

Relativistic recoil effects for energy levels in a muonic atom within a Grotch-type approach. I. General approach

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Recently we calculated relativistic recoil corrections to the energy levels of the low-lying states in muonic hydrogen induced by electron vacuum polarization effects. The results were obtained by Breit-type and Grotch-type calculations. The former were described in our previous papers in detail, and here we present the latter. The Grotch equation was originally developed for pure Coulomb systems and allowed to express the relativistic recoil correction to order $(Z\alpha)^4 m^2/M$ in terms of the relativistic nonrecoil contribution $(Z\alpha)^4 m$. Certain attempts to adjust the method to electronic vacuum polarization took place in the past, however, the consideration was incomplete and the results were incorrect. Here we present a Grotch-type approach to the problem and in a series of papers consider relativistic recoil effects in order $\alpha(Z\alpha)^4 m^2/M$ and $\alpha^2(Z\alpha)^4 m^2/M$. That is the first paper of the series and it presents a general approach, while two other papers present results of calculations of the $\alpha(Z\alpha)^4 m^2/M$ and $\alpha^2(Z\alpha)^4 m^2/M$ contributions in detail. In contrast to our previous calculation, we address now a variety of states in muonic atoms with a certain range of the nuclear charge Z .

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I. INTRODUCTION

Spectroscopy of light muonic atoms was used for a while and provided us with certain important data on the nuclear structure. It was based on a study of the emission lines and had limited accuracy. Recently, the first successful laser-spectroscopy measurement on muonic hydrogen has opened a new generation of experiments. The experiment performed at Paul Scherrer Institut (PSI) delivered the value of the Lamb shift in muonic hydrogen and allowed one to determine the proton charge radius with unprecedented accuracy. Unexpectedly, that measurement has led to one of the currently largest controversies in quantum electrodynamics (QED)-related experiments. A strong discrepancy between the value of the proton charge radius obtained from muonic hydrogen [1] and that in ordinary hydrogen [2] is of about 5 standard deviations. Meantime, the latter value is in perfect agreement with a recent electron-proton scattering result [3].

That circumstance has renewed interest in spectroscopy of muonic atoms. The low l states and, mostly, the $1s$ and $2s$ states are sensitive to the finite-nuclear-size effects and have been used for a while to determine the charge radius for a broad range of nuclei from hydrogen [1] to uranium [4].

Higher- l states are also of interest for more “metrological” measurements. In particular, the $3d_{5/2}-2p_{3/2}$ transition in muonic ^{24}Mg and ^{28}Si was used in [5] to determine m_μ/m_e . A similar measurement was also performed in pionic atoms to determine the pion mass. In such experiments one has to deal with x-ray transitions and then there is a problem in calibration

of the x-ray standards. In [6] the $5f-4g$ transition in pionic nitrogen and the $6h-5f$ one in pionic neon were compared with $5f-4g$ transitions in muonic oxygen.

Higher- l states can also be of interest due to antiprotonic helium spectroscopy. At present, highly accurate data are available only for a three-body system, which includes a nucleus, antiproton, and electron [7,8]. While the antiproton in a circular or a near circular state is rather immune against annihilation, the electron “protects” the antiprotonic state from collision quenching. Still, a possibility for a two-body antiprotonic helium ion has not been given up and such a system may be of experimental interest in the future.

In this situation a theoretical study of low-lying states of circular states, such as $2p, 3d, 4g, 5f, 6h$ is of practical interest. Since the muon mass is substantially higher than the electron mass, one has to pay attention to recoil effects.

To find recoil contributions to energy levels of a hydrogenic atom one can apply various approaches and, in particular, a Grotch-type one.

A calculation of recoil corrections to order m/M is possible in hydrogenic atoms exactly [9] (see also [10]) without any expansion in $Z\alpha$. The result consists of two contributions; one is a result of one-photon exchange in an effective Dirac equation, while the other takes into account multiphoton exchanges.

It is the one-photon exchange that was first derived in [11] without any expansion in $Z\alpha$. The Grotch equation is an efficient way to derive from the one-photon-exchange term the result which allows one to combine a few important features of theory of the energy levels and to obtain a result which incorporates

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(1) the leading nonrelativistic term (i.e., a result of the Schrödinger-Coulomb problem) exactly in m/M ;

(2) the complete relativistic series for infinitely heavy nucleus (i.e., a result of the Dirac-Coulomb problem) exactly in $(Z\alpha)$;

(3) the leading relativistic recoil correction to energy in order $(Z\alpha)^4 m^2/M$.

On the other hand, the electronic vacuum polarization (eVP) effects and, in particular, the Uehling potential, play a crucial role in the theory of energy levels in muonic atoms. It is important to be able to calculate relativistic and recoil corrections to them for a variety of levels.

Recently, such a relativistic recoil contribution of order $\alpha(Z\alpha)^4 m^2/M$ was considered in various approaches for low-lying states in light muonic atoms [12–14] (see also [15–17] for earlier evaluations). Results on $\alpha^2(Z\alpha)^4 m^2/M$ can be found in [18].

Here, we rederive the Grotch equation for a pure Coulomb problem and generalize it for a broad class of potentials. The generalized approach allows one to find relativistic recoil eVP corrections in the first and second order in α , which are studied in subsequent papers [19,20].

II. ONE-PHOTON EXCHANGE IN TWO-BODY BOUND SYSTEMS

The Coulomb bound two-body systems have a binding energy of order $(Z\alpha)^2 m$, where α is the fine structure constant, Z is the nuclear charge, m is the mass of the orbiting particle, i.e., the lighter one in the bound system. Throughout the paper we apply relativistic units in which $\hbar = c = 1$. These energy levels have various corrections due to the relativistic, recoil, and QED effects and due to the nuclear structure.

The $(Z\alpha)^2 m$ term can be found by many different methods, while the methods to derive the corrections often depend on the nature of those corrections. A certain class of the corrections can be expressed in terms of the potentials and one can expect that for their evaluation it is possible to adjust approaches used for pure Coulomb calculations.

The potential corrections and, in particular, those presented by the Uehling potential, are dominant QED effects for light and medium- Z muonic atoms. Here we develop an effective approach to study relativistic recoil corrections in the first order in the electronic vacuum polarization.

