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The Lamb Shift in Helium from a Self-Consistent Field Theory of Electrodynamics

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Abstract

In this paper we present the results of an investigation of the finite self-consistent field theory of electrodynamics applied earlier to the calculation of the Lamb shift in hydrogen (Sachs & Schwebel, 1961; Sachs, 1972), now applied to the problem of the Lamb shift in the low-lying states of Helium. We construct the covariant nonlinear field equations of this theory for Helium, from the Lagrangian formalism. In the linear approximation, the Hamiltonian associated with this field theory for the two-electron atom is set up. It is equivalent to the Breit Hamiltonian plus two extra terms. This generalization is a direct consequence of the two-component spinor formalism of the factorization of the Maxwell theory of electromagnetism that is contained in this theory of electrodynamics (Sachs, 1971). Thus, the energy spectrum predicted for the Helium atom is the spectrum predicted by the Breit Hamiltonian, shifted by amounts in the different energy states according to the effects of the extra terms in the Hamiltonian. The latter can be associated with the corrections to the Helium spectrum that are conventionally attributed to the Lamb shift. The level shifts for the 1^1S and 2^3S states are calculated using the Foldy-Wouthuysen transformation, with the generalization of Charplvy for the two-electron atom. The results are found to be in close agreement with the experimental values for the energy shifts not predicted by the Dirac theory, and with the theoretical values predicted by quantum electrodynamics.

1. *Introduction*

In order to display the success of the present-day theory of quantum electrodynamics, one need but mention the calculations of the Lamb shift and the anomalous magnetic moment of the electron. However, the theory does suffer from some undesirable features. First, divergences appear which must be removed by the renormalization method—a scheme of calculation that is not demonstrably mathematically consistent. Second, the formalism of quantum electrodynamics does not give results in closed form.

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The self-consistent field theory of electrodynamics developed by Sachs (1972) and Sachs & Schwebel (1961) has been applied to the hydrogen atom and shows that the extra energy levels associated with the Lamb splitting are naturally predicted by the theory. This is due to extra terms that appear in the field equations. The existence of these terms is a consequence of the factorization of Maxwell's equations into a pair of uncoupled two-component spinor equations. (Sachs, 1971). In the linear approximation for the matter field equations, the extra terms lead to an extra contribution to the Dirac Hamiltonian for hydrogen. The prediction of the Lamb splittings $(3S_{1/2} - 3P_{1/2})$ and $(2S_{1/2} - 2P_{1/2})$ by these terms was found to be within 1.0% of the experimental values, and as accurate as the values predicted by quantum electrodynamics.

Continuing this line of study, we investigate this theory's prediction in regard to the helium spectrum. The method of calculation applied uses the Foldy-Wouthuysen type of transformation for the Dirac equation, for the two-electron atom, including the extra terms predicted by this theory (Charplvy, 1953). The extra terms appear here as an addition to the Breit Hamiltonian for Helium (Breit, 1929).

The results of the perturbation calculations for the energy shift of the ionization energy of Helium, for the lowest state of parahelium and orthohelium, due to these extra terms, are then compared with the experimental values of the Lamb shift of Helium, and with the theoretical values determined from quantum electrodynamics.

2. *The Field Equations for the Helium Atom*

2.1. *The Construction of Field Equations*

In this section, we construct a Lagrangian density function for the Helium atom, from which the relativistically covariant field equations can be derived, in accordance with the principle of least action.

The Lagrangian density depends explicitly on the Maxwell field spinors $\phi_\alpha^{(1)}$, $\phi_\alpha^{(1)\dagger}$, $\phi_\alpha^{(2)}$, $\phi_\alpha^{(2)\dagger}$, for the electromagnetic field intensities of the two electrons, $\phi_\alpha^{(n)}$, $\phi_\alpha^{(n)\dagger}$ for those of the Helium nucleus, the Dirac field bispinors $\psi^{(1)}$, $\bar{\psi}^{(1)}$, $\psi^{(2)}$, $\bar{\psi}^{(2)}$, for the dynamical field variables of the two electrons, $\bar{\psi}^{(n)}$, $\psi^{(n)}$, for the dynamical variables of Helium nucleus, and on their respective first derivatives.

These Maxwell field spinors satisfy the factorized electromagnetic field equations for this system as follows:‡

$$\sigma_\mu \partial_\mu \phi_\alpha^{(p)} = e^{(p)} \bar{\psi}^{(p)} \Gamma_\alpha \psi^{(p)} \tag{2.1.1}$$

‡ The notations used are:

$$\partial_\mu \left(= \frac{\partial}{\partial x} \right) = \{\partial_0 = -i\partial_t; \partial_k\} \qquad x = \{x_0 = it; x_k\}, \qquad \boldsymbol{\alpha} = i\gamma_0 \Upsilon$$

$$\gamma_\mu = \{\gamma_0; \gamma_k\}, \qquad \gamma_0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} = \beta \qquad \gamma_k = -i \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0 \end{pmatrix} \qquad k = 1, 2, 3$$

$\bar{\psi} \equiv \psi^\dagger \gamma_0$ and σ_k are Pauli matrices, $\hbar = c = 1$.

where $p = 1, 2, n$, $\alpha = 1, 2$, and

$$e^{(p)}\bar{\psi}^{(p)}\Gamma_1\psi^{(p)} = 4\pi i e^{(p)}\begin{pmatrix} \bar{\psi}^{(p)}(-\gamma_0 + i\gamma_3)\psi^{(p)} \\ \bar{\psi}^{(p)}(i\gamma_1 - \gamma_2)\psi^{(p)} \end{pmatrix}$$

$$e^{(p)}\psi^{(p)}\Gamma_2\psi^{(p)} = 4\pi i e^{(p)}\begin{pmatrix} \bar{\psi}^{(p)}(-i\gamma_1 - \gamma_2)\psi^{(p)} \\ \bar{\psi}^{(p)}(\gamma_0 + i\gamma_3)\psi^{(p)} \end{pmatrix}$$

