Gauge Dependence of Four-Fermion QED Green Function and a Breakdown of Gauge Invariance in Atom-Like Bound State Calculations

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Abstract

We derive a relation between four-fermion QED Green functions of different covariant gauges which defines the gauge dependence completely. We use the derived gauge dependence to check the gauge invariance of atom-like bound state calculations. We find that the existing QED procedure does not provide gauge invariant binding energies. A way to a corrected gauge invariant procedure is pointed out.

1 Introduction

QED gives a successful description of atom-like bound states. The recent measurement of the positronium life-time [1] seems to remove the only discrepancy between theory and experiment in this field. Still, one can scrutinize general basis of the existing theory which involves far from trivial assumptions. The main one is that excited states correspond to simple poles of four-fermion QED Green function [2, 3, 4]. In fact, one cannot prove it because of instability of excited states. Next, more technical, is that Bethe-Salpeter kernel is regular in total energy of fermions near the poles. Combination of the above assumptions leads to the generally accepted prescriptions (see, for example, [2]) for calculation of bound state parameters. Needless to say, any numerical success yielded by these rules supports but cannot prove the assumptions.

Let us explain why it is doubtful that the above assumptions hold. To this end, consider propagator of a charged particle. Naively, one would expect that it has a simple pole at the particle mass. But it is well known (see, for example [5]) that radiation of massless photons causes branch point singularity instead of the simple pole. One should expect the similar effect for atom-like bound states. The only difference is that two-particle bound state is a dipole. Consequently, one expects the radiation to be less important. This expectation is in accord with the successes of the standard approach to the atom-like bound states.

The aim of this paper is to demonstrate that the main assumption—correspondence of excited states to simple poles of the Green function—is in contradiction with gauge invariance. More precisely, we will show that the assumption leads to a gauge dependence in the

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pole positions, i.e., in observable energy level shifts. We will estimate the leading contribution to the derivative of level shifts over gauge-fixing parameter. It will turn out that the gauge dependence is too weak to be seen in calculations performed up to now.

It may seem that there is an opposite statement in the literature. Namely, it was found in [6] that level shifts of the standard procedure are gauge invariant. The difference between [6] and the present paper lies in the assumptions on the Green function properties which were used in the study of gauge invariance. In fact, derivation of [6] is based on the above assumptions which we do not use in our analysis. To be specific, in the first of two papers [6] it was pointed out that derivatives of the Green function over gauge parameter contain branch points in the total energy of the pair. The authors conclude, seemingly using the assumption that the only relevant singularities are simple poles, that these branch points should be shifted from the poles corresponding to the bound states. In the present work we allow the possibility that the Green function have branch points and simple poles of coinciding positions. In the second paper of [6], an explicit form of the level shifts was used to prove their gauge invariance. The derivation is algebraic in nature and employs implicitly the second assumption—namely, that Bethe-Salpeter kernels and their energy derivatives are finite at the poles. (In notations of [6], that means finiteness of \( k^{(i)}, \dot{k}^{(i)}, \ddot{k}^{(i)}, \ldots \)) Again, we do not use any assumption on the Bethe-Salpeter kernels in our work (in fact, we even don’t need these objects) and arrive at an opposite result. One may conclude that some of the quantities \( k^{(i)}, \dot{k}^{(i)}, \ddot{k}^{(i)}, \ldots \) of [6] are ill-defined. Indeed, more close analysis proves [7], that, say, \( k^{(5)} \) is infra-red divergent. We should stress that one would run into these singularities in the Bethe-Salpeter kernels only in a calculation of level shifts of order \( \alpha_{11} \).

The latter may give a wrong impression that one can safely use the standard prescriptions for level shift calculations up to order \( \alpha_{11} \). The real range of applicability of the standard prescriptions can be found only from a comparison with new, corrected prescriptions. We have not them in our possession. So, the only claim of the present paper is that the standard prescriptions break down in order \( \alpha_{11} \).

