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RECOIL CORRECTION IN THE DIRAC–COULOMB PROBLEM

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Recoil Correction in the Dirac-Coulomb Problem

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ABSTRACT

The expression for the first recoil correction to the Dirac-Coulomb spectrum is obtained employing the gauge invariance.

Relativistic two-body problem in quantum electrodynamics has been exactly solved in the only limiting case $m/M \to 0$, $\alpha \to 0$ at fixed $Z\alpha$ (here M and m are masses of the constituents, $Z|e|$ and e are their electric charges, $\alpha = e^2/\hbar c$ is the fine structure constant, $\hbar = c = 1$). In this limit, an infinitely heavy nucleus holds still being the source of the constant in time Coulomb field. A wavefunction of the system reduces to that of the light particle, the electron, and obeys the Dirac equation in the Coulomb field,

$$(\vec{\alpha}\vec{p} + \beta m + V_C - E)\,\psi = 0. \tag{1}$$

Expressions for the first (linear in m/M) recoil corrections to energies of the Dirac-Coulomb bound states were obtained several years ago by V.M. Shabaev [1, 2]. He used the perturbation theory in $Z\alpha$, summing up contributions of a given order in $Z\alpha$, linear in m/M. The present note is devoted to a simple derivation of the Shabaev's result, with only minor reference to the perturbation theory.

As a guiding principle we will use the gauge invariance of QED. To begin with, let us generalize the equation (1) to an arbitrary gauge. Since $V_C = Z\alpha D_{00}$[1], and an infinitely heavy particle at rest can emit (or absorb) only zero component of the vector potential, we have:

$$\{\alpha_\mu\,(p_\mu - Z\alpha D_{\mu 0}) + \beta m\}\,\psi = 0, \tag{2}$$

where $\alpha_0 = 1$ by definition, $p_0 = E$. The Dirac-Coulomb spectrum, that is the mutual arrangement of the Green's function singularities at the complex E plane[2], is certainly gauge-invariant.

[1] $D_{\mu\nu}$'s make up the photon propagator.
[2] We consider only gauges with $D_{\mu 0}$ constant in time, so that E is the integral of motion.

Now let us take into account the motion and interaction of the nucleus to first order in $1/M$. They are described by the term

$$\frac{\left(\vec{P} - Z|e|\vec{A}\right)^2}{2M} \tag{3}$$

in the Hamiltonian of the system[3]. Here $\vec{P}$ is the operator of a nucleus momentum, while $\vec{A}$ is the vector potential operator acting at the nucleus site. Due to M in the denominator, $\vec{A}$ can be taken to act at the origin.

In order to find the first recoil correction to an energy of the electron we need to average the above expression over the corresponding Dirac-Coulomb eigenfunction. There is no problem with the vector potential operator — it emits (absorbs) photons which are absorbed (emitted) by the electron. Difficulties emerge when one tries to determine how the operator $\vec{P}$ acts on the electron wavefunction. In fact, the simple relation $\vec{P} = -\vec{p}$ holds in the nonrelativistic limit only, when the problem is truly two-body. The relativistic electron can propagate in both time directions so that at a fixed time slice one has a number of electrons and positrons with the total momentum equal to $-\vec{P}$.

To get rid of the problem we will start with the operator

$$\frac{\left(Ze\vec{A}\right)^2}{2M}, \tag{4}$$

whose expectation value can be easily expressed in terms of the known solution to the Dirac-Coulomb problem. Being only the part of the nucleus Hamiltonian (3), the operator (4) is by no means gauge-invariant. This is also true for its expectation value. The basic idea is to reconstruct a gauge-invariant expression for the total energy correction from its known noninvariant part.

Taking the expectation value of (4) over fluctuations of the electromagnetic field we are left with

$$\Delta E_{\vec{A}^2} = \frac{(Z\alpha)^2}{M} \int \frac{i\,d\omega}{2\pi} \left\langle \alpha_\mu D_{\mu J}(\omega) G(E-\omega) D_{J\nu}(-\omega) \alpha_\nu \right\rangle . \tag{5}$$

Diagrammatically the right-hand side of this equation is shown in Fig.1.

[3] The interaction of the electron with a nucleus proper magnetic moment, formally of the order $1/M$, is taken into account straightforwardly, so we do not discuss it here.

