Level Shifts in Helium. Three Body Forces

G. F. FILIMONOV
Moscow State University

(Submitted to JETP editor November 13, 1955
J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 311–315 (February, 1957)

A fourth order expression containing three–body forces is obtained for a two–field interaction Hamiltonian. An expression is obtained for the energy matrix element of triple collisions between two electrons and an α-particle, and computations are performed for the $1^1 S$ state of helium. The resulting shift is found to be 1.02 ± 0.15 cm^{-1} and does not remove the discrepancy between theory and experiment. Some effects which might be invoked to bring the theory into agreement with experiment are discussed.

THE presence of a three–body interaction in a system of three particles does not lead to divergences and the Hamiltonian is conveniently written in the Schrödinger representation. In order to do this, let us apply Eq. (1.8) of a previous article* for $N=4$ [2].

$$(i\partial/\partial t + \mathcal{H}_3)\psi(\mathbf{r}, t) = 0; \qquad (1)$$

$$\mathcal{H}_3 = e^{-iS_3}[e^{-iS_2}(e^{-iS_1}\mathcal{H}e^{iS_1})e^{iS_2}]e^{iS_3}.$$

As in Ref. 1, the resulting Hamiltonian for the system

$$\mathcal{H} = H_0 + H_1^{tr} + H_2^l,$$

contains the Hamiltonians for the free fields (H_0), the interaction of the particles with transverse photons (H_1^{tr}), and the Coulomb interaction (H_2^l). In the case of helium, these terms (excluding their operators S_k (see reference 1) consist of the following parts:

$$H_0 = H_{0e} + H_{0\alpha} + H_{0\gamma}, \quad H_1^{tr} = H_{1e}^{tr} + H_{1\alpha}^{tr};$$
$$S_1 = S_{1e} + S_{1\alpha}, \quad H_2^l = H_{2ee}^l + H_{2\alpha\alpha}^l + H_{2e\alpha}^l;$$
$$S_2 = S_{2ee} + S_{2\alpha\alpha} + S_{2e\alpha},$$

where H_{0e}, $H_{0\alpha}$, $H_{0\gamma}$, are respectively the Hamiltonians for free electrons, α-particles, and photons; H_{1e}^{tr}, $H_{1\alpha}^{tr}$ and H_{2ee}^l, $H_{2\alpha\alpha}^l$, $h_{2e\alpha}^l$ are the Hamiltonian interactions for electrons and α-particles with transverse photons, and the Coulomb interaction between electrons, between α-particles, and between electrons and α-particles.

It follows from Eq. (2) that the 1st and 2nd order Hamiltonians, even for two fields interacting through a third, consist of physically different types of terms. Thus, expanding the phase factors in $\mathcal{H}_3$ into $S_1, S_2, \ldots$, leads to a complicated expression in which the same processes are denoted by terms of different structure. For example, the transverse part of the two–body interaction between electrons and α-particles consists in this case of two terms.

$$-\frac{i}{2}[S_{1e}, H_{1\alpha}^{tr}] - \frac{i}{2}[S_{1\alpha}, H_{1e}^{tr}].$$

The expression for the 4th order Hamiltonian may be rid of redundant terms and thereby simplified in the following manner; instead of expanding Eq. (1) in terms of $S_1, S_2 \ldots$, expand it first in terms of S_{1e} for example, then $S_{1\alpha}$, $S_{2e\alpha}$, $S_{2\alpha\alpha}$ and so on. The transverse part of the two body interaction then becomes

$$-i[S_{1e}, H_{1\alpha}^{tr}].$$

Carrying out such an expansion of the phase factors in Eq. (1), leads to the following expression for H_4

$$H_4 = H_{4ee} + H_{4\alpha\alpha} + H_{4e\alpha}, \qquad (3)$$

where

$$H_{4ee} = \frac{(-i)^2}{2!}\Big[S_{1e}, \Big[S_{1e}, H_{2ee}^l - \frac{i}{4}[S_{1e}, H_{1e}^{tr}]\Big]\Big] - \frac{i}{2}[S_{2ee}, H_{2ee}], \qquad (4)$$

$$H_{4\alpha\alpha} = \frac{(-i)^2}{2!}\Big[S_{1\alpha}, \Big[S_{1\alpha}, H_{2\alpha\alpha}^l - \frac{i}{4}\Big[S_{1\alpha}, H_{1\alpha}^{tr}\Big]\Big]\Big] - \frac{i}{2}[S_{2\alpha\alpha}, H_{2\alpha\alpha}] \qquad (5)$$

describe the interactions of electrons and α-particles among themselves and with transverse photons (H_{4ee} and $H_{4\alpha\alpha}$ differ only in their indices); the term