Electronic vacuum polarization (eVP) effects are responsible for the Uehling potential, but even for the relativistic recoil contribution one has to go somewhat beyond just the Uehling potential, just as for the calculation of the $(Z\alpha)^4 m^2/M$ term one has to go beyond a pure Coulomb field. Here M is the nuclear mass and appearance of the m/M ratio indicates that recoil effects are involved.

Throughout the paper we consider a pointlike nucleus; however, in many situations the finite-nuclear-size effects can be treated as a small perturbation and, specifically, for low- Z calculations and for a high- l medium- Z case. In any case, the finite nuclear size affects the interaction between the muon and the nucleus; however, the effect can be still described as a kind of potential and the results obtained below can be in part adjusted for the extended nuclei.

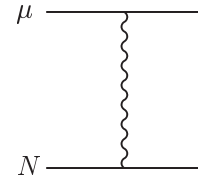


FIG. 1. The leading one-photon-exchange diagram. It is responsible for the contributions to orders $(Z\alpha)^2 m$ and $(Z\alpha)^4 m$.

Relativistic recoil effects contribute to one-photon exchange as well as to many-photon exchanges. The Coulomb and Uehling potentials correspond to a dominant contribution in one-photon exchange.

The one-photon contribution for the Coulomb case and Uehling term are depicted in Figs. 1 and 2, respectively. They are responsible for the entire nonrelativistic contribution to orders $(Z\alpha)^2 m$ and $\alpha(Z\alpha)^2 m$, respectively.

Those contributions can be described by a potential. They partly include recoil effects in a sense, that one has to use the reduced mass $m_R = mM/(m + M)$ in calculations. The result for the Uehling correction can be achieved analytically in terms of elementary functions [21,22]. The potential approach can be also applied for a relativistic evaluation with the Dirac wave functions. For the Uehling potential the energy with the Dirac wave functions is known in closed analytic terms [23,24].

Indeed, as far as the wave functions for Schrödinger-Coulomb and Dirac-Coulomb problems and the dispersion presentation of the Uehling potential, such as

$$V_U(r) = -\frac{\alpha(Z\alpha)}{\pi} \int_0^1 dv \rho_e(v) \frac{e^{-\lambda r}}{r}, \quad (1)$$

where

$$\lambda = \frac{2m_e}{\sqrt{1-v^2}}, \quad \rho_e(v) = \frac{v^2(1-v^2/3)}{1-v^2}, \quad (2)$$

are well known, a numerical calculation has never been a problem (see, e.g., [12,13,15]). Nevertheless, analytic evaluations allow one to find various useful asymptotics [22–24].

We note that the Uehling potential is smaller than the Coulomb potential roughly by a factor of α/π in any kinematic area. Similarly, we see that the eVP potential related to the second-order correction possesses the same property—it is smaller than the Coulomb exchange in any kinematic area by a factor of $(\alpha/\pi)^2$. Since general behavior of the eVP-induced potentials is somewhat similar to the $(\alpha/\pi)V_C(r)$ and $(\alpha/\pi)^2 V_C(r)$, we can hope that whatever we use for a pure Coulomb problem, it may be adjusted for eVP effects, including the relativistic recoil.

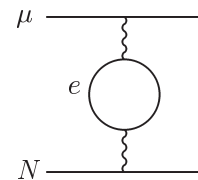


FIG. 2. The one-photon-exchange diagram for the eVP contributions. It is responsible for the the Uehling-potential corrections to orders $\alpha(Z\alpha)^2 m$ and $\alpha(Z\alpha)^4 m$.

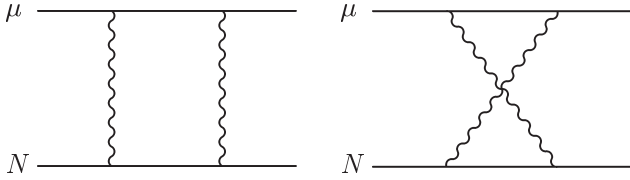


FIG. 3. The leading two-photon-exchange diagrams. In case of any practical calculations, there should be subtraction terms due to the nonperturbative nature of the Coulomb exchange for the bound state problem; meanwhile some one-photon-“reducible” contributions can appear. Those are not shown here. In certain gauges and, in particular, in the Feynman gauge the two-photon-exchange term contributes to order $(Z\alpha)^4 m^2/M$, while in the Coulomb gauge it contributes only to order $(Z\alpha)^5 m^2/M$.

Meanwhile, neither a complete calculation of the one-photon exchange (Figs. 1 and 2) can be identically presented in terms of a potential, nor can the two-photon exchange (Figs. 3 and 4) be in general ignored.

The approach developed by Grotch and Yennie [11] allowed one to resolve this problem for exchange by free photons (Figs. 1 and 3) and here [14] we generalize it, following our previous paper, for the case of the eVP contributions.

At first, we have to address a question of a possibility to use a certain relativistic equation with a kind of effective potential for a calculation of recoil effects.

The one-photon-exchange contribution can be evaluated with the help of the photon propagator, which in the Coulomb gauge takes the form,

$$D_{00}^C = -\frac{1}{\mathbf{k}^2}, \quad D_{i0}^C = 0, \quad D_{ij}^C = -\left(\delta_{ij} - \frac{k_i k_j}{\mathbf{k}^2}\right) \frac{1}{k^2}, \quad (3)$$

where $k^2 = k_0^2 - \mathbf{k}^2$. Note that only the static part of D_{00} produces a contribution in the nonrecoil limit and thus is responsible for an electrostatic potential. The other components of the photon propagators in general depend on the choice of the gauge and they are not directly related to D_{00} . For this reason the complete one-photon contribution cannot in general be expressed in terms of an electrostatic potential.

