# One-photon annihilation in the Ps<sup>-</sup> ion and the angular $(e^-, e^-)$ correlation in two-electron ions

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Various properties of the Ps<sup>-</sup> ion in its bound ground  $({}^{1}S)$  state are calculated from a very accurate explicitly correlated wave function. From the expectation value for the triple delta function  $\langle \delta_{321} \rangle = | \psi(0,0,0) |^2$  we estimate the one-photon annihilation rate  $\Gamma_{\gamma}$  in the Ps<sup>-</sup> ion and show that  $\Gamma_{\gamma} \ll \Gamma_{3\gamma} \ll \Gamma_{2\gamma}$ . The statistical angular correlation coefficients are analyzed for the series of two-electron ions  $(e^-e^-Z^+)$  which includes T<sup>-</sup>, D<sup>-</sup>, H<sup>-</sup>, Mu<sup>-</sup> and Ps<sup>-</sup>.

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# I. INTRODUCTION

The existence of the positronium [1] negative ion  $Ps^$ as a bound state has been well known since the early papers of Wheeler [2] and Hylleraas [3]. A decade ago it was created and studied in the laboratory by Mills [4,5]. Its various properties have been the subject of intensive theoretical investigations [6–17]. A comparison of all results (up to 1990) for these properties of the  $Ps^-$  ion may be found in Ref. [14].

Now we consider a number of other properties of the positronium negative ion. Our first interest is related to the expectation value of the triple Dirac delta function  $\langle \delta_{321} \rangle = | \psi(0,0,0) |^2$ . Its value is needed to determine the probability of the internal conversion of  $\gamma$  quanta in the Ps<sup>-</sup> ion. Such a process can play a definite role in some problems of nuclear physics (see, e.g., [18] and references therein) as well as in metal physics (see, e.g., [19]). The internal conversion of  $\gamma$  quanta in the Ps<sup>-</sup> ion was considered previously by Misawa and Mills [20] and by Chu and Pönisch [18].

In addition, we investigate the nature of the angular correlation between the electrons in the Ps<sup>-</sup> ion and its differences from that in the related series of two-electron anions  $(e^-e^-Z^+)$ . We shall do this by using the statistical angular correlation coefficients [21,22].

In the present calculations we used the exponential variational expansion in the relative interparticle coordinates  $r_{32}$ ,  $r_{31}$ , and  $r_{21}$ . In the case of the ground state in the Ps<sup>-</sup> ion with L = 0 (<sup>1</sup>S state), it is of the form [10,23,24]

$$\psi_{L=0}(r_{32}, r_{31}, r_{21})$$

$$= (1 + P_{21}) \sum_{i=1}^{N} C_i \exp(-\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21}), \quad (1.1)$$

where  $P_{21}$  is the permutation operator, and N is the number of terms in the expansion [25]. The subscripts 1 and 2 denote the electrons, while 3 designates the positron. The linear parameters  $C_i$  must be determined by the solution of the variational (eigenvalue) problem. The nonlinear parameters (quadrature points)  $\alpha_i, \beta_i, \gamma_i$  (i = 1, ..., N)are generated in a quasi-random manner [10,23], respectively, from the real intervals  $[0, A_2], [B_{1,i}, B_2], [G_{1,i}, G_2]$ as follows:

$$\begin{split} \alpha_{i} &= \langle\!\langle \frac{1}{2}i(i+1)\sqrt{2}\rangle\!\rangle A_{2}, \\ \beta_{i} &= \langle\!\langle \frac{1}{2}i(i+1)\sqrt{3}\rangle\!\rangle (B_{2}-B_{1,i}) + B_{1,i}, \\ \gamma_{i} &= \langle\!\langle \frac{1}{2}i(i+1)\sqrt{5}\rangle\!\rangle (G_{2}-G_{1,i}) + G_{1,i}, \end{split}$$

where  $\langle\!\langle x \rangle\!\rangle$  is the fractional part of x.

