

The Spectrum of Positronium in External Fields

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The energy of interaction of the positronium atom with external electric and magnetic fields is calculated up to terms of order v^2/c^2 . The splitting of the spectral lines of the positronium atom in weak and strong electric and magnetic fields is investigated.

1. INTRODUCTION

IN the passage of positrons through matter, the formation of a metastable compound of an atomic type is possible, in addition to the processes of scattering and annihilation¹⁻⁵. The simplest such atomic system is positronium. Recently, positronium has been observed experimentally^{6,7}, while the fine structure of the lowest energy level has also been investigated in some detail^{8,9}.

As was shown in references 1 and 10, a number of effects can be investigated for the positronium atom within the framework of the Pauli approximation for the wave functions, with inclusion of terms of the order of v^2/c^2 . The present work is concerned with the study of some properties of the positronium atom in constant external magnetic and electric fields (both strong and weak), with the same order of accuracy (to v^2/c^2). To these limits of accuracy, the results obtained with the aid of the equation for coupled states¹¹, agree with the results obtained by the much simpler

methods used below (in this connection, see also reference 12).

The positronium atom is a metastable system. It can decay either into three gamma rays (ortho-positronium), or into two gamma rays (para-positronium)²⁻⁵. Investigation of the annihilation radiation (annihilation spectrum), along with a study of the spontaneous radiation (optical spectrum), can play an additional role in the study of the distribution of the energy levels of the system. As will be shown below, the external field changes the spectrum of the decay times which are related to the individual energy levels.

We begin by finding the interaction energy of the positronium atom with an external electromagnetic field. Then we shall consider the energy spectrum of the positronium atom in weak and strong external fields (magnetic and electric).

2. THE INTERACTION ENERGY OF POSITRONIUM WITH AN EXTERNAL FIELD

In calculating the interaction energy in the presence of an external electromagnetic field, it is necessary to divide the scalar and vector potentials into the internal potentials $\Phi_i, \vec{\Phi}_i$ which describe the interaction processes of the electron and positron, and the potentials $\Phi_e, \vec{\Phi}_e$ which arise from the external electric and magnetic fields. Then the total potentials will be given by

$$\Phi = \Phi_i + \Phi_e, \quad (1)$$

$$\vec{\Phi} = \vec{\Phi}_i + \vec{\Phi}_e. \quad (2)$$

In a similar way, the energy of the system can be written in the form

¹ A. A. Sokolov and V. N. Tsytoich, J. Exper. Theoret. Phys. USSR **24**, 253 (1953)

² I. Ia. Pomeranchuk, Dokl. Akad. Nauk SSSR **60**, 213 (1948)

³ E. M. Lifshitz, Dokl. Akad. Nauk SSSR **60**, 21 (1948)

⁴ D. D. Ivanenko and A. A. Sokolov, Dokl. Akad. Nauk SSSR **61**, 51 (1948)

⁵ A. I. Mukhtarov, Dissertation, Moscow State Univ., 1950

⁶ M. Deutsch, Phys. Rev. **82**, 455 (1951)

⁷ M. Deutsch, Phys. Rev. **83**, 866 (1951)

⁸ M. Deutsch and E. Dulit, Phys. Rev. **84**, 601 (1951)

⁹ M. Deutsch and Brown, Phys. Rev. **85**, 1047 (1952)

¹⁰ V. B. Berestetskii, J. Exper. Theoret. Phys. USSR **19**, 1130 (1949)

¹¹ E. E. Salpeter and H. A. Bethe, Phys. Rev. **84**, 1232 (1951)

¹² V. N. Tsytoich, J. Exper. Theoret. Phys. USSR **28**, 113 (1955); Soviet Phys. **1**, 163 (1955)

$$V = V_{\text{kin}} + V_i + V_e, \tag{3}$$

where

$$V_e = -e \int \psi^+ (\Phi_e - \vec{\alpha} \vec{\Phi}_e) \psi d^3x, \tag{4}$$

$$V_{\text{kin}} = \int \psi^+ (c\vec{p}\vec{\alpha} + \rho_3 mc^2) \psi d^3x, \tag{5}$$

$$\psi = \sum_n C_n e^{-icK_n t} \psi_n. \tag{6}$$

The interaction energy V_i for positronium is given, for example, by Sokolov and Tsytovich¹. From the permutation relations for C_n , it follows that

$$V_e = -e \sum_n C_n^+ C_n V_{n, n}, \tag{7}$$

where

$$V_{n_1, n_2} = \int \psi_{n_1}^+ (\Phi_e - \vec{\alpha} \vec{\Phi}_e) \psi_{n_2} d^3x \tag{8}$$

with analogous relations for V_{kin} . We obtain the energy of interaction with the external field by subtracting the energy of the vacuum in the external field from the energy V_e possessed by the electron and positron.

Quantities pertaining to the electron and the positron will be denoted by the indices 1 and 2, respectively. Wave functions which describe the motion of the electron correspond to positive energy, and those describing the motion of the positron to negative energy. Instead of taking electronic functions of negative energy for describing the motion of the positron, we make the transition to positron functions of positive energy by the scheme discussed in reference 1. In this case we have

$$\psi_{-e, -E}^+ \vec{\alpha} \psi_{-e, -E}^- \rightarrow \psi_{+e, E}^+ \vec{\alpha}_2 \psi_{+e, E}^-, \tag{9}$$

$$\psi_{-e, E}^+ \vec{\alpha} \psi_{-e, E}^- \rightarrow \psi_{-e, E}^+ \vec{\alpha}_1 \psi_{-e, E}^-, \tag{10}$$

$$\psi_{-e, -E}^+ \rho_3 \psi_{-e, -E}^- \rightarrow - \psi_{+e, E}^+ \rho_{32} \psi_{+e, E}^-, \tag{11}$$

$$\psi_{-e, E}^+ \rho_3 \psi_{-e, E}^- \rightarrow \psi_{-e, E}^+ \rho_{31} \psi_{-e, E}^-. \tag{12}$$