We should anticipate a question on the gauge dependence of the ground level shift which follows from our general formulas. Indeed, there is no doubt that ground level of bound system, if it exists, corresponds to a simple pole of the Green function. But since perturbations mix it with excited states, the lack of consistent picture for exited states causes inconsistency in its description as well.

The last reservation we should make is on the dependence of the effect under consideration on the masses of bounded particles. To simplify the interim formulae, we consider only fermion-antifermion bound states. But all can be generalized for arbitrary mass ratio. The mass in the final formulae becomes then the reduced mass of the pair. Thus, we claim that even for the case of infinite mass of the heavier particle, i.e., when it can be replaced by the external Coulomb field, the effect survives. We expect that this case may be the most appropriate one to try to develop new, corrected prescriptions for level shift calculations.

Turning to a description of the present work itself, its main technical means is an explicit form of gauge dependence of the four-fermion QED Green function. We found a relation between the Green functions of different covariant gauges which defines the gauge dependence completely. The derivation is nonperturbative and the relation may present some interest in itself. It turns out that the gauge dependence has a simple form in the space-time representation. To use it, we formulate a procedure of extraction of level shifts form the Green
function in \( x \)-representation. Comparison of the gauge dependence of the Green function with the extraction procedure allows us to find the gauge dependence of the level shifts. We conclude pointing out a possible way to a corrected gauge invariant procedure of level shift calculations.

Next section contains a derivation of the evolution in the gauge-fixing parameter; section 3 comprises a brief recall of the extraction procedure and an utilization of the general evolution formula from section 2 for an analysis of gauge-dependence of the extraction; in the last, fourth, section we point out the reason for the gauge dependence and a way to the correct procedure.

## 2 Evolution in Gauge-Fixing Parameter

Let us consider the four-fermion QED Green function

\[
G_\beta(x_f, \overline{x}_f, x_i, \overline{x}_i) \equiv i \int D\psi D\bar{A} \exp \left( iS_{QED}(\beta) \right) (\overline{\psi}(\overline{x}_f)\psi(x_f))(\overline{\psi}(x_i)\psi(\overline{x}_i)),
\]

where \( x_f(\overline{x}_f) \) is a coordinate of outgoing particle (antiparticle) and \( x_i(\overline{x}_i) \) is the same for ingoing pair. The definition of gauge-fixing parameter \( \beta \) is given by corresponding photon propagator:

\[
D_{\mu\nu}(\beta, x) = \int \frac{dk}{(2\pi)^4} \left( -g_{\mu\nu} + \frac{\beta k_{\mu}k_{\nu}}{k^2} \right) \frac{i}{k^2} e^{ikx}.
\]

Our aim is to study the dependence of \( G_\beta \) on \( \beta \). To this end, it is useful to consider a Green function in external photon field, \( G(A) \), which is a result of integration over the fermion field in the rhs of eq. (1). From the one hand, it is simply connected to the Green function:

\[
G_\beta = \left( e^{L_\beta} G(A) \right)_{A=0} \cdot L_\beta \equiv \frac{1}{2} \frac{\delta}{\delta A_\mu} D_{\mu\nu}(\beta) \frac{\delta}{\delta A_\nu}.
\]

(In this formula each \( L_\beta \) generates a photon propagator; the dependence on the coordinates of ingoing and outgoing particles is suppressed for brevity.) From the other hand, \( G(A) \) is simply connected to a gauge invariant object \( G_{inv}(A) \):

\[
G(A) = G_{inv}(A) \exp \left( ie \int_{x_f}^{x_i} A_\mu dx^\mu - ie \int_{\overline{x}_i}^{\overline{x}_f} A_\mu d\overline{x}^\mu \right). \tag{4}
\]

The gauge invariance of \( G_{inv} \) means that it is independent of the longitudinal component of \( A \):

\[
\partial_\mu \frac{\delta}{\delta A_\mu} G_{inv}(A) = 0 \tag{5}
\]

and is a consequence of gauge invariance of the combination

\[
\overline{\psi}(x) \exp \left( ie \int_y^x A_\mu dz^\mu \right) \psi(y). \tag{6}
\]