The one-photon contribution in the Coulomb gauge can be reduced for the m/M correction to its static approximation (i.e., neglecting the k_0 dependence) and thus to several potential-like terms because

(1) there is no k_0 dependence in D_{00} and thus no retardation effects are involved (if they were involved, that still would be of reduced importance because they are proportional to k_0^2/\mathbf{k}^2 and for atomic energy levels that would lead to

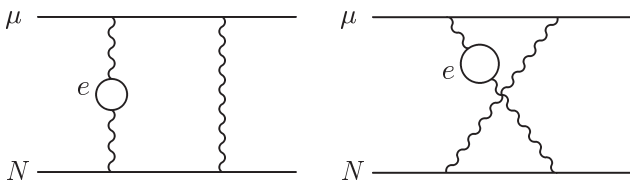


FIG. 4. Two-photon-exchange diagrams for the eVP contribution. Subtraction terms and reducible contributions are omitted. In certain gauges the two-photon-exchange effects contribute to order $\alpha(Z\alpha)^4 m^2/M$.

relativistic corrections proportional to $(m/M)^2$, while here we are interested in the m/M correction only);

(2) $D_{i0} = 0$;

(3) D_{ij} involves lower components of the spinor for the nucleus and thus the contribution is proportional to at least m/M , which means that the retardation effects in the D_{ij} term are of order $(m/M)^2$ or higher and negligible.

In the next sections we apply the static approximation to the one-photon exchange and develop an effective potential equation, first for a pure Coulomb problem and next for a perturbed Coulomb problem.

The remaining question is about two-photon-exchange contributions for the $(Z\alpha)^4 m^2/M$ correction. [In any effective Dirac equation approach, and we follow such an approach since we are to find a Grotch-type effective Dirac equation, it is assumed that certain two-photon-exchange subtractions take place (see, e.g., [29] for detail).] This question was reviewed, e.g., in [14]. The two-photon contributions are of at least order $(Z\alpha)^5 m^2/M$ in the Coulomb gauge because

(1) there is no k_0 dependence in D_{00} and thus there is no photon pole in two-photon exchange with two D_{00} components;

(2) $D_{i0} = 0$, and thus there is no contribution which involves one D_{i0} photon and one D_{00} photon.

That is sufficient to avoid any potential $(Z\alpha)^4 m^2/M$ contribution.

III. GROTCHEQUATION AND ITS SOLUTION FOR THE COULOMB BOUND SYSTEMS

Once we are limiting our consideration to one-photon contribution in a static approximation (i.e., at $k_0 = 0$), we can derive the Grotch equation for the free one-photon exchange (Fig. 1) in order, after that, to generalize it step by step for a more general case, including the eVP contributions. Our consideration closely follows the original one by Grotch and Yennie [11].

Here we give a brief reminder of the derivation of the Grotch equation and its solution in order to describe every step which we will need to adjust to eVP contributions.

The Grotch equation [11] is one of several effective Dirac equations for a two-particle system. It is important to reproduce the two most important features of any system of two fermions with an orbiting particle much lighter than the nucleus. The electron in ordinary hydrogen and the muon in muonic hydrogen are such particles. It is useful to consider the orbiting particle within a full relativistic consideration, while treating the nucleus in the leading nonrelativistic approximation. As a result, we may derive an equation, which correctly reproduces its limits, both the Schrödinger-Coulomb equation with the reduced mass and the Dirac-Coulomb equation with the original mass of the muon (or electron). Indeed, the equation is also supposed to take into account certain relativistic recoil corrections. The uncertainty in the calculation of the static one-photon contribution is of order $(Z\alpha)^4 (m/M)^2 m$. The two-photon contribution is of order $(Z\alpha)^5 m^2/M$.

The desired equation is of the form of Dirac equation for a muon,

$$[\widehat{P}_n - \widehat{p}_N - m - \widetilde{V}_{1\gamma}] \Psi_n = 0, \quad (4)$$

where $\hat{A} = \gamma_{[\mu]}^\nu A_\nu$ and $P_n = (E_n, \mathbf{0})$ (here A^ν is an arbitrary vector, ν is a relativistic 4-index, while μ stands for a muon.)

This is an equation in the center-of-mass system. While the equation is for the muon energy and wave function, the quantized energy E_n is for the two-body system and we should subtract from the whole 4-momentum P_n the nuclear 4-momentum $p_N = (\sqrt{M^2 + \mathbf{p}^2}, -\mathbf{p})$, where \mathbf{p} is the muon momentum.

To obtain a one-particle equation from a two-body one it was suggested that one can present the two-body wave function $\Psi_{\mu N}$ in terms of the free nuclear spinor and the muon wave function ψ ,

$$\Psi_{\mu N} = \begin{pmatrix} 1 \\ -\frac{\mathbf{p} \cdot \boldsymbol{\sigma}_N}{2M} \end{pmatrix} \psi. \quad (5)$$

This suggestion is not just an approximation in a sense that one can construct a perturbation theory and systematically take into account all the corrections required for a certain level of accuracy. The nuclear on-shell corrections are of relativistic nature for the nucleus and thus they are of higher order in m/M and $Z\alpha$ than the leading recoil effects we study. The off-shell corrections can be found through many-photon exchange diagrams and a proper choice of gauge can eliminate them in the leading recoil order.

The effective potential $\tilde{V}_{1\gamma}$ results from the static part of the one-photon exchange averaged over the nuclear part of the wave function in (5). In the momentum space we find

$$\begin{aligned} \tilde{V}_{1\gamma}(\mathbf{q}, \mathbf{p}) &= -i\gamma_\mu^0 \gamma_N^0 (Z\alpha) \left(1, -\frac{\boldsymbol{\sigma}_N \cdot \mathbf{q}}{2M}\right) \\ &\times [i\gamma_N^0 \gamma_\mu^0 D_{00}(\mathbf{k}) + i\gamma_N^i \gamma_\mu^j D_{ij}(\mathbf{k})] \begin{pmatrix} 1 \\ -\frac{\boldsymbol{\sigma}_N \cdot \mathbf{p}}{2M} \end{pmatrix} \\ &= -\frac{Z\alpha}{\mathbf{k}^2} \left\{ 1 + \frac{1}{2M} \left[\boldsymbol{\alpha}_\mu \cdot (\mathbf{p} + \mathbf{q}) \right. \right. \\ &\quad \left. \left. - \frac{(\boldsymbol{\alpha}_\mu \cdot \mathbf{k})(\mathbf{k} \cdot (\mathbf{p} + \mathbf{q}))}{\mathbf{k}^2} \right] \right. \\ &\quad \left. - \frac{1}{2M} [\mathbf{k} \times i\boldsymbol{\sigma}_N] \cdot \boldsymbol{\alpha}_\mu + O\left((Z\alpha)^4 \left(\frac{m}{M}\right)^2 m\right) \right\}, \end{aligned} \quad (6)$$

where $\mathbf{k} = \mathbf{p} - \mathbf{q}$. Here, the neglected term is not $O((Z\alpha)^4(m/M)^2 m)$ by itself, but it represents an operator, the matrix element of which over the atomic wave function is $O((Z\alpha)^4(m/M)^2 m)$.

