Analysis of the Dirac-Coulomb problem in the free-particle representation

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The problem of an electron bound by a Coulomb field of strength $\alpha = Z\alpha'$ ($\alpha' \approx 137^{-1}$) is considered in the free-particle representation of the Dirac equation in momentum space. It is shown explicitly how $O(\alpha^5)$ contributions to the energies for all s-wave states that come from the relativistic free-particle kinetic energy and from the modified Coulomb interaction are canceled by a contribution from electron-positron pair formation. The relativistic correction to the momentum-space Schrödinger wave function is also shown to remove an unwanted $O(\alpha^6 \ln\alpha)$ energy dependence that arises in lowest-order perturbation theory. The work shows how to perform more accurate calculations in semirelativistic quasipotential approaches that are commonly used in quark models.

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While the problem of an electron (or any other massive, charged fermion) bound by an external Coulomb field can be solved exactly using the Dirac equation, a considerable interest remains in approximate treatments that avoid the difficulty of negative-energy solutions. There are valid reasons for such an interest both for the single-particle problem exemplified by the difficulty to approximate solutions variatonally [1] as well as for the many-electron problem, for which the so-called continuum dissolution problem arises [2]. Of course, one can avoid the pitfalls of the presence of negative-energy solutions and perform successfully a multiconfiguration Dirac-Fock scheme to attack the many-electron problem [3]. Nevertheless, the curiosity remains whether the relativistic bound-state problem can be attacked in a Schrödinger-like fashion. Further motivation for such an endeavor comes from the two-particle positronium problem, for which the covariant approach present one with major fundamental difficulties. In a Schrödinger-like approach the aim is to work with a single equation—usually an integral equation in momentum space—that contains only positive-energy eigenvalues and thus can be treated variationally. Whether the energy eigenvalues that are bounded from below represent upper bounds to the exact (field-theoretic) eigenvalues represents a separate problem.

It is straightforward to derive a relativized Schrödinger equation for the two-particle problem for each J^{PC} symmetry sector. It amounts to a single-channel reduction of the 16-component Salpeter equation [4], which represents an energy eigenvalue problem and singles out the center-of-mass frame of reference. It contains the free relativistic kinetic energy of a particle $\omega_p = \sqrt{p^2 + m^2}$ (we employ natural units $\hbar = c = 1$) and a potential energy that results from the sandwiching of the Coulomb potential between positive-energy projectors. If the coupling to the small component is ignored, the so-called "no-pair" equation emerges [5]. Such no-pair equations were investigated for pairs of spin-0 and spin-$\frac{1}{2}$ particles of different mass [6] and later the discussion was extended to treat transverse photon exchange as well [7–9]. These results were obtained within a Hamiltonian variational Fock-space method, which was shown to be powerful enough to treat couplings of the two-photon continuum [10].

It was shown recently [11] how the Dirac equation can be transformed exactly into a single-component representation in which the no-pair equation emerges as a limit and the presence of virtual positron-electron pairs is represented by multidimensional kernels in the integral equation. The no-pair wave equation for fermions is known to have an energy spectrum that agrees to $O(\alpha^4)$ with the Dirac spectrum, but contains an $O(\alpha^5)$ contribution for the s states. It was conjectured that this contribution would be canceled by the simplest virtual-pair contribution depicted in the language of old-fashioned time-ordered perturbation theory in Fig. 1 [5]. In addition, a perturbative analysis based on the exactly known Schrödinger solution in momentum space displays an $O(\alpha^6 \ln\alpha)$ dependence of the eigenenergy.

The aim of the present paper is to demonstrate explicitly how the no-pair equation is corrected by a single virtual-pair contribution. We analyze the Dirac equation in a free-particle representation, which is equivalent to the Feshbach-Villars representation of the Klein-Gordon equation. For the latter a successful resolution of the equivalent, technically somewhat simpler problem was obtained recently [12]. In this representation one still deals with positive- and negative-energy solutions, but one can perturbatively eliminate the $E < 0$ solutions, which is equivalent to the transformation to a single $E > 0$ equation [11].