A substitution of eq. (4) into eq. (3) yields

\[
G_\beta = \left( e^{L_\beta} G_{inv}(A) \exp \left( ie \int_{x_f}^{x_i} A_\mu dx^\mu - ie \int_{\overline{x}_i}^{\overline{x}_f} A_\mu d\overline{x}^\mu \right) \right)_{A=0}. \tag{7}
\]
Let us take a $\beta$-derivative of both sides of this equation:

$$
\frac{\partial}{\partial \beta} G_\beta = \left( e^{L_\beta(\partial_\beta L_\beta)} G_{\text{inv}}(A) \exp \left( i e \int_{x_f}^{x_i} A_\mu dx^\mu - i e \int_{x_i}^{x_i} A_\mu dx^\mu \right) \right)_{A=0}.
$$

To get an evolution equation, one needs to express the rhs of this equation in terms of $G_\beta$. It is possible because $(\partial_\beta L_\beta)$ commutes with $G_{\text{inv}}(A)$ and gives a $c$-factor when acts on the consequent exponential. So, eq. (8) transforms itself into

$$
\frac{\partial}{\partial \beta} G_\beta(x_f, \overline{x}_f, x_i, \overline{x}_i) = F(x_f, \overline{x}_f, x_i, \overline{x}_i)G_\beta(x_f, \overline{x}_f, x_i, \overline{x}_i),
$$

where we have restored the $x$-dependence and used $F$ to denote the action of $(\partial_\beta L_\beta)$ on the exponential:

$$
(\partial_\beta L_\beta) \exp \left( i e \int_{x_f}^{x_i} A_\mu dx^\mu - i e \int_{x_i}^{x_i} A_\mu dx^\mu \right) \equiv F(x_f, \overline{x}_f, x_i, \overline{x}_i) \exp \left( i e \int_{x_f}^{x_i} A_\mu dx^\mu - i e \int_{x_i}^{x_i} A_\mu dx^\mu \right).
$$

An explanation is in order: In deriving eq. (9) we have used a commutativity of $(\partial_\beta L_\beta)$ and $G_{\text{inv}}(A)$; it is a direct consequence of gauge invariance of $G_{\text{inv}}$ (see eq. (3) for a definition of $L_\beta$ and eq. (2) for $\beta$-dependence of $D_{\mu\nu}$).

The solution of eq. (9) for $\beta$-evolution is

$$
G_\beta(x_f, \overline{x}_f, x_i, \overline{x}_i) = \exp \left( (\beta - \beta_0)F(x_f, \overline{x}_f, x_i, \overline{x}_i) \right) G_{\beta_0}(x_f, \overline{x}_f, x_i, \overline{x}_i).
$$

To get the final answer one needs an explicit view of $F$ from eq. (11): It is easily deduced from the $F$-definition (11) and the following representation for the longitudinal part of the photon propagator:

$$
\partial_\beta D_{\mu\nu}(\beta, x) = -\frac{1}{16\pi^2} \partial_\mu \partial_\nu \ln((x^2 - i\varepsilon)m^2),
$$

where $m$ is an arbitrary mass scale which is fixed, for definiteness, on the fermion mass. Then, up to an additive constant,

$$
F = \frac{\alpha}{4\pi} \left( \frac{1}{m^4(x_f - \overline{x}_f)^2(x_i - \overline{x}_i)^2} + \ln \frac{(x_f - x_i)^2(\overline{x}_f - \overline{x}_i)^2}{(x_f - \overline{x}_f)^2(\overline{x}_f - x_i)^2} \right).
$$

Substituting eq. (13) into eq. (11), we get our final answer for $\beta$-evolution:

$$
G_\beta(x_f, \overline{x}_f, x_i, \overline{x}_i) = \left[ \frac{Z(x_f - x_i)^2(\overline{x}_f - \overline{x}_i)^2}{m^4(x_f - \overline{x}_f)^2(x_i - \overline{x}_i)^2(x_f - \overline{x}_f)^2(\overline{x}_f - x_i)^2} \right]^{1/2} G_{\beta_0}(x_f, \overline{x}_f, x_i, \overline{x}_i).
$$