Finally, the following equation is obtained:

$$\left\{ E - c\vec{p}_1 \vec{\alpha}_1 - \rho_{31} mc^2 - c\vec{p}_2 \vec{\alpha}_2 - \rho_{32} mc^2 + \frac{e^2}{r} - U^B - U^0 \right. \tag{13}$$

$$\left. + e (\Phi_1 - \vec{\alpha}_1 \vec{\Phi}_1) - e (\Phi_2 - \vec{\alpha}_2 \vec{\Phi}_2) \right\} \psi = 0,$$

which is valid only for computation of effects of the order v^2/c^2 inclusively. In this approximation, we can make the transition from the 16 component wave function

$$\psi = \begin{pmatrix} \varphi_{11} \varphi_{12} \\ \varphi_{21} \varphi_{22} \end{pmatrix}, \tag{14}$$

where

$$\varphi_{11} = \begin{pmatrix} \psi_{11} \psi_{12} \\ \psi_{21} \psi_{22} \end{pmatrix}; \quad \varphi_{12} = \begin{pmatrix} \psi_{13} \psi_{14} \\ \psi_{23} \psi_{24} \end{pmatrix};$$

$$\varphi_{21} = \begin{pmatrix} \psi_{31}, \psi_{32} \\ \psi_{41}, \psi_{42} \end{pmatrix}; \quad \varphi_{22} = \begin{pmatrix} \psi_{33}, \psi_{34} \\ \psi_{43}, \psi_{44} \end{pmatrix},$$

to a four component one by expressing the small components $\phi_{12}, \phi_{21}, \phi_{22}$ in terms of the larger ϕ_{11} . We note that in Eq. (13), we put the Breit part of the interaction U^B in a form employed by Araki¹³. This form can also be written as

$$U^B = \frac{e^2}{2} [\vec{\alpha}_1 \vec{\nabla}] \left[\frac{\mathbf{p}_2}{mc} - \frac{\hbar}{2mc} [\vec{\sigma}_2 \vec{\nabla}], \vec{\nabla} \right] \frac{r}{2} \tag{15}$$

$$+ \frac{e^2}{2} \left[\frac{\mathbf{p}_1}{mc} + \frac{\hbar}{2mc} [\vec{\sigma}_1 \vec{\nabla}], \vec{\nabla} \right] [\vec{\alpha}_2 \vec{\nabla}] \frac{r}{2},$$

and we obtain the exchange interaction U^0 as¹⁴

$$U^0 = \pi \frac{e^2 \hbar^2}{m^2 c^2} \frac{3 + \vec{\sigma}_1 \vec{\sigma}_2}{2} \delta(\mathbf{r}). \tag{16}$$

Here

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad r = |\mathbf{r}|.$$

Moreover, the normalizing condition must be satisfied:

$$\int (\varphi_{11}^+ \varphi_{11} + \varphi_{12}^+ \varphi_{12} + \varphi_{21}^+ \varphi_{21} + \varphi_{22}^+ \varphi_{22}) d^3x_1 d^3x_2 = 1. \tag{17}$$

¹³ Araki, Progr. Theor. Phys. 6, 379 (1951)

¹⁴ V. B. Berestetskii and L. D. Landau, J. Exper. Theoret. Phys. USSR 19, 673 (1949)

We therefore introduce the normalized four component function χ , related to ϕ_{11} by the equation

$$\phi_{11} = \left(1 - \frac{p_1^2}{8m^2c^2} - \frac{p_2^2}{8m^2c^2}\right) \chi. \quad (18)$$

Bearing in mind that

$$V_{nn'} = \int \text{Spur } \psi_n^+ U \psi_{n'} d^3x_1 d^3x_2, \quad (19)$$

we obtain the following formulas for the transition to the four component wave function χ :

$$\psi^+ (c \mathbf{p}_k \vec{\alpha}_k + \rho_{3k} mc^2 - mc^2) \psi \quad (20)$$

$$\rightarrow \chi^+ \left(\frac{p_k^2}{2m} - \frac{p_k^4}{8m^3c^2} - \frac{e^2}{2mc^2} \vec{\Phi}_k^2 \right) \chi;$$

$$\psi^+ (\vec{\alpha}_k \vec{\Phi}_k) \psi \quad (21)$$

$$\rightarrow \chi^+ \left\{ \left(\mathbf{p}_k + \frac{e_k}{c} \vec{\Phi}_k + \frac{\hbar}{2i} \nabla_k + \frac{\hbar}{2} [\vec{\sigma}_k \nabla_k] \right) \frac{\vec{\Phi}_k}{mc} \right\} \chi;$$

$$\psi^+ \vec{\Phi}_k \psi \rightarrow \chi^+ \left\{ \vec{\Phi}_k + \frac{\hbar^2 \nabla_k^2 \vec{\Phi}_k}{8m^2c^2} - \frac{\hbar}{4m^2c^2} \vec{\sigma}_k [\mathbf{p}_k \nabla_k] \vec{\Phi}_k \right\} \chi. \quad (22)$$

Here

$$k = 1, 2; \quad e_1 = -e_2 = e.$$

\mathbf{p}_1 and \mathbf{p}_2 operate only on the wave function χ , and $\vec{\nabla}_1$ and $\vec{\nabla}_2$ only on the potentials $\vec{\Phi}_1, \vec{\Phi}_2, \vec{\Phi}_1, \vec{\Phi}_2$.

From Eqs. (20), (21) and (22), we obtain the energy of interaction (and also the kinetic energy) of the electron and positron in the presence of an external field, with accuracy to terms of order v^2/c^2 :

$$\begin{aligned} U = & \frac{\left(\mathbf{p}_1 + \frac{e}{c} \vec{\Phi}_1\right)^2}{2m} + \frac{\left(\mathbf{p}_2 - \frac{e}{c} \vec{\Phi}_2\right)^2}{2m} \quad (23) \\ & - \frac{p_1^4}{8m^3c^2} - \frac{p_2^4}{8m^3c^2} - e\Phi_1 + e\Phi_2 \\ & + \frac{e\hbar}{2mc} \left\{ \vec{\sigma}_1 \mathbf{H}_1 - \vec{\sigma}_2 \mathbf{H}_2 \right\} + \frac{e\hbar}{4m^2c^2} \vec{\nabla}_1 \vec{\Phi}_1 [\vec{\sigma}_1 \mathbf{p}_1] \\ & - \frac{e\hbar}{4m^2c^2} \vec{\nabla}_2 \vec{\Phi}_2 [\vec{\sigma}_2 \mathbf{p}_2] - \frac{e\hbar^2}{8m^2c^2} \nabla_1^2 \vec{\Phi}_1 \\ & + \frac{\hbar^2 e}{8m^2c^2} \nabla_2^2 \vec{\Phi}_2 + V^B + V^0 - \frac{e^2}{r}. \end{aligned}$$