The Lagrangian density can be constructed from three parts: $L = L_D + L_M + L_I$. The first part is the usual 'free field' Dirac Lagrangian density,

$$L_D = \sum_{p=1}^{n} [\bar{\psi}^{(p)}(\gamma_\mu \partial_\mu + m^{(p)})\psi^{(p)} + (-\partial_\mu \bar{\psi}^{(p)}\gamma_\mu + m^{(p)}\bar{\psi}^{(p)})\psi^{(p)}] \tag{2.1.2}$$

The second part contains an interaction term which couples the Maxwell field variables to the Dirac field variables through the source term $\bar{\psi}^{(p)}\Gamma_\alpha\psi^{(p)}$. This is the part that gives rise to the Maxwell field equations (2.1.1), when variation is carried out with respect to the Maxwell (spinor) field variables. The form of this part of Lagrangian is as follows:

$$L_M = i g_m \sum_{p \neq q = 1}^{n} \sum_{\alpha = 1,2} (-1)^\alpha \phi_\alpha^{(p)\dagger}(\sigma_\mu \partial_\mu \phi_\alpha^{(q)} - 2e^{(q)}\bar{\psi}^{(q)}\Gamma_\alpha\psi^{(q)}) + \text{h.c.} \tag{2.1.3}$$

where g_m is the extra fundamental constant in this theory, previously determined (Sachs, 1972). The value is $g_m = (2{\cdot}087 \pm 0{\cdot}001) . 10^{-14}$ cm.

The third part contains the conventional interactions which couple the velocity fields of the particles, except for the omission (by this theory) of self-interactions ($p = q$),

$$L_I = -\sum_{p \neq q = 1}^{n} e^{(p)}e^{(q)}\bar{\psi}^{(p)}\gamma_\mu\psi^{(p)} \int \bar{\psi}^{(q)}\gamma_\mu\psi^{(q)}G(x - x')\, d^4x \tag{2.1.4}$$

where the Green's function $G(x - x')$ satisfies D'Alembert's equation

$$\Box G(x - x') = -4\pi\delta(x - x')$$

The total action function whose vanishing variation gives the behavior of the Helium system is

$$A = \iint_{t'}^{t''} L\, d^3x\, dt \tag{2.1.5}$$

The field equations for Helium are now derived from the above action in accordance with the principle of least action, giving the following equations in ψ:

$$[\gamma_\mu \partial_\mu + I_{11} + I_{12} + I_{21} + I_{22} + m_e]\psi^{(1)} = 0 \qquad (2.1.6)$$

$$[\gamma_\mu \partial_\mu + I'_{11} + I'_{12} + I'_{21} + I'_{22} + m_e]\psi^{(2)} = 0 \qquad (2.1.7)$$

$$[\gamma_\mu \partial_\mu + I_n + M_n]\psi^{(n)} = 0 \qquad (2.1.8)$$

where m_e, M_n are the electron and Helium nuclear mass respectively[†], and

$$I_{11}(x) = -(e^2)\gamma_\mu \int \bar{\psi}^{(2)}\gamma_\mu \psi^{(2)} G(x - x')\, d^4x' = i\gamma_\mu e \int J_\mu^{(2)}(x') G(x - x')\, d^4x'$$

$$I_{12}(x) = 2e^2\gamma_\mu \int \bar{\psi}^{(n)}\gamma_\mu \psi^{(n)} G(x - x')\, d^4x' = 2i\gamma_\mu e \int J_\mu^{(n)}(x') G(x - x')\, d^4x'$$

$$I_{21}(x) = ig_m . (-e) \sum_{\alpha=1}^{2} (-1)^\alpha [\phi_\alpha^{(2)\dagger}(x) . \Gamma_\alpha - (\gamma_0 \Gamma_\alpha{}^\dagger \gamma_0) . \phi_\alpha^{(2)}(x)]$$

$$I_{22}(x) = ig_m . (-e) \sum_{\alpha=1}^{2} (-1)^\alpha [\phi_\alpha^{(n)\dagger}(x) . \Gamma_\alpha - (\gamma_0 \Gamma_\alpha{}^\dagger \gamma_0) . \phi_\alpha^{(n)}(x)]$$

$I'_{11}, I'_{12}, I'_{21}, I'_{22}$ are obtained by interchanging 1 and 2.

$$\begin{aligned} I_n(x) = & -\gamma_\mu(2e) \int (-e)\bar{\psi}^{(1)}\gamma_\mu \psi^{(1)} G(x - x')\, d^4x' - \gamma_\mu(2e) \int \\ & \times (-e)\bar{\psi}^{(2)}\gamma_\mu \psi^{(2)} G(x - x')\, d^4x' \\ & + ig_m(2e) \left\{ \sum_{\alpha=1}^{2} (-1)^\alpha [\phi_\alpha^{(1)\dagger} . \Gamma_\alpha - (\gamma_0 \Gamma_\alpha{}^\dagger \gamma_0) . \phi_\alpha^{(1)}] \right. \\ & \left. + \sum_{\alpha=1}^{2} (-1)^\alpha [\phi_\alpha^{(2)\dagger} . \Gamma_\alpha - (\gamma_0 \Gamma_\alpha{}^\dagger \gamma_0) . \phi_\alpha^{(2)}] \right\} \end{aligned}$$

2.2. *The Partial Linearization of Field Equations*

We now show that the solution of (2.1.8) can be approximated by the following stationary form $\psi^{(n)} = e^{-iM_n t} f(\mathbf{r}) s$, where s is the constant four-component spinor such that $s^\dagger s = 1$. Dividing (2.1.8) by M_n we have

$$\left(\frac{1}{M_n} \gamma_0 \partial_0 - \frac{1}{M_n} \gamma_k \partial_k + \frac{I_n}{M_n} + 1 \right) \psi^{(n)} = 0 \qquad (2.2.1)$$

[†] For the purpose at hand, we write the (spinor) equation for the He^3 nucleus. This makes no difference in the calculation that follows for the atomic spectrum of He, as the approximation will be used that is equivalent to infinite nuclear mass.