This effective potential includes a nuclear-spin-dependent term which is responsible for the hyperfine splitting. It is of order $(Z\alpha)^4 m^2/M$. However, experimentally and theoretically the hyperfine structure effects are well separated from the Lamb shift effects. We consider this term as a perturbation and neglect the hyperfine-interaction term (i.e., we average over the nuclear spin).

Once we average the results over the nuclear spin, i.e., over the hyperfine structure, we note that all the remaining nuclear-spin effects appear only in order $(m/M)^2$ (see, e.g., [25–28]) and thus this derivation, started for the nuclear spin 1/2, is now valid for a nucleus with an arbitrary spin.

That is the last crucial step to obtain the Grotch equation [11] and we arrive at that in coordinate space,

$$\begin{aligned} &\left(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + \frac{\mathbf{p}^2}{2M} + V_C + \frac{1}{2M} \{ \boldsymbol{\alpha} \cdot \mathbf{p}, V_C \} \right. \\ &\quad \left. + \frac{1}{4M} [\boldsymbol{\alpha} \cdot \mathbf{p}, [\mathbf{p}^2, W_C]] \right) \psi(r) = E \psi(r), \end{aligned} \quad (7)$$

where the operator W_C appears due to taking into account the D_{ij}^C components of the photon propagator. It is essential that it can be expressed in a certain way through V_C , which is defined through D_{00}^C . In particular, for free one-photon-exchange (Fig. 1) and the relation between the Coulomb gauge is of the form,

$$W_C(\mathbf{k}) = -\frac{2V_C(\mathbf{k})}{\mathbf{k}^2}. \quad (8)$$

For the case of the Coulomb gauge one finds in coordinate and momentum space,

$$V_C(r) = -\frac{Z\alpha}{r}, \quad V_C(\mathbf{k}) = -\frac{4\pi Z\alpha}{\mathbf{k}^2}, \quad (9)$$

and

$$W_C(r) = -Z\alpha r, \quad W_C(\mathbf{k}) = \frac{8\pi Z\alpha}{\mathbf{k}^4}. \quad (10)$$

While the leading part of D_{00}^C in any gauge should produce the Coulomb term V_C , the shape of the Hamiltonian in Eq. (7) and a particular shape of W_C depends on the gauge chosen.

The effective equation above can be solved in a closed analytic form after applying a series of transformations [11]. We start with rearranging the Hamiltonian,

$$\begin{aligned} H &= \left(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + \frac{\mathbf{p}^2}{2M} + V_C + \frac{1}{2M} \{ \boldsymbol{\alpha} \cdot \mathbf{p}, V_C \} \right. \\ &\quad \left. + \frac{1}{4M} [\boldsymbol{\alpha} \cdot \mathbf{p}, [\mathbf{p}^2, W_C]] \right), \end{aligned} \quad (11)$$

as following

$$H = H_0 + \delta H + O\left((Z\alpha)^4 \frac{m^3}{M^2}\right), \quad (12)$$

where

$$H_0 = H_1 + \frac{H_1^2 - m^2}{2M} + \frac{1}{4M} [H_1, [\mathbf{p}^2, W_C]], \quad (13)$$

$$H_1 = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + V_C \frac{1 - \beta m/M}{1 - (m/M)^2}, \quad (14)$$

and

$$\delta H = -\left(\frac{V_C^2}{2M} + \frac{1}{4M} [V_C, [\mathbf{p}^2, W_C]] \right). \quad (15)$$

The correction, neglected in (12), is indeed an operator; its matrix elements over bound states are of order $O((Z\alpha)^4 \frac{m^3}{M^2})$, which is explicitly shown in (12). In this sense Eq. (12) is not correct as an operator identity, but it is sufficiently valid for all matrix elements for the bound states.

We note that due to the relation between V_C and W_C (8) the last term vanishes for the Coulomb potential in the Coulomb

gauge,

$$\delta H = 0. \quad (16)$$

To solve Eq. (7) within the required accuracy is the same as to solve the equation,

$$H_0 \psi_0 = E_0 \psi_0, \quad (17)$$

where $E = E_0$ and $\psi = \psi_0$ for the pure Coulomb case.

To deduce E_0 and ψ_0 we should first find a solution of equation,

$$H_1 \psi_1 = E_1 \psi_1. \quad (18)$$

Looking for it in the form,

$$\psi_1 = (1 + \beta \xi) \tilde{\psi}, \quad (19)$$

one finds that $\tilde{\psi}$ is a solution of an effective one-particle Dirac-Coulomb equation,

$$\left[\boldsymbol{\alpha} \cdot \mathbf{p} + \beta \tilde{m} - \frac{\tilde{Z}\alpha}{Z\alpha} V_C(r) \right] \tilde{\psi} = \tilde{E} \tilde{\psi}, \quad (20)$$

with an effective mass,

$$\tilde{m} = \frac{m \left(1 - \frac{E_1}{M}\right)}{\sqrt{1 - \left(\frac{m}{M}\right)^2}}, \quad (21)$$

and an effective Coulomb coupling constant,

$$\tilde{Z}\alpha = \frac{Z\alpha}{\sqrt{1 - \left(\frac{m}{M}\right)^2}} = Z\alpha \left[1 + O\left(\left(\frac{m}{M}\right)^2\right) \right], \quad (22)$$

where

$$\xi = \frac{M}{m} \left(1 - \sqrt{1 - \left(\frac{m}{M}\right)^2} \right) = \frac{m}{2M} \left[1 + O\left(\left(\frac{m}{M}\right)^2\right) \right]. \quad (23)$$

The solutions of Eq. (20) are similar to the well-known solutions of the conventional Dirac-Coulomb equation (see, e.g., [30]), with the only difference being that the parameters m and $Z\alpha$ must be replaced by effective values \tilde{m} and $\tilde{Z}\alpha$, defined in (21) and (22).

