Vacuum Polarization Contribution to Hydrogen and Positronium Energies

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Relative order $\alpha(Z\alpha)^3$ shift of the energy levels induced by the vacuum polarization is reexamined for a bound system of two particles with masses $m$ and $M$. Recent results for hydrogen and for positronium are shown to contain an error due to the inadequate procedure of the infrared divergence handling. Numerically, the correction to the ground state energy constitutes 0.647 kHz for hydrogen and 46.7 kHz for positronium.

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I. INTRODUCTION

The radiative correction of the relative order $\alpha(Z\alpha)^3$ to the energies of positronium and the radiative-recoil correction of the relative order $\alpha(Z\alpha)^3 \frac{m}{M}$ to the hydrogen energies should be taken into account when one compares the recent experimental results with the QED predictions. An attempt to calculate such the corrections, induced by the vacuum polarization, was undertaken in Ref. [3] for hydrogen. In Ref. [4], the same correction was calculated for a two-body system of particles with an arbitrary mass ratio and the result was applied to hydrogen and positronium.

In the present note the calculation of the vacuum polarization correction is reexamined with the purpose to clarify the issue of the infrared regularization. Such a regularization is necessary for a control over the linear infrared divergence arising in the course of the calculation and through which the leading order correction reveals itself.

In order to separate the contribution of the leading order, which comes from the atomic scale, from the next-to-leading one, saturated by the relativistic scale, we introduce the auxiliary parameter $\lambda'$, $mZ\alpha \ll \lambda' \ll m$. Subtracting the Yukawa potential from the Coulomb one,

$$-\frac{Z\alpha}{r} \rightarrow -\frac{Z\alpha}{r} + \frac{Z\alpha}{r} e^{-\lambda'r},$$

we find the contribution to the energy due to the range of $r$’s satisfying $\frac{1}{\lambda'} < r \sim \frac{1}{mZ\alpha}$. On the other hand, the subtracted contribution is saturated by the short range, $\frac{1}{\lambda'} > r \sim \frac{1}{m}$. In the sum of two contributions, the dependence on the parameter $\lambda'$ is cancelled away.

Below we use a standard scheme of calculations, taking the vacuum polarization into account by means of the substitution

$$\frac{g_{\mu\nu}}{k_0^2 - k^2} \rightarrow \frac{g_{\mu\nu}}{k_0^2 - k^2 - \lambda^2},$$
for a propagator of the photon, which polarizes vacuum. An energy correction which thus becomes a function of \( \lambda \) is then integrated over \( \lambda \) with a density of intermediate states \( \rho(\lambda) \), which equals

\[
\frac{2\alpha \lambda^2 + 2m^2}{3\pi \lambda^3} \sqrt{1 - \frac{4m^2}{\lambda^2}} \theta(\lambda - 2m)
\]  

(3)

for a free particle-antiparticle pair.

II. ORDER \( m\alpha(Z\alpha)^4 \) CONTRIBUTION

If bounded particles are non-relativistic, vacuum polarization manifests itself primarily due to the Coulomb field. Since the atomic momentum is much less than a mass \( \lambda \) of the particle-antiparticle pair, this momentum can be neglected in the right-hand side of (4), so that an effective potential induced by the Coulomb vacuum polarization, at fixed \( \lambda \) turns out to be

\[
V_\lambda(r) = -\frac{4\pi Z\alpha}{\lambda^2} \delta(r),
\]

(4)

while the corresponding (lowest-order) contribution to an atom’s energy is

\[
E_{LO}(\lambda) = -\frac{4\pi Z\alpha |\psi(0)|^2}{\lambda^2}.
\]

(5)

After the integration with respect to \( \lambda \) with the weight function (3) it turns into

\[
\Delta E_{LO} = -\frac{4\alpha Z\alpha |\psi(0)|^2}{15m^2}.
\]

(6)

Now let us find the correction to this result induced by the modification of the Coulomb potential at short ranges (recall that \( \lambda' \gg mZ\alpha \)),

\[
-\frac{Z\alpha}{r} \rightarrow -\frac{Z\alpha}{r} + \frac{Z\alpha}{r} e^{-\lambda'r}.
\]

(7)
To this end we calculate the average value of the operator \([\mathcal{H}]\) over the state, whose wave function is perturbed by the short-range correction to the Coulomb potential \([\mathcal{H}]\):

\[
\mathcal{E}_\lambda = \left\langle \psi(r') \left| V_\lambda(r') \mathcal{G}(r', r|E) \frac{Z \alpha e^{-\lambda r}}{r} \right| \psi(r) \right\rangle + \text{c.c.} \tag{8}
\]