The operator $\gamma_k \partial_k / M_n$ corresponds to the ratio of kinetic energy of He nucleus to its rest energy. Since the recoil energy of He nucleus is negligible compared to its rest energy, we can neglect this term. The operator I_n/M_n corresponds to the ratio of Helium binding energy to the Helium nuclear rest energy. This also can be assumed small enough to be neglected. Therefore equation (2.2.1) takes the form (in the rest frame of the He nucleus):

$$\left(\frac{1}{M_n}\gamma_0\partial_0 + 1\right) e^{-iM_n t} f(\mathbf{r}) = 0 \tag{2.2.2}$$

$f(r)$ can be chosen arbitrarily without altering the validity of equation (2.2.2). Appealing to the physical argument that leads to the assumption of stationary point Helium nucleus, we take

$$|f(\mathbf{r})|^2 = \delta(\mathbf{r}) \tag{2.2.3}$$

$\delta(\mathbf{r})$ is the three-dimensional delta function. This leads to:

$$\bar{\psi}^{(n)}\gamma_k\psi^{(n)} = 0, \qquad \bar{\psi}^{(n)}\gamma_0\psi^{(n)} = \delta(\mathbf{r})$$

In the limit of stationary Helium nucleus and sufficiently small momentum transfer between the interacting electrons, compared with mc, the specification of each electron of the He atom can be made with respect to their own private space-time coordinate frames. This is because in a first approximation, the equations for the two electron waves may be considered separately. Thus x goes to x_1 in $I_{11}, I_{12}, I_{21}, I_{22}$ and x goes to x_2 in $I'_{11}, I'_{12}, I'_{21}, I'_{22}$. Inserting (2.2.3) into I_{12} we have

$$I_{12} = \frac{2e^2\gamma_0}{r_1}, \qquad \text{Similarly } I'_{12} = \frac{2e^2\gamma_0}{r_2} \tag{2.2.4}$$

These are just the Coulomb potential.

Before I_{22} can be determined explicitly, we must know the form of the spinor solution $\phi_\alpha^{(n)}$ of the Maxwell's field equations for the nucleus. Putting (2.2.3) into (2.1.1), we have:

$$\sigma_\mu\partial_\mu\phi_1^{(n)} = -4\pi i\,.(2e)\,\delta(\mathbf{r})\begin{pmatrix}1\\0\end{pmatrix} \tag{2.2.5a}$$

$$\sigma_\mu\partial_\mu\phi_2^{(n)} = +4\pi i.\,(2e)\,\delta(\mathbf{r})\begin{pmatrix}0\\1\end{pmatrix} \tag{2.2.5b}$$

The solutions are (Sachs, 1971)

$$\phi_1^{(n)}(x) = -\frac{2ie}{r^3}\begin{pmatrix}z\\x+iy\end{pmatrix}, \qquad \phi_2^{(n)}(x) = \frac{2ie}{r^3}\begin{pmatrix}x-iy\\-z\end{pmatrix} \tag{2.2.6}$$

Finally, substituting these solutions into I_{22}, we obtain:

$$I_{22} = 16\pi i g_m 2e^2 \frac{(\mathbf{r}_1 \times \mathbf{\Upsilon})_3}{r^3} \tag{2.2.7}$$

We now proceed to solve the spinor Maxwell's equations for the two electrons. The Green's function for the two-component spinor equations is (Sachs, 1971)

$$S(x - x') = \frac{1}{(2\pi)^4} \int \frac{-i\bar{\sigma}_\rho k_\rho}{k_\mu{}^2} e^{ik_\mu(x_\mu - x'_\mu)}\, d^4k, \qquad \bar{\sigma}_\rho = (\sigma_0; -\boldsymbol{\sigma}) \tag{2.2.8}$$

Thus,

$$S(x - x') = \frac{1}{(2\pi)^4} \bar{\sigma}_\rho \frac{\partial}{\partial x'_\rho} \int \frac{e^{ik_\mu(x_\mu - x'_\mu)}}{k_\mu{}^2}\, d^4k$$

Because

$$\frac{1}{4\pi^3} \int \frac{e^{ik_\mu(x_\mu - x'_\mu)}}{k_\mu{}^2}\, d^4k = \frac{1}{R} \delta(t' + R - t)$$

$S(x - x')$ can be written explicitly as

$$S(x - x') = \frac{1}{(4\pi)} \left\{ \sigma_0 \frac{1}{R(t')} \delta'(t' + R - t) - \boldsymbol{\sigma}.\hat{r}_{xx'} \left[-\frac{1}{R^2(t')} \delta(t' + R - t) \right] \right\}$$

where (2.2.9)

$$R \equiv |\mathbf{r}_{xx'}| \equiv |\mathbf{r} - \mathbf{r}'(t')|, \qquad \hat{r}_{xx'} \equiv \frac{\mathbf{r}_{xx'}}{R}$$

and

$$\delta'(t' + R(t') - t) \equiv \frac{d}{df} \delta(f - t)$$

The solutions are as follows:

$$\phi_\alpha^{(p)}(x) = \int S(x - x') \Upsilon_\alpha^{(p)}(x')\, d^4x' \qquad p = 1, 2 \tag{2.2.10}$$

where

$$\Upsilon_1^{(p)}(x') = -4\pi i \begin{pmatrix} \rho + j_3 \\ j_1 + ij_2 \end{pmatrix}, \qquad \Upsilon_2^{(p)}(x') = -4\pi i \begin{pmatrix} j_1 - ij_2 \\ \rho - j_3 \end{pmatrix}$$

$$\rho(\mathbf{r}', t') = -e\delta(\mathbf{r} - \mathbf{r}'(t'))$$

$$\mathbf{j}(\mathbf{r}', t') = -e\mathbf{V}\delta(\mathbf{r} - \mathbf{r}'(t'))$$

