

Precise nonvariational calculation of the two-photon annihilation rate of the positronium negative ion

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A direct (nonvariational) solution of the Schrödinger equation for the ground state of the positronium negative ion is obtained with the correlation-function hyperspherical-harmonic (CFHH) method. Given the proper correlation function chosen from physical considerations, the CFHH method generates wave functions accurate in the whole range of interparticle distances that lead, in turn, to precise estimates of the expectation values of the Hamiltonian and of different functions of interparticle distances. The correlation function used was chosen to have proper electron-positron and electron-electron cusps as well as asymptotic behavior. The inclusion of 225 hyperspherical functions yields the nonextrapolated ground-state energy value of 0.262 005 058 atomic units, which is lower than the nonextrapolated energy values 0.262 004 895 and 0.262 005 056 calculated in works of Ho [J. Phys. B **16**, 1503 (1983)] and Bhatia and Drachman [Phys. Rev. A **28**, 2523 (1983)] but higher than the best variational value 0.262 005 069 obtained by Petenlenz and Smith [Phys. Rev. A **36**, 5125 (1987)]. The accuracy of our value of $2.086\,10 \pm 0.000\,06 \text{ nsec}^{-1}$ for the two-photon annihilation rate is higher by an order of magnitude than obtained in the previous literature.

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The correlation-function hyperspherical-harmonic (CFHH) method, unifying the correlation-function approach [1] with the hyperspherical-harmonic method [2], was introduced a few years ago by Haftel and Mandelzweig [3–9]. The method provides a very accurate direct (nonvariational) solution of the Schrödinger equation for different three-body systems and cures the main pitfall of the variational method—the necessity of guessing the mathematical form of the wave function, which can result in a low-quality wave function even in cases where hundreds of variational parameters generate extremely precise energies [10]. Given the proper correlation function, chosen from physical considerations, the CFHH method yields wave functions accurate in the whole range of interparticle distances [8,9]. This leads, in turn, to precise estimates of the expectation values of the Hamiltonian and of different functions of interparticle distances [4–7,9]. Variational wave functions, on the other hand, are often accurate only in the region where the probability density is high. The Green's-function Monte Carlo method, which is applied, for example, to calculate the ground state of the three-body mesomolecular $d\bar{t}\mu$ system [11], does not have these limitations, but its extension to the excited states is very difficult because any small admixture of the ground state in the impor-

tance function will eventually dominate the numerical simulation.

In the CFHH method, which is elaborated in detail in Ref. [6], one writes the wave function as a product of two factors,

$$\psi = \chi \phi, \quad (1)$$

where χ is the “correlation factor” and ϕ is expanded in the usual hyperspherical-harmonic (HH) functions. If the correlation factor χ is chosen to describe the singular features of ψ (like cusps), the HH expansion for ϕ should be rapid. The solution for ϕ proceeds as in the usual HH method, except that the potential V is replaced by an effective velocity-dependent potential V' ,

$$V' = V - \frac{1}{2} \frac{\nabla^2 \chi}{\chi} - (\nabla \ln \chi) \nabla, \quad (2)$$

where ∇ is the six-dimensional gradient operator and V in our case is the sum of the pair Coulomb potentials. In the previous calculations [3–9], the simplest spatially symmetric correlation factor

$$\chi = \exp(f), \quad f = -\gamma(r_1 + r_2) - \delta r_3, \quad (3)$$

with parameters γ and δ chosen for each given system from physical considerations, was employed, yielding

surprisingly accurate wave function for ground and excited states of considered three-body Coulomb systems [2–9]. We denote by M, Z the ratios of masses and charges of the nonidentical particle 3 to those of like particles 1, 2, whose mass and charge are set to unity. The interparticle distances r_i are in the odd-man-out notation. The usual choice [2–9] of parameters γ, δ was based on the requirement of the absence of the Coulomb singularities in the effective potential [cusp parametrization $\gamma = MZ/(M+1), \delta = -0.5$] or on their partial absence [γ is chosen to be $MZ/(M+1)$ to remove the Coulomb singularities between particles 1, 3 and 2, 3, while δ is taken to be zero—uncorrelated cusp parametrization] or some positive number (cusp-asymptotic parametrization) to make the correlation function fall off at large distances between particles 1 and 2 in order to facilitate the correct asymptotic behavior of the wave function [7].