The Breit part of the energy V^B , and the exchange energy V^0 which determines the fine structure in the absence of field, were found earlier by Berestetskii and Landau¹⁴:

$$\begin{aligned} V^B = & 4\pi\mu_0^2 \delta(\mathbf{r}) + \frac{e}{2mc} \mu_0 \frac{1}{r} \left\{ \vec{\sigma}_1 [\mathbf{r}\mathbf{p}_1] - \vec{\sigma}_2 [\mathbf{r}\mathbf{p}_2] \right\} \quad (24) \\ & + \frac{e^2}{2m^2c^2} \left\{ \frac{1}{r} \mathbf{p}_1 \mathbf{p}_2 + \frac{x_n x_{n'} p_{1n} p_{2n'}}{r^3} \right\} \\ & - \frac{e}{mc} \mu_0 \frac{1}{r^3} \left\{ \vec{\sigma}_2 [\mathbf{r}\mathbf{p}_1] - \vec{\sigma}_1 [\mathbf{r}\mathbf{p}_2] \right\} \\ & + \mu_0^2 \left\{ \frac{8\pi}{3} (\vec{\sigma}_1 \vec{\sigma}_2) \delta(\mathbf{r}) + \frac{3(\vec{\sigma}_1 \mathbf{r})(\vec{\sigma}_2 \mathbf{r}) - \vec{\sigma}_1 \vec{\sigma}_2 r^2}{r^5} \right\}; \\ V^0 = & 4\pi\mu_0^2 \frac{3 + \vec{\sigma}_1 \vec{\sigma}_2}{2} \delta(\mathbf{r}). \quad (25) \end{aligned}$$

Here $\mu_0 = e\hbar/2mc$ and $\vec{\sigma}_1$ and $\vec{\sigma}_2$ are the double row matrices of Pauli; in Eqs. (23), (24) and (25), p_i act both on the wave function χ , and on the potential Φ .

3. THE ENERGY SPECTRUM OF POSITRONIUM IN A WEAK MAGNETIC FIELD

In the presence of a constant external magnetic field $H = H_z = \text{const}$, the energy of interaction of positronium with the external magnetic field can be obtained for Eq. (23)

$$U^H = \frac{e\hbar H}{2mc} (\sigma_{1z} - \sigma_{2z}) + \frac{e^2 H^2}{16m^2 c^2} (x^2 + y^2). \quad (26)$$

In a weak magnetic field ($\mu_0 H < \alpha^2 e^2 / r_0$) the second term of Eq. (26) is negligibly small ($< \alpha^4 e^2 / r_0$) in comparison with the first. Therefore, it is sufficient in computing the energy spectrum in this case to find the various matrix elements of the energy:

$$U_1^H = \frac{e\hbar H}{2mc} (\sigma_{1z} - \sigma_{2z}). \quad (27)$$

With the help of the wave functions found in the absence of field, for example, in reference 1, we have*

$$\begin{aligned} V_a^a = V_b^b = V_c^c = V_d^d = V_b^c \\ = V_b^d = V_c^d = 0, \quad (28) \end{aligned}$$

* Here and below, indices are used (see reference 1, A. A. Sokolov and V. N. Tsytovich, J. Exper. Theoret. Phys. USSR 24, 253 (1953)).

$$V_a^b = 2\mu_0 H \sqrt{\frac{l^2 - m^2}{l(2l+1)}} (1 - \delta_{l0}), \quad (29)$$

$$V_a^c = 2\mu_0 H \frac{m}{\sqrt{l(l+1)}} (1 - \delta_{l0}), \quad (30)$$

$$V_a^d = 2\mu_0 H \sqrt{\frac{(l+1)^2 - m^2}{(l+1)l(2l+1)}}. \quad (31)$$

taken for identical values of the quantum numbers m, n, l in the initial and final states.

The matrix elements of the fine structure (energy $U^B + U^0$) are determined by the formula (see reference 1):

$$E = -\frac{Rh}{2n^2} + \Delta E; \quad (32)$$

$$\Delta E = \frac{Rh}{2n^2} \left\{ \frac{11\alpha^2}{16n^2} + \frac{4\alpha^2}{n} \varepsilon \right\},$$

The matrix elements (29), (30) and (31) are

$$\begin{aligned} \varepsilon^0 &= -\frac{1}{4(l+1/2)} && \text{for state a} \\ \varepsilon^1 &= \varepsilon^0 + \frac{7}{12}\delta_{l0} + \frac{(1-\delta_{l0})}{8(l+1/2)} \begin{cases} -\frac{1}{l(l+1)} & \text{for state b} \\ -\frac{3l-1}{l(2l-1)} & \text{for state c} \\ \frac{3l+4}{(l+1)(2l+3)} & \text{for state d} \end{cases} \end{aligned} \quad (33)$$

where ε^0 pertains to the para-state and ε^1 to the ortho-state*. Here

$$Rh = me^4 / 2\hbar^2, \quad \alpha = e^2 / \hbar c. \quad (34)$$

Solving the corresponding secular equations with the aid of the matrix elements of Eqs. (29) - (33), we can find the energy spectrum:

1. $l = 0$. Here the wave functions of the ortho-state with $m = \pm 1$ are not distorted (for $l = 0$, we have only solutions of the form d), while the wave functions of the ortho-state with $m = 0$ are distorted, whence (see also reference 10):

$$\varepsilon^H = -\frac{5}{24} \pm \sqrt{\left(\frac{7}{24}\right)^2 + \left(\frac{\mu_0 H n^3}{R\hbar\alpha^2}\right)^2}, \quad (35)$$

and the energy is found with the help of Eq. (32).