*Here and below, we use the notation of Ref. 1, without further comment.

quired matrix element

$$\Delta^3 E_n = \langle n | : H'_{4e\alpha} : | n \rangle, \qquad (10)$$

which represents the correction to the nth energy level of a helium atom due to three-body forces. Expression (3) is too complex and cannot be solved exactly. Therefore we shall take advantage of the smallness of the effect we are investigating, and we shall simplify (10) by replacing : $H'_{4e\alpha}$: by its nonrelativistic approximation. It is convenient to use the diagonal representation of the field operators, wherein the Hamiltonian for the free photons is in diagonal form.*

Carrying out the required transformation, we find

$$\Delta^3 E_n = \frac{-Zq^4}{(4\pi)^3 m} \int dx_1\, dx_2\, dx_4 \qquad (11)$$

$$\times \Bigg\{ 4 \frac{\partial}{\partial x_{4i}} \psi^*_{ab}(x_2, x_{41}) \frac{\partial}{\partial x_{2j}} \psi_{ab}(x_{21}, x_4)$$

$$\times \left(\frac{1}{x_4} - \frac{1}{x_2}\right) \varepsilon\,(x_{24} x_1^0) \frac{\delta_{ij} - x^0_{1i} x^0_{1j}}{x_1^2}$$

$$- 2i \Bigg[\frac{\partial}{\partial x_4} \psi^*_{ab}(x_2, x_{41}) \left(\frac{[x_1^0 \sigma_a]}{x_4} - \frac{[x_1^0 \sigma_b]}{x_2} \right)$$

$$+ \psi^*_{ab}(x_2, x_{41}) \left(\frac{[x_1^0 \sigma_b]}{x_4} - \frac{[x_1^0 \sigma_a]}{x_2} \right) \frac{\partial}{\partial x_2} \Bigg]$$

$$\times \psi_{ab}(x_{21}, x_4) \frac{\delta\,(x_{24} x_1^0)}{x_1^2}$$

$$+ \frac{\partial}{\partial x_2} \left(\psi^*_{ab}(x_2, x_{41}) [\sigma_a [x_1^0 \sigma_b]] \psi_{ab}(x_{21}, x_4) \right)$$

$$\times \left(\frac{1}{x_4} - \frac{1}{x_{41}} \right) \frac{\delta\,(x_{24} x_1^0)}{x_1^2} \Bigg\},$$

where $\delta\,(a)$ is a delta function, $\epsilon\,(a)$ is a sign function, and $\psi_{ab}\,(x_2, x_4)$ is the wave function for a three particle system in the center of mass coordinates. Its space part may be identified for the $1^1 S$ state of helium with the Hylleraas function or with the screened wave function. There is no sense in using Hartree's method in Eq. (11), for although this method yields the best value to the zero approximation E_n^0, it leads to nonorthogonal wave functions and various potentials for the electrons thus excluding a consistent application of perturbation theory.

The integrals in (11) are very complicated and can only be evaluated approximately. They were computed graphically for the $1^1 S$ state of helium making use of the three–term Hylleraas functions and it was found that

$$\Delta^3 E = (1.02 \pm 0.15)\ \text{cm}^{-1}, \qquad (12)$$

which is beyond the present limits of experimental uncertainty.

The main contribution to this quantity arises from the third term of (11), and is due to the spin–spin part of the interaction. It contributes 1.1 ±0.13 cm^{-1} to $\Delta^3 E$.

The first term in (11) represents the orbit–orbital part of the interaction, and yields a small correction to this quantity, viz., –0.09 ± 0.03 $cm.^{-1}$ The second term of (11) represents the spin–orbital part of the interaction and cannot contribute to a shift of the stationary levels.