In the present calculations we have used the following values of the constants:  $A_2 = 1.157, B_2 = 0.783, G_2 = 0.819$ . To choose the points  $B_{1,i}$  and  $G_{1,i}$  for each *i* we used the prescription

$$B_{1,i} = -\kappa \alpha_i = -0.075 \alpha_i,$$
  

$$G_{1,i} = -\kappa \min(\alpha_i, \beta_i)$$
  

$$= -0.375 \min(\alpha_i, \beta_i), if \beta_i \ge 0,$$
  

$$G_{1,i} = -\beta_i, if \beta_i < 0.$$
(1.2)

The parameters  $\beta_i$  and  $\gamma_i$  can be negative (for each *i*), but the following three sums must always be positive in order to guarantee square integrability, i.e.,  $\alpha_i + \beta_i > 0$ ,  $\alpha_i + \gamma_i > 0$ , and  $\beta_i + \gamma_i > 0$ .

### **II. EXPECTATION VALUES**

In Table I we present the expectation values (in atomic units) of some useful characteristics for the Ps<sup>-</sup> ion for N = 700,800, and 850. Other properties coincide (with good accuracy) with the values which have been obtained by us for the Ps<sup>-</sup> ion in Ref. [15]. It should be mentioned that almost all of the properties of the Ps<sup>-</sup> ion in Table I have never been calculated before. The quantity  $\langle f \rangle$  is the expectation value of the following (always positive) integrand in relative  $(r_{31}, r_{32}, r_{21})$  or perimetric coordinates  $(u_1, u_2, u_3)$ :

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N	700	800	850
$\langle r_{21}^3 \rangle$	1265.5804473	1265.5804476	1265.5804481
$\langle r_{31}^3 \rangle$	607.29562920	607.29562942	607.29562969
$\langle r_{21}^4 \rangle$	21054.45337	21054.45339	21054.45341
$\langle r_{31}^4 \rangle$	9930.638663	9930.638679	9930.638691
$\langle (\mathbf{r_{31}} \cdot \mathbf{r_{32}}) \rangle$	1.8296203008	1.8296203015	1.8296203018
$\langle (\mathbf{r}_{31} \cdot \mathbf{r}_{21}) \rangle$	46.589316917	46.589316920	46.589316925
$\langle \cos(\mathbf{r_{31}}\cdot\mathbf{r_{32}}) \rangle$	0.019769632810	0.019769632813	0.019769632814
$\langle \cos(\mathbf{r}_{31} \cdot \mathbf{r}_{21}) \rangle$	0.591981701154	0.591981701152	0.591981701150
$\langle  abla_1 \cdot  abla_2  angle$	0.0017289583	0.0017289585	0.0017289583
$\langle \nabla_1 \cdot \nabla_3 \rangle$	0.0031730276	0.0031730280	0.0031730274
$\langle \frac{1}{2} \nabla_1^2 \rangle$	0.066619294535	0.066619294535	0.066619294535
$\langle \frac{1}{2} \nabla_3^2 \rangle$	0.128766481159	0.128766481159	0.128766481159
η	$0.328 \times 10^{-10}$	$0.260 \times 10^{-10}$	$0.230 \times 10^{-10}$
$\langle f \rangle$	0.050933258779	0.050933258779	0.050933258779
$\langle \delta_{321} \rangle$	$0.358974 \times 10^{-4}$	$0.358995 \times 10^{-4}$	$0.358996 \times 10^{-4}$
$\langle \delta_{31} \rangle$	0.0207331996	0.0207332003	0.0207331988
$\langle \delta_{21} \rangle$	$0.1709989 \times 10^{-3}$	$0.1709984 \times 10^{-3}$	$0.1709981 \times 10^{-3}$
$\Delta r_{21}$	0.5244551626	0.5244551625	0.5244551626
$\Delta r_{31}$	0.7788947611	0.7788947611	0.7788947611
-E	0.2620050702321	0.2620050702324	0.2620050702326