In weak fields we have the quadratic effect:

$$\varepsilon^{0H} = \varepsilon^0 - \frac{12}{7} \left(\frac{\mu_0 H n^3}{R\hbar\alpha^2}\right)^2, \quad (36)$$

$$\varepsilon^{1H} = \varepsilon^1 + \frac{12}{7} \left(\frac{\mu_0 H n^3}{R\hbar\alpha^2}\right)^2. \quad (37)$$

* It was noted by Berestetskii [e.g., see reference 10, V. B. Berestetskii, J. Exper. Theoret. Phys. USSR 19, 1130 (1949)] that for $n > 3$, it is necessary to consider the nondiagonal matrix elements of the form $V_{j-1}^{j+1} = \text{const} (r^{-3})_{j-1}^{j+1}$. As calculation shows, $(r^{-3})_{n, j-1}^{n, j+1} \equiv 0$, and therefore the validity of Eq. (33) is not limited by the condition $n < 4$.

2. $l \neq 0$. The Matrix elements (29), (30) and (31) distort the wave functions of the ortho- and para-states. The allowed values of m for a given l for the para-state are $m = 0, \pm 1, \dots, \pm l$. Therefore, the ortho-states with m which do not fall into this interval in a weak magnetic field are not distorted ($\varepsilon^{1H} = \varepsilon^1$). For the states with m falling in this interval, we have

$$\varepsilon^{0H} = \varepsilon^0 - \left(\frac{2\mu_0 H n^3}{R\hbar\alpha^2}\right)^2 \quad (38)$$

$$\times \frac{(2l+1) \{ (7l^2 + 7l - 3) - m^2(9l^2 + 9l - 3) \}}{(3l+4)(3l-1)};$$

$$\varepsilon_b^{1H} = \varepsilon_b^1 - \left(\frac{2\mu_0 H n^3}{R\hbar\alpha^2}\right)^2 \times \frac{2l-1}{3l-1} (l^2 - m^2); \quad (39)$$

$$\varepsilon_c^{1H} = \varepsilon_c^1 - \left(\frac{2\mu_0 H n^3}{R\hbar\alpha^2}\right)^2 (2l+1) m^2; \quad (40)$$

$$\varepsilon_d^{1H} = \varepsilon_d^1 + \left(\frac{2\mu_0 H n^3}{R\hbar\alpha^2}\right)^2 \frac{2l+3}{3l+4} \{ (l+1)^2 - m^2 \}, \quad (41)$$

where ε_b^{1H} (as also ε_b^1) does not exist for $|m|=l$.

4. THE ENERGY SPECTRUM OF POSITRONIUM IN A STRONG MAGNETIC FIELD

We can now consider the case of strong fields, for which $\mu_0 H > \alpha^2 e^2 / r_0$ and also $\mu_0 H < e^2 / r_0$. In this case, it is necessary to consider the energy U_1^H exactly, while the energy

$$U_2^H = \frac{e^2}{16m^2c^2} H^2 (x^2 + y^2) \quad (42)$$

can be regarded as a perturbation.

First, we consider the field for which the energy of Eq. (42) is small in comparison with the fine structure. We find the wave functions of positronium, considering the energy U_1^H .

The eigenfunctions of the commuting operators

$$\hat{H}\psi \equiv \left(\frac{p^2}{m} - \frac{e^2}{r} + \mu_0 H (\sigma_{1z} - \sigma_{2z}) \right) \psi = E\psi, \quad (43)$$

$$J_z \psi \equiv \left([\mathbf{r}\mathbf{p}]_z + \frac{\hbar}{2} \sigma_{1z} + \frac{\hbar}{2} \sigma_{2z} \right) \psi = \hbar m \psi, \quad (44)$$

$$M^2 \psi \equiv ([\mathbf{r}\mathbf{p}]^2) \psi = \hbar^2 l(l+1) \psi, \quad (45)$$

$$s_{1z} = \frac{\hbar}{2} \sigma_{1z}; \quad s_{2z} = \frac{\hbar}{2} \sigma_{2z}, \quad (46)$$

have the form

$$\psi^I = N_{l, m-1} \begin{pmatrix} Y_l^{m-1} & 0 \\ 0 & 0 \end{pmatrix} R_{n, l}, \quad (47)$$

$$\psi^{II} = N_{l, m} \begin{pmatrix} 0 & Y_l^m \\ 0 & 0 \end{pmatrix} R_{n, l}, \quad (48)$$

$$\psi^{III} = N_{l, m} \begin{pmatrix} 0 & 0 \\ Y_l^m & 0 \end{pmatrix} R_{n, l}, \quad (49)$$

$$\psi^{IV} = N_{l, m+1} \begin{pmatrix} 0 & 0 \\ 0 & Y_l^{m+1} \end{pmatrix} R_{n, l}. \quad (50)$$

Here $N_{l, m} = \sqrt{\frac{2l+1}{4\pi} \frac{1}{(l+m)!(l-m)!}}$, and $Y_l^{m'}$

and $R_{n, l}$ are written in the notation of reference 1.

The corresponding energy values are

$$E_n^{I0} = -\frac{Rh}{2n^2}, \quad (51)$$

$$E_n^{II0} = -\frac{Rh}{2n^2} + 2\mu_0 H, \quad (52)$$

$$E_n^{III0} = -\frac{Rh}{2n^2} - 2\mu_0 H, \quad (53)$$

$$E_n^{IV0} = -\frac{Rh}{2n^2}. \quad (54)$$

States I, IV correspond to spin projections directed along the z axis. The magnetic moments in these states are oppositely directed, and hence these states do not interact with the magnetic field. In states II and III, on the other hand, the magnetic moments are parallel (spins anti-parallel), and, corresponding to this case, the coefficient 2 appears in Eqs. (52) and (53).

It is easy to see that, in spite of the fact that the expressions for the energy (52), (53) depend linearly on the field, linear splittings will not be observed in the optical spectra. From Eqs. (47)-(50), it follows that the optical transitions between levels (51), (52), (53) and (54) are forbidden. Thus, in a strong magnetic field the linear Zeeman effect will not be observed in the optical spectra. The role of the magnetic field in the approximation under consideration reduces to a shifting of the levels which do not appear in the optical spectrum.

The spectrum of positronium in a strong magnetic field is, if we do not consider the fine structure, the usual spectrum of the hydrogenlike atom ($r_0 = 2\hbar^2/me^2$). However, the fine structure of the spectrum will be different than in the absence of the field, since the magnetic field changes the eigenfunctions of the stationary states [Eqs. (47)-(50)]. These functions are classified according to the values of the projection of the electron and positron spins in the direction of the magnetic field. In the computation of the matrix elements of the energy of the fine structure [Eqs. (24) and (25)] with the aid of the wave functions I, II, III and IV, it should be recalled that the states I and IV are degenerate.