and where $\mathbf{r}'(t')$ is the position of the electron at the retarded time. Thus, with these source terms we obtain

$$\phi_1^{(2)}(x) = ie \left\{ \sigma_0 \frac{1}{K} \frac{d}{dt'} \left[\begin{pmatrix} 1 + V_{1z} \\ V_{1x} - V_{1y} \end{pmatrix} \frac{1}{KR} \right] \right.$$

$$- \boldsymbol{\sigma}.\hat{r}_{xx'}\left[-\frac{1}{KR^2}\begin{pmatrix} 1+V_{1z} \\ V_{1x}-iV_{1y}\end{pmatrix}+\frac{1}{K}\frac{d}{dt'}\left[\frac{1}{KR}\begin{pmatrix} 1+V_{1z} \\ V_{1x}+V_{1y}\end{pmatrix}\right]\right]\Bigg\}$$

where (2.2.11)

$$K \equiv \frac{dt}{dt'} = 1 + \frac{\hat{r}_{xx'}.\mathbf{V}}{c}$$

(If now we put c into the equations.)

We have

$$\phi_1^{(2)}(x) = ie\left[\boldsymbol{\sigma}.\hat{r}_{xx'}\begin{pmatrix}1\\0\end{pmatrix}\frac{1}{KR^2}\right] + 0\left(\frac{\mathbf{V}}{c}\right) + 0\left(\frac{V^2}{c^2}\right)$$

$$\simeq -\frac{ie}{KR^3}\begin{pmatrix} z-z' \\ (x-x')+i(y-y')\end{pmatrix} \tag{2.2.12}$$

Similarly,

$$\phi_2^{(2)}(x) \simeq \frac{ie}{KR^3}\begin{pmatrix}(x-x')-i(y-y') \\ -(z-z')\end{pmatrix} \tag{2.2.13}$$

The substitution of (2.2.12) and (2.2.13) into I_{21} leads to

$$I_{21} \simeq -i16\pi g_m e^2 \frac{(\mathbf{r}_{12}x\Upsilon)_3}{Kr_{12}^3}\ \ddagger \tag{2.2.14}$$

The velocity of the two electrons in He atom is the order of $c\alpha$, $\alpha \equiv e^2/\hbar c$ so $K \simeq 1$ in I_{21}.

3. *The Hamiltonian for Helium*

It is the main purpose of this paper to investigate the contribution to the Helium spectrum due to these extra electromagnetic interactions involving g_m. Thus, it is not necessary here really to solve exactly the two non-linear coupled field equations for the two electrons. From the physical point of view, we can construct a total Hamiltonian for He from terms in these two field equations, such that

$$H\Psi = -E\psi \tag{3.1}$$

where

$$H = H_0 + H_{11} + H_{12} + H_{21} + H_{22}$$

$$E = \beta_1\frac{\partial}{\partial x_{10}} + \beta_2\frac{\partial}{\partial x_{20}}, \qquad H_0 = (\boldsymbol{\alpha}_1 . \mathbf{p}_1 + \boldsymbol{\alpha}_2 . \mathbf{p}_2)c + (\beta_1+\beta_2)mc^2$$

[‡] Because $\mathbf{r}_{xx'}$ goes to $\mathbf{r}_{12}$ in I_{21}.

with

$$H_{11} = \tfrac{1}{2}(\beta_1 I_{11} + \beta_2 I'_{11})$$
$$H_{12} = \beta_1 I_{12} + \beta_2 I'_{12}$$
$$H_{21} = \tfrac{1}{2}(\beta_1 I_{21} + \beta_2 I'_{21})$$
$$H_{22} = \beta_1 I_{22} + \beta_2 I'_{22}$$

Ψ is now the He wave function that has 16 components.

The physical meaning of the various terms in the Hamiltonian is as follows:

H_0 is the free particle Dirac Hamiltonian.

H_{11} is the sum of the Coulomb interaction between the two electrons and the Breit interaction term (Breit, 1929) which is, up to the order of (V^2/c^2),

$$H_{11} \simeq -\frac{e^2}{r_{12}} + \frac{e^2}{2}\left[\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r_{12}} + \frac{(\boldsymbol{\alpha}_1 \cdot \mathbf{r}_{12})(\boldsymbol{\alpha}_1 \cdot \mathbf{r}_{12})}{r_{12}^3}\right] \tag{3.2}$$

H_{12} is the Coulomb potential of the two electrons due to the Helium nucleus.

H_{21} is the extra electromagnetic coupling term between the two electrons.

H_{22} is the extra electromagnetic coupling term of the two electrons due to the nucleus.

These two terms do not have any counterpart in the standard vector-tensor representation of the Maxwell's formalism.

We see that, without the terms H_{21} and H_{22}, this wave equation is just the Breit equation for He. Therefore the energy spectrum, without considering the contribution of these two terms, will be the same as that from the conventional Dirac theory. We now investigate whether these two extra terms will give the correct shift to the energy levels of He, replacing the usual quantum electrodynamical contributions associated with the Lamb shift.

Since these two terms are much smaller than the total energy of He atom,‡ first-order perturbation theory will be sufficient for calculating the energy shift.

