Publ. Astron. Obs. Belgrade No. 99 (2020), 51 - 54 *Contributed Paper*

HYPERFINE SPLITTING OF THE LOWEST STATE ENERGY OF POSITRONIUM IN STRONG ELECTRIC FIELD

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Abstract. The lowest state energy of positronium in an external electric field is calculated in the range of field strengths belonging to the tunnelling and over-the-barrier ionization regimes, using the wave-packet propagation method and the complex-rotation method. It is found that the hyperfine splitting of this level in the tunnelling domain decreases by increasing the field strength, but in the over-the-barrier domain the additional splitting occurs for triplet states.

1. INTRODUCTION

The electron-positron (e^-e^+) bound system, known as positronium (Ps), is an unstable exotic atom due to a non-negligible probability for annihilation of its constituents (see e.g. Rich et al. 1981). The lifetimes of the singlet (1^1S_0) and triplet (1^3S_1) components of the ground-state of Ps, the so-called para-positronium (p-Ps) and orto-positronium (o-Ps), are 125 ps and 142 ns, respectively. The ground state energy of Ps is about half of that of hydrogen ($E \approx -6.8\,\mathrm{eV}$), but its hyperfine splitting (HFS) $E_{\text{o-Ps}} - E_{\text{p-Ps}} = 0.845\,\mathrm{meV}$, when compared to that for hydrogen, is more than three orders of magnitude larger. This splitting is a consequence of two spin-dependent interactions: (i) the spin-spin coupling (the interaction of individual magnetic momenta of e^- and e^+) and (ii) ”the annihilation force” (the possibility of virtual annihilation and re-creation of the e^-e^+ pair, see Deutsch, 1952).

However, when positronium is placed in an electric field, another kind of instability arises – the ionization of Ps by the field. In this case the Coulomb potential of e^-e^+ pair and the external electric field form a potential (Stark) barrier through which the system can decay by tunnelling. The limiting case of this process when the barrier is suppressed below the energy of the atomic state, which takes place at very strong fields, is usually referred to as over-the-barrier ionization (OBI). The HFS of energy levels of Ps, on the other hand, is not directly affected by the external electric field. A weak dependence of HFS on electric field, however, occurs due to the change of form of the lowest state wave function of positronium when the field increases. In order to calculate this effect and the influence of electric filed generally, we apply two different numerical methods: the wave-packet propagation (WP) method and the complex-rotation (CR) method, used previously in the studies of ordinary atoms in strong fields (see Bunjac et al., 2017; Milošević and Simonović, 2015).

2. THE MODEL

2. 1. INTERACTION WITH ELECTRIC FIELD

The first step in the analysis of electric field effects on the positronium lowest levels will be the calculation of energies and ionization rates without the HFS terms. The corresponding unperturbed Hamiltonian describing the relative motion of the e^-e^+ pair, placed in the external electric field of strength F, reads (in atomic units)

$$H_0 = -\frac{1}{2\mu}\nabla^2 - \frac{1}{r} - Fz, \tag{1}$$

where r is the inter-particle distance, z is its component in the field direction and μ is the reduced mass which for positronium takes the value 1/2. When $F \neq 0$ the Coulomb potential $-1/r$ and the external field form the potential barrier with the saddle point of hight $V_{\mathrm{sp}} = -2\sqrt{F}$ located at $\mathbf{r}_{\mathrm{sp}} = (0, 0, 1/\sqrt{F})$. Since the potential energy outside the barrier asymptotically tends to $-\infty$, the system can decay by tunnelling at any energy E. Therefore, all bound states of the field-free atom become resonant (autoionizing) states when $F \neq 0$.

As it was already mentioned in Introduction, two ionization regimes can be distinguished: (i) the tunnel ionization (tunnelling) regime, when $E < V_{\mathrm{sp}}$, and (ii) over-the-barrier ionization (OBI) regime, when $E > V_{\mathrm{sp}}$. Here we consider the lowest resonant state which in the limit $F \to 0$ approaches the ground state of the field-free atom. The value of the field strength which separates the ionization regimes F^* is the root of equation $E(F^*) = V_{\mathrm{sp}}(F^*) \equiv -2\sqrt{F^*}$. Using numerically determined values for the lowest state energy, this equation gives $F^* = 0.016\,\mathrm{a.u.}$ for Ps. Thus, the tunnelling and OBI take place for: (i) $F < F^*$ and (ii) $F > F^*$, respectively.