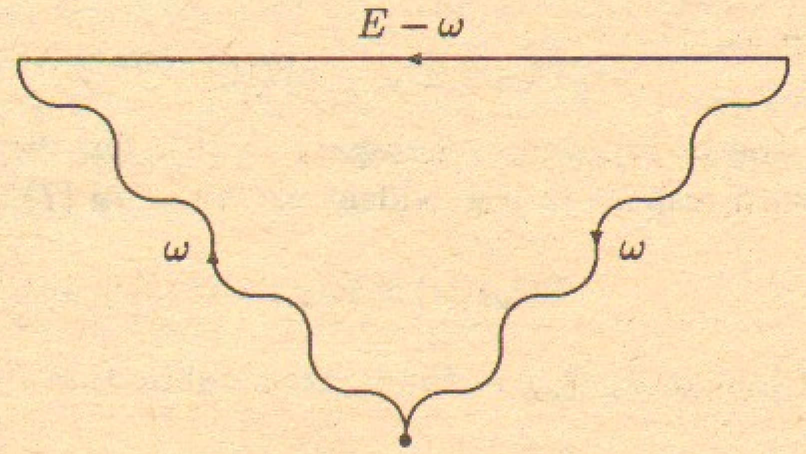

Fig.1. "Seagull" contribution to the recoil.

The solid line depicts G, the Green's function for the Dirac equation in the Coulomb field, wiggly lines represent photon propagators $D_{\mu J}$ and $D_{J\nu}$. As far as a gauge is not fixed, it is convenient to make difference between Lorentz indices corresponding to a nucleus interaction vertex (upper case) and those corresponding to an electron vertex (lower case). Overall factor $1/M$ allows us to take the limit $M \to \infty$ everywhere else. In particular, the remaining photon propagators connecting the electron line with the nucleus one and not shown explicitly in Fig.1, have the upper case index equal to zero (see (2)). As usual, Latin indices run from 1 to 3, Greek ones run from 0 to 3. For the sake of brevity and later convenience, only the integral over energy flowing along the loop is written down explicitly. E in (5) is the energy of a Dirac-Coulomb eigenstate we average over.

Turn now to the gauge transformation properties of (5). The above discussion of the Dirac equation in the Coulomb field shows that $\Delta E_{\vec{A}^2}$ is invariant with respect to a gauge transformation at the electron site,

$$\delta D_{\mu\Lambda} = \nabla_\mu \varphi_\Lambda , \tag{6}$$

where φ_Λ are arbitrary (linear in time) functions. Hence, it remains to recover the invariance with respect to the transformation at the opposite 'end' of D, attached to the nucleus line, namely

$$\delta D_{\mu J} = \nabla_J \varphi_\mu . \tag{7}$$

Trying to do this we cannot use components of D with a spatial upper case index. Actually, those components of D emerge in an expression for the energy correction due to the operator $\vec{A}$ acting at the nucleus site. Since the quadratic in $\vec{A}$ effect is already taken into account by (5), the only thing that can help us reads

$$\alpha_\mu D_{\mu 0} = D_{00} - \alpha_l D_{l0}. \tag{8}$$

It does not spoil the invariance with respect to (6). On the other hand, its gauge variation with respect to the evident extension of (7),

$$\delta D_{\mu 0}(\omega) = i\omega\varphi_\mu, \tag{9}$$

does compensate that of $\alpha_\mu D_{\mu J}$ in the linear combination

$$\alpha_\mu D_{\mu J}(\omega) + \frac{1}{\omega}\alpha_\mu i\,[\nabla_J, D_{\mu 0}(\omega)]. \tag{10}$$

By this means the gauge-invariant expression for the recoil correction takes the form:

$$\Delta E = \frac{(Z\alpha)^2}{M}\int\frac{i\,d\omega}{2\pi}\left\langle\alpha_\mu\left(D_{\mu J}(\omega) + \frac{1}{\omega}i\,[\nabla_J, D_{\mu 0}(\omega)]\right)\right.$$
$$\left. G(E-\omega)\left(D_{J\nu}(-\omega) - \frac{1}{\omega}i\,[\nabla_J, D_{0\nu}(-\omega)]\right)\alpha_\nu\right\rangle. \tag{11}$$

Recall that $\alpha_0 = 1$. Unfortunately, this expression is meaningless until we define how to treat the new singularity at $\omega = 0$.

As soon as the gauge invariance is maintained we can choose the mostly convenient gauge. Without question this is the Coulomb one. Then the total energy shift (11) is naturally broken up into four terms:

$$\Delta E = \Delta E_{CC} + \Delta E_{CM} + \Delta E_{MC} + \Delta E_{MM}, \tag{12}$$

the last of which is nothing but the Coulomb gauge version of $\Delta E_{\vec{A}^2}$ (see (5) and Fig.1), i. e. the double magnetic exchange contribution to the energy shift. The third and the second terms comprise the correction arising due to a single magnetic exchange. Their origin at (3) is the term $-Z|e|(\vec{P}\vec{A} + \vec{A}\vec{P})/2M$. Finally, the pure Coulomb contribution ΔE_{CC} is just the mean value of the nucleus 'kinetic energy' $\vec{P}^2/2M$.

