QED
and ortho- and para- positronium mass difference

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Abstract

Bound state problem in the relativistic QED is investigated by the functional integral methods. The ortho- para- positron mass difference is calculated. Contribution of the "nonphysical" time variable turned out to be important and leads to the nonanalytic dependence of the bound state mass of the order $\alpha^{\frac{2}{3}}$. It is shown that the relativistic and non-relativistic QED gives different results for this mass shift. In addition so-called abnormal states as "time excitations" arise.

Sequential application of relativistic QED to bound state problem is in contradiction with real ortho- and para- positronium bound states.

The conclusion: the relativistic QED is not suited to describe real bound states correctly.

1 Introduction.

We believe that the relativistic quantum electrodynamics (QED) is a uniquely correct universal theory giving an exhaustive description of all interactions between electrons and photons including possible bound states like positronium. Only our inability to calculate something out of perturbation method does not permit us to obtain all the desired details. Earlier, some scientists considered that QED should have its own applicability region. A short review of the history and the development of quantum field theory is done in [1]. Supporting these doubts we will show in this paper that the sequential use of the standard QED does not give a correct description of the positronium spectra, namely, the ortho- para- positronium mass difference.

First of all let us realize what is the status of bound states in non-relativistic quantum mechanics (QM) and relativistic quantum field theory (QFT).

The total Hamiltonian $H = H_0 + gH_I$ can be constructed in QM and QFT. However, in QM H is a well defined operator, so that the non-relativistic Schrödinger equation is mathematically correct and time development of a quantum system can be described. Solutions of the Schrödinger equation contain both free and bound states. One can remark that in QM a bound state (positronium) is created by real particles (electron-positron), i.e. constituent particles are on mass shell.

In QFT the Fock space $\mathcal{F}$ is defined by the noninteracting free Hamiltonian H_0 and contains the free particles only. However, H_I is not defined on $\mathcal{F}$. As a result, the bound state as an eigenvalue problem of the relativistic Schrödinger equation on the Fock space cannot be formulated mathematically in a correct way (see [2]). Besides, the time development of quantum field system cannot be obtained. The only way to overcome these problems is to construct the S-matrix which contains all elastic and inelastic scattering amplitudes of free particles from the time $t \to -\infty$ to the time $t \to \infty$. It is important that the S-matrix is a unitary operator on the Fock space. It means that the bound states like positronium, which is a unstable particle,

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cannot belong to any Fock space in principle. In addition, our computing abilities are restricted to the perturbation theory.

Nevertheless, we believe that the S-matrix amplitudes should contain some correct information on possible bound states. The simplest way to realize this idea is to postulate that a bound state is a simple pole of an elastic scattering amplitude of constituent particles with appropriate quantum numbers. It means, that the amplitudes out of mass shell and out of perturbation approach should be calculated. Standard methods to go out of perturbation calculations are reduced to sum appropriate classes of Feynman diagrams and this summation can be formulated in a form of integral equations. The best known approaches are the Bethe-Salpeter and Schwinger-Dyson equations. The important difference comparable with the nonrelativistic case is that bound states in these equations are created by particles which are out of mass shell so that the role of time becomes important.

One remark on these equations. We know that the perturbation series are asymptotic series so that the problem is how to sum them? The exact amplitudes should have some singularity at the point $\alpha = 0$ in QED (see [3]). What is a precise character of this singularity is not known up to now. Standard perturbation expansions are connected with Feynman diagrams. Usual methods are reduced to summation of an appropriate class of Feynman diagrams. Result of a summation of any definite class of Feynman diagrams is a kind of geometrical progression, i.e. it is an analytic function at the point $\alpha = 0$. However, it should be stressed that the generally accepted point of view - non-perturbed behavior is a sum of a definite class of Feynman diagrams - is not true.

One of probably successful proposals to calculate the relativistic corrections to bound state problem is the so-called non-relativistic QED (NRQED) (see [4]). The basic idea is that the QM is correct, only non-relativistic momenta are responsible for bound state properties. In other words, the Hamiltonian should not depend on time and the problem is to find somehow relativistically small corrections to the non-relativistic Coulomb potential. The basic idea is that for small coupling constants the Born approximation is a good approximation which is directly defined by the Fourier transform of the potential. The aim is to extract from the relativistic S-matrix some relativistic corrections to non-relativistic Hamiltonian. The hypothesis is that the scattering amplitudes in the non-relativistic Schrödinger theory and the relativistic S-matrix theory should coincide in the low energy limit. The procedure is to write down the non-relativistic Lagrangian with a set of all possible terms, and coefficients in front of them are calculated by identification with appropriate amplitudes of relativistic S-matrix. This prescription allows one to remove effectively time out of the relativistic equations, in other words, to place all intermediate particles on their mass shell. It seems NRQED is supported by experimental data.