The energies E_1 are related to the known eigenvalues of the effective equation (20), \tilde{E} , by the equation,

$$\tilde{E} = \frac{E_1 - \frac{m^2}{M}}{\sqrt{1 - \left(\frac{m}{M}\right)^2}}. \quad (24)$$

The eigenvalues and eigenfunctions of Hamiltonian H_0 in Eq. (7), according to (12), are related to E_1 and ψ_1 , as

$$E_0 = E_1 + \frac{E_1^2 - m^2}{2M} \quad (25)$$

$$= \tilde{E} + \frac{\tilde{E}^2 + m^2}{2M} + O\left(\frac{m^3}{M^2}\right), \quad (26)$$

$$\psi_0 = N \left[1 - \frac{1}{4M} [\mathbf{p}^2, W_C] + O\left(\left(\frac{m}{M}\right)^2 (Z\alpha)^4\right) \right] (1 + \beta \xi) \tilde{\psi}, \quad (27)$$

where N is a normalization constant, for which one can find (see, e.g., [31])

$$N^2 = \frac{1}{1 + 2\xi \tilde{E}/\tilde{m} + \xi^2} \quad (28)$$

$$= 1 - \frac{m}{M} + \frac{(Z\alpha)^2 m}{2n^2 M} + O\left(\left(\frac{m}{M}\right)^2\right) + O\left(\frac{m}{M} (Z\alpha)^4\right). \quad (29)$$

This evaluation is not yet completed. We note that the energy E_0 is expressed in terms of E_1 (25), and the latter in terms of \tilde{E} (24). Meanwhile, \tilde{E} is a function of \tilde{m} (21) and $\tilde{Z}\alpha$ (22). The effective mass \tilde{m} in its turn depends on E_1 as follows from Eq. (21).

To proceed further, we note that for the Dirac-Coulomb problem,

$$E_{\text{DC}} = f_C(Z\alpha) m, \quad (30)$$

and thus the value of

$$\tilde{F} = \frac{\tilde{E}}{\tilde{m}}, \quad (31)$$

being equal to $f_C(\tilde{Z}\alpha)$, does not depend on the effective mass of the orbiting particle \tilde{m} , while the effective charge $\tilde{Z}\alpha$, as follows from Eq. (22), does not depend on energy. This allows simplifications.

Applying Eqs. (31) and (21) to (24), we obtain

$$E_1 = m \frac{\tilde{F} + \frac{m}{M}}{1 + \frac{m}{M} \tilde{F}}, \quad (32)$$

and, using (25),

$$E_0 = m + m \left(1 - \frac{m}{M}\right) (\tilde{F} - 1) - \frac{m^2}{2M} (\tilde{F} - 1)^2 \frac{\left(1 - \frac{m}{M}\right) \left(1 + \frac{m}{M} + 2\frac{m}{M} \tilde{F}\right)}{\left(1 + \frac{m}{M} \tilde{F}\right)^2}.$$

Since

$$\tilde{F} - 1 = O((Z\alpha)^2),$$

we can efficiently expand

$$E_0 = m + m \left(1 - \frac{m}{M}\right) (\tilde{F} - 1) - \frac{m^2}{2M} (\tilde{F} - 1)^2 \frac{\left(1 - \frac{m}{M}\right) \left(1 + 3\frac{m}{M}\right)}{\left(1 + \frac{m}{M}\right)^2} + O\left(m \left(\frac{m}{M}\right)^3 (Z\alpha)^6\right), \quad (33)$$

$$\tilde{m} = m \sqrt{\frac{1 - \frac{m}{M}}{1 + \frac{m}{M}}} \left[1 - \frac{\frac{m}{M}}{1 + \frac{m}{M}} (\tilde{F} - 1) + \frac{\left(\frac{m}{M}\right)^2}{\left(1 + \frac{m}{M}\right)^2} (\tilde{F} - 1)^2 + O\left(\left(\frac{m}{M}\right)^3 (Z\alpha)^6\right) \right]. \quad (34)$$

For the pure Coulomb problem it is sufficient to transform Eq. (33), neglecting terms of order $(Z\alpha)^4(m/M)^2m$. We note, comparing F and

$$F = f_C(Z\alpha),$$

that we have to distinguish between $\tilde{Z}\alpha$ and $Z\alpha$ only in the leading term of $(\tilde{F} - 1)$,

$$F = 1 + \left(\frac{Z\alpha}{\tilde{Z}\alpha}\right)^2 (\tilde{F} - 1) + O\left((Z\alpha)^4 \left(\frac{m}{M}\right)^2 m\right).$$

As a result, we eventually find for the Coulomb problem,

$$E = m + m_R(F - 1) - \frac{m_R^2}{2M}(F - 1)^2, \quad (35)$$

which has corrections only of order $(Z\alpha)^4(m/M)^2m$.

Here we have taken into account that for a pure Coulomb problem $\delta H = 0$ and thus the eigenvalues of the Hamiltonians H in Eq. (11) and H_0 in Eq. (13) are the same, i.e., $E = E_0$.

This evaluation, following [11], eventually presents eigenvalues and eigenfunctions of the Grotch equation (7) in terms of the well-known solution of the Dirac-Coulomb problem (see, e.g., [30]), but with effective parameters \tilde{m} and $\tilde{Z}\alpha$. We briefly overview those solutions in Appendix A (see, e.g., [30] for details).

We note that the Grotch equation (7) and its solution (35) is a complete account of the static one-photon exchange, once we average over the nuclear spin. The relativistic energies (see, e.g., [30]) are listed in Appendix A. We have not evaluated the wave functions, but it is more appropriate to perform such an evaluation once we clarify what accuracy is required. The energy levels (35) by themselves are obtained without any need for explicit expressions for the wave functions. However, once we step out from a pure Coulomb case the wave functions will be required; however, they are to appear in calculations of a small perturbation and do not need a high accuracy.

