

# Hyperfine splitting of the lowest state energy of positronium in strong electric field

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## 1. The model

### 1.1. Interaction with electric field

The Hamiltonian describing the relative motion of a two-particle system consisting of one electron ( $m_1 = 1$ ,  $q_1 = -1$ ) and another particle of the opposite charge ( $q_2 = +1$ ), placed in an external electric field, reads (in atomic units)

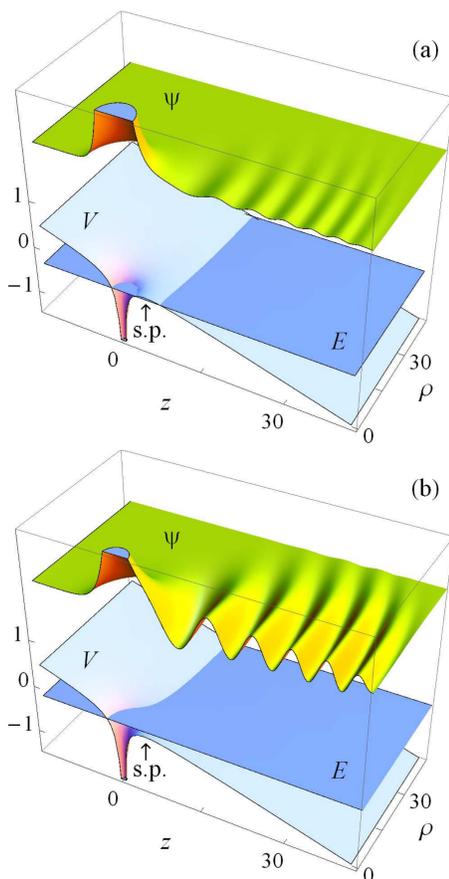
$$H = -\frac{p^2}{2\mu} - \frac{1}{r} - Fz, \quad (1)$$

where  $F$  is the field strength and  $\mu = m_1 m_2 / (m_1 + m_2)$  is the reduced mass. For the hydrogen atom (H) this mass is  $\mu = 1$  (in the approximation of infinitely heavy nucleus), whereas for positronium (Ps) it takes the value  $\mu = 1/2$ .

The Coulomb potential  $-1/r$  and the external field form the potential barrier (see Figure 1) whose saddle point position and height are

$$z_{sp} = 1/\sqrt{F} \quad V_{sp} = -2\sqrt{F}. \quad (2)$$

As a consequence, the system of any binding energy decays either by tunnelling through or over the barrier, i.e. all states become resonant (autoionizing).



**Figure 1.** Potential  $V = -1/r - Fz$  (bottom, light blue), the lowest energy level  $E$  (bottom, dark blue) and the real part of wave function  $\psi$  (top, green) corresponding to the lowest resonant state at the field strength  $F = 0.05$  a.u. ( $\approx 2.571 \times 10^{10}$  V/m) for: (a) hydrogen ( $\mu = 1$ ,  $E = -0.5061$  a.u.) and (b) positronium ( $\mu = 1/2$ ,  $E = -0.2846$  a.u.). The vertical arrow shows the position of the saddle point (s.p.) of the potential barrier. Note that at this field strength the ionization of hydrogen realizes by tunnelling, while in the case of positronium it is over-the-barrier ionization.

ionization regimes:

**tunnel ionization** (TI) takes place if  $E < V_{sp}$ ,

**over-the-barrier ionization** (OBI) occurs if  $E > V_{sp}$ ,

where  $E$  is the energy of the system in a given state. Here we consider the ionization from the lowest state.

Since both  $E$  and  $V_{sp}$  depend on the field strength, the TI and OBI occur for  $F < F^*$  and  $F > F^*$ , respectively, where  $F^*$  is the solution of the equation

$$E(F^*) = V_{sp}(F^*) \equiv -2\sqrt{F^*}. \quad (3)$$

### 2.1. The spin-spin and annihilation interaction

The interactions which lead to the energy splitting between the o-Ps and p-Ps ground states, the spin-spin coupling and the annihilation interaction, are described by two additional terms in the Hamiltonian for relative motion (Berestetskii et al., 1982)

$$V_{ss} = \frac{\alpha^2}{4} \left[ \frac{3(\vec{\sigma}_1 \cdot \mathbf{r})(\vec{\sigma}_2 \cdot \mathbf{r})}{r^5} - \frac{\vec{\sigma}_1 \cdot \vec{\sigma}_2}{r^3} + \frac{8\pi}{3} \vec{\sigma}_1 \cdot \vec{\sigma}_2 \delta(\mathbf{r}) \right], \quad (4)$$

$$V_{ann} = \frac{\pi\alpha^2}{2} (3 + \vec{\sigma}_1 \cdot \vec{\sigma}_2) \delta(\mathbf{r}). \quad (5)$$

Here  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  is the relative radius vector of  $e^-e^+$  pair,  $\vec{\sigma}_{1,2}$  are the Pauli matrices describing the spin of these two particles and  $\alpha = 1/137.036$  is the fine-structure constant. In analogy with ordinary atoms, this energy splitting is called the hyperfine splitting (HFS), although for Ps it is of the same order as the fine structure corrections.

