Analysis of the Klein-Gordon Coulomb problem in the Feshbach-Villars representation

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We consider the problem of a massive charged scalar particle bound in a given external Coulomb field of charge Z with varying strength parameter $\alpha = Z\alpha'$ ($\alpha' \approx 137^{-1}$) in the Feshbach-Villars (FV) representation. It is shown how the expansion in α of the momentum space integral equations can be handled to reproduce the exactly known spectrum up to some given order in α. In particular, it is shown in detail how the $O(\alpha^5)$ contributions to the ground-state energy that arise in the truncated FV equations from the kinetic and potential energies are canceled by virtual pair contributions. The findings are of relevance to quasipotential approaches to the relativistic few-body problem.

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I. INTRODUCTION

In this paper we consider the seemingly trivial problem of a massive spin-0 particle bound by an external Coulomb field. The problem has an exact solution that is presented in many textbooks. We are, however, interested in analyzing the problem using an alternative formulation of the Klein-Gordon equation, namely the Feshbach-Villars (FV) representation [1].

The motivation for this obviously more complicated undertaking of solving a pair of integral equations in momentum space is twofold.

(i) The FV formulation admits an interpretation of the two wave functions that appear as the particle- and antiparticle states in the free-field limit. Thus, one can interpret the appearing contributions and isolate virtual pair effects. It has been shown formally in the Dirac-Coulomb problem both at the level of quantum mechanics and field theory that, as a result of covariance (Z graphs in time-ordered perturbation theory), the Dirac equation contains the effects of virtual electron-positron pairs [2]. These pairs are related to the exchange of Coulomb photons. Virtual pairs associated with vacuum polarization are not considered here, as we do not include the exchange of transverse photons. In this contribution we demonstrate *explicitly* how the pair contribution is required to remove, in the energy, a dependence on an uneven order in the coupling constant $\alpha = Z\alpha'$, where $\alpha' \approx 137^{-1}$ is the fine-structure constant and A is the nuclear charge. An $O(\alpha^5)$ contribution is apparently present in the FV equations, both due to the kinetic-energy operator $E_p = c\sqrt{p^2 + m^2c^2}$ and the potential kernel.

(ii) Relativistic few-body problems are treated commonly by quasipotential approaches that use the kinetic-energy operator E_p in momentum space, e.g., Refs. [3–11]. The strange result, that this operator gives an odd-order $O(\alpha^5)$ contribution in the positronium spectrum, has been known for some time [11], but a proper analysis has not been performed. It was conjectured in the Dirac-Coulomb case that this contribution would be canceled by virtual pair effects [11]. A proper way of removing the unwanted $O(\alpha^5)$ contribution in a quasipotential approach, therefore, is of interest.

We chose the sin-0 particle problem for a start, as the FV representation is established in this case and a quasipotential approach is known to have a common lowest-order $O(\alpha^4)$ accurate limit [4]. The method can, however, also be used for the fermionic case [3].

II. THEORY

Our aim in this contribution is to elucidate the origin of *all* the corrections of order α^5 as well as some higher ones to the total energy and work out a method for their evaluation. As a model system we consider a massive scalar particle in the external Coulomb field described by the Klein-Gordon equation. The momentum-space particle-antiparticle representation of the Klein-Gordon equation [1] resembles the main features of the relativistic equations derived in various approaches [3,11], being at the same time relatively simple and exactly solvable.

In the Feshbach-Villars representation [2], the Klein-Gordon equation for the s-wave state of a particle in the static $-Z\alpha'/r$ field reads ($\hbar = c = m = 1$)

$$(\omega_p - E)u(p) = \frac{\alpha}{\pi}\int_0^\infty dq \frac{q}{p}\ln\left|\frac{p+q}{p-q}\right| \left[\frac{\omega_p + \omega_q}{\sqrt{\omega_p\omega_q}}u(q) + \frac{\omega_p - \omega_q}{2\sqrt{\omega_p\omega_q}}v(q)\right], \tag{1a}$$

$$-(\omega_p + E)v(p) = \frac{\alpha}{\pi}\int_0^\infty dq \frac{q}{p}\ln\left|\frac{p+q}{p-q}\right| \left[\frac{\omega_p - \omega_q}{2\sqrt{\omega_p\omega_q}}u(q) + \frac{\omega_p + \omega_q}{2\sqrt{\omega_p\omega_q}}v(q)\right]. \tag{1b}$$