We remember that the energy levels (25) and (35) and wave functions (27) obtained above reproduce correctly:

(1) the leading nonrelativistic term (i.e., a result of the Schrödinger-Coulomb problem with the reduced mass) exactly in m/M ;

(2) the relativistic corrections (exactly in $Z\alpha$) for a infinitely heavy nucleus (i.e., a result of the Dirac-Coulomb problem);

(3) the leading relativistic recoil correction to energy in order $(Z\alpha)^4m^2/M$.

The result for the energy has to contain also various higher-order contributions $(Z\alpha)^k m^2/M$ ($k \geq 6$), which, without being a complete result, still have a certain sense, since it is sometimes clear how to upgrade them to a complete result [9,10].

IV. CONSIDERATION OF AN ARBITRARY NONRELATIVISTIC-TYPE POTENTIAL

Let us consider now a potential, which is a sum of the Coulomb potential and a “nonrelativistic-type potential”:

$$V = V_C + V_N.$$

The “nonrelativistic-type potential” $V_N(r)$ is such a potential that the leading nonrelativistic correction to energy is of order $\varepsilon(Z\alpha)^2m$ and the leading relativistic correction is of order $\varepsilon(Z\alpha)^4m$, while the leading correction to the wave function is of relative order ε both for nonrelativistic and relativistic behavior. It is understood that ε is a small but finite parameter, such as α/π , and that the potential $V_N(r)$ is smaller than the Coulomb potential in any area by a factor of ε .

We consider such a potential as a nonrelativistic-type potential, because its relativistic correction, similarly to the case of pure Coulomb potential, can be found through a relativistic expansion, which treats relativistic corrections as additional effective terms of a Hamiltonian of a nonrelativistic Schrödinger equation. Such a consideration is valid, e.g., for the eVP effects in muonic atoms, but not valid for eVP effects in ordinary atoms.

For consideration of $V_C + V_N$ in comparison with a pure Coulomb problem [11], reviewed in the previous section, one should take into account the following:

(1) It is not necessary that $\varepsilon(Z\alpha)^4m^2/M$ contributions can be calculated in the one-photon-exchange approximation. We suggest that it is valid for all $\varepsilon(Z\alpha)^4m^2/M$ terms, and that sets a constraint on effects which may be taken into account by the method developed here. This question is common for Grotch-type and Breit-type calculations and was discussed for one-loop eVP corrections in [14]. As explained there, there is a gauge, where the eVP contribution can be calculated within such an approximation.

(2) Rigorously speaking, there is no such a thing as just “potential.” One has to deal with a generalized one-photon exchange. The correction can be due to the photon propagator correction (as it is in the case of eVP effects), nuclear structure, etc. While its D_{00} component in a static regime is related to a “potential” for the external field approximation, the result for the other terms depends on the nature of the correction. There is no single rule on how to express the complete effect in terms of V_N . Here, we suggest that the expression (7) holds for the one-photon contribution in order up to $\varepsilon(Z\alpha)^4m^2/M$. The Hamiltonian is of the form,

$$H = \left(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + \frac{\mathbf{p}^2}{2M} + V + \frac{1}{2M} \{ \boldsymbol{\alpha} \cdot \mathbf{p}, V \} + \frac{1}{4M} [\boldsymbol{\alpha} \cdot \mathbf{p}, [\mathbf{p}^2, W]] \right), \quad (36)$$

where

$$W = W_C + W_N, \quad (37)$$

and an appropriate W_N term is to be found.

Furthermore, we suggest that in general the behavior of W_N is somewhat similar to that of εW_C , and the order of magnitude of related matrix elements can be found from that similarity. It is essential that in some way the last term in the Hamiltonian resulted from the lower (smaller) component of the nuclear spinor, so the related matrix elements are of order $(Z\alpha)^4m^2/M$ and may additionally contain ε .

All that apparently sets another constraint on interactions which can be described by means of a Grotch-type equation. What is important for our purposes is that for the eVP contributions we deal with a certain correction to the photon

propagator, the equation (7) is valid, and the appropriate function W_N can be explicitly found (see [14,19,20]).

(3) Next we note that the addition to the Hamiltonian, defined in Eq. (15), which vanishes in the pure Coulomb case, does not in the general situation:

$$\delta H = - \left(\frac{V^2}{2M} + \frac{1}{4M} [V, [\mathbf{p}^2, W]] \right) \neq 0. \quad (38)$$

In the former, pure Coulomb, case this addition was equal to zero. It consisted of two operators, matrix elements of which are of order $(Z\alpha)^4 m^2/M$:

$$\left\langle \frac{V^2}{2M} \right\rangle - \left\langle \frac{1}{4M} [V, [\mathbf{p}^2, W]] \right\rangle = O \left((Z\alpha)^4 \frac{m^2}{M} \right).$$

These are operators which have a nonvanishing matrix element between upper-upper (large-large) components of the muon spinor. To obtain the leading term of order $(Z\alpha)^4 m^2/M$ it is sufficient to work with the nonrelativistic wave functions ψ_{NR} . So, the equations for the Hamiltonian and the energy are now

$$H = H_0 + \delta H, \quad (39)$$

$$H_0 = H_1 + \frac{H_1^2 - m^2}{2M} + \frac{1}{4M} [H_1, [\mathbf{p}^2, W]], \quad (40)$$

$$H_1 = \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + V \frac{1 - \beta m/M}{1 - (m/M)^2}, \quad (41)$$

where we neglect the terms of order $(Z\alpha)^4 (m/M)^2 m$, and

$$E = E_0 + \delta E, \quad \delta E = \langle \psi_{\text{NR}} | \delta H | \psi_{\text{NR}} \rangle. \quad (42)$$

Since δE is already of order $\varepsilon (Z\alpha)^4 m^2/M$, only the linear corrections are necessary and the nonrelativistic wave function is that of the problem with H_0 .