TABLE I. The expectation values in atomic units of some properties for the ground bound state of the  $Ps^-$  ion. The subscripts 1 and 2 denote the electrons, while 3 designates the positron. N is the number of basis functions used.

$$\langle f \rangle = \langle \psi \mid f \mid \psi \rangle = \left\langle \psi \mid \frac{u_1}{r_{32}} \frac{u_2}{r_{31}} \frac{u_3}{r_{21}} \middle| \psi \right\rangle + \int \int \int \mid \psi(r_{31}, r_{32}, r_{21}) \mid^2 \frac{u_1}{r_{32}} \frac{u_2}{r_{31}} \frac{u_3}{r_{21}} r_{31} r_{32} r_{21} dr_{31} dr_{32} dr_{21} \\ \times \int \int \int \mid \psi(u_1, u_2, u_3) \mid^2 u_1 u_2 u_3 du_1 du_2 du_3,$$

$$(2.1)$$

where  $u_i = \frac{1}{2}(r_{ij} + r_{ik} - r_{jk})$ , and (i, j, k) = (1, 2, 3). The last equation can be considered, in principle, as the connection between two possible types of coordinates for the three-body systems (i.e., relative and perimetric co-ordinates, respectively).

It can be shown that for an arbitrary three-body Coulomb system the equality

$$\langle \cos(\mathbf{r}_{31} \cdot \mathbf{r}_{32}) \rangle + \langle \cos(\mathbf{r}_{21} \cdot \mathbf{r}_{31}) \rangle$$

$$+\langle \cos(\mathbf{r}_{21} \cdot \mathbf{r}_{32}) \rangle = 1 + 4\langle f \rangle \quad (2.2)$$

must be obeyed. For the considered symmetric case (in particles 1 and 2) this takes the form

$$\langle \cos(\mathbf{r}_{31} \cdot \mathbf{r}_{32}) \rangle + 2 \langle \cos(\mathbf{r}_{21} \cdot \mathbf{r}_{31}) \rangle = 1 + 4 \langle f \rangle. \tag{2.3}$$

The dimensionless Pearson correlation coefficients  $\Delta r_{31}$ and  $\Delta r_{21}$  presented in Table I are of the form

$$\Delta r_{ij} = [\langle r_{ij}^2 \rangle - \langle r_{ij} \rangle^2]^{\frac{1}{2}} / \langle r_{ij} \rangle, \qquad (2.4)$$

where (ij) = 31 or 21. The uncertainty in  $r_{31} = r_{32}$ is  $\approx 78\%$  and in  $r_{21}$  is  $\approx 52\%$ . They are similar to the corresponding values in H<sup>-</sup> and other three-body systems with two electrons.

The virial factor  $\eta$  is

$$\eta = \left| 1 + \frac{2\langle T \rangle}{\langle V \rangle} \right|, \qquad (2.5)$$

where  $\langle T \rangle$  is the expectation value of the kinetic energy, while  $\langle V \rangle$  is the expectation value of the potential energy. The deviation of the parameter  $\eta$  from zero indicates the quality of the wave function used [when  $\eta = 0$  the virial theorem holds exactly (see, e.g., [26])]. In the present calculations  $\eta$  never deviated from zero by more than  $1 \times 10^{-10}$ .

Now we consider some applications of the formulas given above in the general theory of the two-electron anions such as  $e^-e^-Z^+$ . Let  $\lambda$  designate the mass ratio  $m_Z/m_e$  or  $m_Z$ , since in atomic units  $m_e = 1$ . As is well known [22], the statistical angular correlation coefficient  $\tau = \langle \cos(\mathbf{r}_{31} \cdot \mathbf{r}_{32}) \rangle$  is negative for the  $^{\infty}\mathrm{H}^-$  ion  $(\lambda = \infty)$ , while inspection of Table I reveals that for the Ps<sup>-</sup> ion  $(\lambda = 1)$  it is positive. Therefore, an intermediate  $\lambda_0$  must exist in which the equalities