4. *Energy Shift of He Due to H_{22}*

This two-particle Hamiltonian in the above section can be reduced to the non-relativistic limit by the Foldy–Wouthusen type of transformation. The variational wave function will be used for the perturbation calculations. The reduced Hamiltonian, up to the order of α^2, given by Chaplevy (1953) is as follows (in atomic units):

$$H_R = -\frac{1}{\alpha^2} + (\epsilon\epsilon) - \frac{\alpha^2}{2}\left[(o\epsilon)^2 + (\epsilon o)^2\right]$$

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‡ Because the order of g_m is only $\simeq 10^{-14}$ cm.

$$
\begin{aligned}
&+\frac{\alpha^4}{8}\,[[(o\epsilon),(\epsilon\epsilon)],(o\epsilon)]+\frac{\alpha^4}{8}\,[[(\epsilon o),(\epsilon\epsilon)],(\epsilon o)]\\
&+\frac{\alpha^6}{8}\,[(o\epsilon)^4+(\epsilon o)^4]+\frac{\alpha^4}{4}(oo)^2\\
&+\frac{\alpha^4}{8}\,[[(o\epsilon),(oo)]_+,(\epsilon o)]_+ +\frac{\alpha^4}{8}\,[[(\epsilon o),(oo)]_+,(o\epsilon)]_+\\
&-\frac{\alpha^6}{16}\,[(o\epsilon),(\epsilon o)]^2\\
&-\frac{\alpha^6}{8}\,[(o\epsilon)^2,(\epsilon o)^2]_+ -\frac{\alpha^6}{8}\,[(\epsilon o)(o\epsilon)^2(\epsilon o)+(o\epsilon)(\epsilon o)^2(o\epsilon)] \qquad (4.1)
\end{aligned}
$$

where $(o\epsilon)$ is the operator in the Hamiltonian odd with respect to the first electron and even with respect to the second, in the Dirac matrix $\boldsymbol{\alpha}$, and

(ϵo)—(even, odd)
$(\epsilon\epsilon)$—(even, even)
(oo)—(odd, odd)

$[a, b]$ and $[a, b]_+$ are the commutator and the anticommutator respectively. For our case,

$$(\epsilon\epsilon)=\frac{2}{r_1}+\frac{2}{r_2}-\frac{1}{r_{12}} \qquad (4.2a)$$

$$(oo)=\frac{1}{2}\frac{(\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)}{r_{12}}+\frac{1}{2}\frac{1}{r_{12}^3}(\boldsymbol{\alpha}_1\cdot\mathbf{r}_{12})(\boldsymbol{\alpha}_2\cdot\mathbf{r}_{12}) \qquad (4.2b)$$

$$(\epsilon o)=\frac{1}{\alpha}(\boldsymbol{\alpha}_2\cdot\mathbf{p}_2)+\frac{K}{r_2^3}(\mathbf{r}_2\times\boldsymbol{\alpha}_2)_3 \qquad (4.2c)$$

$$(o\epsilon)=\frac{1}{\alpha}(\boldsymbol{\alpha}_1\cdot\mathbf{p}_1)+\frac{K}{r_1^3}(\mathbf{r}_1\times\boldsymbol{\alpha}_1)_3 \qquad (4.2d)$$

where

$$K\equiv 16\pi(g_m/\lambda_c)(2\alpha)^2, \qquad \lambda_c\equiv\frac{\hbar}{mc}$$

The reduced Hamiltonian, H_R, up to the order of α^2, is just equal to the conventional Breit Hamiltonian in approximate reduced form, plus the additional term Q: Thus,

$$H_R=H_{RO}+H_B+Q \qquad (4.3)$$

with

$$H_{RO} = \frac{\nabla_1^2}{2} + \frac{\nabla_2^2}{2} + \frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{r_{12}}$$

$$H_B = H_B(1) + H_B(2)$$

$$Q = Q(1) + Q(2)$$

where H_B is the conventional Breit Hamiltonian in approximate reduced form (Charplvy, 1954)

$$\begin{aligned} H_B(1) = & -\frac{1}{\alpha^2} + \frac{\alpha^2}{8} p_1{}^4 + \frac{\alpha^2}{4}\left[\frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{r_{12}} + \frac{(\mathbf{r}_{12} \cdot \mathbf{p}_1)(\mathbf{r}_{12} \cdot \mathbf{p}_2)}{r_{12}^3}\right] \\ & + \frac{\alpha^2}{4} \boldsymbol{\sigma}_1 \cdot \left(\mathbf{E}_1 + \frac{\mathbf{r}_{12}}{r_{12}^3}\right) \times \mathbf{p}_1 + \frac{\alpha^2}{8} . 4\pi\delta(\mathbf{r}_{12}) \\ & - \frac{\alpha^2}{4}\left[\frac{i(\mathbf{r}_{12} \cdot \mathbf{p}_1)}{r_{12}^3} - \frac{2\boldsymbol{\sigma}_2 . (\mathbf{r}_{12} \times \mathbf{p}_1)}{r_{12}^3} - 4\pi i \delta(\mathbf{r}_{12})(\mathbf{r}_{12} \times \mathbf{p}_1)\right] \\ & - \frac{\alpha^2}{8}\left[\frac{\boldsymbol{\sigma}_1 . \boldsymbol{\sigma}_2}{r_{12}^3} - \frac{3(\boldsymbol{\sigma}_1 . \mathbf{r}_{12})(\boldsymbol{\sigma}_2 . \mathbf{r}_{12})}{r_{12}^5} - \frac{8\pi}{3}(\boldsymbol{\sigma}_1 . \boldsymbol{\sigma}_2)\delta(\mathbf{r}_{12})\right] \\ & - \frac{\alpha^2}{8}\left[\frac{3}{r_{12}^2} - \frac{2\boldsymbol{\sigma}_1 . \boldsymbol{\sigma}_2}{r_{12}^2} + \frac{(\boldsymbol{\sigma}_1 . \mathbf{r}_{12})(\boldsymbol{\sigma}_2 . \mathbf{r}_{12})}{r_{12}^4}\right] \end{aligned}$$

$H_B(2) = H_B(1)(\mathbf{r}_1 \to \mathbf{r}_2, \boldsymbol{\sigma}_1 \to \boldsymbol{\sigma}_2$, etc.), and

$$\begin{aligned} Q(1) = -\frac{\alpha^2}{2}\Bigg\{ & \frac{K^2}{r_1{}^6}(\mathbf{r}_1 \times \boldsymbol{\alpha}_1)_3{}^2 + \frac{1}{\alpha}(\boldsymbol{\alpha}_1 . \mathbf{p}_1)\left[\frac{K}{r_1{}^3}(\mathbf{r}_1 \times \boldsymbol{\alpha}_1)_3\right] \\ & + \frac{1}{\alpha}\frac{K}{r_1{}^3}(\mathbf{r}_1 \times \boldsymbol{\alpha}_1)_3(\boldsymbol{\alpha}_1 . \mathbf{p}_1)\Bigg\} \end{aligned}$$

$Q(2) = Q(1)(\mathbf{r}_1 \to \mathbf{r}_2, \boldsymbol{\alpha}_1 \to \boldsymbol{\alpha}_2$, etc.).