Another quantum field idea is that a bound state is defined by an asymptotic behavior of the vacuum mean value of the corresponding relativistic currents (see, for example, [5]) with desired quantum numbers:

$$\langle 0|\mathbf{J}(x)\mathbf{J}(0)|0\rangle = \sum_n \langle 0|\mathbf{J}(x)|n\rangle \langle n|\mathbf{J}(0)|0\rangle = \sum_n e^{-E_n|x|}|\langle 0|\mathbf{J}(0)|n\rangle|^2$$
$$\sim e^{-M_{min}|x|}|\langle 0|\mathbf{J}(0)|min\rangle|^2 \quad \text{for} \quad |x| \to \infty. \tag{1}$$

This formula gives a possibility to calculate the mass of the lowest bound state $|min\rangle$ if $M_{min} < 2m$. Essentially, the space of states $\{|n\rangle\}$ is supposed to contain possible bound states although we saw that the Fock space cannot contain unstable bound states. These vacuum mean values (1) can be represented in closed forms by functional methods. The functional methods permit one to get formally the exact representations for Green functions which are not connected directly with Feynman diagrams, so that it is possible to go out of standard perturbation expansions using asymptotic methods. Development of functional methods permits one to get the exact character of non-analyticity at the point $\alpha = 0$ and to clarify the role of "time" in

bound state formation. Exactly this approach will be used in this paper.

The practically unique experimental object to investigate the bound state problems is the positronium which is the result of pure QED interaction. On the one hand, the positronium is not a stable state. It cannot belong to the asymptotic Fock space. Nevertheless, it exists. The binding energy of positronium itself is not measured with great accuracy but the mass difference of two possible states, ortho-positronium (1^3S_1) and para-positronium (1^1S_0), is known with very large accuracy

$$\Delta\epsilon = \epsilon_{ortho} - \epsilon_{para} = 203.38910\ GHz = \frac{7}{12}\alpha^4 m_e \cdot 0.99512...$$

The main contribution can be explained by the non-relativistic Breit potential approach (see, for example, [6]) taking into account scattering and annihilation channels

$$\Delta\epsilon = \epsilon_{ortho} - \epsilon_{para} = \frac{7}{12}\ \alpha^4 m_e, \qquad \frac{7}{12} = \left(\frac{1}{3}\right)_{scatt} + \left(\frac{1}{4}\right)_{annih}.$$

If we apply the relativistic current formula (1) to the positronium problem, we can write

$$\langle 0|\mathbf{J}(x)\mathbf{J}(0)|0\rangle = \sum_{particles} e^{-iE_n|x|}|\ \langle 0|\mathbf{J}(0)|n\rangle\ |^2 + \sum_{photons} e^{-iE_n|x|}|\ \langle 0|\mathbf{J}(0)|n\rangle\ |^2$$

where

$$\sum_{particles} e^{-iE_n|x|}|\ \langle 0|\mathbf{J}(0)|n\rangle\ |^2 \sim e^{-M_{lowest}|x|}$$

and annihilation channel looks like

$$\sum_{photons} e^{-iE_n|x|}|\ \langle 0|\mathbf{J}(0)|n\rangle\ |^2 \sim \frac{1}{|x|^2}$$

It means that the annihilation channel does not take part in the bound state formation in contradiction with the non-relativistic potential approach.

Another point: we want to understand what is the role of TIME in formation of bound states.

In this paper we apply functional methods to calculate the asymptotic behavior of vacuum mean value (1) of relativistic currents for positronium and clarify the role of time in the formation of bound states.

2 Two-point Green function

All our calculations will be performed in the Euclidean space. The Lagrangian of the electron field ψ and the electromagnetic photon field A_μ looks like

$$\begin{aligned} L(x) &= -\frac{1}{4}F^2_{\mu\nu}(x) + (\overline{\psi}(x)[i(\hat{p} + e\hat{A}(x)) - m]\psi(x)), \\ F_{\mu\nu}(x) &= \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x). \end{aligned} \tag{2}$$

The object of our interest is the gauge invariant two-point Green function

$$\mathbf{G}_\Gamma(x-y) \ = \ \iint \frac{D\overline{\psi}D\psi DA}{C} e^{\int dx\ L(x)} (\overline{\psi}(x)\Gamma\psi(x))(\overline{\psi}(y)\Gamma\psi(y)) \tag{3}$$

Here Γ is a Dirac matrix which defines the local vertex with quantum numbers of the state $J_\Gamma = (\overline{\psi}\Gamma\psi)$. We have for para-positronium $\Gamma = i\gamma_5$ and for ortho-positronium $\Gamma = \gamma_\mu$.