In the free-particle representation [13], the Dirac equation for an electron in the static Coulomb field reads ($m = 1$, m is the electron mass)

$$(\omega_p - E)u(\mathbf{p}) = \frac{\alpha}{2\pi^2}\int \frac{d^3q}{(\mathbf{p}-\mathbf{q})^2} f(p,q)\left[\left[1 + \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\omega_p+1}\frac{\boldsymbol{\sigma}\cdot\mathbf{q}}{\omega_q+1}\right]u(\mathbf{q}) + \left[\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\omega_p+1} - \frac{\boldsymbol{\sigma}\cdot\mathbf{q}}{\omega_q+1}\right]v(\mathbf{q})\right], \tag{1a}$$

$$-(\omega_p + E)v(\mathbf{p}) = \frac{\alpha}{2\pi^2}\int \frac{d^3q}{(\mathbf{p}-\mathbf{q})^2} f(p,q)\left[\left[\frac{\boldsymbol{\sigma}\cdot\mathbf{q}}{\omega_q+1} - \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\omega_p+1}\right]u(\mathbf{q}) + \left[1 + \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\omega_p+1}\frac{\boldsymbol{\sigma}\mathbf{q}}{\omega_q+1}\right]v(\mathbf{q})\right]. \tag{1b}$$

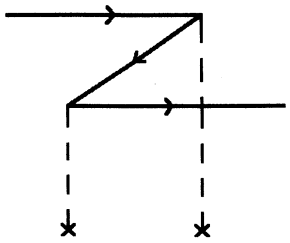

FIG. 1. Time-order perturbation-theory diagram depicting virtual-pair production by a massive particle in an external Coulomb field.

Here E is the total energy of the particle, $\alpha = Z\alpha' \approx Z/137$ is the coupling constant, σ is the set of Pauli matrices [14], $\omega_p = \sqrt{1+p^2}$, and

$$f(p,q) = \{[(\omega_p+1)(\omega_q+1)]/4\omega_p\omega_q\}^{1/2} . \quad (2)$$

The functions $u(p)$ and $v(p)$ represent amplitudes for the particles and antiparticles in the field-free limit, respectively. The amplitudes $u(p)$ and $v(p)$ differ from those used in Ref. [13] by a factor of $\sqrt{2\omega_p/(\omega_p+1)}$, which transforms the equation's kernel to a symmetrical form [11]. We denote the spin-up and spin-down components by plus and minus signs: $u^T(\mathbf{p}) = (u_+(\mathbf{p}), u_-(\mathbf{p}))$ and $v^T(\mathbf{p}) = (v_+(\mathbf{p}), v_-(\mathbf{p}))$. We consider now the s-wave states with the energy [15]

$$E_n = (1+\{\alpha^2/[(n-1+\sqrt{1-\alpha^2})^2]\})^{-1/2}$$
$$= 1 - \frac{\alpha^2}{2n^2} - \frac{\alpha^4}{2n^3}\left[1-\frac{3}{4n}\right] + O(\alpha^6) , \quad \alpha \to 0 . \quad (3)$$

Let us introduce the scaled variable $x = p/\alpha$. The Schrödinger equation for the nonrelativistic Coulomb particle

$$\left[\frac{x^2}{2} + E_0\right] u^{(0)}(x) = \frac{1}{2\pi^2}\int \frac{d^3y}{(\mathbf{x}-\mathbf{y})^2} u^{(0)}(y) \quad (4)$$

follows from (1), when the limit $\alpha \to 0$ is taken for fixed $x = p/\alpha$:

$$u_+(\alpha x) = u^{(0)}(x) + \cdots , \quad \alpha \to 0 \quad (5)$$

$$E = 1 - \alpha^2(E_0 + \cdots) , \quad (6)$$

while all the other components vanish. The s-wave solution corresponding to eigenenergies $E_{0n} = 1/2n^2$ are, in particular [13],

$$u^{(0)}_{n=1}(x) = A_1/(x^2+1)^2 , \quad (7)$$

$$u^{(0)}_{n=2}(x) = A_2(4x^2-1)/(4x^2+1)^3 , \quad (8)$$

etc. The normalization constants A_n are fixed by the condition

$$\int d^3p [u^{(0)}(p/\alpha)]^2 = 1 . \quad (9)$$

Combining Eq. (1a) for the component $u_+(p)$ and Eq. (4), we write out the exact expression for the correction to the energy as

$$E = 1 - \alpha^2/2n^2 + N^{-1}(E_1^k + E_1^u + E_1^v) , \quad (10)$$

where we have isolated a "kinetic-energy" contribution

$$E_1^k = \int d^3p\, u^{(0)}\left[\frac{p}{\alpha}\right]\left[\omega_p - 1 - \frac{p^2}{2}\right] u_+(p) , \quad (11)$$