Here \(\mathcal{G}(r', r|E)\) is the reduced Green’s function of the Schrödinger equation in the Coulomb field, \(\psi(r)\) is the solution of this equation. To the lowest order in \(Z \alpha\), we can disregard the Coulomb interaction in \(\mathcal{G}\) and the atomic momentum as compared with \(\lambda\):

\[
\mathcal{G}(0, r|E) \to -\frac{2\mu}{4\pi r}, \quad \psi(r) \to \psi(0), \tag{9}
\]

\((\mu = mM/(m + M)\) is the reduced mass) and obtain

\[
\mathcal{E}_\lambda = \frac{4\pi(Z \alpha)^2}{\lambda^2} |\psi(0)|^2 \frac{4\mu}{\lambda^2}. \tag{10}
\]

\section*{II. ORDER \(m\alpha(Z \alpha)^5\) CONTRIBUTION}

In the next-to-leading order, let us consider the double photon exchange accounting for vacuum polarization by one of these photons. According to the Feynman’s rules, corresponding contribution to the energy at fixed \(\lambda\) is

\[
\mathcal{E}(\lambda, \lambda') = -2(Z \alpha)^2 \psi^2 \int \frac{dk_0}{2\pi i} \int \frac{d^3k}{(2\pi)^3} \frac{4\pi}{k^2 - k'^2} \frac{4\pi}{k^2 - k'^2} \left\langle \frac{(1 + \gamma_0)m + \gamma_0 k_0 - \gamma k}{k^2 - \omega^2} \gamma_\nu \right\rangle \left\langle \frac{(1 + \gamma_0)M - \Gamma \nu k_0 + \Gamma k}{k^2 - \Omega^2} \Gamma_\mu - (\mu \leftrightarrow \nu, M \leftrightarrow -M) \right\rangle. \tag{11}
\]

This expression can be represented graphically as two fermion lines connected by two photon ones. The first and the second terms in the angle brackets correspond to the graphs with uncrossed and crossed photon propagators, respectively. In \([\mathcal{H}], k^2 = k'^2, \]

\[
\mathcal{K} = \sqrt{k_0^2 - \lambda^2}, \quad \mathcal{K}' = \sqrt{k_0^2 - \lambda'^2};
\]
\[
\omega = \sqrt{k_0^2 + 2mk_0}, \quad \Omega_\pm = \sqrt{k_0^2 \pm 2Mk_0};
\]

\(\gamma_\mu (\Gamma_\mu)\) are the Dirac matrices for the light (heavy) particle. The parameter \(\lambda\) will be used below as a mass of the virtual pair, in accord with (2), while the parameter \(\lambda'\) is introduced to regularize the otherwise infrared divergent integral in (11). Two possible ways to insert \(\lambda\) and \(\lambda'\) into the photon propagators are accounted for in (11) by the overall factor 2. Choosing \(\lambda, \lambda' \gg mZ\alpha\), we can neglect atomic momenta so that taking the average over a bound state reduces to that over the Pauli spinors which is denoted by angle brackets, together with the multiplication by \(\psi^2 \equiv |\psi(0)|^2\). The spinor averages are trivial:

\[
\langle \gamma_\mu (1 + \gamma_0) \gamma_\nu \gamma_\nu \rangle \langle \Gamma_\mu(\nu)(1 + \Gamma_0) \Gamma_\nu(\mu) \rangle = 4,
\]

\(12\)

\[
\langle \gamma_\mu \gamma_0 \gamma_\nu \rangle \langle \Gamma_\mu(\nu)(1 + \Gamma_0) \Gamma_\nu(\mu) \rangle = \langle \gamma_\mu (1 + \gamma_0) \gamma_\nu \rangle \langle \Gamma_\mu(\nu) \Gamma_0 \Gamma_\nu(\mu) \rangle = 2,
\]

\(13\)

\[
\langle \gamma_\mu \gamma_0 \gamma_\nu \rangle \langle \Gamma_\mu(\nu)\Gamma_0 \Gamma_\nu(\mu) \rangle = 4 \mp 2\sigma\sigma',
\]

\(14\)

\[
\langle \gamma_\mu \gamma_\nu \rangle \langle \Gamma_\mu(\nu)\Gamma\Gamma_\nu(\mu) \rangle = -6 \pm 4\sigma\sigma'.
\]

\(15\)

Before proceeding further, let us consider the analytic properties of the integrand in (11) as a function of \(k_0\). The photon propagators have the poles at the points \(\pm \sqrt{k^2 + \lambda^2}\) and \(\pm \sqrt{k^2 + \lambda'^2}\). After the integration over \(k\) these poles turn into the cuts that go from \(-\infty\) to \(-\lambda\) (\(-\lambda'\)) and from \(\lambda\) (\(\lambda'\)) to \(\infty\). Similarly, the light fermion propagator gives rise to the cuts \((-\infty, -2m]\) and \([0, \infty)\). The heavy fermion propagator in the second term of (11), which corresponds to the graph with crossed photon lines, gives rise to the cuts \((-\infty, -2M]\) and \([0, \infty)\). Finally, the heavy fermion propagator in the first term, corresponding to the graph with uncrossed photon lines, produces the cuts \((-\infty, 0]\) and \([2M, \infty)\).