After integration over the electron fields ψ and $\overline{\psi}$ we get

$$\mathbf{G}_\Gamma(x-y) = \mathbf{B}_\Gamma(x-y) + \mathbf{H}_\Gamma(x-y), \tag{4}$$

where (we neglect electron loops)

$$\mathbf{B}_\Gamma(x-y) = \int \frac{DA}{C} e^{-\frac{1}{2}(A_\mu D^{-1}_{\mu\nu} A_\nu)} \cdot \mathrm{Tr}[\Gamma S(x,y|A)\Gamma S(y,x|A)], \tag{5}$$

and

$$\mathbf{H}_\Gamma(x-y) = \int \frac{DA}{C} e^{-\frac{1}{2}(A_\mu D^{-1}_{\mu\nu} A_\nu)} \cdot \mathrm{Tr}[\Gamma S(x,x|A)] \cdot \mathrm{Tr}[\Gamma S(y,y|A)].$$

Here $S(x,y|A)$ is the electron propagator in the external field A_μ:

$$S(x,y|A) = \frac{1}{i(\hat{p} + e\hat{A}(x)) - m}\delta(x-y) \tag{6}$$

The loop $\mathbf{B}_\Gamma$ contains all possible $(\overline{\psi}\Gamma\psi)$-bound states. If the mass of the lowest state $M_\Gamma < 2m$, then the asymptotic behavior of this loop for large $|x-y|$ looks like

$$\mathbf{B}_\Gamma(x-y) \sim e^{-M_\Gamma|x-y|} \tag{7}$$

where M_Γ is the mass of the lowest state in the current $(\overline{\psi}\Gamma\psi)$, i.e. the mass of a possible bound state. This mass can be calculated by the formula

$$M_\Gamma = -\lim_{|x|\to\infty} \frac{1}{|x|} \ln \mathbf{B}_\Gamma(x) = 2m - \epsilon_\Gamma. \tag{8}$$

Here ϵ_Γ defines the binding energy of the lowest bound state. Our aim is to calculate the functional integral (5) in the limit $|x-y| \to \infty$ and to find M_Γ, according to (8).

The loop $\mathbf{H}$ describes so the called annihilation channel and contains long-range contributions of photons:

$$\mathbf{H}_\Gamma(x-y) \sim \frac{1}{|x-y|^2}$$

This term does not contain any bound state.

3 The electron propagator

The electron propagator (6) can be represented by the functional integral (see, for example, [9, 10]):

$$S(x,y|A) = [i(\hat{p}_x + e\hat{A}(x)) + m] \int\limits_0^\infty \frac{ds}{8\pi^2 s^2} e^{-\frac{1}{2}\left[m^2 s + \frac{(x-y)^2}{s}\right]}$$
$$\cdot \int \frac{D\eta}{C} e^{-\int\limits_0^s dt \frac{\dot{\eta}^2(t)}{2} + ie\int\limits_0^s dt \dot{z}_\mu(t) A_\mu(z(t))} \mathrm{T}_t \left\{ e^{\frac{e}{4}\int\limits_0^s dt \sigma_{\mu\nu}(t) F_{\mu\nu}(z(t))} \right\}, \tag{9}$$

$$z(t) = x\frac{t}{s} + y\left(1 - \frac{t}{s}\right) + \eta(t).$$

The boundary conditions are $\eta(0) = \eta(\alpha) = 0$. The symbol T_t means the time-ordering of the matrix $\sigma_{\mu\nu}(\tau)$ to the time variable t.