$$\tau_0 = \langle \cos(\mathbf{r}_{31} \cdot \mathbf{r}_{32}) \rangle = 0, \qquad (2.6)$$
$$\langle \cos(\mathbf{r}_{21} \cdot \mathbf{r}_{31}) \rangle = 0.5 + 2\langle f \rangle$$

hold exactly. The determination of this point  $\lambda_0$  where  $\tau$  vanishes is of definite interest, since for such a system it is expected that there is orthogonality between the position vectors of each of the electrons with respect to the positive particle, or that the electrons are completely independent of each other. However, the complete independence is not the case for the considered systems.

From the definition,  $\tau$  is bounded between +1 and -1, i.e.,  $-1 \leq \tau \leq +1$ . If  $\tau = +1$ , there is perfect positive

correlation where the position vectors are expected to coincide, whereas  $\tau = -1$  is perfect negative correlation with the electrons expected to be at diametrical positions with respect to the "nucleus." In Ps<sup>-</sup>, the electrons tend to be on the same side of the "nucleus" while in  $^{\infty}H^{-}$  they tend to be on opposite sides.

The numerical results in atomic units for the total energies E as well as  $\langle f \rangle, \langle \Delta r_{31} \rangle$ , and  $\langle \Delta r_{21} \rangle$  are presented in Table II for a number of systems in the range of  $1 \leq \lambda \leq \infty$ . Table III contains the values of the various correlation coefficients as well as  $\langle \delta(\mathbf{r}_{31}) \rangle$ . Table IV (see [27]) contains  $\langle r_{31} \rangle, \langle r_{21} \rangle, \langle r_{31}^2 \rangle$ , and  $\langle r_{21}^2 \rangle$ , while Table V contains  $\langle \nabla_1 \cdot \nabla_2 \rangle, \langle \nabla_1 \cdot \nabla_3 \rangle, \langle \mathbf{r}_{31} \cdot \mathbf{r}_{32} \rangle$ , and  $\langle \mathbf{r}_{31} \cdot \mathbf{r}_{21} \rangle$  for the same systems. From the results for  $\tau$  in Table III we have determined the  $\lambda_0$  value as  $\approx 1.385$ . Of course,  $\lambda_0$ does not correspond to the beginning of a real physical process in the  $e^-e^-Z^+$  ion.  $\tau$  assesses angular correlation for primarily small separations of the "nucleus" from the electrons, i.e., the inner region of the electron distribution. We have calculated two other angular correlation coefficients,  $\tau_{\mathbf{r}}$  and  $\tau_{\mathbf{p}}$ :

$$\tau_{\mathbf{r}} = \frac{\langle \mathbf{r}_{31} \cdot \mathbf{r}_{32} \rangle}{\langle r_{31}^2 \rangle} \tag{2.7}$$

 $\operatorname{and}$ 

$$\tau_{\mathbf{p}} = \frac{\langle \nabla_1 \cdot \nabla_2 \rangle}{\langle \nabla_1^2 \rangle}.$$
(2.8)

The former is more sensitive to intermediate separations of the electrons from the nuclei than is  $\tau$ .  $\tau_{\mathbf{p}}$  assesses angular correlations at intermediate momenta. Inspection of Table III reveals that  $\tau_{\mathbf{r}}$  vanishes for  $\lambda \approx 2.35$ , while  $\tau_{\mathbf{p}}$  vanishes for  $\lambda \approx 1.4$ , which is very close to  $\lambda_0 \approx 1.385$  for which  $\tau$  vanishes.

All these measures decrease monotonically with  $\lambda$  between  ${}^{\infty}\mathrm{H}^{-}$ , where they are negative, and Ps<sup>-</sup>, where they are positive. In this region of  $\lambda$  variation,  $1 \leq \lambda \leq \infty$ ,  $\tau$  is always smaller than  $\tau_{\mathbf{r}}$ .

