Z\right](\delta+4\gamma)+(1+\delta)(5\gamma^2+4\gamma\delta+\delta^2)\right], \quad (5)$$

and (iii) proper asymptotic behavior of the correlation function [asymptotic parametrization[14]

$$\gamma=\sqrt{M|E|/(M+1)}\,,$$

where $\delta=0$]. Here M is the ratio of the mass of the nonidentical particle to that of like particles. Clearly, the cusp parametrization is expected to work best for small systems, such as the ground-state helium atom, where electrons are close to a nucleus and to each other. The asymptotic or variational parametrizations should be most appropriate for loosely bound and clustered systems, such as the positronium negative ion considered here, where particles are located far away from each other. This system is adequately represented as a positronium core with an extra loosely bound and nearly uncorrelated electron. An alternative description could be given by the uncorrelated cusp parametrization $\gamma=MZ/(M+1)$, $\delta=0$. This last choice takes care of the singularity of interaction between close particles and neglects those between distant particles. It turned out to be an excellent choice for excited helium,[13] and it was natural also to consider it in the present computation.

The eigenvalues[12] E for the positronium negative ion, obtained with different sets of parameters (γ,δ), are given in Table I. The table allows us to choose the parametrization that corresponds to the fastest convergence. This turns out to be the uncorrelated-parametrization. The asymptotic, variational, and uncorrelated-variational parametrizations [the last one is obtained by variation of γ in (5) with δ fixed at zero value] give, obviously, far less accurate results. Table II summarizes the eigenvalues E of Eq. (2) and the expectation values of the true Hamiltonian $H=-\frac{1}{2}\nabla^2+V$ (which, in our approach, are not automatically equal to each other[12]) obtained by inclusion into the expansion of ϕ, 49, 81, 121, and 169 hyperspherical functions, corresponding to maximum global angular momenta $K_m=24$, 32, 40, and 48, respective-

TABLE II. Eigenvalues E and expectation values $\langle H\rangle$ (a.u.) of the Hamiltonian operator for the ground state of the positronium negative ion when the uncorrelated cusp parameters are employed. The number of digits indicates the numerical precision of the calculated value. The last entry gives the result of the variational calculations (Refs. 1, 2, 4, 5, and 7).

K_m	24	32	40	48	Variational
$-E$	0.261 964 226	0.262 025 526 4	0.262 009 899	0.262 002 413 0	0.261 995 6[a]
$-\langle H\rangle$	0.262 000	0.262 003 4	0.262 004 47	0.262 004 857	0.262 001 1[b]
					0.262 004 895[c]
					0.262 005 065[d]
					0.262 005 070[e]

[a]Reference 1.
[b]Reference 2.
[c]Reference 4.
[d]Reference 5.
[e]Reference 7.

TABLE III. Expectation values (a.u.) of various functions of interparticle distances for the ground-state positronium negative ion. The number of digits indicates the numerical precision of the calculated value. The table contains also variational results (Refs. 1, 4, 5, 6, and 7).

K_m	N	r_{13}^{-2}	r_{13}^{-1}	$\delta(r_{13})$	r_{13}	r_{13}^{2}	$(r_{13}r_{23})^{-1}$
24	49	0.279 23	0.339 89	0.020 712	5.483	48.31	0.091 05
32	81	0.279 335 8	0.339 751	0.020 741 3	5.497 1	48.63	0.090 843 3
40	121	0.279 332 0	0.339 809 4	0.020 737 5	5.491 082	48.459	0.090 917 11
48	169	0.279 309 7	0.339 831 3	0.020 730 3	5.488 352	48.379 317	0.090 949 23
Variational			0.339 8[a]	0.020 713[a]	5.489 1[a]	48.393 6[a]	
			0.339 821 02[b]	0.020 730[c]	5.506[d]	48.415 2[e]	
				0.020 733[c]	5.489 633 3[b]	48.75[d]	
						48.418 936[b]	

K_m	N	r_{12}^{-2}	r_{12}^{-1}	$\delta(r_{12})$	r_{12}	r_{12}^{2}	$(r_{12}r_{13})^{-1}$
24	49	0.036 11	0.155 81	0.000 188 97	8.536	92.98	0.060 78
32	81	0.035 979 2	0.155 483	0.000 184 094 9	8.563 2	93.60	0.060 629 5
40	121	0.036 017 95	0.155 602 0	0.000 181 826 9	8.551 381	93.258	0.060 684 08
48	169	0.036 034 51	0.155 654 3	0.000 180 151 7	8.546 111 29	93.100 697 0	0.060 707 79
Variational			0.155 6[a]	0.000 171 29[c]	8.547 6[a]	93.128 3[a]	
			0.155 631 90[b]	0.000 171 5[c]	8.580[d]	93.171 4[e]	
					8.548 580 8[b]	93.94[d]	
						93.178 633[b]	

[a]Reference 4.
[b]Reference 7.
[c]Reference 5.
[d]Reference 1.
[e]Reference 6.

ly. Table III displays expectation values of various functions of interparticle distances. The results in both Tables II and III are calculated with the uncorrelated cusp parametrization.

The convergence pattern of the energy values in the Table II indicates that our final ground-state energy 0.262 004 86 computed as the expectation value of the Hamiltonian for $K_m = 48$ has an error only in the seventh decimal place. With this precision it agrees very well with the values given by the most sophisticated variational calculations,[4,5,7] which use hundreds of variational parameters. The agreement among averages of powers of interparticle distances calculated by us and by the variational method is also very good and on the same level as the agreement among different variational calculations. Our value of 0.020 730 for the electron density $\langle \delta(\mathbf{r}_{13}) \rangle$ at the position coincides exactly with the value obtained by Bhatia and Drachman[6] under the restriction of the correlation factor being symmetric under interchange of the electrons, a condition which was also employed in the present work. However, as follows from Table III, the probability $\langle \delta(\mathbf{r}_{12}) \rangle$ of two electrons to be found at the same point is rather different in our present direct calculation and the variational calculation.[5] This could reflect the difficulty of reproducing the electron-electron cusp (not taken into account explicitly in the exponential correlation factors in both computations) with the help of the sum of smooth continuous terms.

Summing up, we have solved directly the three-body Schrödinger equation for the positronium negative ion with the help of the correlation function hyperspherical method. Our present results show that this method provides a very accurate solution not only for the system of two light and one heavy particle, such as the helium atom,[12–14] but also for the system of particles with comparable masses. Our positronium ion ground-state energy and expectation values agree very well with the results of the most recent variational calculations,[4–7] and the two-photon annihilation rate of 2.0858 nsec^{-1} coincides precisely with that calculated in Ref. 5. Our results were obtained with the correlation function which contains the electron-positron cusps exactly. This guarantees a smoothness of the factor ϕ and therefore a fast convergence of the hyperspherical expansion. In particular, the correct analytic structure of the wave function ψ is assured in the vicinity of the electron-positron coalescence points. This renders a very accurate $\delta(\mathbf{r}_{13})$ expectation value, which depends solely on the values of the wave function at the coalescence points. Hence our annihilation rate should be rather reliable. The expected increase in the experimental precision[9] would allow us to test this number and the present understanding of quantum electrodynamic corrections.

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