2. 2. THE SPIN-SPIN COUPLING 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)

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

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

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

$$H = H_0 + V_{\mathrm{ss}} + V_{\mathrm{ann}} = H_0 + V_{\mathrm{hfs}}. \tag{4}$$

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

$$V_{\text{hfs}} = \frac{\alpha^2}{2r^3}\left[3(\mathbf{S}\cdot\mathbf{e}_r)^2-\mathbf{S}^2\right]+\pi\alpha^2\left(\frac{7}{3}\mathbf{S}^2-2\right)\delta(\mathbf{r}). \tag{5}$$

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

$$(\mathbf{S}\cdot\mathbf{e}_r)^2 = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \hline 0 & \frac{1}{4}(\cos2\vartheta+3) & -\frac{\sin2\vartheta\, e^{i\varphi}}{2\sqrt{2}} & \frac{1}{2}\sin^2\vartheta\, e^{2i\varphi} \\ 0 & -\frac{\sin2\vartheta\, e^{-i\varphi}}{2\sqrt{2}} & \sin^2\vartheta & \frac{\sin2\vartheta\, e^{i\varphi}}{2\sqrt{2}} \\ 0 & \frac{1}{2}\sin^2\vartheta\, e^{-2i\varphi} & \frac{\sin2\vartheta\, e^{-i\varphi}}{2\sqrt{2}} & \frac{1}{4}(\cos2\vartheta+3) \end{array}\right), \tag{6}$$

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

$$(\mathbf{S}^2)_{SM_S,S'M'_S} = S(S+1)\,\delta_{SS'}\delta_{M_SM'_S}. \tag{7}$$

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 (6) and (7) is zero, in the singlet case the spin-dependent terms in Eq. (5) vanish and V_{hfs} reduces to

$$V_{\text{hfs}}^{(S=0)} = -2\pi\alpha^2\delta(\mathbf{r}). \tag{8}$$

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

$$V_{\text{hfs}}^{(S=1)} = \frac{\alpha^2}{2r^3}\left[3[(\mathbf{S}\cdot\mathbf{e}_r)^2]_{1M_S,1M_S}-2\right]+\frac{8}{3}\pi\alpha^2\delta(\mathbf{r}). \tag{9}$$

3. RESULTS

The lowest state energy of positronium, calculated using the model without the HFS terms by the WP and CR methods, is shown in Fig. 1(a) in the range of the field strengths from $F = 0$ to 0.25 a.u. ($\approx 1.286\times10^{11}$ 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 (see Klaiman, 2010).

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. (9) 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

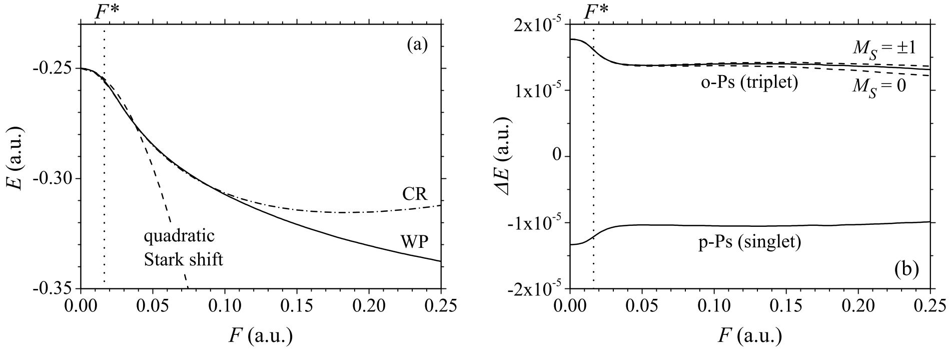

Figure 1: (a) Dependence of the lowest state energy E of positronium on the strength of external electric field F obtained numerically using the wave-packet method (WP) and the complex-rotation method (CR), respectively. For comparison the Stark shift expansion up to the quadratic term is shown (dashed line). The vertical dotted line marks the field strength F^* dividing the tunnelling and OBI domains. (b) 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 ($\Delta E_{\text{p-Ps,o-Ps}} = E_{\text{p-Ps,o-Ps}} - E$), as functions of the field strength. The dashed lines represent the values for o-Ps which are obtained using the complete expression (9) for $M_S = 0$ and $M_S = \pm 1$ separately, whereas the full line is obtained using only the term with delta-function.

which validates Eq. (9) as a good approximation. 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. 1(a), are presented in Fig. 1(b). 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. This behaviour 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 $E_{\text{hfs}}(F) \approx \frac{14}{3}\pi\alpha^2|\psi(0;F)|^2$, 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.

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