We obtain the same values of the matrix elements for the energy which contains the correction for the dependence of mass on velocity (see references 1 and 14), and the energy which describes the Breit correction, as in the absence of the field (see references 1 and 10). The matrix elements of the energy of spin-orbit interaction

$$V_3 = \frac{3\mu_0^2}{\hbar r^3} [\mathbf{r}\mathbf{p}] (\vec{\sigma}_1 + \vec{\sigma}_2) \quad (55)$$

have the form

$$E_3 = \frac{Rh}{2n^2} \frac{3\alpha^2}{4n} \frac{1 - \delta_{l0}}{l(l+1)(l+1/2)} s(m-s), \quad (56)$$

where s characterizes the magnitude of the projection of the total spin in the direction of the magnetic field, and is given by

$$s = \begin{cases} 1 & \text{for state I,} \\ 0 & \text{for states II and III} \\ -1 & \text{for state IV} \end{cases} \quad (57)$$

The diagonal matrix elements of the energy of spin-spin interaction

$$V_4 = \mu_0^2 \left\{ \frac{8\pi}{3} \delta(\mathbf{r}) (\vec{\sigma}_1 \vec{\sigma}_2) + \frac{3(\vec{\sigma}_1 \mathbf{r})(\vec{\sigma}_2 \mathbf{r}) - (\vec{\sigma}_1 \vec{\sigma}_2) r^2}{r^5} \right\} \quad (58)$$

have the form

$$E_4 = \frac{Rh}{2n^2} \left\{ \frac{\alpha^2}{3n} (2s^2 - 1) \delta_{l0} - \frac{\alpha^2 (2s^2 - 1) (1 - \delta_{l0})}{8n(l+1)(l+1/2)(l+3/2)} \left[1 - \frac{3}{2} \frac{l^2 - (m-s)^2}{l(l-1/2)} \right] \right\}. \quad (59)$$

Moreover, for $l > 0$, it is necessary to consider the nondiagonal elements (58) (for the degenerate states I, IV)

$$\left(V_4 \right)_{I}^{IV} = - \frac{Rh}{2n^2} \frac{3\alpha^2}{16n} \times \frac{V(l^2 - m^2)((l+1)^2 - m^2)}{l(l+1)(l+1/2)(l-1/2)(l+3/2)}, \quad (60)$$

which express the superposition of states I and IV for values of m common to states I and IV, i.e., for

$$m = -(l-1) \dots 0 \dots (l-1). \quad (61)$$

For the remaining values of m , states I and IV are unmixed:

$$m = \pm l, \pm(l+1). \quad (62)$$

It is evident that from the matrix elements (56)-(60) that the fine structure in the case under consideration depends on the magnetic quantum number m which characterizes the magnitude of the projection of the total momentum along the direction of the magnetic field.

Finally, we get for the matrix elements of the specific exchange energy (25)

$$E_5 = \frac{Rh}{2n^2} \frac{\alpha^2}{2n} (s^2 + 1) \delta_{l0}. \quad (63)$$

Thus the exchange energy in the states with identical directions of spin projections is twice as great as the exchange energy in the states with opposed projection directions. We note for comparison that in the absence of a magnetic field, the exchange energy of the para-state is zero, while that of the ortho-state is equal to

$$E_5 = \frac{Rh}{2n^2} \frac{\alpha^2}{n}. \quad (64)$$

General formulas for the fine structure can also be obtained. From the invariance of the energy (24), (25) relative to changes of sign of the charge (electron changed to positron and vice versa) it follows that the fine structure of the two states of opposite directions of the projections is the same. We obtain the formula for the fine structure in the form

$$E = E^0 + \Delta E. \quad (65)$$

Here E^0 is defined by Eqs. (51)-(54), and

$$\Delta E = \frac{Rh}{2n^2} \left\{ \frac{11\alpha^2}{16n^2} + \frac{\alpha^2}{n} \epsilon \right\}, \quad (66)$$

where

$$\epsilon_0 = \delta_{l0} - \frac{1}{l+1/2} + \frac{1}{8(l+1)(l+1/2)(l+3/2)} \quad (67)$$

$$\times \left(1 - \frac{3}{2} \frac{(l^2 - m^2)(1 - \delta_{l0})}{l(l-1/2)} \right),$$

$$\epsilon_{1,-1} = \frac{7}{3} \delta_{l0} - \frac{1}{l+1/2} - \frac{(7l+9)(1 - \delta_{l0})}{8l(l+1)(l+1/2)(l+3/2)} \quad (68)$$

$$+ \frac{3}{16l} \frac{(1 - \delta_{l0})}{l(l+1)(l-1/2)(l+1/2)(l+3/2)}$$

$$\times [l^2 - m^2 - 1$$

$$\pm \sqrt{m^2(4l^2 + 4l - 1)^2 + (l^2 - m^2)((l+1)^2 - m^2)}].$$

The quantity ϵ_0 corresponds to opposite directions of the projections of the electron and positron spins along the magnetic field, and $\epsilon_{1,-1}$ to identical directions of the projections; the two possible signs in Eq. (68) correspond to two possible superpositions of the states with identical projection directions $[-(l-1) \leq m \leq l-1]$: for $m = l, l-1$, one takes the upper sign; for $m = -l, -(l+1)$, the lower sign (superposition is absent in the last two cases).

For the remaining states ($n = 1, l = 0$) we obtain

$$\epsilon_{1,-1} = 1/3, \quad \epsilon_0 = -5/6. \quad (69)$$

The coincidence of the fine structure of the fundamental state ($n = 1$) in a strong magnetic field with the fine structure of the lowest ortho-state in the absence of a magnetic field is connected with the parity of the mean values of the energy of

spin-spin interaction and the exchange energy (splitting at $n = 0$ is brought about only by the presence of just this interaction).

The difference ϵ_0 [see Eq. (69)] from the fine structure of the para-system for $H = 0$ ($\epsilon^0 = -2$) is connected with the appearance of a non-vanishing exchange energy ($\epsilon = 1/2$) in strong fields and with a decrease in the amount of spin-spin interaction ($\epsilon = -1/3$ instead of $\epsilon = -1$).