In the first order in ε we need only pure Coulomb wave functions (see Appendix A), since we explicitly took into account that δH , which vanishes in the pure Coulomb case, has to be proportional to ε . To second order in ε we have to construct the nonrelativistic wave function perturbatively. Such a problem can be successfully resolved for many problems numerically.

The solution suggests that the effective energy \tilde{E} depends on the effective mass \tilde{m} , and the actual energy E_0 is expressed in terms of \tilde{E} . Meantime, the effective mass \tilde{m} depends on the energy E_0 . In the case of the pure Coulomb problem, the ratio,

$$\frac{\tilde{E}}{\tilde{m}} = \tilde{F},$$

does not depend on the effective mass and as a result we can disentangle \tilde{E} and \tilde{m} . In the general case, the ratio \tilde{E}/\tilde{m} depends on \tilde{m} and, through it, it depends on energy E_0 . This can be resolved only through expansion over the relativistic effects.

We have to apply expressions (33) and (34) studied above, where now the solution of the Dirac equation with potential V is of the form,

$$E = f_D(Z\alpha, Z\alpha m/\mu) m, \quad (43)$$

and

$$\tilde{F} = f_D(\tilde{Z}\alpha, \tilde{Z}\alpha \tilde{m}/\mu),$$

where f_D is a dimensionless energy of the Dirac equation with V and

$$\tilde{F} - 1 = O((Z\alpha)^2).$$

In contrast to the pure Coulomb case the dimensionless energy f_D depends on the effective mass through a dimensionless parameter $\tilde{Z}\alpha \tilde{m}/\mu$. This is possible if the potential V_N depends on the dimensional parameter μ . While calculating various integrals over the wave function the scale parameter of the potential, say, ‘‘radius’’ ($\sim 1/\mu$), is naturally compared with the atomic Bohr radius ($\sim 1/Z\alpha m$). For instance, in the case of eVP corrections in muonic atoms $\mu = m_e$ and the related parameter is $\sim 1.5Z$.

Next we note [see Eq. (34)] that

$$\tilde{m} = m_0 \left(1 + O \left(\frac{m}{M} (\tilde{F} - 1) \right) + \dots \right),$$

where m_0 is the result in the limit $Z\alpha \rightarrow 0$. The relativistic part is already proportional to $(Z\alpha)^4 m$ and it is sufficient to apply m_0 there. The nonrelativistic part is of order $(Z\alpha)^2 m$ and a correction of relative order $(Z\alpha)^2 m/M$ is important in the leading approximation, while higher powers of m/M are to be neglected here.

The result of the expansion with all terms required is

$$\begin{aligned} \tilde{m} &= m_R \sqrt{1 - \left(\frac{m}{M} \right)^2} \left[1 - \frac{m}{M} (\tilde{F} - 1) \right] \\ &= m_R \sqrt{1 - \left(\frac{m}{M} \right)^2} - \frac{m}{M} E_{\text{NR}}, \end{aligned} \quad (44)$$

where E_{NR} is the nonrelativistic part of the energy for the Schrödinger problem with V . As we mentioned, any further m/M corrections in the second term are unimportant and in particular, we can choose to calculate E_{NR} with a muon mass m or with the reduced mass m_R .

The effective mass is not included in \tilde{F} and F directly, but only in a combination,

$$\tilde{Z}\alpha \tilde{m} = Z\alpha m_R \left[1 - \frac{E_{\text{NR}}}{M} \right]. \quad (45)$$

Thus we find

$$\begin{aligned} \tilde{F} - 1 &= \frac{(Z\alpha)^2}{(\tilde{Z}\alpha)^2} (f_D(\tilde{Z}\alpha, \tilde{Z}\alpha \tilde{m}/\mu) - 1) \\ &= \frac{(Z\alpha)^2}{(\tilde{Z}\alpha)^2} \left\{ f_D(\tilde{Z}\alpha, Z\alpha m_R/\mu) - 1 \right. \\ &\quad \left. - \frac{E_{\text{NR}}}{M} \kappa \frac{\partial}{\partial \kappa} f_D(\tilde{Z}\alpha, \kappa) \right\}, \end{aligned} \quad (46)$$

where for the following it is useful to introduce

$$\kappa = \frac{Z\alpha m_R}{\mu}.$$

One can treat the first two terms in (46) separately, introducing

$$F_0 - 1 = \frac{(Z\alpha)^2}{(\tilde{Z}\alpha)^2} \{ f_D(\tilde{Z}\alpha, Z\alpha m_R/\mu) - 1 \},$$

which now does not depend on \tilde{m} . The energy can also be split into two terms:

$$E_0 = E^{(1)} + E^{(2)},$$

with the first term similar to the one for the pure Coulomb case [cf. Eq. (35)]

$$E^{(1)} = m + m_R(F_0 - 1) - \frac{m_R^2}{2M}(F_0 - 1)^2. \quad (47)$$

For the second term we note that $(f_D - 1)$ is the leading nonrelativistic contribution to the energy and with a sufficient accuracy we can approximate

$$f_D(\widetilde{Z}\alpha, Z\alpha m_R/\mu) - 1 = \frac{E_{\text{NR}}}{m_R},$$

and thus

$$E^{(2)} = -\frac{m_R^2}{2M} \frac{\partial}{\partial \ln \kappa} \left(\frac{E_{\text{NR}}}{m_R} \right)^2. \quad (48)$$

Eventually we arrive at the identity for the complete energy,

$$E = m + m_R(F_0 - 1) - \frac{m_R^2}{2M}(F_0 - 1)^2 - \frac{m_R^2}{2M} \frac{\partial}{\partial \ln \kappa} \left(\frac{E_{\text{NR}}}{m_R} \right)^2 - \langle \psi_{\text{NR}} | \left(\frac{V^2}{2M} + \frac{1}{4M} [V, [\mathbf{p}^2, W]] \right) | \psi_{\text{NR}} \rangle, \quad (49)$$

which is valid for our purposes and have corrections to order $(Z\alpha)^4 m^3/M^2$ and $\varepsilon(Z\alpha)^4 m^3/M^2$.

For the relativistic recoil term $(Z\alpha)^4 m^2/M$ we choose between applying m_R and m in such a way that it would simplify a comparison with Breit-type calculations of the same corrections (see [14]) for details. A difference between m_R and m in relativistic recoil corrections produces only terms of order $(Z\alpha)^4 (m/M)^2 m$.