To find a prescription according to which the $1/\omega$-singularity should be passed by one can exploit its independence of $Z\alpha$ and analyze the corresponding expression perturbatively in $Z\alpha$, to the lowest nontrivial order. Very natural result for the single-magnetic exchange reads

$$\frac{1}{\omega} \to \frac{1}{2}\left(\frac{1}{\omega - i0} + \frac{1}{\omega + i0}\right). \tag{13}$$

For example, the third term in (12) can be represented diagrammatically by the sum of two graphs shown in Fig.2. There the thick line depicts the propagator $(\pm\omega + i0)^{-1}$ of the infinitely heavy nucleus having the energy $M \pm \omega$, while the dashed line shows the interaction through the Coulomb electric field $Z|e|[\vec{\nabla}, D_{00}]$.

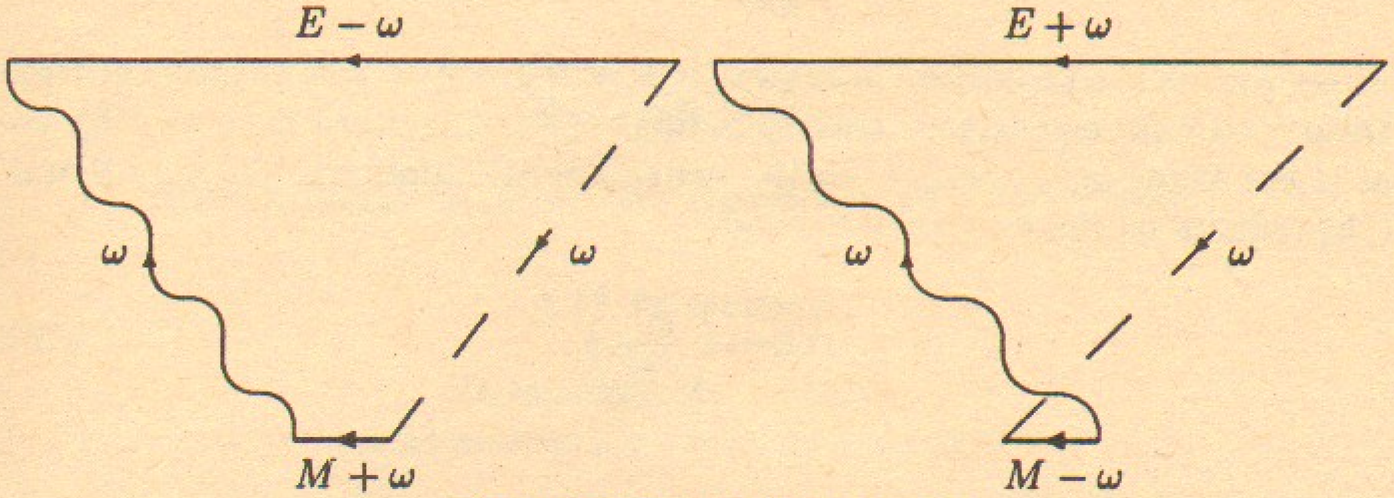

Fig.2. Single magnetic exchange.

Simple perturbative analysis of the pure Coulomb contribution ΔE_{CC} suggests that corresponding prescription has the form:

$$\frac{1}{\omega^2} \to \frac{1}{2}\left(\frac{1}{(\omega - i0)^2} + \frac{1}{(\omega + i0)^2}\right). \tag{14}$$

Actually, here we have the sum of the nucleus propagator derivatives resulting from the expansion of $(\vec{P}^2/2M \pm \omega + i0)^{-1}$. To obtain Feynman diagrams for the pure Coulomb contribution, one need only substitute wiggly lines in Fig.2 for dashed ones as well as the nucleus propagator for its square.

Now, when the integral in (11) is completely defined one can easily check that this expression equals the sum of recoil corrections found by Shabaev in the more straightforward way [1, 2] (in [2], the overall sign of the expression for ΔE_{MM} is corrected).

Recall that our starting point was the expectation value (5). Its perturbative expansion can be readily appreciated to begin with $(Z\alpha)^5$. To be certain that the corresponding expansion for the total correction (11) begins with $(Z\alpha)^2$, let us consider in greater detail the pure Coulomb contribution which alone survives the transition to the nonrelativistic limit. As a byproduct we will see how the expectation value $\left\langle\vec{P}^2/2M\right\rangle$ looks in terms of the solution to the Dirac-Coulomb problem.

Evaluating the integral with respect to ω in ΔE_{CC} according to the prescription (14) together with the standard rules for the Dirac-Coulomb Green's function one readily obtains

$$\Delta E_{CC} = \frac{1}{2M} \langle \vec{p}(\Lambda_+ - \Lambda_-)\vec{p} \rangle , \qquad (15)$$

where $\Lambda_\pm$ are the projection operators to sets of positive- and negative-energy Dirac-Coulomb eigenstates correspondingly. Passing from (11) to (15) we used the Dirac equation (1). In the nonrelativistic limit $\Lambda_+ \to 1$, $\Lambda_- \to 0$ and (15) reduces to the well-known result,

$$\Delta E \to \left\langle \frac{\vec{p}^{\,2}}{2M} \right\rangle . \qquad (16)$$

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