Assuming that the interaction with electric field is fully described by the dipole term  $-Fz$ , the Hamiltonian for positronium in electric field, which takes into account the HFS, reads

$$H = H_0 + V_{ss} + V_{ann} = H_0 + V_{hfs}. \quad (6)$$

Using relations  $\vec{\sigma}_1 \cdot \vec{\sigma}_2 = 2\mathbf{S}^2 - 3$  and  $(\vec{\sigma}_1 \cdot \mathbf{r})(\vec{\sigma}_2 \cdot \mathbf{r}) = 2(\mathbf{S} \cdot \mathbf{r})^2 - r^2$ , where  $\mathbf{S} = (\vec{\sigma}_1 + \vec{\sigma}_2)/2$  is the total spin, and writing  $\mathbf{r} = r\mathbf{e}_r$ , the HFS term becomes

$$V_{hfs} = \frac{\alpha^2}{2r^3} [3(\mathbf{S} \cdot \mathbf{e}_r)^2 - \mathbf{S}^2] + \pi\alpha^2 \left( \frac{7}{3}\mathbf{S}^2 - 2 \right) \delta(\mathbf{r}). \quad (7)$$

The matrix which represents operator  $(\mathbf{S} \cdot \mathbf{e}_r)^2$  in the basis of singlet/triplet spin states  $\{|S, M_S\rangle | S = 0, 1; M_S = -S, \dots, S\rangle\}$  has quasi-diagonal form

$$(\mathbf{S} \cdot \mathbf{e}_r)^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4}(\cos 2\vartheta + 3) & -\frac{\sin 2\vartheta e^{i\varphi}}{2\sqrt{2}} & \frac{1}{2}\sin^2\vartheta e^{2i\varphi} \\ 0 & -\frac{\sin 2\vartheta e^{-i\varphi}}{2\sqrt{2}} & \sin^2\vartheta & \frac{\sin 2\vartheta e^{i\varphi}}{2\sqrt{2}} \\ 0 & \frac{1}{2}\sin^2\vartheta e^{-2i\varphi} & \frac{\sin 2\vartheta e^{-i\varphi}}{2\sqrt{2}} & \frac{1}{4}(\cos 2\vartheta + 3) \end{pmatrix}, \quad (8)$$

while the corresponding matrix of operator  $\mathbf{S}^2$  is diagonal

$$(\mathbf{S}^2)_{SM_S, S'M'_S} = S(S+1) \delta_{SS'} \delta_{M_S M'_S}. \quad (9)$$

Thus, the HFS terms do not couple singlet ( $S = 0$ ) and triplet ( $S = 1$ ) states, but  $V_{ss}$  couples the triplet states with different values of  $M_S$ .

Since the first diagonal element ( $SM_S = S'M'_S = 00$ ) of matrices (8) and (9) is zero, in the singlet case the spin-dependent terms in Eq. (7) vanish and  $V_{hfs}$  reduces to

$$V_{hfs}^{(S=0)} = -2\pi\alpha^2 \delta(\mathbf{r}). \quad (10)$$

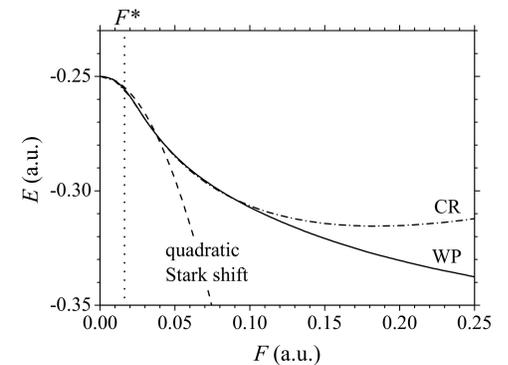
For the triplet case the spin-dependent terms in  $V_{hfs}$  are different from zero. Assuming, however, that their contribution is much smaller than the contribution of the term with delta-function, we neglect the  $M_S$ -coupling and characterize the lowest state by a definite value of quantum number  $M_S$ . In this approximation we keep in the HFS term only diagonal matrix elements  $[(\mathbf{S} \cdot \mathbf{e}_r)^2]_{1M_S, 1M_S}$  and  $(\mathbf{S}^2)_{1M_S, 1M_S} = 2$  and apply the expression

$$V_{hfs}^{(S=1)} = \frac{\alpha^2}{2r^3} [3[(\mathbf{S} \cdot \mathbf{e}_r)^2]_{1M_S, 1M_S} - 2] + \frac{8}{3}\pi\alpha^2 \delta(\mathbf{r}). \quad (11)$$