It is convenient to extract the heavy fermion propagator from the first term of (11),

\[
\frac{1}{k^2 - \omega^2} \frac{1}{k^2 - \Omega_+^2} = \frac{1}{2(M + m)k_0} \left( \frac{1}{k^2 - \omega^2} - \frac{1}{k^2 - \Omega_+^2} \right),
\]

\(16\)
and then to change the sign of the integration variable \(k_0 \to -k_0\) in all terms containing \(1/(k^2 - \Omega_-^2)\). In this way the integral over \(k_0\) is naturally split into two parts. The former one,

\[
\mathcal{E}_{\text{cut}}(\lambda, \lambda') = -2 \left( \frac{Z \alpha^2 \psi^2}{M^2 - m^2} \right) \int_{C_-} \frac{dk_0}{2\pi i} \int \frac{d^3k}{(2\pi)^3} \frac{4\pi}{k^2 - \Omega^2} \frac{4\pi}{k^2 - K^2} \left[ \left( \frac{2Mm}{k_0} + 2m + \frac{m}{M} \frac{2k_0^2 - k^2}{k_0} + \frac{\sigma \sigma'}{3} \frac{3k_0^3 - 2k^3}{k_0} \right) \frac{2M}{k^2 - \Omega^2} - (M \leftrightarrow m) \right],
\]

where \(\Omega \equiv \Omega_+\), is taken over the contour \(C_-\), wrapping the left cut. The latter part is a residue at the \(k_0 = 0\) pole, which appears in terms containing \(k_0^{-1}(k^2 - \Omega_-^2)^{-1}\) after the change \(k_0 \to -k_0\):

\[
\mathcal{E}_{\text{pole}}(\lambda, \lambda') = -2 \left( \frac{Z \alpha^2 \psi^2}{M + m} \right) \frac{4\pi}{\lambda + \lambda'} \left( \frac{2Mm}{\lambda \lambda'} + 1 - \frac{2\sigma \sigma'}{3} \right).
\]

Let us begin with the latter contribution. In (18), the first term in the brackets is singular when one of the lambdas approaches zero. This term is just the regulator contribution subtracted from the leading order correction. In fact, neglecting \(\lambda'\) as compared with \(\lambda\) in the sum \(\lambda + \lambda'\) above, we see that the infrared–singular term in (18) is compensated by the effect of the Coulomb potential modification (10). Hence, only two last terms in the right-hand side of Eq.(18) comprise the genuine order \((Z \alpha)^5\) contribution of the \(k_0 = 0\) pole, so that we can safely set \(\lambda' = 0\) in those terms:

\[
\mathcal{E}_{\text{pole}}(\lambda) = -2 \left( \frac{Z \alpha^2 \psi^2}{M + m} \right) \frac{4\pi}{\lambda} \left( 1 - \frac{2\sigma \sigma'}{3} \right).
\]

Likewise, we can set \(\lambda' = 0\) in the left-cut contribution (17) as far as this procedure does not spoil the infrared convergence of the integral. The integration over \(k\) gives for \(\mathcal{E}_{\text{cut}}(\lambda) \equiv \mathcal{E}_{\text{cut}}(\lambda, 0):

\[
\mathcal{E}_{\text{cut}}(\lambda) = \frac{4(Z \alpha^2 \psi^2}{M^2 - m^2} \int_{C_-} dk_0 \left\{ \left( \frac{2m}{k_0} + \frac{m}{M} \right) \frac{1}{|k_0| + \mathcal{K}} - \left[ \frac{2Mm}{k_0^2} + \frac{m}{3} \left( \frac{4M}{k_0} - 1 \right) \right] \frac{1}{\Omega + \mathcal{K}} - (M \leftrightarrow m) \right\}.
\]