With the help of the wave functions obtained as a result of superposition [see Eq. (60)], the correct selection for optical spectra can easily be found:

$$\Delta l = \pm 1; \quad \Delta m = 0, \pm 1. \quad (70)$$

Furthermore, transitions from states of oppositely directed projections to states of parallel projections, and also between two different states with anti-parallel projections, are forbidden.

Transitions between two states of similarly directed projections are permitted, with the exception of the forbidden transition $m' = 0 \rightarrow m = 0$.

Finally, we consider the quadratic Zeeman effect in strong fields specified by the energy

$$U_2^H = \frac{e^2 H^2}{16 m c^2} (x^2 + y^2). \quad (71)$$

For the matrix elements U_2^H , which are computed with the aid of the wave functions (47) and (50), we obtain:

for diagonal elements

$$E_2^H = \frac{R h (2\mu_0 H n^2)^2}{2n^2 (R h)^2} \frac{5n^2 + 1 - 3l(l+1)}{16(l-1/2)(l+3/2)} \quad (72)$$

$$\times (l^2 + (m-s)^2 + l - 1);$$

for non-diagonal elements

$$(V_2^H)_{s, l}^{s, l-2} = - \frac{e^2 H^2}{64 m c^2} \quad (73)$$

$$\times \frac{V(\overline{l^2 - (m-s)^2})((l-1)^2 - (m-s)^2)}{(l-1/2)V(l+1/2)(l-3/2)} (r^2)_l^{l-2}.$$

We note that the quadratic effect of the energy (71) does not produce a splitting of the fine structure levels, since, even without taking Eq. (71) into account, the fine structure depends on the value of the magnetic quantum number m . According to Eqs. (72) and (73), the energy levels are shifted proportional to the square of the field ($\sim H^2$).

In particular, for the fundamental level ($n = 1$), the shift of all terms is identical. Starting out from this shift [Eq. (72)], we can calculate the diamagnetic susceptibility of the gas of positronium atoms (per mole):

$$\chi = - \frac{N}{\alpha} \left(\frac{\hbar}{m c} \right)^3 = - 4.67 \times 10^{-6} \text{ cm}^3. \quad (74)$$

5. STARK EFFECT IN WEAK ELECTRIC FIELDS

We obtain the energy of interaction of positronium with a constant external electric field \mathcal{E} from Eq. (23) in the form

$$U^{\mathcal{E}} = e \mathcal{E} z + \frac{e \hbar}{4 m^2 c^2} (\vec{\sigma}_1 + \vec{\sigma}_2) [\vec{\mathcal{E}} \mathbf{p}], \quad (75)$$

$$z = z_1 - z_2; \quad |\mathcal{E}| = \mathcal{E}_z = \text{const.} \quad (76)$$

As a system of unperturbed wave functions we take the wave functions of positronium in the absence of external fields. These are found, for example, in reference 1. In weak fields it is sufficient to calculate the matrix elements of the first term of Eq. (75). The matrix element of transition between states corresponding to the values of quantum numbers $s, n, m, l, j \rightarrow s', n', m', l', j'$ we denote by $V_{s, n, m, l, j}^{s', n', m', l', j'}$, in which the index s pertains to the states a, b, c, d (notation in reference 1). We get

$$V_{a, n, m, l, l}^{b, n, m, l+1, l} \quad (77)$$

$$= - \frac{3}{2} m n e \mathcal{E} r_0 \frac{(1 - \delta_{l0})}{V l (2l+1)} \sqrt{\left(\frac{n}{l+1} \right)^2 - 1};$$

$$V_{c, n, m, l, l}^{b, n, m, l-1, l-2} = V_{c, n, m, l, l}^{d, n, m, l+1, l+2} = 0; \quad (78)$$

$$V_{c, n, m, l, l}^{d, n, m, l-1, l} \quad (79)$$

$$= \frac{3}{2} m n e \mathcal{E} r_0 \frac{(1 - \delta_{l0})}{V (l+1) (2l+1)} \sqrt{\frac{n^2}{l^2} - 1};$$

$$V_{b, n, m, l, l-1}^{d, n, m, l+1, l+2} = 0; \quad (80)$$

$$V_{b, n, m, l, l-1}^{d, n, m, l-1, l} \quad (81)$$

$$= - \frac{3}{2} n e \mathcal{E} r_0 \frac{(1 - \delta_{l0})}{(2l+1)(2l-1)} \frac{V \overline{l^2 - m^2}}{(2l+1)(2l-1)} \sqrt{\frac{n^2}{l^2} - 1};$$

$$V_{a, n, m, l, l}^{a, n, m, l+1, l+1} = -\frac{3}{2} ne \mathcal{E} r_0 \frac{V[(l+1)^2 - m^2][n^2 - (l+1)^2]}{V(2l+1)(2l+3)}; \tag{82}$$

$$V_{b, n, m, l, l-1}^{b, n, m, l+1, l} = -\frac{3}{2} ner_0 \mathcal{E} \sqrt{\frac{l+1}{l}} \frac{(1 - \delta_{l0})}{2l+1} \sqrt{(l^2 - m^2)} \sqrt{n^2 - (l+1)^2}; \tag{83}$$

$$V_{c, n, m, l, l}^{c, n, m, l+1, l+1} = -\frac{3}{2} ner_0 \mathcal{E} \frac{V(l+1)^2 - m^2 \sqrt{n^2 - (l+1)^2} V(l+2)}{(l+1) V(2l+1)(2l+3)}; \tag{84}$$

$$V_{d, n, m, l, l+1}^{d, n, m, l+1, l+2} = -\frac{3}{2} ner_0 \mathcal{E} \sqrt{\frac{l+1}{l+2}} \frac{V(l+2)^2 - m^2}{2l+3} \sqrt{n^2 - (l+1)^2}, \tag{85}$$

where

$$r_0 = 2\hbar^2/me^2.$$

Inasmuch as the projection of the total momentum along the z axis is preserved in an electric field, the matrix elements for different m vanish.

In addition to the matrix elements (77)-(85), we must also consider the matrix elements of the fine structure (33). This permits us to examine the Stark effect in weak and strong fields.