We observe that  $\langle f \rangle$  achieves its minimum value for  $\lambda \approx 50$ . The Pearson coefficients are fairly constant for the entire series in the range  $1 \leq \lambda \leq \infty$ . The electronelectron distance uncertainty  $\Delta r_{21}$  achieves its maximum of 55% for  $\lambda \approx 5$ . The electron-"nucleus" distance uncertainty  $\Delta r_{31}$  achieves its maximum value for  $\lambda \approx 3$ .

Another observation is that  $Ps^-$  ( $\lambda = 1$ ) is the energy minimum for this series. It is quite important for the general theory of bound-state spectra in the Coulomb threebody systems with unit charges that there is symmetry

TABLE II. The total energies E, the expectation values of the factor  $\langle f \rangle$  (in atomic units), and the dimensionless Pearson coefficients  $\Delta r_{31}$ ,  $\Delta r_{21}$  for the ground <sup>1</sup>S states of the two-electron ions. The subscripts 1 and 2 denote the electrons, while 3 designates the positively charged "nucleus" ( $\lambda = m_Z$ ).

System $(\lambda)$	- <i>E</i>	$\langle f \rangle$	$\Delta r_{31}$	$\Delta r_{21}$
∞H-	0.527751016523	0.04864886722	0.7886699477	0.5424743756
T-	0.527649048182	0.04864880165	0.7887041003	0.5424884861
D-	0.527598324665	0.04864876913	0.7887210821	0.5424955023
H-	0.527445881093	0.04864867173	0.7887720898	0.5425165768
Mu <sup>-</sup>	0.525054806223	0.04864721513	0.7895664232	0.5428447615
100	0.522209210068	0.04864566288	0.7904975706	0.5432294043
50	0.516793180922	0.04843294699	0.7922262244	0.5439429070
25	0.506320134427	0.04864117285	0.7954003415	0.5452484745
15	0.493051460692	0.04864396156	0.7990836311	0.5467473579
10	0.477483746333	0.04865663814	0.8028875179	0.5482564851
5	0.436497014687	0.04875334999	0.8099159100	0.5506878680
3	0.392141012853	0.04899589514	0.8119736243	0.5502359497
2.5	0.373320338311	0.04915287978	0.8109174461	0.5489078691
2.35	0.366602303945	0.04921770298	0.8102473822	0.5482552045
2.34	0.366133420709	0.04922240677	0.8101947697	0.5482060449
2.33	0.365661778400	0.04922716213	0.8101410752	0.5481561177
2.25	0.361786297843	0.04926715024	0.8096704484	0.5477276041
2	0.348371665880	0.04941845023	0.8076329271	0.5459885851
1.5	0.313675728354	0.04990876248	0.7993649815	0.5395642820
1.4	0.305037054376	0.05005449928	0.7966241452	0.5375132010
1.385	0.303679896901	0.05007829198	0.7961686668	0.5371740879
1.35	0.300447000308	0.05013596250	0.7950564260	0.5363476559
1.25	0.290665616892	0.05031908823	0.7914575155	0.5336895958
1.1	0.274276314100	0.05065581245	0.7846407574	0.5286724117
1.05	0.268288338877	0.05078843665	0.7819053129	0.5266650611
$Ps^{-}$	0.262005070232	0.05093325878	0.7788947611	0.5244551626
$(1.05^{-1})^{\mathbf{a}}$	0.268511907135	0.05108387054	0.7757432057	0.5221399593
$(2.5^{-1})^{a}$	0.379608952236	0.05452454236	0.7037814234	0.4669196521

<sup>a</sup>The notation  $(\lambda^{-1})$  indicates the system  $X^+X^+e^-$  whose properties coincide with those of the charge-conjugated system  $X^-X^-e^+$ .