To date the accuracy of the CFHH method has been verified for ground (1^1S) and excited ($2^1S, 3^1S, 4^1S$, and 5^1S) states of the helium atom [3, 4, 6, 8, 9], for the ground state of mesomolecular $pp\mu, dd\mu$, and $tt\mu$ systems [7], and for the ground state of the positronium negative ion $e^+e^-e^-$ (also denoted Ps^-) [5, 8]. These calculations demonstrate the utility of the method for systems with different mass ratios.

The direct (nonvariational) ground-state solution [3–8] of the Schrödinger equation obtained by the CFHH method has precision comparable to that obtained previously only by elaborate variation calculations. For example, for the maximum global momentum $K_m = 48$, up to nine significant figure precision is obtained for the ground-state energy of the helium atom [4, 6] and seven significant figure accuracy for the positronium ion [5]. The wave functions for the whole range of the interparticle distances, and different expectation values for these systems, have about six and five significant figure precision, respectively. The overall and local quality of the corresponding wave function, which is determined by computation of the absolute value of the relative local deviation $\Delta = (H\psi/E\psi) - 1$ (which defines the quality of the wave function [12]) and of its averages $\langle |\Delta| \rangle$, respectively, is very high [6, 8].

The results of excited-state helium calculations [6–9] show that the simplest correlation factor (3) works very well also for excited states. Indeed, the comparison of the results for $K_m = 48$ and 56 shows that the precision of the expectation values of the Hamiltonian is eight significant figures and of other expectation values five significant figures. The obtained energy values are better than those obtained in variational calculations of Accad, Pekeris, and Schiff [13] with the Hylleraas-type variational wave functions, and in generator-coordinate computations of Thakkar and Smith [14]. They agree well with the most sophisticated variational calculations of Drake [15] and Kono and Hattori [16], who use trial functions constructed with two groups of basis functions, as well as with the results of Frankowsky [17] and Baker, Hill, and Morgan [18], whose basis functions incorporate logarithmic terms. Both of these modifications of the Hylleraas expansion yield more rapidly convergent variational energies.

Improvements in the correlation function used in the CFHH calculation are nevertheless desirable. One cannot simultaneously build in both a satisfactory asymptotic and cusp behavior with the symmetric linear correlation function f , Eq. (3), used in Refs. [3–9]. As a result one has to choose between the inclusion of the cusp behavior, which yields a better short-distance description of the wave function, and the asymptotic behavior, which produces better results for large distances. For example, as one can see from the comparison of Table III of Ref. [4] and Table I of Ref. [9], the convergence of the expectation values of the operator $\delta(r_{12})$, which stresses very small electron-electron distances, in the cusp parametrization $\gamma = 2, \delta = -0.5$ of Ref. [9] (which includes the electron-electron cusp but produces completely wrong asymptotic behavior when r_{12} is going to infinity) is significantly better than in the uncorrelated cusp parametrization $\gamma = 2, \delta = 0$ of Ref. [4] (where this cusp is omitted, in order to improve the asymptotic behavior in r_{12}). The convergence of the expectation values of r_{12}^2 , defined by large electron-electron distances, is worse.

On the whole, the inability of the correlation factor (3) to include the cusp and asymptotic behaviors simultaneously leads to lower quality of the wave functions (higher values of the local deviation Δ) at small or large interparticle distance [8, 9], which in turn leads to less accurate expectation values of the Hamiltonian and of different functions of interparticle distances.

The purpose of this work is to employ a more sophisticated correlation factor χ , in which f is a nonlinear function of interparticle distances, chosen to simultaneously describe both the cusps and the asymptotic behavior. We will utilize it for the calculation of the energy and of the two-photon electron-positron annihilation rate in the ground state of the positronium negative ion Ps^- ($e^+e^-e^-$), a system whose binding energy and decay rate were measured by Mills [19, 20] a few years ago.