Our aim is to calculate the functional integral (5) in the limit $|x| \to \infty$ (we put $y = 0$). For large $x \to \infty$ and small α the saddle-point in the integral over s is realized for $s = \frac{X}{m}$. Putting $\sqrt{x^2} \Rightarrow x_4 = X > 0, \qquad t = \frac{X}{m}\tau$, one can get for $X \to \infty$

$$S(x,0|A) \Rightarrow \frac{\text{const}}{X^{\frac{1}{2}}}(1+\gamma_0)e^{-mX} \cdot \mathcal{S}(x)$$

$$\mathcal{S}(x) = \int \frac{D\eta}{C} e^{-\int\limits_0^X d\tau \ \frac{m\dot{\eta}^2(\tau)}{2} + ie\int\limits_0^X d\tau \ \dot{z}_\mu(\tau)A_\mu(z(\tau))} R[z],$$

$$R[z] = \mathrm{T}_\tau \left\{ e^{\frac{e}{4m}\int\limits_0^X d\tau \ \sigma_{\mu\nu}(\tau)F_{\mu\nu}(z(\tau))} \right\}$$

with $z(\tau) = n\tau + \eta(\tau) = \left\{ \begin{array}{l} \boldsymbol{\eta}(\tau), \\ \tau + \eta_4(\tau). \end{array} \right.$

3.1 Mass of the bound state

The next step is to substitute electron propagators in the form (10) into the representation (5) for the Green function $\mathbf{B}_\Gamma(x)$ and then to integrate over the photon field A. We have for large $X \to \infty$

$$\mathbf{B}_\Gamma(X) \sim e^{-2mX} \iint \frac{D\eta_1 D\eta_2}{C} e^{-\frac{m}{2}\int\limits_0^X d\tau[\dot{\eta_1}^2(\tau)+\dot{\eta}_2^2(\tau)]} \mathcal{F}_\Gamma[X,\eta_1,\eta_2], \tag{10}$$

with

$$\begin{aligned} &\mathcal{F}_\Gamma[X,\eta_1,\eta_2] \qquad (11)\\ &= \int \frac{DA}{C} e^{-\frac{1}{2}(A_\mu D^{-1}_{\mu\nu}A_\nu) + ie\int\limits_0^X d\tau \dot{z}^{(1)}_\mu(\tau)A_\mu(z^{(1)}(\tau)) + ie\int\limits_0^X d\tau \dot{z}^{(2)}_\mu(\tau)A_\mu(z^{(2)}(\tau))} \\ &\cdot \frac{1}{4}\mathrm{Tr}\left[\Gamma \ (1+\gamma_0)\, R[z^{(1)}] \ \Gamma \ (1-\gamma_0)\, R[z^{(2)}]\right]. \end{aligned}$$

We omit here all calculations, they are done in [11]. Finally the desired mass difference can be represented as

$$\delta M = M_{ortho} - M_{para} = \frac{1}{3} \cdot \alpha^4 m \cdot \Delta(\alpha), \tag{12}$$

where

$$\begin{aligned} \Delta(\alpha) = &\lim_{Y\to\infty} \frac{1}{Y} \int\limits_0^Y\!\!\int dv_1 dv_2 \iint \frac{d\mathbf{q}dq}{2\pi^3} \cdot \frac{\mathbf{q}^2 \ e^{iq(v_1-v_2) - \frac{1}{4}[\alpha^2 q^2 + \mathbf{q}^2]|v_1-v_2|}}{\mathbf{q}^2 + \alpha^2 q^2} \\ &\cdot \int \frac{D\boldsymbol{\rho}}{C_{\boldsymbol{\rho}}} e^{-\int\limits_0^Y dv\left[\frac{1}{4}\dot{\boldsymbol{\rho}}^2(v) - \frac{1}{|\boldsymbol{\rho}(v)|}\right]} e^{-\frac{i\mathbf{q}}{2}(\boldsymbol{\rho}(v_1)+\boldsymbol{\rho}(v_2))} \\ &\cdot \int \frac{D\rho}{C_\rho} e^{-\int\limits_0^Y dv\left[\frac{1}{4}\dot{\rho}^2(v) + \frac{\alpha}{8}|\rho(v)|\right]} e^{-\frac{i\alpha q}{2}(\rho(v_1)+\rho(v_2))}. \end{aligned}$$

One can see the mass is defined by the usual Coulomb potential and "time" linear potential which lead to the general spectrum

$$E_{n\kappa} = \left[-\frac{\alpha^2}{n^2} + \alpha^{2+\frac{2}{3}}\epsilon_\kappa\right] m, \qquad n, \kappa = 0, \ 1, \ 2, ... \tag{13}$$

As a result we have the "time excitations" (ϵ_κ is spectrum of the linear potential), or abnormal states, connected with the fourth component of 4-dimensional space. These states appear in solutions of the Bethe-Salpeter equation. Up to now it is not known exactly these states does or does not exist in reality. It is another reason why relativistic QED does not describe correctly the real bound states.