chowing, while a confidence are bounded and on the formation (i.e. 192).							
System $(\lambda)$	$\langle \cos({f r_{31}}\cdot{f r_{32}}) angle$	$rac{\langle (\mathbf{r_{31}}\cdot\mathbf{r_{32}}) angle}{\langle r^2_{31} angle}$	$rac{\langle  abla_1 \cdot  abla_2  angle}{\langle  abla_1^2  angle}$	$\langle \delta({f r}_{31})  angle$			
∞H_	-0.10514769356	-0.0576909764	-0.1067996808	0.164552786			
$T^{-}$	-0.10509720022	-0.0576485590	-0.1067255101	0.164461550			
D-	-0.10507208489	-0.0576274628	-0.1066862610	0.164416176			
Н-	-0.10499660630	-0.0575640770	-0.1065778219	0.164279857			
Mu <sup>-</sup>	-0.10381387809	-0.0565730681	-0.104848985	0.162150596			
100	-0.10240910569	-0.0554014457	-0.1028138957	0.159638380			
50	-0.09974368276	-0.0531944406	-0.0990585421	0.154922159			
25	-0.09461982697	-0.0490094682	-0.0918804475	0.146044228			
15	-0.08818391622	-0.0438559069	-0.0832861726	0.135251375			
10	-0.08070835433	-0.0380042436	-0.0737868912	0.123229903			
5	-0.06137038868	-0.0234300092	-0.0514955885	0.094819954			
3	-0.04085765110	-0.0085402558	-0.0311544658	0.069155282			
2.5	-0.03222332893	-0.0023227070	-0.0235140851	0.059780498			
2.35	-0.02914418872	-0.0000985988	-0.0209121558	0.056643884			
2.34	-0.02892927946	0.0000568766	-0.0207328703	0.056429014			
2.33	-0.02871310305	0.0002133050	-0.0205528830	0.056213410			
2.25	-0.02693662988	0.0015002717	-0.0190851425	0.054461868			
2	-0.02078245006	0.0059844847	-0.0141564578	0.048671994			
1.5	-0.00476154992	0.0179625735	-0.0023936983	0.035585723			
1.4	-0.00073161275	0.0210740480	0.0003386828	0.032731868			
1.385	-0.0000964660	0.0215688871	0.0007614770	0.032297598			
1.35	0.00141893495	0.0227546899	0.0017617478	0.031278351			
1.25	0.00602640336	0.0264072373	0.0047309104	0.028323301			
1.1	0.01383530008	0.0327772066	0.0095245528	0.023793236			
1.05	0.01672074215	0.0351938945	0.0112229748	0.022265407			
$Ps^{-}$	0.01976963281	0.0377872875	0.0129764082	0.020733199			
$(1.05^{-1})^{\mathbf{a}}$	0.02284006226	0.0404422105	0.0147004110	0.022310905			
$(2.5^{-1})^{a}$	0.07900236537	0.0983534309	0.3971597877	0.062190319			

TABLE III. The expectation values of  $\langle \cos(\mathbf{r}_{31} \cdot \mathbf{r}_{21}) \rangle$ ,  $\frac{\langle (\mathbf{r}_{31} \cdot \mathbf{r}_{32}) \rangle}{\langle \mathbf{r}_{31}^2 \rangle}$ ,  $\frac{\langle \nabla_1 \cdot \nabla_2 \rangle}{\langle \nabla_1^2 \rangle}$ , and  $\langle \delta(\mathbf{r}_{31}) \rangle$  (in atomic units) for the ground <sup>1</sup>S states of the two-electron ions. The subscripts 1 and 2 denote the electrons, while 3 designates the positively charged "nucleus" ( $\lambda = m_Z$ ).