Theoretically [21, 22] in the lowest order the two-photon decay rate of this system in atomic units (a.u.) is given by the equation

$$\Gamma = 2\pi\alpha^4 \left[1 - \alpha \left(\frac{17}{\pi} - \frac{19\pi}{12} \right) + \eta_3 \right] \langle \delta(\mathbf{r}_1) \rangle$$

which, in nsec^{-1} , has the form

$$\Gamma = 100.938(0.996824 + \eta_3) \langle \delta(\mathbf{r}_1) \rangle. \quad (4)$$

Here $\langle \delta(\mathbf{r}_1) \rangle$ is the probability of an electron and the positron being at the same point. The number in the parentheses on the right-hand side accounts for radiative and three-photon annihilation corrections [21, 22], and η_3 for bound-state and relativistic effects, which have not yet been calculated in the literature and should be found from the comparison with experiment [20]. The experiment currently gives $2.09 \pm 0.09 \text{ nsec}^{-1}$ and its accuracy could in principle be improved by an order of magnitude. The density $\langle \delta(\mathbf{r}_1) \rangle$ of the electron at the positron was calculated variationally by Ho [23] and Bhatia and Drachman [24], but the obtained values of 0.020713 (Ref. [23]) and 0.020730 and 0.020733 (Ref. [24]) varied strongly not only from work to work, but even in the

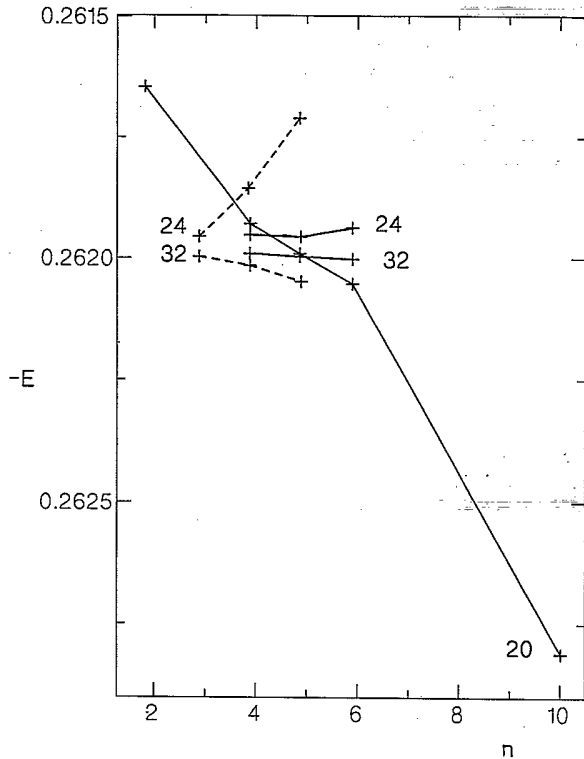


FIG. 1. Dependence of the eigenvalue E , the solution of the CFHHM system of coupled differential equations, on the free parameter n , for two values of the free parameter a_1 , and different maximum values of the global angular momentum K_m . Full lines, $a_1=0$; dashed lines, $a_1=-0.2$. Curves are labeled by the values of K_m . Atomic units (a.u.) are used in all figures.

and parameters a_i have to provide a proper asymptotic description. Parameters c_i determine the start of an asymptotic region. In view of the space symmetry of the wave function $a_1=a_2$, $b_1=b_2$, and $c_1=c_2$.

