

Polarizabilities of the Ps negative ion

A. K. Bhatia and Richard J. Drachman

Heliophysics Science Division, NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771, USA

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We have calculated polarizabilities (α_1 , β_1 , γ_1 , α_2 , β_2 , and γ_2) of Ps^- by the pseudostate method. These parameters can be used to calculate Rydberg states of Ps^- in the presence of an external electron with high quantum numbers N and L . They are also of importance in a system containing Ps^- bound to a proton [PsH] and also Rydberg states of Ps_2 .

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INTRODUCTION

The positronium negative ion (Ps^-), consisting of two electrons and a positron, is particle stable and decays only by e^+ and e^- annihilation into γ rays. Mills [1,2] has produced and detected this ion and measured its lifetime. Bhatia and Drachman [3] have calculated various properties like the ground-state (1S) energy and decay rate. They [4] and Ward *et al.* [5] also calculated its photodetachment cross sections because Mills [1] has suggested that the Ps^- ion could be used to generate positronium (Ps) beams of controlled energy which involves acceleration of Ps^- ions and photodetachment of one electron. In the past we investigated Rydberg states of various two-electron [6] and three-electron systems [7,8] for which generalized polarizabilities of the core are necessary. Now we are interested in analogous Rydberg states involving Ps^- .

The obvious application is to a system containing a Ps ion bound to an external positive charge. One such system is the exotic “atom” composed of Ps^- bound to a proton. This system would have energy levels like those of the hydrogen atom (with a modified Rydberg constant due to the large mass of the ion) but with quantum defects caused by the extended charge distribution of the ion. The polarizabilities would perturb the energy levels and would be most useful for high angular momenta where the high centrifugal barrier would emphasize the long-range part of the potential. Of course, these states would be metastable, or resonant, since other rearrangement thresholds lie below. In addition, there should also be similar resonances in Ps-Ps scattering, where metastable bound states composed of either $\text{Ps}^- + e^+$ or its charge conjugate would be important.

THEORY AND CALCULATIONS

In the past, we calculated the polarizabilities of various two-electron systems [9,10] and calculated the Rydberg states of Li atoms [7]. Similar calculations can be carried out when the core is that of a Ps^- atom and the valence particle is an electron, positron, or a proton. Following the notation of Ref. [9], the interaction between the valence particle and the core can be represented by the following effective potential:

$$U(x) = -\frac{\alpha_1}{x^4} + \frac{6\beta_1 - \alpha_2}{x^6} + \dots, \quad (1)$$

where α_1 and α_2 are the dipole and quadrupole polarizabilities, respectively, and β_1 is the first nonadiabatic coefficient.

There are higher-order terms involving γ_1 , γ_2 , and β_2 which appear in the coefficient of $1/x^8$ [6]. The first-order shift in energy of any hydrogenic valence particle with quantum numbers N and L due to this potential is

$$\Delta_1 = \int d^3x \Psi_{NL}(x) U(x) \Psi_{NL}(x). \quad (2)$$

In Ref. [9], we have given the Hamiltonian for a general mass M of the valence particle. We therefore briefly give the Hamiltonian relative to the center of mass of the system:

$$H = H_c + H_v + V, \quad (3)$$

where H_c and H_v are the Hamiltonian of the core and valence particle, respectively, appropriately scaled for convenience [9]. For application to Ps_2 we set $M=1$ and the resulting Hamiltonian for the core is given by

$$H_c = -\nabla_{\rho_1}^2 - \nabla_{\rho_2}^2 - \frac{2}{3} \nabla_{\rho_1} \cdot \nabla_{\rho_2} - \frac{2}{\rho_1} - \frac{2}{\rho_2} + \frac{2}{|\rho_1 - \rho_2|}, \quad (4)$$

where ρ_1 and ρ_2 are the distances of electrons 1 and 2 from the positron, respectively. The Hamiltonian for the valence positron is given by

$$H_v = -\frac{3}{2} \left[\nabla_x^2 + \frac{2}{x} \right], \quad (5)$$

where x is the distance of the valence positron from the center of mass of the core. The interaction potential has the form

$$V = 3 \left[\frac{1}{\left| \mathbf{x} - \rho_1 + \frac{1}{2}\rho_2 \right|} + \frac{1}{\left| \mathbf{x} - \rho_2 + \frac{1}{2}\rho_1 \right|} - \frac{1}{\left| \mathbf{x} + \frac{1}{2}(\rho_1 + \rho_2) \right|} + \frac{1}{x} \right]. \quad (6)$$