The normalization $Z$ is infinite before the ultraviolet renormalization. After the renormalization it is scheme-dependent and calculable order by order in perturbation theory. We will not need its value in what follows.
3 The Bound State Parameters And The Four-Fermion QED Green Function

The four-fermion QED Green function contains too much information for one who just going to calculate bound-state parameters. One can throw away unnecessary information by putting center of mass space-time coordinate of ingoing pair and relative times of both ingoing and outgoing pairs to zero:

\[ \begin{align*}
G_{(et)\beta}(t, x, r, r') &\equiv G_{\beta}(x_f(t, x, r'), \bar{x}_f(t, x, r'), x_i(r), \bar{x}_i(r)),
\end{align*} \]

where the space-time coordinates depend on a space-time coordinate of the center of mass of the outgoing pair \((t, x)\) and a relative space coordinate of outgoing \((r')\) and ingoing \((r)\) pair. In the case of equal masses

\[ \begin{align*}
x_f &= (t, x + \frac{r'}{2}), & \bar{x}_f &= (t, x - \frac{r'}{2}),
x_i &= (0, \frac{r}{2}), & \bar{x}_i &= (0, -\frac{r}{2}).
\end{align*} \]

\( G_{(et)\beta} \) still contains an unnecessary piece of information — the dependence on the center of mass space coordinate. The natural way to remove it is to go over to momentum representation and put the center of mass momentum to zero. In coordinate representation, which is more convenient for gauge invariance check, we define the propagator \( D_{\beta} \) of the fermion pair:

\[ \begin{align*}
G_{(et)\beta}(t, x, r, r') &\equiv D_{\beta}(t, r', r)\delta(x) + \ldots,
\end{align*} \]

where dots denote terms with derivatives of \( \delta(x) \). It is natural to consider \( D_{\beta} \) as a time dependent kernel of an operator acting on wave-functions of relative coordinate. In what follows we will not make difference between a kernel and the corresponding operator. The naturalness of the above definition of the propagator is apparent in the nonrelativistic approximation:

\[ \begin{align*}
e^{i2mt}D_{\beta}(t) &\approx \sum_{E_0} \theta(t)e^{-iE_0 t}P(E_0),
\end{align*} \]

where the summation runs over the spectrum of nonrelativistic Coulomb problem and \( P(E_0) \) are the projectors onto corresponding subspaces of the nonrelativistic state space. One can obtain eq. (18) keeping leading term in \( \alpha \)-expansion of the lhs if one will keep \( t \propto 1/\alpha^2 \) and \( r', r \propto 1/\alpha \) (see [1, 3]). The subscript on \( E_0 \) is to denote that it will get radiative corrections (see below). The exponential in the lhs is to make a natural shift in energy zero. In what follows we will include the energy shift in the definition of \( D_{\beta}(t) \).

The next step in calculation of radiative corrections to the energy levels is a crucial one: one should make an assumption about the general form of a deformation of the \( t \)-dependence of the rhs of eq. (18) caused by relativistic corrections. A natural guess and the one which leads to the generally accepted rules of calculation of the relativistic corrections to the energy eigenvalues (see, for example [2]) is to suppose that one can contrive oscillating part of the exact propagator \( D_{\beta} \) from the rhs of eq. (18) just shifting energy levels and modifying the operator coefficients \( P(E_0) \):

\[ \begin{align*}
D_{\beta}(t) &= \sum_{E_0 + \Delta E_0} \theta(t)e^{-i(E_0 + \Delta E_0) t}P_{\beta}(E_0 + \Delta E_0) + \ldots.
\end{align*} \]
where dots denote terms which are slowly-varying in time (the natural time-scale here is $1/E_0$). The additional subscript $\beta$ on $P_\beta$ is to denote that oscillating part of $D_\beta(t)$ can acquire a gauge parameter dependence from relativistic corrections.