In the limit of interparticle distance r_k being much larger than r_i (in which case $r_j \approx r_k$) the positronium negative ion Ps^- separates in one of two possible configurations (i) or (ii), consisting either of the bound e^-e^+ (positronium) cluster and a distant electron, or the unbound system of two electrons, interacting with a distant positron, respectively. In configuration (i) the energy of the distant particle is fixed by the binding energy ε_i of the two-particle cluster and by the binding energy ε of the positronium ion and the asymptotic behavior of the Ps^- wave function for $r_k \rightarrow \infty$ ($r_k \gg r_i$) is given by

$$\begin{aligned} \psi &\approx \exp(-\sqrt{2\mu_i\varepsilon_i}r_i)\exp[-\sqrt{2M_i(\varepsilon-\varepsilon_i)}r_k] \\ &\approx \exp[-\sqrt{2M_i(\varepsilon-\varepsilon_i)}r_k]. \end{aligned} \quad (8)$$

Here

$$\mu_i = \frac{m_j m_k}{m_j + m_k} = \frac{1}{2} \quad \text{and} \quad M_i = \frac{m_i(m_j + m_k)}{m_i + m_j + m_k} = \frac{2}{3} \quad (9)$$

are the reduced masses of the cluster constituents and of the cluster and the distant particle, respectively. Equation (8) is written under the assumption that the clustered

particles are in the S state. We have, therefore, in this case the following asymptotic form of the wave function:

$$\psi \approx \exp[-\sqrt{\frac{4}{3}(\varepsilon-\frac{1}{4})}r_k], \quad (10)$$

whose comparison with Eq. (7) gives

$$a_i r_i + a_j r_j + a_k r_k \approx (a_j + a_k) r_k \approx -\sqrt{\frac{4}{3}(\varepsilon-\frac{1}{4})}r_k$$

or, if we identify $\{i, j, k\}$ with $\{1, 2, 3\}$,

$$a_3 = -\sqrt{\frac{4}{3}(\varepsilon-\frac{1}{4})} - a_1. \quad (11)$$

The comparison of the asymptotic form of the wave function corresponding to the configuration (ii) of two electrons and a distant positron with Eq. (7) does not put any restriction on parameters a_1 and a_3 , since the energy of two electrons lying in the continuous spectrum is arbitrary and so is the positron energy. We define, therefore, a_1 as an arbitrary parameter whose optimal value will be found in the process of the computation.

The choice of parameters b_i is straightforward: comparison with Eq. (3) for the positronium ion immediately gives $b_1=b_2=-\gamma=-0.5$, $b_3=-\delta=0.5$. The choice of parameters c_i is more complicated, since the definition of the asymptotic region is somewhat arbitrary. Under the intuitive assumption that the asymptotic region in r_i starts when an interparticle distance is of the order of

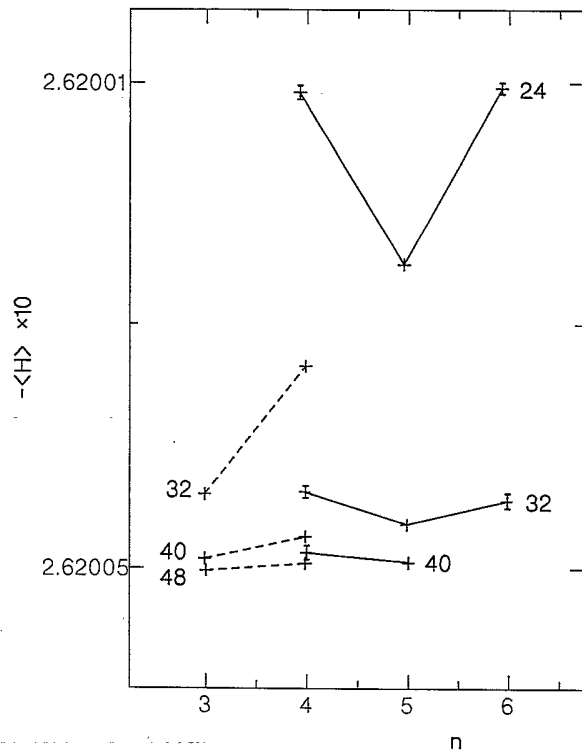


FIG. 2. Dependence of the expectation value of the Hamiltonian on the free parameter n for two values of the free parameter a_1 . Notation is as in Fig. 1. Error bars reflect a conservative estimate of the intrinsic accuracy of the calculations. The main source of inaccuracy is the degree of flatness of the plateau in the dependence of the quadrature on the upper limit of the ρ integration.