\(\mathcal{K}\)
Finally, integrating with respect to $k_0$ and adding up the pole contribution (19), we obtain:

$$\mathcal{E}(\lambda) = -\frac{4(Z\alpha)^2\psi^2}{M^2 - m^2} \left\{ Mm(M - m) \frac{2\pi}{\lambda^3} - \frac{4Mm}{\lambda^2} A\left(\frac{\lambda}{2M}\right) + (M - m) \frac{2\pi \sigma\sigma'}{\lambda} \right\}$$

$$+ \frac{m}{M} \left( \frac{1}{2} + \ln \frac{\lambda}{M} \right) + \sigma\sigma' \left[ \ln \frac{M}{m} - \frac{4}{3} A\left(\frac{\lambda}{2M}\right) \right]$$

$$- \left( \frac{m}{M} + \frac{\sigma\sigma'}{3} \right) \frac{\lambda^2}{2M^2} \left[ A\left(\frac{\lambda}{2M}\right) + \ln \frac{\lambda}{M} \right] - (M \leftrightarrow m). \quad (21)$$

Here

$$A(x) = \theta(1 - x) \frac{\sqrt{1 - x^2}}{x} \cos^{-1} x - \theta(x - 1) \frac{\sqrt{x^2 - 1}}{x} \cosh^{-1} x. \quad (22)$$

From (21), the known results for the vacuum polarization contribution to the hyperfine splitting in muonium [5,6] and positronium [7] can be obtained:

$$\Delta E_{hfs}^{\mu^+e^-} = \alpha(Z\alpha)E_F \left\{ \frac{3}{4} - \frac{m}{M} \left( 2\ln^2 \frac{M}{m} + \frac{8}{3} \ln \frac{M}{m} + \frac{28}{9} + \frac{\pi^2}{3} \right) + O\left(\frac{m^2}{M^2}\right) \right\}; \quad (23)$$

$$\Delta E_{hfs}^{e^+e^-} = \frac{5}{3} \alpha(Z\alpha)E_F. \quad (24)$$

Here

$$E_F = \frac{8\pi Z\alpha\psi^2}{3 \cdot Mm} \quad (25)$$

is the Fermi splitting with the anomalous magnetic moments omitted.

For the spin-independent part of the correction to the energy levels of hydrogen and positronium, we have

$$\Delta E^{e^+e^-} = \frac{4(Z\alpha)^2\psi^2}{Mm} \int_1^\infty dx \rho(x) \left\{ \frac{\pi}{2x^3} - \frac{1}{x^2} + \frac{\sqrt{x^2 - 1}}{x^3} \cosh^{-1} x \right\}$$

$$+ \frac{1}{2} \ln 2x - 2x^2 \ln 2x + 2x\sqrt{x^2 - 1} \cosh^{-1} x \right\}$$

$$= \frac{\alpha(Z\alpha)^2}{\pi} \frac{\psi^2}{Mm} \left( \frac{47\pi^2}{144} - \frac{70}{27} \right) + O\left(\frac{m}{M}\right); \quad (26)$$

$$= \alpha(Z\alpha)^2 \frac{\psi^2}{Mm} \left( \frac{47\pi^2}{144} - \frac{70}{27} \right) + O\left(\frac{m}{M}\right); \quad (27)$$
and
\[
\Delta E^{e^+e^-} = -\frac{2(Z\alpha)^2\psi^2}{m^2} \int_1^\infty dx \rho(x) \left\{ \frac{\pi}{2x^3} - \frac{\cosh^{-1} x}{x^3\sqrt{x^2-1}} - \frac{1}{x^2} - 2 \right. \\
\left. -2\ln 2x + 2x^2\ln 2x - 8x\sqrt{x^2-1}\cosh^{-1} x - 2 \frac{x\cosh^{-1} x}{\sqrt{x^2-1}} \right\} 
\]
\[
= \frac{\alpha(Z\alpha)^2\psi^2}{\pi m^2} \left( \frac{49\pi^2}{288} - \frac{40}{27} \right). 
\]

where
\[
\rho(x) = \frac{\alpha}{3\pi} \frac{2x^2 + 1}{x^4} \sqrt{x^2 - 1}. 
\]

These results differ from those obtained in Refs. [3,4] for hydrogen and in Ref. [4] for positronium. The error made in both works has the same origin – inaccurate treatment of the infrared divergence. In fact, the authors of Refs. [3,4] do not introduce in (11) the parameter \(\lambda'\), which, as we have seen above, regularizes the infrared divergence. Instead, they subtract from the integrand in (11) its asymptotic value at small \(k\)'s. Giving the finite results of Refs. [3,4], this last procedure cannot be correct, since those finite results arise as a difference between two divergent integrals. In contrast, the regularization procedure used in the present work deals with the well-defined finite expressions.

Numerically, the correction (27) constitutes 0.647 kHz for the ground-state energy of hydrogen, while (29) equals 46.7 kHz for the ground-state energy of positronium. In the case of hydrogen, the correction exceeds the uncertainty of the recent measurement [2].

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