Our calculations give

$$\Delta(\alpha) = \sum_{n=1}^{\infty}\sum_{\ell=0}^{n-1}\sum_{\kappa=0}^{?}(-1)^{\ell+\kappa}\Delta_{n\ell\kappa}(\alpha),$$

$$\Delta_{n\ell\kappa}(\alpha) = \frac{32}{\pi^2}\iint\limits_0^\infty \frac{dkdq\ k^4}{k^2+\alpha^2q^2}\cdot\frac{k^2+\alpha^2q^2+1-\frac{1}{n^2}+\alpha^{\frac{2}{3}}(\epsilon_\kappa-\epsilon_0)}{\left(k^2+\alpha^2q^2+1-\frac{1}{n^2}+\alpha^{\frac{2}{3}}(\epsilon_\kappa-\epsilon_0)\right)^2+16q^2}$$

$$\cdot\ (2\ell+1)\mathbf{C}_{nl}^2\left(\frac{k}{2}\right)\left|\mathcal{A}_\kappa\left(\alpha^{\frac{2}{3}}q\right)\right|^2 \qquad (14)$$

Here the functions $\mathcal{A}_\kappa\left(\alpha^{\frac{2}{3}}q\right)$ are corresponding form-factors of the linear "time" potential (see [11]). The numerical results are shown in Table 1.

Table 1. The function $\Delta_{n\ell0}(\alpha)$

$(n\ell)$	(10)	(20)	(21)	(30)	(31)	(32)
$\Delta_{n\ell0}(0)$	1.	0.0987	0.0987	0.0283	0.0307	0.00244
$\Delta_{n\ell0}(\alpha)$	0.9999	0.09868	0.09864	0.02829	0.03071	0.002438
$\Delta_{n\ell1}(\alpha)$	0.96707	0.09387	0.09617	0.2683	0.002986	0.00238
$\Delta_{n\ell2}(\alpha)$	0.01421	0.002089	0.001173	0.0006319	0.0004049	0.00002632

For the function $\Delta(\alpha)$ we get

$$\Delta_0(0) = \sum_{n=1}^{3}\sum_{\ell=0}^{n-1}(-1)^\ell\Delta_{n\ell0}(0) = 1.0,$$

$$\Delta_0(\alpha) = \sum_{n=1}^{3}\sum_{\ell=0}^{n-1}(-1)^\ell\Delta_{n\ell0}(\alpha) = 0.9641,$$

$$\Delta(\alpha) = \sum_{n=1}^{3}\sum_{\ell=0}^{n-1}\sum_{\kappa=0}^{2}(-1)^{\ell+\kappa}\Delta_{n\ell\kappa}(\alpha) = 0.952754.$$

Obviously, this result is in contradiction with the existing experimental number ($\Delta = 0.99512...$).

4 Conclusion

In conclusion, one can say that the functional approach is the best mathematical representation to preserve the gauge invariance. The developed technique of calculations permits one to get accurate results in QED where the coupling constant α is small. The lowest approximation of this functional representation is the pure non-relativistic Feynman path integral representation of the non-relativistic Schrödinger equation with the Coulomb potential. One can see that any regular series for next corrections to α do not exist and these corrections can not be reduced to some terms to the non-relativistic potential in the Schrödinger picture. In other words,the

"nonphysical" time coordinate is important and leads to corrections which is not analytic of the order $\alpha^{\frac{2}{3}}$.

There exists a contradiction in the current algebra formula (1). On one hand, it is supposed that the space of states $\{|n\rangle\}$ can contain possible bound states. However on the other hand, in reality it is the Fock space of free electrons and photons which does not contain any unstable bound states. Nevertheless calculations of the functional representation for an appropriate Green function in the limit $t \to \infty$ indicate that a bound with $M_{bound} < 2m$ does exist really. Besides, the current algebra in QFT excludes influence of the annihilation channel for the bound state formation.

Our calculations show that the role of time is very important and give essential contribution into bound state mass. The next radiation corrections, connected with time excitations, to electromagnetic mass difference to positronium are of the order $\alpha^{\frac{2}{3}}$, i.e. they are to large.

In addition, the "time excitations", or abnormal states arise in QFT calculations but they are not exist in reality.

The experimental value of ortho- para-positronium mass difference is described in the framework of the Breit potential picture with attraction of the annihilation channel. Thus, explanation of experimental value para- ortho- positronium mass difference requires to take into account annihilation channel for effective potential.

One can conclude that in the relativistic QED time corrections are important, but the bound state problem requires the non-relativistic potential description where the time variable does not play any essential role.

The conclusion: the relativistic QED is not suited to describe real bound states correctly.

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