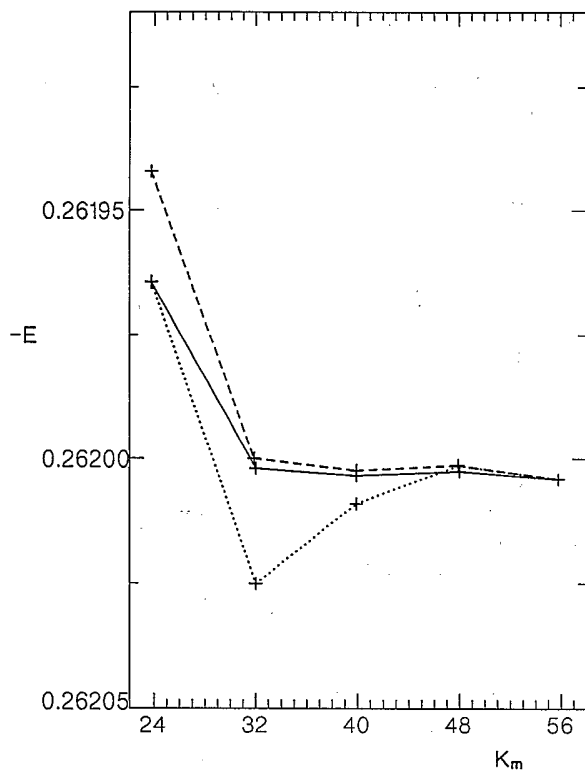


FIG. 3. Dependence of the eigenvalue E on the maximum global angular momentum K_m for two combinations of the free parameters a_1 and n . Full line, $a_1=0$, $n=5$; dashed line, $a_1=-0.2$, $n=3$. Also shown is the result of Ref. [5] in which the uncorrelated cusp parametrization was used (dotted line).

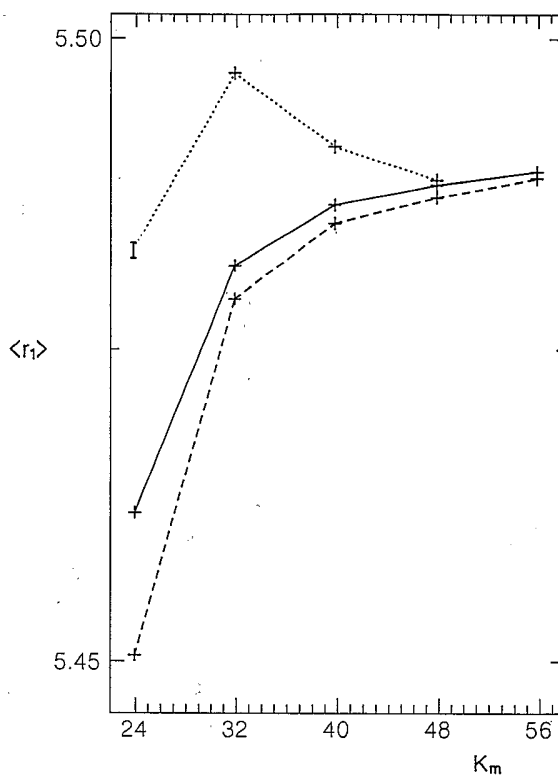


FIG. 5. Dependence of the expectation value of the distance between an electron and the positron $\langle r_1 \rangle$ on K_m (a.u.). The notation is as in Fig. 3.