a potential-energy contribution involving the u_+ amplitude only

$$E_1^u = -\frac{\alpha}{2\pi^2}\int d^3p\, u^{(0)}\left[\frac{p}{\alpha}\right]\int \frac{d^3q}{(\mathbf{p}-\mathbf{q})^2}\left[f(p,q)\left[1+\frac{\mathbf{p}\cdot\mathbf{q}}{(\omega_p+1)(\omega_q+1)}\right]-1\right] u_+(q) , \quad (12)$$

and contributions that depend on the antiparticle amplitudes as well

$$E_1^v = -\frac{\alpha}{2\pi^2}\int d^3p\, u^{(0)}\left[\frac{p}{\alpha}\right]\int \frac{d^3q}{(\mathbf{p}-\mathbf{q})^2} f(p,q)\left[\left[\frac{p_z}{(\omega_p+1)} - \frac{q_z}{(\omega_q+1)}\right] v_+(q) + \left[\frac{p_x - ip_y}{(\omega_p+1)} - \frac{q_x - iq_y}{(\omega_q+1)}\right] v_-(q)\right] . \quad (13)$$

Note that there is no explicit correction in (10) from the particle of the opposite spin $u_-(p)$. The quantity N in Eq. (10) stands for the overlap integral

$$N = \int d^3p\, u^{(0)}(p/\alpha) u_+(p) = 1 + O(\alpha^2) , \quad \alpha \to 0 . \quad (14)$$

The leading corrections to the nonrelativistic binding energy come from E_1^k and E_1^u. Introducing the approximation (5) into Eqs. (11) and (12) yields

$$E_1^k = -(\alpha^4/2n^3)\left[2 - \frac{3}{4n}\right] + \cdots \quad (15)$$

and

$$E_1^u = (\alpha^4/2n^3) + \cdots , \quad (16)$$

yielding the complete α^4 correction in Eq. (3).

To proceed effectively with deriving the corrections of higher order, an expansion of $u_+(p)$ in the limit $\alpha \to 0$ for a fixed p is needed [12] in addition to the expansion (5) for a fixed $x = p/\alpha$. Following Ref. [12] we write

$$u_+(p) = u_0(p) + \cdots , \quad \alpha \to 0 , \quad (17)$$

$$u_0(p) = u^{(0)}(p/\alpha)\xi_0(p) , \quad (18)$$

with $\xi_0(0) = 1$. We demand that in the limit $\alpha \to 0$ the function $u_0(p)$ should satisfy Eq. (1a) for $u_+(p)$ with $u_-(p) = v_+(p) = v_-(p) = 0$. In contrast with the limiting case of Eq. (5), the variable p is now held fixed. Making use of the wave-function asymptotes

$$u^{(0)}(x) \approx (2/n\alpha)^{3/2}(1/\pi x^4) , \quad x \to \infty , \quad (19)$$

we get

$$\xi_0(p) = [(\omega_p+1)^{3/2}]/2\sqrt{2\omega_p} \quad (20)$$

for any s-wave state. The function $u_0(p)$ goes over into the Schrödinger-Coulomb solution $u^{(0)}(p/\alpha)$ only for $p \to 0$.

With the expansion (17) introduced into Eqs. (11) and (12) we arrive after some manipulations at

$$E_1^k=-\frac{5}{8}\frac{\alpha^4}{n^3}+\int d^3p\left[u^{(0)}\left[\frac{p}{\alpha}\right]\right]^2\left[\left[\omega_0-1-\frac{p^2}{2}\right]\xi_0(p)+\frac{p^4}{2}\right]+\cdots=-\frac{5}{8}\frac{\alpha^4}{n^3}+\left[\frac{64}{15\pi}-\frac{16z_1}{\pi}\right]\frac{\alpha^5}{n^3}+E_2^k \quad (21)$$

and

$$E_1^u=\frac{\alpha^4}{2n^3}-\frac{\alpha}{2\pi^2}\int d^3p\,u^{(0)}\left[\frac{p}{\alpha}\right]\int d^3q\,u^{(0)}\left[\frac{q}{\alpha}\right]\frac{1}{(\mathbf{p}-\mathbf{q})^2}$$
$$\times\left[\left[[f(p,q)-1]\xi_0(q)+\frac{p^2+q^2}{8}\right]+\left[\frac{f(p,q)}{(\omega_0+1)(\omega_q+1)}\xi_0(q)-\frac{1}{4}\right]\mathbf{p}\cdot\mathbf{q}\right]+\cdots$$
$$=\frac{\alpha^4}{2n^3}-\frac{16z_2}{\pi}\frac{\alpha^5}{n^3}-\frac{\alpha^6\ln\alpha}{4n^3}+E_2^u\ . \quad (22)$$