In contrast to the pure Coulomb problem in the external field approximation, for which we know the energy and wave functions in closed analytic form, we indeed cannot know them for an arbitrary potential.

For the main term in (49) we need to be able to find the energy of the Dirac equation with potential V and the reduced mass m_R with a required accuracy. For two other terms we need to know only the nonrelativistic results for the related problem of a Schrödinger equation with potential V and the reduced mass m_R .

Both relativistic and nonrelativistic problems can be considered at this stage perturbatively since $\varepsilon \ll 1$ and V_N is a small correction to V_C .

V. CONCLUSIONS

The main result of this paper is that there is a certain kind of potential V for which a calculation of the relativistic effects can be split into two parts. One is a calculation of the energy in the external field approximation for a muon with the mass equal to its reduced mass in the atom. That is a “standard” problem of a Dirac equation for a particle with the mass equal to the reduced mass. This calculation can be, in principle, performed by various means, including numerical solutions.

The second part, which is a nontrivial part of the relativistic recoil correction, can be obtained once we know the nonrelativistic results for the atom with a muon with the reduced mass. That includes certain derivatives. Such a reduction

of the relativistic correction to nonrelativistic calculations essentially simplifies the problem. Roughly speaking, the essential two-body effects are less complicated than the one-particle relativistic problem.

Apparently, a number of problems to be solved for a relativistic muon is limited and we do not expect that a Dirac equation with potential V can be solved exactly. As far as the non-Coulomb term is a perturbation, i.e., for $\varepsilon \ll 1$, we can find all required elements perturbatively.

In particular, in the subsequent paper [19] we apply the developed approach to the eVP corrections in the first order in α , i.e., to the relativistic Uehling correction. In this case, one can expand (49) in $\varepsilon = \alpha/\pi$ and find that all required terms are known in a closed form. In the other subsequent paper [20] the same master equation is applied to the relativistic recoil Källén-Sabry correction, however, none of the eVP related terms are known analytically. So, they are calculated by means of numerical integration. Here, it is still sufficient to work in the first order in $\varepsilon = (\alpha/\pi)^2$. However, the relativistic recoil results of the same order, namely $\alpha^2(Z\alpha)^4 m^2/M$ arise also from double iteration of the Uehling potential, for this case $\varepsilon = \alpha/\pi$, and the second order in ε terms are required in (49). The recoil effects are obtained for these corrections also by means of numerical integration [20].

To conclude, we mention that the condition $\varepsilon \ll 1$ was set only because we are interested in developing a framework for perturbative calculations of the eVP relativistic recoil effects, which are performed in subsequent papers [19,20]. In principle, one can consider any “nonrelativistic-type potential,” but the related Dirac equation should be solved numerically.

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APPENDIX A: SOLUTION OF THE DIRAC EQUATION WITH COULOMB POTENTIAL

The exact relativistic energy for a pure Dirac-Coulomb problem $E_C(nl_j)$ for the nl_j state is of the form (see, e.g., [30]),

$$E_C(nl_j) = f_C(Z\alpha) m, \quad (A1)$$

$$f_C(Z\alpha) = \frac{1}{\sqrt{1 + \frac{(Z\alpha)^2}{(n_r + \zeta)^2}}}, \quad (A2)$$

and¹

$$v = (-1)^{j+l+1/2} (j+1/2), \quad \zeta = \sqrt{v^2 - (Z\alpha)^2}, \\ n_r = n - |v|.$$

¹It is customary to use κ for $(-1)^{j+l+1/2} (j+1/2)$ (cf. [30]), however, κ is used in our papers on muonic atoms for something else.

The wave functions of the Dirac-Coulomb problem are (see, e.g., [30])

$$\psi_{n_j l m}^{(C)}(\mathbf{r}) = \begin{pmatrix} \Omega_{j,l,m}(\mathbf{r}/r) f(r) \\ (-1)^{\frac{1+2l-2j}{2}} \Omega_{j,2j-l,m}(\mathbf{r}/r) g(r) \end{pmatrix}, \quad (\text{A3})$$

where the radial components are

$$\left. \begin{aligned} f \\ g \end{aligned} \right\} = \pm \frac{(2m\eta)^{3/2}}{\Gamma(2\zeta+1)} \sqrt{\frac{(m \pm E_C)\Gamma(2\zeta+n_r+1)}{4Z\alpha m \left(\frac{Z\alpha}{\eta} - \nu\right) n_r!}} \\ \times e^{-m\eta r} (2m\eta r)^{\zeta-1} \\ \times \left\{ \left(\frac{Z\alpha}{\eta} - \nu\right) {}_1F_1(-n_r, 2\zeta+1; 2m\eta r) \right. \\ \left. \mp n_r \times {}_1F_1(1-n_r, 2\zeta+1; 2m\eta r) \right\}. \quad (\text{A4})$$

Here the upper signs correspond to the large component f and lower ones are for the small components g ; ${}_1F_1(a, b; z)$

are confluent hypergeometric functions, Ω_{jlm} is a spherical spinor, and

$$\eta = \sqrt{1 - (E_{n_j}/m)^2} = \frac{Z\alpha}{\sqrt{(n_r + \zeta)^2 + (Z\alpha)^2}}.$$

The leading nonrelativistic contribution to the Dirac-Coulomb wave functions can be expressed in terms of the eigenfunctions of the Schrödinger-Coulomb problem,

$$\Phi_{nlm}^{(C)}(\mathbf{r}) = Y_{lm}(\mathbf{r}/r) R_{nl}(r), \quad (\text{A5})$$

where

$$R_{nl}(r) = \frac{2(Z\alpha m)^{3/2}}{n^{l+2}(2l+1)!} \sqrt{\frac{(n+l)!}{(n-l-1)!}} (2Z\alpha m r)^l e^{-\frac{Z\alpha m r}{n}} \\ \times {}_1F_1\left(-n+l+1, 2l+2; \frac{2Z\alpha m r}{n}\right), \quad (\text{A6})$$

and Y_{lm} are spherical functions.

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