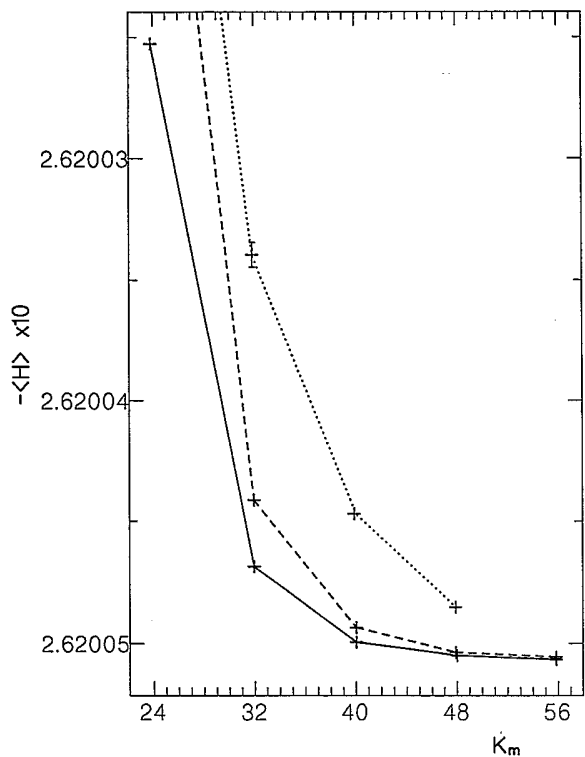


FIG. 4. Dependence of the expectation value of the Hamiltonian operator on K_m . The notation is as in Fig. 3.

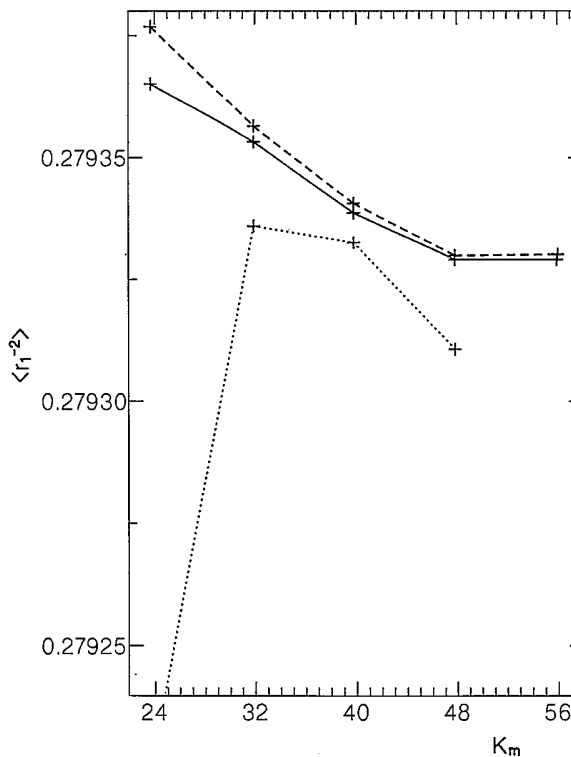


FIG. 6. Dependence of $\langle r_1^{-2} \rangle$ on K_m . The notation is as in Fig. 3.

two to ten times larger than its average value $\langle r_i \rangle$ (taken, for example, from Ref. [5]), we set $c_i = 1/(n \langle r_i \rangle)$, and find the optimal value of n , providing the fastest convergence, in the process of the computation.

The results of the calculations with $a_1 = 0$ and $n = 5$ are given in Table I. The influence of the choice of parameters a_1 and n is illustrated in Figs. 1–8. Before calculating the dependence of the eigenvalue E on the parameter n (Fig. 1), it was necessary to check that the matrix power-series expansion of the effective potential W in the variable ρ converged numerically at the largest values of ρ used in solving the system of coupled differential equations. In the arithmetic with about 16 digit precision, it was found in the case $a_1 = 0$, $n = 4$, that at $\rho = 100$ the leading element of W converges to about 7 digits with the maximum power 52, and at $\rho = 50$ to 10 digits with the maximum power 35. With $n = 5$, the result is 10 digits and 12 digits, with maximum powers 48 and 35, respectively. With $a_1 = -0.2$, $n = 4$, the result is 8 and 11 digits, with maximum powers 56 and 38, respectively. The maximum ρ used in the solution was of the order of 80. However, even for much larger maximum ρ the results are not affected at all by the breakdown of the power series because of the nature of the method of solution, and the small weight large values of ρ carry in the determination of the wave function. The value of ρ at which numerical breakdown of the series occurs is roughly proportional to n , which is apparent from the expression for the correlation function f .