The experimental value of the ionization potential for the $1^1 S$ level of helium is I_0 = 198313 ± 5 cm^{-1} , while latest computations[8,9] lead to theoretical value I_0' = 198304 cm^{-1} if one uses the best value of E_n^0 obtained from an eight–term Hylleraas wave function.

The correction (12) computed in the present article decreases the value of I_0' to

$$I_0'' = I_0' - \Delta^3 E_{1^1S} = 198303\ \text{cm}^{-1} \qquad (13)$$

and cannot bring theory in accord with experiment.

It should be noted that (13) does not by any means contain all 4th order relativistic corrections: Thus, we have not included the effect of the interaction of the atomic electrons through vacuum polarization [see Eq. (4a)] which partly explains discrepancy with experiment. A second important reason for the difference between experimental and theoretical values of I_0 , is that while the Ritz variational method which was used for finding E_n^0 leads to an increase in the absolute value of E_n^0 , there is at present no way of estimating the degree of discrepancy between the value found for E_n^0 and the actual minimum of the Ritz functional. Thus, when comparing the theoretical and experimental values of the $1^1 S$ energy level of helium, it seems in order to use the results obtained with the eight–term function and the corresponding minimal $|E_n^0|$.

In connection with this, there is another important effect which may be responsible for the difference between the experimental and theoretical values of I_0. It consists in the fact that the relativistic

*As is well known, the transition to this representation can be made in thecase of spinors with the aid of the unitary transformation.

$$H_{4e\alpha} = \frac{(-i)^2}{2!}\left[S_{1e}, \left[S_{1e}, H^l_{2e\alpha} - \frac{i}{3}[S_{1e}, H^{tr}_{1\alpha}]\right]\right] + (-i)^2\left[S_{1\alpha}, \left[S_{1e}, H^l_2 - \frac{i}{2}\left[S_{1e}, \frac{2}{3}H^{tr}_{1e} + H^{tr}_{1\alpha}\right]\right]\right] + \frac{(-i)^2}{2!}[S_{1\alpha}, [S_{1\alpha}, H_{2ee} + H_{2e\alpha}]] - i[S_{2ee}, H_{2e\alpha} + H_{2\alpha\alpha}] - i\left[S_{2e\alpha}, \frac{1}{2}H_{2e\alpha} + H_{2\alpha\alpha}\right] \tag{6}$$

describes the interaction between electrons and α-particles, and free photons among themselves. Note that the particular nature of the fields e, α, γ have not yet been specified in equations (3) to (6), and these expressions may be used for describing the general interaction of two fields in the 4th order.

We shall now make use of the Hamiltonian H_4 to obtain the relativistic corrections to the terms of the helium atom. As is well known, the wave functions for He and the zero-order approximation eigenvalues E_n^0 of the Hamiltonian operator are obtained in the Coulomb interaction approximation (see for example Ref. 3). We must therefore omit from Eqs. (3) to (6) all the terms which include only longitudinal components as these have already been included in the zero order approximation. This may be achieved by replacing everywhere S_2 by S_2^{tr}. The Hamiltonian H_4' obtained in this fashion represents a small correction to $(H_0 + H_2^l)$ and is of the same order of magnitude ($\sim 1\ \mathrm{cm}^{-1}$) as the experimental uncertainty. In computing the matrix elements $\langle n | H_4' | n \rangle$, it is justified to keep only the largest terms in H_4', specifically those terms which contain the time component of the current of α-particle, in as much as the terms containing the space components of the current of α-particles lead to a correction ΔE_n which is far below the limits of experimental detection.