## 3. Results

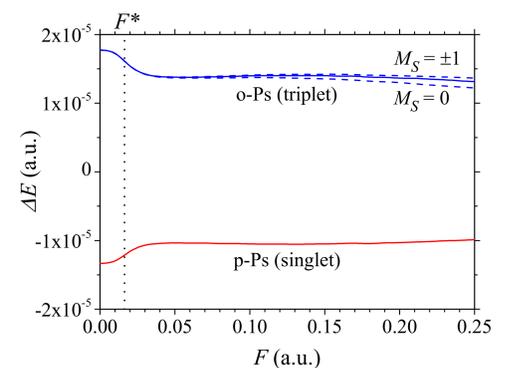
The lowest state energy of positronium, calculated using the model without the HFS terms by the wave-packet (WP) method (see Bunjac et al., 2017) and the complex-rotation (CR) method (see Milošević and Simonović, 2015) methods, is shown in Fig. 2 in the range of the field strengths from  $F = 0$  to 0.25 a.u. ( $\approx 1.286 \times 10^{11}$  V/m).

A difference between results obtained by these two methods, which becomes significant at very strong fields ( $F \gg F^*$ ), indicates that the resonance mean energy  $E$  obtained by the WP method and the real part of complex energy obtained by the CR method do not have the same meaning, particularly for very broad resonances.



**Figure 2.** Dependence of the lowest state energy  $E$  of positronium on the strength of external electric field  $F$  obtained numerically using the wave-packet method (WP) and the complex-rotation method (CR), respectively. For comparison the Stark shift expansion up to the quadratic term is shown (dashed line). The vertical dotted line marks the field strength  $F^*$  dividing the tunnelling and OBI domains.

The lowest state Ps energy with the HFS, i.e. the p-Ps and o-Ps energies as functions of the field strength, are calculated using the CR method. The calculations show that the term in Eq. (11) which is proportional to  $1/r^3$  gives much smaller contribution to the HFS (for about two orders of magnitude) than the term with delta-function. This fact is in agreement with the assumption from the previous section which validates Eq. (11) as a good approximation.



**Figure 3.** Hyperfine splitting of the lowest state energy of Ps in electric field. The p-Ps and o-Ps lowest state energies relative to the unperturbed energy ( $\Delta E_{p-Ps, o-Ps} = E_{p-Ps, o-Ps} - E$ ), as functions of the field strength. The dashed lines represent the values for o-Ps which are obtained using the complete expression (11) for  $M_S = 0$  and  $M_S = \pm 1$  separately, whereas the full line is obtained using only the term with delta-function.

The p-Ps and o-Ps energies (the later with and without the term  $\sim 1/r^3$ ), relative to the unperturbed energy shown in Fig. 2, are presented in Fig. 3. It can be seen that in the tunnelling domain and at the beginning of OBI domain the HFS decreases significantly by increasing the field strength, but for  $F > 2F^*$  it changes slowly taking the values which are 20-25% smaller than the field-free value.

The behaviour shown in Fig. 3 can be explained by the change of form of the lowest state wave function of positronium when it is placed in the field. The HFS in the range  $F < 2F^*$  can be estimated by applying the first order perturbation theory, using  $V_{hfs}$  (without term  $\sim 1/r^3$ ) as the perturbation. This approach gives

$$E_{hfs}(F) \approx \frac{14}{3}\pi\alpha^2 |\psi(0; F)|^2, \quad (12)$$

where  $\psi(0; F)$  is the value of the lowest state wave function of Ps in the field of strength  $F$  for  $r = 0$ . This relation indicates that the observed decrease of HFS when  $F$  increases is a consequence of the decrease of electron density at the positron position ( $|\psi(0; F)|^2$ ), which can be explained by the shift of the density distribution in electric field towards the barrier.

## References

- A. Bunjac, D. B. Popović and N. S. Simonović, *Phys. Chem. Chem. Phys.*, **19**, 19829 (2017).  
V. B. Berestetskii, E. M. Lifshitz, L. P. Pitaevskii, *Quantum electrodynamics, 2nd ed. (Course of theoretical physics, Vol. 4)*, Butterworth-Heinemann, an imprint of Elsevier, Oxford, 1982.  
M. Z. Milošević and N. S. Simonović, *Phys. Rev. A*, **91**, 023424 (2015).