In the large- n limit, the cusp parametrization is

recovered. However, the cusp parametrization, as opposed to the uncorrelated cusp parametrization of Ref. [5], cannot be used at small K_m because the asymptotic constant in the solution for $K_m = 0$, κ^+ and κ^- , as defined in Ref. [9], are complex. This is reflected in the case of the nonlinear correlation function f in the fact that large n , for small K_m , causes the ground-state energy to be driven toward more binding, making it practically disappear in the limit n going to infinity. As is apparent from Figs. 1 and 2, this problem is avoided in the present calculation since the optimum values of n are small. The figures also show that the dependence on a_1 and n diminishes as K_m increases.

The optimum values of the parameter a_k are close to zero, i.e., much smaller in absolute value than the cusp parameters b_k . This is to be expected, since in this way, the terms dominant near the coalescence points [proportional to $(b_k - a_k)$] of the correlation function are multiplied by exponential functions which render them small in the asymptotic regions, with the necessary small corrections by the terms proportional to a_k , which ensure the proper asymptotic behavior.

One immediate gain of the nonlinear correlation function is the increased stability of calculations with respect to the maximum ρ used in the solution of the system of differential equations. At small K_m ($K_m = 20$), the eigenvalue E was stable to 13 digits at maximum ρ about 80; for the linear f (uncorrelated cusp parametrization), E was stable to only 6 digits even for maximum ρ of the order of 500, and the stability set in only at larger K_m .

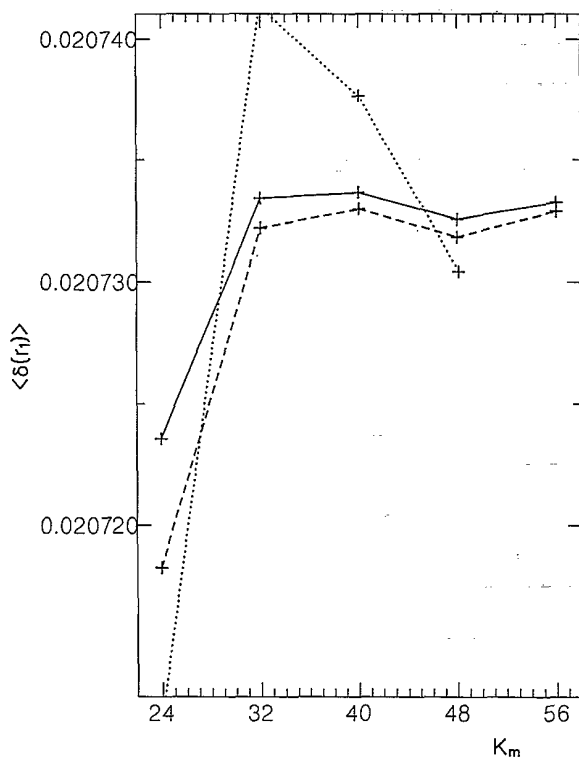


FIG. 7. Dependence of the expectation value of the δ function of the electron-positron distance on K_m . The notation is as in Fig. 3.