We are interested in the case of $x \gg \rho_{1,2}$ and therefore make an expansion in Legendre polynomials,

$$V = \frac{1}{3x^2}(\mathbf{w} \cdot \hat{\mathbf{x}}) + \frac{2}{x^3} \left[\rho_1^2 P_2(\hat{\boldsymbol{\rho}}_1 \cdot \hat{\mathbf{x}}) + \rho_2^2 P_2(\hat{\boldsymbol{\rho}}_2 \cdot \hat{\mathbf{x}}) - \frac{2}{3} w^2 P_2(\hat{\mathbf{w}} \cdot \hat{\mathbf{x}}) \right] + \dots, \quad (7)$$

where $\mathbf{w} = \rho_1 + \rho_2$. We can write the above potential V as a sum of two terms:

$$V = \frac{v_1}{x^2} + \frac{v_2}{x^3}. \quad (8)$$

We use the potential V , in its multipole form, in the second-order perturbation theory and define the various polarizabilities as follows:

$$\alpha_i = \sum_N \frac{\langle 0|v_i|N\rangle\langle N|v_i|0\rangle}{(E_N - E_0)}, \quad (9)$$

$$\beta_i = \sum_N \frac{\langle 0|v_i|N\rangle\langle N|v_i|0\rangle}{(E_N - E_0)^2}, \quad (10)$$

and

$$\gamma_i = \sum_N \frac{\langle 0|v_i|N\rangle\langle N|v_i|0\rangle}{(E_N - E_0)^3}. \quad (11)$$

Because of our previous scaling [9], these polarizabilities are also scaled. For the two electrons in the Coulomb field of the positron, the ground state Ψ_0 is of the Hylleraas form

$$\Psi_0 = e^{-(a\rho_1 + b\rho_2)} \sum_{l,m,n} \rho_1^l \rho_2^m \rho_{12}^n + (1 \leftrightarrow 2). \quad (12)$$

We calculate the sum in the above expressions by the pseudostate method by using a set of normalizable functions to approximate the complete set represented by $|N\rangle$. These too have the Hylleraas form with angular momentum 1 or 2 for the dipole and quadrupole terms, respectively. For $L=1$, we define

$$\Psi_p = -\cos(\theta_{12}/2)(f + \tilde{f})\mathcal{D}_1^{1+} - \sin(\theta_{12}/2)(f - \tilde{f})\mathcal{D}_1^{1-}, \quad (13)$$

where

$$f(\rho_1, \rho_2, \rho_{12}) = e^{-(\gamma\rho_1 + \delta\rho_2)} \rho_1 \sum_{l,m,n} C_{lmn} \rho_1^l \rho_2^m \rho_{12}^n, \quad (14)$$

$$\tilde{f}(\rho_1, \rho_2, \rho_{12}) = f(\rho_2, \rho_1, \rho_{12}). \quad (15)$$

Similarly, for $L=2$ we have

$$\Psi_D = (f + \tilde{f})[-D_2^{0+} + \sqrt{3} \cos(\theta_{12})D_2^{2+}] + \sqrt{3} \sin(\theta_{12})(f - \tilde{f})D_2^{2-} + (g + \tilde{g})[-\cos(\theta_{12})D_2^{0+} + \sqrt{3}D_2^{2+}], \quad (16)$$

where

$$f(\rho_1, \rho_2, \rho_{12}) = e^{-(\gamma\rho_1 + \delta\rho_2)} \rho_1^2 \sum_{l,m,n} C_{lmn}^{(1)} \rho_1^l \rho_2^m \rho_{12}^n, \quad (17)$$

TABLE I. Polarizabilities of Ps^- : α_1 , β_1 , and γ_1 .

N_p	α_1	β_1	γ_1
286	231.320459502	2400.55309516	29596.7045767
364	231.322194343	2400.64847894	29601.0088789
455	231.323050606	2400.69966056	29603.2591674

$$g(\rho_1, \rho_2, \rho_{12}) = e^{-(\gamma\rho_1 + \delta\rho_2)} \rho_1 \rho_2 \sum_{l,m,n} C_{lmn}^{(2)} \rho_1^l \rho_2^m \rho_{12}^n, \quad (18)$$

and

$$\tilde{f}(\rho_1, \rho_2, \rho_{12}) = f(\rho_2, \rho_1, \rho_{12}), \quad (19)$$

$$\tilde{g}(\rho_1, \rho_2, \rho_{12}) = g(\rho_2, \rho_1, \rho_{12}). \quad (20)$$

The rotational harmonics \mathcal{D} appearing in the wave functions have been defined by Bhatia and Temkin [11]. Using these forms, we obtain variational wave functions for the initial 1S state of Ps^- and the set of intermediate pseudostates which, along with their variational energies, are used in expressions (9)–(11) for the polarizabilities. We obtain the ground-state energy $-0.524\,010\,139\,585$ Ry for 615 terms in Ψ_0 when the nonlinear parameters are $a=b=0.88$. The nonlinear parameters for P states are $\gamma=\delta=0.50$, and we show the convergence of α_1 , β_1 , and γ_1 in Table I with respect to the number of terms in the wave function Ψ_p . The polarizability α_1 has a variational lower bound, and therefore it has been optimized with respect to the nonlinear parameters γ and δ . We use the same nonlinear parameters to calculate β_1 and γ_1 .