The numerical constant z_1 and z_2 entering Eqs. (21) and (22) stand for the integrals

$$z_1=\int_0^\infty\frac{dp}{p^2}\frac{\xi_0(p)-1}{(\omega_p+1)^2}\approx0.0566\ , \quad (23)$$

and

$$z_2=\int_0^\infty\frac{dq}{q^4}\left[[\xi_0(q)=1][f(0,q)-1]+\frac{q^2}{4}\right]\approx0.2934\ . \quad (24)$$

In Eqs. (21) and (22) all the terms coming from the function $u_0(p)$ from Eq. (18) that are of the order of α^6 and higher are collected into the terms E_2^k and E_2^u, respectively. These E_2 terms incorporate also the terms coming from the correction to the function $u_0(p)$,

$$\Delta_1u_+(p)=u_+(p)-u_0(p)\ . \quad (25)$$

Let us now calculate the antiparticle correction (13). Using either of the approximations (5) or (17) in Eq. (1b) we obtain in the limit $\alpha\to0$ the first-order approximations for the wave-function components associated with negative energy that describe antiparticles

$$v_+(p)=\left[\frac{2\alpha^5}{n^3}\right]^{1/2}\frac{f(p,0)}{(\omega_p+1)^2}\frac{p_z}{p}+\cdots\ , \quad (26)$$

$$v_-(p)=\left[\frac{2\alpha^5}{n^3}\right]^{1/2}\frac{f(p,0)}{(\omega_p+1)^2}\frac{p_x+ip_y}{p}+\cdots\ . \quad (27)$$

Substituting (26) and (27) into (13), respectively, yields

$$E_1^v=(4/3\pi)(\alpha^5/n^3)+E_2^v\ . \quad (28)$$

Collecting the α^5 contributions from Eqs. (21), (22), and (28) we obtain a perfect cancellation of these terms

$$\left[\left[\frac{64}{15\pi}-\frac{16z_1}{\pi}\right]-\frac{16z_2}{\pi}+\frac{4}{3\pi}\right]\frac{\alpha^5}{n^3}=0\ , \quad (29)$$

where the identity $z_1+z_2=7/20$ was used.

In order to obtain all the terms of the order $\alpha^6\ln\alpha$ in the expansion of the energy E, we have to derive a correction to $u_0(p)$. The function $\Delta_1u_+(p)$ from (25) obeys the equation

$$(\omega_0-E)\Delta_1u_+(p)$$
$$=\frac{\alpha}{2\pi^2}\int\frac{d^3q}{(\mathbf{p}-\mathbf{q})^2}f(p,q)\left[1+\frac{\mathbf{p}\cdot\mathbf{q}}{(\omega_0+1)(\omega_q+1)}\right]$$
$$\times\Delta_1u_+(q)+U_1(p)+V_1(p)\ , \quad (30)$$

where

$$U_1(p)=-(\omega_p-E)u_0(p)+\frac{\alpha}{2\pi^2}\int\frac{d^3q}{(\mathbf{p}-\mathbf{q})^2}f(p,q)$$
$$\times\left[1+\frac{\mathbf{p}\cdot\mathbf{q}}{(\omega_p+1)(\omega_q+1)}\right]u_0(q) \quad (31)$$

and

$$V_1(p)=\frac{\alpha}{2\pi^2}\int\frac{d^3q}{(\mathbf{p}-\mathbf{q})^2}f(p,q)$$
$$\times\left[\frac{p_zv_+(q)+(p_x-ip_y)v_-(q)}{(\omega_p+1)}-\frac{q_zv_+(q)+(q_x-iq_y)v_-(q)}{(\omega_q+1)}\right]\ . \quad (32)$$

Equations (31) and (32) together with Eqs. (26) and (27) yield the limiting the expression

$$U_1(p)+V_1(p)=\frac{\alpha^{7/2}}{4n^{3/2}p\sqrt{\omega_p(\omega_p+1)}}+\cdots\ ,\quad \alpha\to0\ . \quad (33)$$