We consider a weak electric field ($er_0 \mathcal{E} n^3 / 2R\hbar\alpha^2 \ll 1$). Inasmuch as there is no l degeneracy in positronium, in contrast to hydrogen-like atoms, the linear Stark effect will not be observed in weak fields, except for the multiple levels n^3P_2 and n^3D_2 , which are split, proportional to the field, into five equally spaced levels.

In the calculation of the Stark effect in weak fields, we shall obtain an approximate solution

of the cumbersome secular equation by expanding ΔE in powers of \mathcal{E} (the electric field):

$$\Delta E_\sigma^m = E_\sigma + \lambda_\sigma^m \mathcal{E} + \mu_\sigma^m \mathcal{E}^2, \tag{86}$$

where E_σ is the fine structure energy (the index denotes the term of the fine structure); furthermore, the amount of splitting depends on the characteristic values m of the projection of the total momentum in the direction of the field. The quantities λ_σ^m , with the exception of those for the states n^3P_2 and n^3D_2 , are equal to zero. We obtain the following formulas for splitting:

1. For $n = 1$, splitting is absent;
2. For $n > 1$, we have

$$\Delta E_\sigma^m = E_\sigma + \epsilon_\sigma^m \frac{2R\hbar\alpha^2}{n^3} \left(\frac{e\mathcal{E}r_0 n^3}{2R\hbar\alpha^2} \right)^2, \tag{87}$$

where ϵ_σ^m is given by Table I.

TABLE I

$\sigma \backslash m$	0	± 1	± 2	± 3
2^1S_0	-27	×	×	×
2^3P_0	-36 : 5	×	×	×
2^3P_1	0	-108 : 7	×	×
2^1P_1	27	0	×	×
2^3P_2	-720 : 23	-540 : 23	0	×
2^3S_1	4428 : 115	6264 : 161	×	×
3^3S_0	-162	×	×	×
3^3P_0	-18468 : 115	×	×	×
3^3P_1	-405 : 2	-41553 : 112	×	×
3^1P_1	-243	-1215 : 4	×	×
3^3D_1	4779 : 46	1863 : 16	×	×
3^3P_2	-42795 : 46	7485 : 23	-210	×
3^3D_2	405 : 2	7485 : 23	-210	×
3^1D_2	405	1215 : 4	0	×
3^3D_3	756	672	420	0
3^3S_1	26568 : 115	37584 : 161	×	×

Equation (87) does not take into account the linear Stark effect for the multiple levels n^3P_2 and n^3D_2 , for which there is an additional energy, besides that of Eq. (87):

$$\Delta E = \frac{V\sqrt{3}}{4} me \mathcal{E} r_0 \sqrt{\frac{n^2-4}{5}}, \quad (88)$$

where $m = 0, \pm 1, \pm 2$, while the wave functions of the states n^3P_2 and n^3D_2 are mixed for $m = \pm 1, \pm 2$. For the case $m = 0$, the wave functions are not mixed, and the level is not shifted. However, in the following approximation (the effect proportional to \mathcal{E}^2) this multiple level divides into two, corresponding to the states n^3P_2 and n^3D_2 .

6. THE STARK EFFECT IN STRONG ELECTRIC FIELDS

Neglecting the fine structure, we can write

$$\left(E + \frac{e^2}{r} - \frac{p^2}{m} - e\mathcal{E}z \right) \psi = 0. \quad (89)$$

Then, in the first approximation of excitation theory, we have

$$E = -\frac{Rh}{2n^2} + 3 \frac{\hbar^2}{me^2} e\mathcal{E}n(n_1 - n_2). \quad (90)$$

Here $n_1 - n_2$ is the electric quantum number. Thus, in strong electric fields (as also in hydrogen-like atoms) the linear Stark effect must be considered. By virtue of Eq. (90), this effect is four times larger, in relative units, in positronium than in hydrogen (correspondingly, the quadratic Stark effect is 16 times larger, and the third order effect 64 times larger).

To find the fine structure of the Stark effect in strong fields, we solve the secular equation with the matrix elements (77)-(85) and (33), (34) in an approximation distinct from Eq. (86), expanding the desired difference in a power series inverse in the field:

$$\begin{aligned} \Delta E_k^m = \Delta E_h + \frac{Rh}{2n^2} \left\{ \frac{11}{16} \frac{\alpha^2}{n^2} - \frac{4\alpha^2}{n} \varepsilon_k^m \right\} \\ + \lambda_k^m \left(\frac{2Rh\alpha^2}{n^3 e r_0 \mathcal{E}} \right)^2 \frac{2Rh\alpha^2}{n^3} + \dots \end{aligned} \quad (91)$$

Here ΔE_k is determined by Eq. (90). The third and subsequent terms of Eq. (91) describe the field-dependent fine structure. In the approximation

under discussion ($2Rh\alpha^2/n^3 e r_0 \mathcal{E} \ll 1$) this represents a very small correction to the field-independent fine structure which is described by the second term of Eq. (91).

We shall write out here only the quantities ϵ_k^m for the field-independent part of the fine structure. For ϵ_k^m we have Table II ($n = 1, 2, 3$)*.

For certain levels ($2^3P_2, 2^1P_1, 2^3P_1, 3^3D_3, 3^1D_2$) there exist such states ($m = \pm 2, \pm 1, 0, \pm 3, \pm 2$, correspondingly) which do not interact with the electric field. They therefore pertain to fixed Stark components for the levels of the fine structure. The fine structure of these levels, in contrast to the rest, do not depend on the field at all. For the remaining Stark components ($\Delta E_k = \pm 3 e r_0 \mathcal{E}, \pm \frac{1}{2} e r_0 \mathcal{E}, \pm 9 e r_0 \mathcal{E}, \dots$), the coincidence of the fine structure for components of different sign takes place only if we do not consider the field-dependent part of the fine structure. For $n = 2$, the central component is split into 5 sublevels, and the edge component into 3. For $n = 3$, the central component splits into 7 levels, the next into 5, and the edge into 3, etc.