<sup>a</sup>See footnote of Table II.

between symmetric systems  $X^+X^+Z^-$  (or  $X^-X^-Z^+$ ) with  $\lambda = 1 + \varepsilon$  and with  $\lambda = 1 - \varepsilon$  (where  $\varepsilon \ge 0$  in both cases) in the neighborhood of the Ps<sup>-</sup> ion, i.e., when  $\varepsilon \approx 0$  (actually  $\varepsilon \le 1 \times 10^{-8}$ ). Following [15] we could expect such a symmetry for the total energies and, perhaps, for a few of the properties. However, it is interesting that a number of the characteristics in such systems coincide with each other with very good accuracy.

## **III. POSITRON ANNIHILATION**

The rate,  $\Gamma_{2\gamma}$ , of the regular two-photon positron annihilation in Ps<sup>-</sup> was measured by Mills [5] and calculated by a number of authors (see e.g., [15] and references therein). We consider now the rate of one-photon annihilation,  $\Gamma_{\gamma}$ .  $\Gamma_{\gamma}$  is proportional to  $\langle \delta_{321} \rangle$ , i.e.,

$$\Gamma_{\gamma} = \zeta \times \frac{16}{3} \pi^2 \alpha^3 m_e^{-5} \langle \delta_{321} \rangle$$
  
=  $\zeta \times 2.397 \, 82 \times 10^3 \langle \delta_{321} \rangle$ , (3.1)

where  $\langle \delta_{321} \rangle$  is in atomic units. There is not agreement in the literature as to the value of the proportionality constant,  $\zeta$ . Chu and Pönisch [18] find  $\zeta = 1$ , while Misawa and Mills [20] find  $\zeta = 2$ . Use of our value of  $\langle \delta_{321} \rangle$  from Table I yields the respective values  $\Gamma_{\gamma} = 0.08608 \text{ sec}^{-1}$  for  $\zeta = 1$  and 0.1719 sec<sup>-1</sup> for  $\zeta = 2$ . Our value for  $\langle \delta_{321} \rangle$  is slightly smaller than the values previously obtained by Bhatia and Drachman, Ho, and Misawa and Mills (all of their values are presented in Ref. [18]).

It is interesting to compare  $\Gamma_{\gamma}$  with  $\Gamma_{2\gamma}$  and  $\Gamma_{3\gamma}$  for the Ps<sup>-</sup> ion. The expression for  $\Gamma_{2\gamma}$  in the Ps<sup>-</sup> ion takes the form (see [28,29])

$$\Gamma_{2\gamma} = 2\pi \alpha^4 c a_0^{-1} \langle \delta_{31} \rangle$$
  
= 100.939 429 7 × 10<sup>9</sup>  $\langle \delta_{31} \rangle$  sec<sup>-1</sup>, (3.2)

where  $c = 0.299792458 \times 10^9$  m sec<sup>-1</sup>,  $a_0 = 0.529177249 \times 10^{-10}$  m, and  $\alpha = 0.729735308 \times 10^{-2}$  [all data from CODATA 1986 (see, e.g., [30])]. The subscript 1 denotes the electron, while 3 designates the positron. By using the very-accurate expectation value for  $\langle \delta_{31} \rangle$  from Table I we estimate the value of  $\Gamma_{2\gamma}$  for the Ps<sup>-</sup> ion as  $\approx 0.20928 \times 10^{10}$  sec<sup>-1</sup>.

Likewise, with the use of the approximate relation [31]

$$\Gamma_{3\gamma}(\mathrm{Ps}^{-}) = [\Gamma_{3\gamma}(\mathrm{Ps})/\Gamma_{2\gamma}(\mathrm{Ps})]\Gamma_{2\gamma}(\mathrm{Ps}^{-}) \approx 0.881\,455\,7\times10^{-3}\Gamma_{2\gamma}(\mathrm{Ps}^{-}),$$
(3.3)

we estimate the three-photon annihilation rate for the  $Ps^-$  ion as  $\approx 0.1845 \times 10^7 sec^{-1}$ . In this equation  $\Gamma_{2\gamma}(Ps)$  and  $\Gamma_{3\gamma}(Ps)$  denote the two-photon (and three-photon,

respectively) annihilation rates for the two-body neutral system Ps (data from Ref. [32]). Thus in the case of the Ps<sup>-</sup> ion the inequalities  $\Gamma_{\gamma}(Ps^{-}) << \Gamma_{3\gamma}(Ps^{-}) << \Gamma_{2\gamma}(Ps^{-})$  are obeyed.