It is observed that the perturbation operator Q diverges at the origin as r^{-4}. Therefore, in order to ensure that the wave function shall have proper behavior at the origin that would lead to a convergent matrix element for the perturbation operators that depend on r^{-n} $(n \geqslant 2)$, let us redefine the unperturbed and the perturbing Hamiltonian by adding and substracting the term $f(r_1, r_2)$ such that

$$f(r_1, r_2) = \frac{1}{2}\left[-\frac{\mathscr{K}'^2}{r_1^4} - \frac{\mathscr{K}'^2}{r_2{}^4}\right] \tag{4.4}$$

where $\mathscr{K}' \equiv \mathscr{K}\alpha$.

With this choice of $f(r_1, r_2)$ we get the new unperturbed wave function

$$\psi_0' = \psi_0 \exp\left(-\frac{\mathscr{K}'}{r_1} - \frac{\mathscr{K}'}{r_2}\right)$$

where

$$\psi_0 \text{ satifies } H_{RO}\psi_0 = -E_{RO}\psi_0$$
$$\psi_0' \text{ satifies } H_{RO}'\psi_0' = -E_{RO}\psi_0'$$

with

$$H_{RO}' = H_{RO} + f(r_1, r_2)$$

and the new perturbation operator $Q' = Q - f(r_1, r_2)$.

4.1. *Ground State* $(1\,^1S)$*-Parahelium*

We can evaluate the matrix elements in Q' by using the 6-parameter Hylleraas variational wave function (Hylleraas, 1929)

$$\psi_0 = e^{-(A/2)s}(1 + C_1u + C_2t^2 + C_3s + C_4s^2 + C_5u^2) \quad \text{(Unnormalized)}$$

where $s = r_1 + r_2, t = r_1 - r_2, u = r_{12}$,

$C_1 = 0{\cdot}353808, \quad C_2 = 0{\cdot}128521, \quad C_3 = -0{\cdot}100828$
$C_4 = 0{\cdot}033124, \quad C_5 = -0{\cdot}031799$

and $A = 3{\cdot}64$.

The various terms in the matrix element of Q' can be written out explicitly as follows (in atomic units):

$$Q_1' = -S^\dagger\psi_0'\frac{\alpha^2K^2}{r_1^6}(\mathbf{r}_1 \times \boldsymbol{\alpha}_1)_3^2\psi_0'S + S^\dagger\psi_0'\frac{K'^2}{r_1^4}\psi_0'S + Q_1'(2)$$

$$= \frac{K^2\alpha^2}{r_1^4}\cos^2\theta_1 . \psi_0'^2 + \frac{K^2\alpha^2}{r_2^4}\cos^2\theta_2 . \psi_0'^2 \qquad (4.1.1a)$$

Here,

$$S = \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \alpha(2)\beta(1)], \qquad \alpha = \begin{pmatrix}1\\0\end{pmatrix}, \qquad \beta = \begin{pmatrix}0\\1\end{pmatrix}$$

$$Q_2' = S^\dagger\psi_0'\frac{(\boldsymbol{\alpha}_1 . \mathbf{p}_1)}{\alpha}\left[\frac{K\alpha^2}{r_1^3}(\mathbf{r}_1 \times \boldsymbol{\alpha}_1)_3\right]\psi_0'S + Q_2'(2)$$

$$= -2K\alpha\psi_0'\frac{1}{r_1^3}\frac{\partial\psi_0'}{\partial\phi_1} - 2K\alpha\psi_0'\frac{1}{r_2^3}\frac{\partial\psi_0'}{\partial\phi_2} \qquad (4.1.1b)$$

$$Q_3' = S^\dagger\psi_0'\left[\frac{K\alpha^2}{r_1^3}(\mathbf{r}_1 \times \boldsymbol{\alpha}_1)_3\right]\frac{(\boldsymbol{\alpha}_1 . \mathbf{p}_1)}{\alpha}\psi_0'S + Q_3'(2)$$

$$= Q_2' \qquad (4.1.1c)$$

From symmetry, it is seen that the Q'_2 and Q'_3 terms vanish when integrating over the azimuthal angles ϕ_1 and ϕ_2.

We thus arrived at the energy shift $(\Delta E_{22})_{1^1S}$ as follows:

$$(\Delta E_{22})_{1^1S} = \frac{K^2\alpha^2N^2}{2}\int \frac{\cos^2\theta_1}{r_1^4}\psi_0'^2\,d\tau + \frac{K^2\alpha^2N^2}{2}\int \frac{\cos^2\theta_2}{r_2^4}\psi_0'^2\,d\tau$$

where N^2 is the normalization constant

$$N^2 = (\langle\psi'_0|\psi'_0\rangle)^{-1}$$
$$d\tau = d^3r_1 . d^3r_2$$

By carrying out the integration (Yu, 1974), we obtain $(\Delta E_{22})_{1^1S} \simeq 4{\cdot}8\ \text{cm}^{-1}$.