The conjecture (19) could be proven if the bound states were the eigenstates of the Hamiltonian. But being unstable they are not. We will see that the conjecture (19) contradicts gauge invariance. Still it turns out extremely useful—the relativistic corrections calculated with it are in agreement with the experiment. Is it possible that another ansatz may be used instead of eq. (19) preserving its advantage of success is an open question.

Let us see how one can use eq. (19) in energy level calculations. It is quite sufficient to consider $D_\beta(t)$ on relatively short times when $\Delta E_0 t \ll 1$, $E_0 t \sim 1$. For such times one can approximate $D_\beta$ expanding the rhs of eq. (19) over $\Delta E_0 t$:

$$D_\beta(t) \approx \sum_{E_0} \theta(t) e^{-iE_0 t} \sum_k t^k A_{\beta}^{(k)}(E_0), \quad (20)$$

where

$$A_{\beta}^{(k)}(E_0) = \sum_{\Delta E_0} \left( -i \Delta E_0 \right)^k \frac{1}{k!} P_\beta(E_0 + \Delta E_0). \quad (21)$$

An extraction of these objects from the perturbation theory is an interim step in the level shift calculations. (Here we should mention that in calculation practice $A_{\beta}^{(k)}(E_0)$ are extracted in momentum representation — i.e. not as coefficients near the powers of time but as the ones near the propagator-like singularities $(E - E_0 + i\varepsilon)^{-k+1}$.) To come nearer to the level shift values, useful objects are

$$A_{\beta}^{(k)} \equiv \sum_{E_0} A_{\beta}^{(k)}(E_0) t^k k!. \quad (22)$$

Namely, as notations of eq. (21) suggest, eigenvalues of $A_{\beta}^{(0)}$ should be equal to normalizations of bound state wave functions which are driven from unit by relativistic corrections while the eigenvalues of $A_{\beta}^{(k)}$ should be energy shifts to the $k$-th power times corresponding normalizations. Thus, the eigenvalues of

$$S_{\beta}^{(k)} \equiv \left[ A_{\beta}^{(0)} \right]^{-1} A_{\beta}^{(k)} + A_{\beta}^{(k)} \left[ A_{\beta}^{(0)} \right]^{-1} \quad (23)$$

should be just energy shifts to the $k$-th power. Thus, we define

$$S_{\beta} \equiv S_{\beta}^{(1)} \quad (24)$$

to be the energy shift operator: its eigenvalues are the energy level shifts caused by relativistic corrections. Our aim is now to check $\beta$-independence of $S_{\beta}$ eigenvalues.

Some notes are in order: If the conjecture (19) is true $A_{\beta}^{(0)}$ should commute with $S_{\beta}^{(k)}$ and the following relation should hold:

$$S_{\beta}^{(k)} = [S_{\beta}]^k. \quad (25)$$

We will use it in what follows. Another thing to note is that relativistic corrections affect the form of the scalar product of wave functions and, thus, one should add a definition of
operator products to the formal expressions (23), (25). But the level of accuracy to which we will operate permits us not to go into this complication and use the operator products as they are in the nonrelativistic approximation — i.e. as the convolution of the corresponding kernels.

The way to the gauge invariance check of the energy shift calculations is clear now: Using the gauge evolution relation (14) one should find the $\beta$-dependence of $S_\beta$ and then of its eigenvalues. As $S_\beta$ is defined in eqs. (24), (23) through $A^{(k)}_\beta$'s which are, in turn, defined in eq. (20) through the propagator $D_\beta$, the first step is to simplify eq. (14) to the reduced case of zero relative time and total momentum of the fermion pair:

$$D_\beta(t, r', r) = \left[ \frac{(1 - (r' - r)^2/(4t^2))}{(1 - ((r' + r)^2)/(4t^2))} \right]^{\frac{\alpha}{2\pi}}(\beta - \beta_0) \times$$

$$\left[ \frac{Z}{m^2 r'^2 m^2 r^2} \right]^{\frac{\alpha}{2\pi}}(\beta - \beta_0) D_{\beta_0}(t, r', r).$$

(26)

The factor in the square brackets of the second line is time-independent and further factorizable on factors depending on either ingoing or outgoing pair parameters. This reduce the influence of this factor to a change in the normalization of states. Being interested in gauge invariance of energy shifts, we omit this factor in what follows. Let us turn to the analysis of the influence of the factor in the first line of eq. (26).