Accordingly, we can write the following approximate expression for the component of H_4' capable of producing in helium a measurable change in E_n°:

$$H'_{4ee} \approx \frac{(-i)^2}{2!}\left[S_{1e}, [S_{1e}, H^l_{2ee}]\right] - \frac{i}{2}[S^{tr}_{2ee}, H^l_{2ee}]; \tag{4a}$$

$$H'_{4\alpha\alpha} \approx 0; \tag{5a}$$

$$H'_{4e\alpha} \approx \frac{(-i)^2}{2!}[S_{1e}, [S_{1e}, H^l_{2e\alpha}]] - i[S^{tr}_{2ee}, H^l_{2e\alpha}]. \tag{6a}$$

The effect of triple collisions of an α-particle and two electrons will be included in $H'_{4e\alpha}$. As already stated, it does not lead to an "ultraviolet catastrophe" and can conveniently be written in the Schrödinger representation. The operators which appear in it have the following explicit form (see Refs. (1) and (4):

$$S_{1e} = \frac{-q}{4i\pi^{3/2}} \times \int \frac{d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{k}}{\sqrt{k}}\,\delta(\mathbf{k} - \mathbf{p}_{12})\,\frac{a_i(\mathbf{k})\,\psi_1^*\alpha_i\psi_2 - a_i^*(\mathbf{k})\,\psi_2^*\alpha_i\psi_1}{k - \varepsilon_1 + \varepsilon_2}, \tag{7}$$

$$S^{tr}_{2ee} = \frac{-q^2}{4i(2\pi)^3}\int \frac{d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{p}_3 d\mathbf{p}_4}{p_{12}}\,\delta(\mathbf{p}_{12} + \mathbf{p}_{34}) \times :\frac{\psi_1^*\alpha_i\psi_2\psi_3^*\alpha_j\psi_4 - \psi_4^*\alpha_j\psi_3\psi_2^*\alpha_i\psi_1}{\varepsilon_2 + \varepsilon_4 - \varepsilon_1 - \varepsilon_3}:\frac{\delta_{ij} - p^0_{12i}p^0_{12j}}{p_{12} - \varepsilon_1 + \varepsilon_2} + A; \tag{8}$$

$$H^l_{2e\alpha} = \frac{-Zq^2}{(2\pi)^3} \times \int \frac{d\mathbf{p}_1 d\mathbf{p}_2 d\mathbf{P}_1 d\mathbf{P}_2}{p_{12}^2}\,\delta(\mathbf{p}_{12} + \mathbf{P}_{12}) : \psi_1^*\psi_2\Phi_1^*\Phi_2 : \frac{E_1 + E_2}{2\sqrt{E_1E_2}}. \tag{9}$$

Here and from now on, $a_i(\mathbf{k})$ denotes an annihilation operator for transverse photons with momentum $\mathbf{k}$, polarized in the i direction ($i = 1,2,3$); $\psi_{k\alpha} = \psi_\alpha(\mathbf{p}_k)$ ($\Phi_{k\alpha} = \Phi_\alpha(\mathbf{P}_k)$) denote annihilation operators for electrons (α-particles) with momentum $\mathbf{p}_k$ ($\mathbf{P}_k$); A which appears in S^{tr}_{2ee} contains the photon operators; the two dot symbols denotes a normal product of field operators;

$$\mathbf{p}_{ab} = \mathbf{p}_a - \mathbf{p}_b, \quad \mathbf{p}^0_\alpha = \mathbf{p}_\alpha / p_\alpha;$$

$$E_k = \sqrt{\mathbf{P}_k^2 + M^2}, \quad \varepsilon_k = \pm\sqrt{\mathbf{p}_k^2 + m^2};$$

M, m are the masses of the α-particles and the electrons; α, β are Dirac matrices; ab, $[ab]^{\cdot}$, $[abc]$ denote respectively scalar vector, and triple scalar products; the units are such that $c = \hbar = 1$, $q = \sqrt{4\pi}$.

Substituting operators (7) to (9) into Equation (6a), and keeping only normal products, we find the recorrections contained in (13), were computed with a simple Hylleraas function instead of the eight–term function; thus there is no guarantee that the value of some of these terms would not change if they were evaluated with an eight–term function. This is especially true of the orbit–orbital part of the 2nd order relativistic correction,[8] where not only the magnitude, but even the sign depends on the choice of wave function. Furthermore, one should evaluate more correctly the Lamb shift in the electric field of the nucleus; this has been done so far using screened wave functions.