4.2. *The Excited State (2^3S)-Orthohelium*

In the triplet S state of lowest energy for orthohelium, the terms,

$$(\boldsymbol{\alpha}_i . \mathbf{p}_i)\left[\frac{K\alpha}{r_i^3}(\mathbf{r}_i \times \boldsymbol{\alpha}_i)_3\right] \quad \text{and} \quad \frac{K\alpha(\mathbf{r}_i \times \boldsymbol{\alpha}_i)_3}{r_i^3}(\boldsymbol{\alpha}_i . \mathbf{p}_i), \qquad i = 1, 2$$

give vanishing matrix elements, independent of the spin states of the electrons, therefore the only non-vanishing matrix element is still

$$\frac{\cos^2\theta_1}{r_1^4} + \frac{\cos^2\theta_2}{r_2^4}$$

Because of the larger separation of the electrons from the nucleus, the energy shift of this state should be smaller than that of 1^1S state. The simple wave function, the antisymmetrized product of two hydrogen–like wave function with nuclear charge Z_i and Z_a for the inner and outer electron, will be sufficient for calculating the matrix element. The wave function is (Bethe & Salpeter, 1957),

$$\psi'_0 = [\exp(-z_i r_2 - \tfrac{1}{2}z_a r_1)(\tfrac{1}{2}z_a r_1 - 1) - \exp(-z_a r_2 - \tfrac{1}{2}z_i . r_1)$$
$$\times (\tfrac{1}{2}z_a r_2 - 1)]\exp\left(-\frac{K'}{r_1} - \frac{K'}{r_2}\right) \tag{4.2.1}$$

where $z_i \simeq 2{\cdot}01, z_a \simeq 1{\cdot}53$.

With this wave function we find (Yu, 1974) the energy shift from the term

$$\frac{\cos^2\theta_1}{r_1^4} + \frac{\cos^2\theta_2}{r_2^4}$$

to be $(\Delta E_{22})_{2^3S} \cong 3{\cdot}5\ \text{cm}^{-1}$.

5. *The Lamb Shift of Helium*

What we will compare from theory, with the experimental results, is what is usually referred to as the Lamb shift in the ionization energy of He. That is the difference of energy shift with the corresponding energy levels of He^+ and He atom. Because, previously, we assumed that those extra terms are the replacements of the usual quantum electrodynamics contributions, the energy shift to the ionization energy due to those extra terms will be associated with Lamb shift of Helium. Therefore we first have to calculate the energy shift due to this kind of extra term for He^+, which is (Sachs, 1972)

$$\Delta E(\mathrm{He}^+) = \tfrac{64}{3}\pi \frac{(2\alpha)^2}{[(S+N)+(2\alpha)^2]}\left(\frac{g_m}{\lambda_c}\right) mc^2 . I \tag{5.1}$$

where

$$I = (\eta z\alpha)^{-1} \int_0^\infty \frac{FG}{\rho^2} \exp\left(-\frac{2K}{\rho}\right) d\rho$$

with

$$\eta = \int_0^\infty (G^2 + F^2) \exp\left(-\frac{2K}{\rho}\right) d\rho, \qquad \rho = \eta r$$

$$K = \frac{16\pi}{[(S+N)+(2\alpha)^2]^{1/2}}\left(\frac{g_m}{\lambda c}\right)(2\alpha)^2$$

$$F = \mathrm{e}^{-\rho} \sum_{u=0}^{\infty} \rho^{S+u} a_u$$

$$G = \mathrm{e}^{-\rho} \sum_{u=0}^{\infty} \rho^{S+u} b_u$$

$$S \equiv \sqrt{[k^2 - (2\alpha)^2]}, \qquad k = \pm (j + \tfrac{1}{2})$$

The principal quantum number $n = N + k, N = u$. For the 1*S* state of He^+ we have $F \simeq a_0 \rho \mathrm{e}^{-\rho}, G \simeq a_0 \alpha F$. Thus we obtain the result: $\Delta E(\mathrm{He}^+) \simeq 3{\cdot}4\ \mathrm{cm}^{-1}$.

Next, we shall investigate the contribution of the operator H_{21} to the energy shift. H_{21} is proportional to $1/r_{12}^2$ and H_{22} is proportional to $1/r_1{}^2$ and $1/r_2{}^2$. The interaction strength in H_{21} is one-half of that in H_{22}. For the $1\,^1S$ state, from Pekeris' results (Pekeris, 1959),

$$\left\langle \frac{1}{r_{12}^2} \right\rangle \simeq \frac{1}{5}\left\langle \frac{1}{r_1{}^2} \right\rangle = \frac{1}{5}\left\langle \frac{1}{r_2{}^2} \right\rangle$$

Hence the energy shift due to H_{21}, $(\Delta E)_{21}$, is approximately one-tenth of $(\Delta E)_{22}$. That is, $(\Delta E)_{21}$ is roughly $-0{\cdot}5$ cm^{-1}. For the 2^3S state,

$$\left\langle \frac{1}{r_{12}^2} \right\rangle \simeq \frac{1}{40} \left\langle \frac{1}{r_1^2} \right\rangle = \frac{1}{40} \left\langle \frac{1}{r_2^2} \right\rangle.$$

Hence the energy shift due to H_{21} for this state can be neglected.

Finally, the energy shift associated with the Lamb shift is

$$\Delta E_J = \Delta E(\mathrm{He}^+) - (\Delta E)_{22} - (\Delta E)_{21} \qquad (5.2)$$

For the 1^1S state: $\Delta E_J = 3{\cdot}4$ cm^{-1} $- 4{\cdot}8$ cm^{-1} $- (-0{\cdot}5)$ cm^{-1} $= -0{\cdot}9$ cm^{-1}.
For the 2^3S state: $\Delta E_J = 3{\cdot}4$ cm^{-1} $- 3{\cdot}5$ cm^{-1} $= -0{\cdot}1$ cm^{-1}.

6. *Comparison and Discussion*

The aim of this analysis has been to determine whether or not the generalized theory of electrodynamics which is incorporated in Sachs' self-consistent field theory might lead to a prediction in the fine structure of Helium that could be comparable with the contribution that is conventionally attributed to radiative corrections, according to quantum electrodynamics. This is the very small correction in the conventional theory of the Helium atom, leading to energy level shifts in the low-lying states of the order of 1 cm^{-1}, that are necessary to obtain agreement between theory and experiment.