Let us represent the function $\Delta_1u_+(p)$ for $\alpha\to0$ at a fixed p as

$$\Delta_1u_+(p)\approx u_1(p)=u^{(0)}(p/\alpha)\xi_1(p)\ . \quad (34)$$

The function $\xi_1(p)$, as obtained from solving Eqs. (30), (33), and (34) for $\alpha\to0$, reads

$$\xi_1(p)=(\pi/8)[(\omega_p+1)/2\omega_p]^{1/2}p\alpha\ . \quad (35)$$

Naturally, the function $\xi_1(p)$ is dependent on the particle-antiparticle coupling that determines the antipar-

ticle contribution $V_1(p)$ to the inhomogeneous term in Eq. (30). We remark, however, that the linear behavior of the function $\xi_1(p)$ for small momenta is governed solely by the p^{-1} behavior of $U_1(p)$ in Eq. (31) and is thus independent of the antiparticle term $V_1(p)$. The resulting expansion of the solution $u_+(p)$ takes the form

$$u_+(p)=\frac{A\alpha^4}{(p^2+\alpha^2)^2}\frac{(\omega_p+1)^{3/2}}{2\sqrt{2\omega_p}}\left[1+\frac{\pi}{4}\frac{\alpha p}{\omega_p+1}+\cdots\right], \quad \alpha\to 0 . \tag{36}$$

We are now ready to determine the corresponding corrections to the energy E. We find that

$$E_2^k=\int d^3p\, u^{(0)}\left[\frac{p}{\alpha}\right]\left[\omega_p-1-\frac{p^2}{2}\right]u_1(p)+\cdots=\frac{\alpha^6\ln\alpha}{2n^3}+O(\alpha^6) , \tag{37}$$

$$E_2^u=-\frac{\alpha}{2\pi^2}\int d^3p\, u^{(0)}\left[\frac{p}{\alpha}\right]\int\frac{d^3q}{(\mathbf{p}-\mathbf{q})^2}\left[f(p,q)\left[1+\frac{\mathbf{p}\cdot\mathbf{q}}{(\omega_p+1)(\omega_q+1)}\right]-1\right]u_1(q)=-\frac{\alpha^6\ln\alpha}{4n^3}+O(\alpha^6) , \tag{38}$$

and

$$E_2^v=O(\alpha^6) . \tag{39}$$

It is essential to note that the corrections of order $\alpha^6\ln\alpha$ in Eqs. (37) and (38) are independent of the coupling to the antiparticle sector, being determined by the behavior of the function $u_1(p)$ in the region of small p only, which is independent of that coupling. Combining Eqs. (22), (37), and (38) shows that the corrections of order $\alpha^6\ln\alpha$ cancel perfectly.

Thus, for the energy to be calculated correctly at order α^5, one has to take into account the particle-antiparticle interaction in the first order of perturbation theory. However, the correct α^5 contributions from E^k and E^u that are canceling the effect of virtual pairs cannot be obtained easily from the zeroth-order nonrelativistic Coulomb wave functions. Instead one has to make use of an appropriate zeroth-order solution to the integral equation given by Eqs. (17), (18), and (20). Furthermore, the second term in the large parentheses in (36) is required to obtain a perfect cancellation between the $\alpha^6\ln\alpha$ contributions. As a result, one can get the energy E correctly up to α^6 already after the first iteration.

We consider now briefly the relativistic corrections for the states with nonzero angular momentum. Due to centrifugal barrier, the wave functions for these states are less singular at the origin in the coordinate-space representation as compared to the ones for the s-wave states. That manifests itself in a faster decrease of the wave function at high momenta, e.g., as p^{-5} for the p-wave states [13]. As a result, no terms of order α^5 or $\alpha^6\ln\alpha$ are present in the expansions of expression (11)–(13) for these higher partial waves. The terms of uneven power in α which will eventually appear in such expansions, like α^7 terms for the p-wave states, may be treated using the same technique.

For practical atomic physics applications of the method one has to deal with the problem of finite nuclear size, i.e., radius R_0. This can be done perturbatively as R_0 represents an additional small parameter. The first-order nonrelativistic correction can be calculated in coordinate space and is of order $R_0\alpha^4$ for a simple cutoff Coulomb potential. To estimate the relativistic corrections a careful analysis along the lines of this paper can be performed in p space.

We hope that the free-particle representation approach may be found useful for estimating energy corrections in the case of small molecules and ions. Implying that fairly accurate nonrelativistic momentum-space wave functions are obtained, one would expect that using the improved wave functions [Eq. (36)] and taking antiparticles into account will provide accurate results for relativistic energy corrections.

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