As for the relativistic corrections whose sign does not depend on the choice of wave function, for example the spin–spin part of the two and three–body interactions, it may be expected that the use of an eight–term Hylleraas function instead of the simpler one will not produce a noticeable change in the numerical values of these small quantities; this is indicated, for example, by the fact that in computing E_n^0 with various Hylleraas functions, the results were found to differ only in the fourth place.

On the basis of this analysis it may be expected that including the effects discussed above will lead to agreement between theoretical and experimental value for I_0 within the limits of experimental accuracy.

In conclusion the author wishes to express his gratitude to Iu. M. Shirokov for his continued interest in this analysis and to V. N. Ts'itovich for checking the formula.

---

1 G. F. Filimonov and Iu. M. Shirokov, J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 99 (1957); Soviet Phys. JETP 5, 84 (1957).

2 Here and below we use the notation of Ref. 1 without further explanation.

3 H. Bethe, *Handbuch der physik* (J. Springer, Berlin, 1933), Vol. 24, No. 1.

4 G. Wentzel, *Quantum Theory of Fields* (Intersciences Publishers, Inc., New York, 1949).

5 H. S. Snyder, Phys. Rev. 78, 98 (1950).

6 As is well known, this may be realized in the case of spinors by means of a unitary transformation [see L. L. Fouldy and S. A. Wouthuysen, Phys. Rev. 78, 29 (1950)].

7 J. Hopfield, Astrophys. J. 72, 133 (1930).

8 A. M. Sessler and H. M. Foley, Phys. Rev. 92, 1321, 1322 (1953).

9 H. A. S. Eriksson, Z. Physik 109, 762 (1938).

10 Chandrasekhar, Elbert, and Herzberg, Phys. Rev. 91, 1172 (1953).

Translated by M. A. Melkanoff
65

SOVIET PHYSICS JETP VOLUME 5, NUMBER 2 SEPTEMBER, 1957

Non-Linear Theory of Betatron Oscillations in a Strong Focusing Synchrotron

Iu. F. Orlov

(Submitted to JETP editor November 15, 1955)
J. Exptl. Theoret. Phys. (U.S.S.R.) 32, 316–322 (February, 1957)

A new method has been developed for investigating betatron resonances. Parametric resonances are investigated.

---

1. EQUATIONS OF MOTION

THE equations describing betatron oscillations about some plane periodic orbit in a strong focussing synchrotron[1] have the following form:

$$\frac{d^2r}{d\theta^2}+\frac{1}{P}\left(\frac{l}{2\pi}\right)^2\frac{\partial H}{\partial r}r =\frac{1}{P}\left(\frac{l}{2\pi}\right)^2\left\{\frac{1}{\rho}(P-\rho H_0)-\delta\left(\frac{\partial H}{\partial r}\right)r -\frac{\partial H}{\partial z}z -\sum_{n\geqslant 2}\frac{\partial^n H}{\partial r^n}\left[\frac{r^n}{n!}-\frac{r^{n-2}z^2}{2!\cdot(n-2)!}+\frac{r^{n-4}z^4}{4!\,(n-4)!}-\cdots\right]\right\}; \quad (1)$$

$$\frac{d^2z}{d\theta^2}-\frac{1}{P}\left(\frac{l}{2\pi}\right)^2\frac{\partial H}{\partial r}z=\frac{1}{P}\left(\frac{l}{2\pi}\right)^2\left\{H_{\rho_0}+\delta\left(\frac{\partial H}{\partial r}\right)z -\frac{\partial H}{\partial z}r+\sum_{n\geqslant 2}\frac{\partial^n H}{\partial r^n}\left[\frac{r^{n-1}z}{(n-1)!}-\frac{r^{n-3}z^3}{3!\,(n-3)!}+\cdots\right]\right\}, \quad (2)$$

where r denotes the radial and z the vertical deviation of the particles from their periodic orbit; $\rho(\theta)$ is the radius of the orbit. The "angle" θ changes by 2π over a period length l; $\partial H/\partial r$ is the gradient of the magnetic field, $\delta(\partial H/\partial r)$ is the error in the gradient; $1/P = e/cp$, where p is the momentum of the particles. The series of unessential terms in (1) and (2) are discarded; we neglect H_θ in the frequency.