This factor is close to unit in the atomic scale $r', r \sim 1/\alpha$, $t \sim 1/\alpha^2$. We will use its approximate form:

$$\text{Factor} \approx 1 + \frac{\alpha}{2\pi} (\beta - \beta_0) \frac{r'r}{t^2} + O(\alpha^5).$$

(27)

One can read the dependence of $A^{(k)}_\beta$ on $\beta$ from eqs. (20), (24), (27) as

$$A^{(k)}_\beta \approx A^{(k)}_{\beta_0} - \frac{\alpha}{2\pi} \frac{(\beta - \beta_0)}{(k + 1)(k + 2)} r A^{(k+2)}_{\beta_0} r,$$

(28)

where $r$ is the vector operator of relative position of interacting particles. The mixing of different $A^{(k)}_\beta$'s with a change in the gauge parameter is due to the presence of $1/t^2$ in the rhs of eq. (27). Finally, using the definition (24), relations (25) and the fact that $A^{(0)} \approx 1$

(29)

in the nonrelativistic approximation one can derive the following $\beta$-dependence of $S_\beta$:

$$S_\beta \approx S_{\beta_0} - \frac{\alpha}{2\pi} (\beta - \beta_0) \left( \frac{1}{6} r S^3_{\beta_0} r - \frac{1}{4} S_{\beta_0} r S^2_{\beta_0} r - \frac{1}{4} r S^2_{\beta_0} r S_{\beta_0} \right).$$

(30)

Treating the term in the last line of the rhs of the above relation as a perturbation, one can get an approximate value of the $\beta$-dependent piece of the energy shift just averaging the perturbation with respect to the corresponding eigenstate of $S_{\beta_0}$.

Thus, we get for the leading order of $\beta$-derivative of an energy shift the following representation:

$$\left( \frac{\partial}{\partial \beta} \Delta_\beta \right)_L = -\frac{\alpha}{2\pi} \left( \frac{1}{6} \langle r S^3_L r \rangle - \frac{1}{4} \langle S_L r S^2_L r \rangle - \frac{1}{4} \langle r S^2_L r S_L \rangle \right),$$

(31)
where \(\langle \ldots \rangle\) means averaging with respect to the corresponding nonrelativistic eigenstate and the subscript \(L\) means the leading order in \(\alpha\)-expansion.

Eq. (31) is sufficient to define an order in \(\alpha\) in which the energy shifts become gauge dependent:

\[
\left( \frac{\partial}{\partial \beta} \Delta_{\beta} \right)_L \sim \alpha^{11}.
\]

Here we have taken into account that \(r \sim 1/\alpha\) and \(S_L \sim \alpha^4\).

To have a gauge dependence in any observable is clearly unacceptable. In the next section we will see how one should correct the above procedure of energy shift extraction from the QED Green function to get rid of the gauge dependence of energy shifts.

4 A Way Out

The procedure recalled in the previous section is based on the conjecture (19). A consequence of this conjecture is the gauge dependence of energy shifts of eq. (31). One can conclude that the conjecture is wrong. In particular, as one can infer from eq. (26), the operator coefficients near the oscillating exponentials in eq. (19) should get a time dependence from relativistic corrections. Even if in some gauge they are time independent, the gauge parameter evolution should generate a dependence which in the leading order in \(\alpha\) reduce itself to the following replacement in eq. (19):

\[
P_{\beta}(E_0 + \Delta_{E_0}) \rightarrow P_{\beta}(E_0 + \Delta_{E_0}) + \frac{\Sigma_{\beta}(E_0)}{t^2}.
\]

That \(\Sigma_{\beta}(E_0)\) has nothing to do with energy shifts but will give contributions to \(A_{\beta}^{(k)}(E_0)\)'s from eq. (21). Being gauge dependent these contributions lead to the gauge dependence of energy shifts.