It can be shown easily that the polarizability α_1 has a lower bound. We can calculate variational upper bound to the ground-state energy due to an applied electric field as follows. Choose the trial function of the form

$$|\Psi\rangle = |0\rangle + \sum_p C_p |p\rangle \quad (21)$$

and the Hamiltonian

$$H = H_0 + \lambda z, \quad (22)$$

where λ is a parameter proportional to the electric field \mathcal{E} . We have

$$\langle 0|H_0|0\rangle = E_0, \quad \langle p|H_0|p'\rangle = E_p \delta_{pp'}, \quad (23)$$

and

$$\langle 0|p\rangle = 0, \quad \langle 0|z|0\rangle = 0, \quad \langle p|p'\rangle = \delta_{pp'}. \quad (24)$$

We define the total energy by

$$\bar{E} = \frac{\langle \Psi|H\Psi\rangle}{\langle \Psi|\Psi\rangle}, \quad (25)$$

and the total wave function satisfies

$$\langle \Psi|\Psi\rangle = 1 + \sum_p C_p^2. \quad (26)$$

The numerator of Eq. (25) can be written as

$$\begin{aligned}
\langle \Psi | H | \Psi \rangle &= \left[\langle 0 | + \sum_{p'} C_{p'} \langle p' | \right] [H_0 + \lambda z] \left[|0\rangle + \sum_p C_p |p\rangle \right] \\
&= \langle 0 | H_0 | 0 \rangle + \sum_{pp'} C_p C_{p'} \langle p' | H_0 | p \rangle \\
&\quad + \lambda \left[\langle 0 | z \sum_p C_p | p \rangle + \sum_{p'} C_{p'} \langle p' | z | 0 \rangle \right], \quad (27)
\end{aligned}$$

which implies

$$\bar{E} = \frac{E_0 + \sum_p C_p^2 E_p + 2\lambda \left[\sum_p C_p \langle 0 | z | p \rangle \right]}{1 + \sum_p C_p^2}, \quad (28)$$

which is an upper bound on \bar{E} . To optimize \bar{E} , we can calculate $\frac{\partial \bar{E}}{\partial C_p}$ which for $\frac{\partial \bar{E}}{\partial C_p} = 0$ gives

$$C_p = \frac{- \left(1 + \sum_{p'} C_{p'}^2 \right) \lambda \langle 0 | z | p \rangle}{E_p \left(1 + \sum_{p' \neq p} C_{p'}^2 \right) - E_0 - \sum_{p' \neq p} C_{p'}^2 E_{p'} - 2\lambda \sum_{p'} C_{p'} \langle 0 | z | p' \rangle}. \quad (29)$$

This indicates that C_p is of the order of λ . If λ is small, then

$$C_p = \frac{\lambda \langle 0 | z | p \rangle}{E_0 - E_p}. \quad (30)$$

Substituting this value of C_p into Eq. (28), simplifying and retaining terms of the order of λ^2 , we find

$$\bar{E} = E_0 + \lambda^2 \sum_p \frac{|\langle 0 | z | p \rangle|^2}{E_0 - E_p}. \quad (31)$$

This is still an upper bound on \bar{E} . Polarizability is defined in terms of the second-order energy shift as

$$\Delta_2 = -\frac{1}{2} \alpha_1 \mathcal{E}^2. \quad (32)$$

Consider an electric field produced by a point charge (Ze):

TABLE II. Polarizabilities of Ps^- : α_2 , β_2 , and γ_2 .

N_{sd}	α_2	N_{pp}	β_2	γ_2
120	2381.87400781	84	11585.9124706	126578.66942
165	2383.53370234	120	11590.4226644	126686.716004
220	2385.52905893	165	11591.3318978	126711.918561

$$\mathcal{E} = -\frac{Ze}{r^2}. \quad (33)$$

This gives

$$\Delta_2 = -\frac{1}{2} \alpha_1 \frac{Z^2 e^2}{r^4}. \quad (34)$$

Letting $r = \bar{r} a_0$, we get

$$\Delta_2 = -\frac{1}{2} \alpha_1 \frac{Z^2 e^2}{\bar{r}^4 a_0^4} = \Delta \bar{E} \frac{e^2}{2a_0}, \quad (35)$$

where

$$\Delta \bar{E} = -\frac{\alpha_1 Z^2}{a_0^3 \bar{r}^4}, \quad (36)$$

which shows that α_1 is in the units of a_0^3 and

$$\alpha_1 = \sum_p \frac{\langle 0 | z | p \rangle \langle p | z | 0 \rangle}{E_p - E_0}, \quad (37)$$

which is a lower bound (notice the change in sign of the denominator).

Similarly, it can be shown that α_2 has a lower bound. We therefore optimize α_2 with respect to the nonlinear parameters and use the same parameters in the calculation of β_2 and γ_2 . As noted above, Ψ_D consists of two types of terms pp and sd . For α_2 , the total number of terms is given by $N_d = N_{pp} + N_{sd}$. We keep $N_{pp} = 120$ and show the convergence with respect to N_{sd} in Table II. For β_2 and γ_2 , we keep $N_{sd} = 220$ and vary N_{pp} . The convergence is shown in Table II.

As indicated earlier in Eq. (2), these parameters can be used to calculate the energy shifts and therefore the Rydberg states of Ps^- in the presence of another electron in higher states with quantum numbers N and L .

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