Obviously, one-photon annihilation in the Ps<sup>-</sup> ion could proceed as the regular two-photon annihilation, followed by internal conversion of one of the two emitted  $\gamma$ quanta by the second (remaining) electron. Therefore, one can write from quantum-electrodynamical considerations

$$\Gamma_{\gamma} = W_{2\gamma,\gamma}^{c} \Gamma_{2\gamma} = 2\alpha \xi \frac{\langle \delta_{321} \rangle}{\langle \delta_{31} \rangle} \Gamma_{2\gamma}$$
$$= 2\alpha \xi \langle \delta_{321} \rangle \times 100.939\,429\,7 \times 10^{9} \text{sec}^{-1}, \qquad (3.4)$$

where  $W_{2\gamma,\gamma}^c$  is the conversion coefficient,  $\alpha$  is the finestructure constant, 2 is the number of  $\gamma$  quanta being emitted, and  $\xi$  is a dimensionless parameter which must be determined from accurate quantum-electrodynamics calculations. The value of the conversion coefficient  $W_{2\gamma,\gamma}^c$  can be found from the present values of  $\Gamma_{\gamma}$  and  $\Gamma_{2\gamma}$ . We find  $W_{2\gamma,\gamma}^c \approx 4.113 \times 10^{-11} \zeta$ . The constant  $\xi$  in the last equation equals  $1.62758 \times 10^{-6} \zeta$ .

### **IV. CONCLUSIONS**

In conclusion we emphasize that the internal conversion of  $\gamma$  quanta in the Ps<sup>-</sup> ion differs significantly in many aspects from such well-known phenomena as the Auger effect for atoms and ions (the internal conversion of x rays), or the internal conversion of the nuclear  $\gamma$  quanta on the atomic shells. The main difference is the presence of only one body (electron) and one photon in the final state. Obviously, further investigations of this phenomenon may give new information about processes in polyelectronic mixtures and systems.

Previously it was found that the statistical angular correlation coefficients were negative for the ground  ${}^{1}S$ states of H<sup>-</sup>, He, Li<sup>+</sup>, and the other two-electron atomic ions [22]. The only examples of positive angular correlation coefficients were for the excited  $2{}^{1}P$  states of Li<sup>+</sup>, Be<sup>2+</sup>, etc. We have found that the ground  ${}^{1}S$  state in the Ps<sup>-</sup> ion exhibits positive angular correlation. In the series of two-electron ions of total charge -1, there exist "nuclear" mass values for which each of the angular correlation coefficients vanishes. This indicates that the position vectors of the electrons with respect to the "nucleus" are expected to be orthogonal to one another for these mass values. The fact that the various angularcorrelation coefficients do not all vanish for the same mass values reflects that they probe different regions.

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$$\psi_{L=0}(r_{32}, r_{31}, r_{21}) = (1 + P_{21})\exp(-\alpha r_{32} - \beta r_{31} - \gamma r_{21})$$

where  $r_{ij}$  [(ij) = (32), (31), (21)] are the relative coordinates. The optimized values of the parameters  $\alpha, \beta$ , and  $\gamma$  equal 0.520 1386, 0.1479152, and -0.0059907, respectively. The optimized energy is -0.256 692 004 87 atomic units. This single exponential function in the relative coordinates is sufficient to obtain the bound ground state with L = 0 in the case of an arbitrary Coulomb three-body symmetric system with unit charges such as  $X^+X^+Y^-$  (or  $X^-X^-Y^+$ ). For more details see A.M. Frolov, V.H. Smith, Jr., and J. Komasa, J. Phys. A **26**, 6507 (1993).

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