The way to the correct procedure is to throw away terms like \(\Sigma_{\beta}(E_0)/t^2\) prior to the definition of the energy shift operator. Thus, a necessary step in the process of extracting energy shifts from the QED Green function (and the one which necessity is not recognized in the standard procedure) is to calculate and subtract contributions like the last term in the rhs of eq. (33) from the propagator of the fermion pair.

Below we report on a calculation of \(\Sigma_{\beta}(E_0)\) from eq. (33). The most economical way to calculate it is to note that the energy dependence of the Fourier transform of the corresponding contribution to the propagator is

\[
(E - E_0) \ln(-(E - E_0 + i\varepsilon))
\]

and that it comes from diagrams describing radiation and subsequent absorption of a soft photon with no change in the level \(E_0\) of the radiating and absorbing bound state. Similar contributions (with another power of energy before the \(\log\) ) are well known for the propagator of a charged fermion [5].

It may be worth to note here that contribution of eq. (34) vanishes at \(E = E_0\). This explains why such contributions are insignificant for practical calculations of the present day
accuracy. In particular, one can neglect them, despite the log-singularity, in the resonance
scattering calculations and preserve the classic results of [9].

The first step in our calculation is to present the pair propagator in the following form:

\[ D_\beta(t) \approx \left( e^{L_s e^{i \epsilon A(t)}} D_{\text{inv}}(t, A) e^{-i \epsilon A(0)} \right)_{A=0}, \quad (35) \]

where \( L_s \) is the same as in eq. (3) except a restriction on the momentum of photon propagator — the range of its variation is restricted to the soft region which border is of order of atomic
binding energies; the exponentials with gauge potential are originated from the ones in eq. (4); \( D_{\text{inv}} \) is a descendant of \( G_{\text{inv}} \) from (7): to go over from \( G_{\text{inv}} \) to \( D_{\text{inv}} \) one should make all
pairing of non-soft photons in \( G_{\text{inv}} \) and all the reductions of space-time coordinates which
was involved in going over from the \( G_\beta \) of eq. (1) to the \( D_\beta \) of eq. (17); at last, all gauge
potentials in eq. (35) are taken at zero of space coordinate in accord with the \( \delta(x) \) of eq. (17). The difference between the lhs and the rhs of eq. (35) does not contribute to the term
under the calculation.

The leading in the nonrelativistic approximation contribution to \( D_{\text{inv}} \) is the same as
for \( D_\beta \) — it is just the propagator of the nonrelativistic Coulomb problem. We explicitly
calculate the leading contribution to the dependence of \( D_{\text{inv}}(t, A) \) on the gauge potential
in its expansion over soft momenta of the external photons. Not surprisingly, the dipole
interaction of the pair with the external photon field arises in this approximation:

\[ D_{\text{inv}}(t, A) \approx \left( \frac{i}{\partial t} - H_c + e r \mathcal{E}(t) \right)^{-1}, \quad (36) \]

where \( H_c \) is the Hamiltonian of the nonrelativistic Coulomb problem and \( \mathcal{E} \) is the strength
of the electric field:

\[ \mathcal{E}(t) \equiv -\dot{A}(t) + \nabla A_0(t). \quad (37) \]

Substituting eq. (36) in eq. (35) and keeping terms with only one soft photon propagator
we get expressions which sum contains the term under calculation:

\[ e^2 \left( L_s r A(t) D_{\text{nr}}(t) r A(0) \right)_{A=0}, \quad (38) \]

\[ e^2 \left( L_s \int d\tau_1 d\tau_2 D_{\text{nr}}(t - \tau_1) r \mathcal{E}(\tau_1) D_{\text{nr}}(\tau_1 - \tau_2) r \mathcal{E}(\tau_2) D_{\text{nr}}(\tau_2) \right)_{A=0}, \quad (39) \]

\[ i e^2 \left( L_s \int d\tau D_{\text{nr}}(t - \tau) r \mathcal{E}(\tau) D_{\text{nr}}(\tau) r A(0) \right) \right. \]

\[ \left. - \left. - r A(t) D_{\text{nr}}(t - \tau) r \mathcal{E}(\tau) D_{\text{nr}}(\tau) \right) \right)_{A=0}, \quad (40) \]

where \( D_{\text{nr}}(t) \) is the propagator of the nonrelativistic Coulomb problem from the rhs of eq.
(18).