To compare the theoretical predictions according to the results in the preceding chapter with experiment, reference may be made to Herzberg's (1958) observations of the ionization potential of Helium. He compared his results with the theoretical values obtained from relativistic wave mechanics for the two-electron atom—the Breit Hamiltonian, also including mass-polarization correction. He then attributed the difference between these theoretical predictions and his observations to radiative effects. The calculations of these radiative effects according to quantum electrodynamics agreed with Herzberg's results for this difference.

However, the present theory also predicts the Helium spectrum from the Dirac formalism for the two-electron atom, including the Breit terms, as well as extra (generalized) electromagnetic terms, but without the radiative terms present. It is then the aim in this investigation to see if the theory proposed might also feasibly account for this required correction in the spectrum of Helium, instead of evoking the radiative effects. If so, then the general form of this theory would have to be tested against quantum electrodynamics in further applications.

Herzberg's ionization potentials were to have the following values:

$$J_{\mathrm{exp}}(\mathrm{He}^4) = 198310{\cdot}82 \pm 0{\cdot}15 \text{ cm}^{-1}$$

$$J_{\mathrm{exp}}(\mathrm{He}^3) = 198300{\cdot}32 \pm 0{\cdot}15 \text{ cm}^{-1}$$

Taking into account the isotope shift of $10{\cdot}50 \pm 0{\cdot}05$ cm^{-1} and using Perkeris' theoretical value, from his variation calculation with 203 parameters,

$J_{\text{th}}(\text{He}^4) = 198312{\cdot}01\ \text{cm}^{-1}, J_{\text{th}}(\text{He}^3) = 198301{\cdot}54\ \text{cm}^{-1}$, Herzberg obtained the following 'experimental' values of the Lamb shift for the ground state,

$$\Delta E_j(\text{He}^4) = -1{\cdot}19 \pm 0{\cdot}15\ \text{cm}^{-1}$$

$$\Delta E_j(\text{He}^3) = -1{\cdot}23 \pm 0{\cdot}15\ \text{cm}^{-1}$$

If we take the ionization potential of Helium from Pekeris (1962) theoretical value from solving a determinant of order 1078,

$$J_{\text{th}}(\text{He}^4) = 198312{\cdot}026\ \text{cm}^{-1}$$

then, comparing with Herzberg's ionization potential, we obtain the corresponding 'experimental' values for the ground state

$$\Delta E_J(\text{He}^4) = -1{\cdot}21 \pm 0{\cdot}15\ \text{cm}^{-1}$$

$$\Delta E_J(\text{He}^3) = -1{\cdot}25 \pm 0{\cdot}15\ \text{cm}^{-1}$$

The present calculation from this theory gives

$$\Delta E_J(1^1S) \simeq -0{\cdot}9(5)\ \text{cm}^{-1}$$

For the 2^3S state of Helium, Herzberg's experimental ionization potential is $38454{\cdot}73 \pm 0{\cdot}05\ \text{cm}^{-1}$. The corresponding Perkeris (1962) theoretical value is $38454{\cdot}8274\ \text{cm}^{-1}$. Thus the 'experimental' Lamb shift for this state is $-0{\cdot}10 \pm 0{\cdot}05\ \text{cm}^{-1}$. This present calculation gives

$$\Delta E_J(2^3S) \simeq -0{\cdot}10\ \text{cm}^{-1}$$

For the 2^1S state of Helium, Herzberg's experimental value is $32033{\cdot}26 \pm 0{\cdot}03\ \text{cm}^{-1}$. The corresponding result of Pekeris (1962) is $32033{\cdot}318\ \text{cm}^{-1}$. Thus the 'experimental' Lamb shift is $-0{\cdot}06 \pm 0{\cdot}03\ \text{cm}^{-1}$. The present calculation gives

$$E_J(2^1S) \simeq -0{\cdot}10\ \text{cm}^{-1}$$

We can see that, to the accuracy used here, the results of present calculations are the same order of magnitude as the experimental values for the required shifts. However, there is some discrepancy. Part of this discrepancy probably comes from the assumption of a stationary point charge nucleus, without taking account of the charge distribution of Helium nucleus. A better approximation to the solution of more coupled field equations that describe the system may inprove the results and would contribute to the difference in the Lamb shifts in He^4 and He^3.

Other sources of error are: the approximations used when evaluating the intergrals $I_{11}, I_{12}, I_{21}, I_{22}$ (Yu, 1974), the cut-off for the reduced Hamiltonian to the order of α^2, the approximation used for the wave function in the calculations of the matrix elements required in this study. It may be pointed out, however, that a wave function using many more terms in its perturbation expansion would not improve the results of the present paper very much. A more accurate calculation, taking these possible errors into account, would be needed to make comparison with the experimental result in the second decimal place—which is the accuracy of the experimental values. Thus, the present approximate agreement suggests that the Sachs formulation is indeed correct.

According to quantum electrodynamics, the total radiative correction (the Lamb shift) to the ionization potential energy of Helium for the ground state is $-1{\cdot}341 \pm 0{\cdot}05\ \mathrm{cm}^{-1}$ (Kabir & Salpeter, 1957). The radiative shifts for the 2^1S and 2^3S states, according Suh and Zaidi, as quoted in Pekeris (1962), are $-0{\cdot}104 \pm 0{\cdot}014\ \mathrm{cm}^{-1}$ and $-0{\cdot}109 \pm 0{\cdot}009\ \mathrm{cm}^{-1}$, respectively.

We see that our results are also close to theirs. However, the results of this paper come from a theory that is fundamentally different from quantum electrodyanmics both in concepts and formalism. From this theory, the dynamical and electromagnetic coupling of the electron-nucleus system alone leads to correct predictions of the Lamb shift. Thus the theoretical interpretation of the Lamb shift is not necessarily a consequence of the assumptions of quantum electrodynamics. The implication then follows that the self-consistent field theory should be compared with quantum electrodynamics in still further applications.

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