7. PROBABILITIES OF ANNIHILATION OF POSITRONIUM IN EXTERNAL ELECTRIC AND MAGNETIC FIELDS

We first consider the probability of annihilation in an electric field. It is easy to see that the matrix elements of the energy U of interaction of the positronium atom with external electric field [see Eq. (75)] are diagonal relative to the spin variable. Therefore, the electric field does not produce transitions between the ortho- and para-states (does not mix them). The para-states are annihilated into two photons, the ortho-states into three (see references 2 and 5). The change in the annihilation probability for the presence of an electric field is connected with the fact that the electric field changes the value of the quantum number l , whereas the annihilation is possible only for $l = 0$. The mixing can be found from the secular equations which are solved above. We note that for $n = 1$ the linear Stark effect is absent, and the probability of annihilation of these levels does not change upon the inclusion of the electric field. For much higher levels ($n > 1$), we have

$$\psi_\sigma^m = \sum_{\sigma'} C_{\sigma\sigma'}^m \psi_{\sigma'}. \quad (92)$$

* The value of ϵ for 3^3D_3 is not included in the Table and is determined by Eq. (33).

TABLE II

n	$\Delta E h$	m		
		0	± 1	± 2
2	0	$\frac{31}{120}, \frac{5}{24}$	$\frac{19}{120}, \frac{1}{6}$	$\frac{13}{120}$
2	$\pm 3e r_0 \mathcal{E}$	$\frac{1}{20}, \frac{1}{3}$	$\frac{3}{80}$	\times
3	0	$\frac{17}{420}, \frac{7}{30}$	$\frac{69 \pm \sqrt{1373}}{840}$	$\frac{41}{420}, \frac{1}{10}$
3	$\pm \frac{9}{2} e r_0 \mathcal{E}$	$\frac{19}{120}, \frac{157}{840}$	$\frac{737}{7560}, \frac{2}{15}$	$\frac{41}{420}$
3	$\pm 9e r_0 \mathcal{E}$	$\frac{17}{210}, \frac{4}{15}$	$\frac{287}{3780}$	\times

TABLE III

σ	m	α		
		± 2	± 1	0
2^3S_1	\times	\times	$-\frac{4546368}{25921} w_3$	$-\frac{2388528}{13225} w_3$
2^3P_2	0	\times	$\frac{64800}{529} w_3$	$\frac{86400}{529} w_3$
2^1P_1	\times	\times	0	$81w_2$
2^3P_1	\times	\times	$\frac{2592}{49} w_3$	0
2^3P_0	\times	\times	\times	$\frac{432}{25} w_3$
2^1S_0	\times	\times	\times	$-81w_2$

Here m is the magnetic quantum number and the index σ denotes the state a, b, c, d (see reference 1). The coefficients $C_{\sigma\sigma'}^m$ can be found in the two cases under consideration: weak and strong fields.

By way of an example, we take the case $n = 2$. In computing the annihilation probability, it is sufficient to know $|C_{S, 2S_{1/2}}|^2$. In weak fields, we will classify the state with the aid of symbols in the absence of the field. The changes in annihilation probability can be found by means of the formula

$$\Delta w_{\sigma}^m = \alpha_{\sigma}^m \left(\frac{4 e r_0 \mathcal{E}}{R h \alpha^2} \right)^2, \tag{93}$$

where the α_{σ}^m are given in Table III.

Here w_3 and w_2 are the probabilities of three photon and two photon annihilation for $n = 2$. The change in the annihilation probability, compared with the case $\mathcal{E} = 0$, is proportional to the square of the electric field, and depends on the position of the level of the fine structure [the numerical coefficients in Table III correspond to Eq. (33)].

As was shown in reference 1, the states 2^3S_1 and 2^1S_0 are metastable in relation to the optical transitions. Annihilation is much more probable for them, since their lifetimes are $8\tau_3$ and $8\tau_2$, respectively, whereas τ_3 and τ_2 are the lifetimes of the fundamental state of positronium ($n = 1$), relative to three photon (ortho-positronium) and

two photon (para-positronium) annihilation.

With the inclusion of the electric field the levels 2^2S_1 and 2^1S_0 cease to be metastable relative to optical transitions. An estimate, made with the aid of Eq. (92), shows that the metastability is removed for relatively weak fields, when the energy in the external electric field is approximately an order of magnitude smaller than the splitting of the fine structure. In strong electric fields, we find that, for $n = 2$, the annihilation probability of the central Stark component (states of five levels in the fine structure) is zero. The edge Stark components consist of three sublevels, one of which corresponds to para-state, the other two to ortho-state. For the annihilation probability of the para-level ($E \sim \pm 3er_0 \mathcal{E}$) we get $\frac{1}{2}w_2$, and for the ortho-level $\frac{1}{2}w_3$, where w_2 and w_3 are the two and three photon annihilation probabilities in the absence of the field. Thus, in a strong electric field the lifetime, relative to annihilation, is the same for para-positronium as for ortho-positronium ($n = 2$).

We now consider the case of a magnetic field. The effect of a weak magnetic field on the annihilation probability was investigated in reference 1. In a strong magnetic field, the spin states of positronium are characterized by the magnitudes of the projections of the electron and positron spins in the direction of the magnetic field. It is easy to see⁵ that the lifetime of the fundamental state, with oppositely directed spin projections on the magnetic field, relative to two photon annihilation, is twice as large as for $H = 0$:

$$\tau_2^H = 2.5 \times 10^{-10} \text{ sec.} \quad (94)$$

Moreover, the states of opposing projection directions can annihilate into three photons, whence the

lifetime of the fundamental state ($n = 1$) relative to three photon annihilation is twice as great as the lifetime of ortho-state for $H = 0$:

$$\tau_3^H = 2.8 \times 10^{-7} \text{ sec.} \quad (95)$$

One out of about 1120 atoms with states having uniform directions of projections decays into three photons. From the selection rule (70), it is easy to see that the S states for $n = 2$ are metastable relative to the optical transitions. Because of this, their annihilation is much more probable. The lifetimes, relative to the two and three photon annihilations, of the metastable ($n = 2$) state with opposing directions of spin projections are equal to

$$\tau_2^{1H} = 2 \times 10^{-9} \text{ sec and } \tau_3^{1H} = 2.24 \times 10^{-6} \text{ sec.} \quad (96)$$

For states with uniform directions of projections, two photon annihilations are forbidden. The lifetime relative to three photon annihilation for the fundamental state ($n = 1$) is

$$\tau_3 = 1.4 \times 10^{-7} \text{ sec} \quad (97)$$

and for the metastable state ($n = 2$)

$$\tau_3^1 = 1.12 \times 10^{-6} \text{ sec} \quad (98)$$

are equal to the corresponding times for $H = 0$.

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