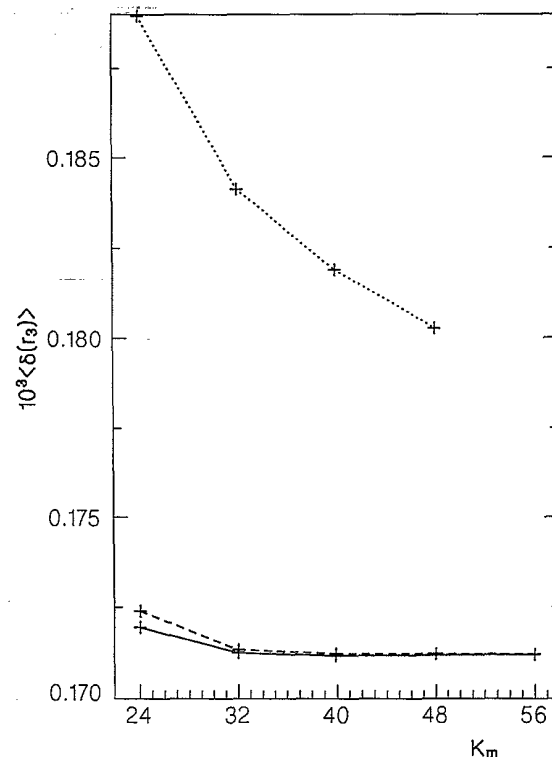


FIG. 8. Dependence of the expectation value of the δ function of the electron-electron distance on K_m . The notation is as in Fig. 3.

Without the need to include very large values of ρ , one stays within the numerical convergence radius of the matrix power series for the effective potential W .

From Fig. 4 it is apparent that to reach the same accuracy of the expectation value of the Hamiltonian operator, $K_m=36$ with the nonlinear correlation function equivalent to $K_m=48$ with uncorrelated cusp parametrization, the number of coupled equations being 100 and 169, respectively.

Figure 5 shows that the correlation function (5) produces rather smooth convergence patterns with increasing K_m for the expectation value of the distance between an electron and the positron. The convergence curve for this expectation value calculated in Ref. [5] with the linear correlation function shows less smooth behavior. The same distinction between linear and nonlinear correlation function calculations is even more apparent in Fig. 6, showing the convergence of the inverse-square interparticle distances, and in Fig. 7, showing the convergence of the δ -function operator in interparticle distance, which are especially sensitive to the values of the wave function at double coalescence points. The expectation values of other powers of the distance between an electron and the positron as well as of various powers of the distances between two electrons show a very similar pattern. In addition Fig. 8 shows the sensitivity of the wave function to the inclusion of the repulsive cusp behavior between the two electrons. Moreover, Figs. 3–8 illustrate the superior convergence properties of the present calculations using the correlation function (5) over the earlier calculations which used the linear version [5].

Summing up, in this paper we show that the use of a general nonlinear correlation function (5) for the positronium negative ion improves significantly the accuracy of the CFHH method. This is our first application of the

nonlinear correlations. In order to improve the accuracy of the calculations we also increase here the value of maximum global momentum up to $K_m=56$. This increases from 169 to 225 the number of basis hyperspherical harmonic functions and the corresponding coupled equation. The inclusion of 225 hyperspherical functions together with the correlation factor (5) yields the ground-state energy of 0.262 005 058 a.u. The substitution of our value of $\langle\delta(r_3)\rangle=0.020\,733\,0\pm 0.000\,000\,6$ (where an error evaluation follows from the comparison of the results for $K_m=40, 48,$ and 56) into Eq. (4) gives a value of $(2.086\,10+2.092\,75\eta_3)\pm 0.000\,06\text{ nsec}^{-1}$ for the two-photon annihilation rate. The neglect of the η_3 correction, expected to be very small, yields $2.086\,10\pm 0.000\,06\text{ nsec}^{-1}$.

From Table I one can see that our nonextrapolated $K_m=56$ energy value 0.262 005 058 is lower than the nonextrapolated energy values 0.262 004 895 and 0.262 005 056 calculated in works of Ho [23] and Bhatia and Drachman [24] but higher in the eighth significant figure than the best variational value 0.262 005 069 obtained by Petelenz and Smith [26]. This is in agreement with the result of a comparison of values of $\langle H \rangle$ for $K_m=56$ and for $K_m=48$ which indicates that the accuracy of our present direct calculation of the energy is at least eight significant figures. The previously obtained nonvariational energy values of 0.2620 and 0.262 021 7 a.u. calculated, respectively, by the direct solution of the Schrödinger equation with the help of the hyperspherical coordinates method [27,28] and by the orthogonal collation method of numerical solution of the Faddeev equations [29], have an accuracy of four significant figures. The accuracy of the present estimate of the decay rate is higher by an order of magnitude than that obtained in the literature until now.

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