The next step is to pick out a contribution of a level \( E_0 \) in eqs. (39), (39), (40). That is
achievable by the replacement

\[ D_{\text{nr}}(t) \to e^{-i E_0 t} \theta(t) P(E_0). \quad (41) \]
The last ingredient that one needs to calculate eqs. (38), (39), (40) is the time dependence of the soft photon propagators. It can be deduced from eq. (2) as

\[
(L_s A_i(t_1) A_j(t_2)) = \theta \left( (t_1 - t_2)^2 > t_c^2 \right) \frac{\delta_{ij}}{4\pi^2(t_1 - t_2)^2},
\]

\[
(L_s A_i(t_1) E_j(t_2)) = \theta \left( (t_1 - t_2)^2 > t_c^2 \right) \frac{\delta_{ij}}{2\pi^2(t_1 - t_2)^3},
\]

\[
(L_s E_i(t_1) E_j(t_2)) = \theta \left( (t_1 - t_2)^2 > t_c^2 \right) \frac{\delta_{ij}}{\pi^2(t_1 - t_2)^4}.
\] (42)

Here the $\theta$-functions are to account for the softness of the participating photons ($t_c \sim 1/E_0$).

Taking eq. (42) into account we get the following contributions from eqs. (38), (39), (40):

\[
(38) \rightarrow \frac{1}{t^2} \theta(t) e^{-iE_0 t} \pi \left( -1 + \frac{\beta}{2} \right) rP(E_0)r,
\]

\[
(39) \rightarrow \frac{1}{t^2} \theta(t) e^{-iE_0 t} \frac{2}{3} P(E_0)rP(E_0)rP(E_0),
\]

\[
(40) \rightarrow \frac{1}{t^2} \theta(t) e^{-iE_0 t} \frac{\alpha}{\pi} \left( rP(E_0)rP(E_0)rP(E_0) - rP(E_0)rP(E_0) \right).
\] (43)

The sum of the above terms yields the result of our calculation:

\[
\Sigma_\beta(E_0) = \frac{\alpha}{\pi} \left( \frac{2}{3} P(E_0)rP(E_0)rP(E_0) + (-1 + \frac{\beta}{2}) rP(E_0)r + i(P(E_0)rP(E_0)r - rP(E_0)rP(E_0)) \right).
\] (44)

One can explicitly check that $\beta$-dependence of $\Sigma_\beta(E_0)$ is the right one — i.e. if one subtracts the $\Sigma$-term from the propagator before the definition of the energy shift operator, the latter becomes gauge independent. Another observation is that the $\Sigma$-term cannot be killed by any choice of the gauge (in contrast to the case of charged fermion propagator where an analogous term is equal to zero in the Yennie gauge).

Summing up, in this paper we derived a relation between QED Green functions of different gauges. We used it to check the gauge invariance of the energy shift operator. It turns out to be gauge dependent. This fact forced us to recognize that energy shifts are not one, and the only one, source for the positive powers of time near the oscillating exponentials in the propagator of the pair. We found a particular additional source of the positive powers of time which is responsible for the gauge dependence of the naive energy shift operator. We conclude with an observation that at the moment we have not a clear definition of the energy shift operator — to get it one needs a criterion for picking out contributions to the positive powers of time originating from the energy shifts.

The author is grateful to A. Kataev, E. Kuraev, V. Kuzmin, A. Kuznetsov, S. Larin, Kh. Nirov, E. Remiddi, V. Rubakov, D. Son, P. Tinyakov for helpful discussions. This work was supported in part by Russian Foundation for Basic Research, project no. 94-02-14428.
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