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Here E is the total energy of the particle, $\alpha = Z\alpha' \approx Z/137$ is the coupling constant, and $\omega_p = \sqrt{1+p^2}$. The functions $u(p)$ and $v(p)$ represent amplitudes for the particles and antiparticles in the field-free limit, respectively. The energy E, known from the exact solution of the Klein-Gordon equation in the coordinate representation, is given by

$$E = \left[1 + \frac{\alpha^2}{(1/2+\sqrt{1/4-\alpha^2})^2}\right]^{-1/2}$$
$$= 1 - \tfrac{1}{2}\alpha^2 - \tfrac{5}{8}\alpha^4 - \tfrac{21}{16}\alpha^6 + \cdots, \quad \alpha \to 0 \ . \tag{2}$$

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

$$\left[\frac{x^2}{2} + E_0\right] u^{(0)}(x) = \frac{1}{\pi}\int_0^\infty dy \frac{y}{x} \ln\left|\frac{x+y}{x-y}\right| u^{(0)}(y) \tag{3}$$

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

$$u(\alpha x) = u^{(0)}(x) + \cdots, \quad \alpha \to 0 \tag{4}$$

$$E = 1 - \alpha^2(E_0 + \cdots) \ . \tag{5}$$

Equation (3) has the ground-state solution

$$u^{(0)}(x) = \frac{A}{(x^2+1)^2} \tag{6}$$

for the eigenenergy $E_0 = \frac{1}{2}$. We set $A = 2^{3/2}\alpha^{-3/2}\pi^{-1}$ in order that $u^{(0)}(p/\alpha)$ be normalized as

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

Combining Eq. (1a) and Eq. (3) for $x = p/\alpha$ we write out the exact expression for the correction to the energy as

$$E = 1 - \alpha^2/2 + E_1^k + E_1^{uu} + E_1^{uv} \ , \tag{7}$$

where we have isolated a "kinetic-energy" contribution

$$E_1^k = N^{-1}\int d^3p u^{(0)}\left[\frac{p}{\alpha}\right]\left[\omega_p - 1 - \frac{p^2}{2}\right] u(p) \ , \tag{8}$$

a contribution involving the u amplitude only,

$$E_1^{uu} = N^{-1}\int d^3p u^{(0)}\left[\frac{p}{\alpha}\right]\left[-\frac{\alpha}{\pi}\right] \times \int_0^\infty dq \frac{q}{p}\ln\left|\frac{p+q}{p-q}\right| \frac{\omega_p+\omega_q}{2\sqrt{\omega_p\omega_q}} u(q) \ , \tag{9}$$

and a contribution that depends on the v amplitude as well,

$$E_1^{uv} = N^{-1}\int d^3p u^{(0)}\left[\frac{p}{\alpha}\right]\left[-\frac{\alpha}{\pi}\right] \times \int_0^\infty dq \frac{q}{p}\ln\left|\frac{p+q}{p-q}\right| \frac{\omega_p-\omega_q}{2\sqrt{\omega_p\omega_q}} v(q) \ . \tag{10}$$

Here N stands for the overlap integral

$$N = \int d^3p u^{(0)}(p/\alpha) u(p) = 1 + \cdots, \quad \alpha \to 0 \ . \tag{11}$$

To obtain the first-order correction in perturbation theory, we make use of the approximations $u(p) \approx u^{(0)}(p/\alpha)$ and

$$v(p) \approx -\frac{1}{\omega_p+1}\frac{\alpha}{\pi}\int_0^\infty dq \frac{q}{p}\ln\left|\frac{p+q}{p-q}\right| \frac{\omega_p-\omega_q}{2\sqrt{\omega_p\omega_q}} u^{(0)}\left[\frac{q}{\alpha}\right]$$
$$\approx -\frac{A\alpha^4}{4\sqrt{\omega_p}(\omega_p+1)^2}, \quad \alpha \to 0 \ , \tag{12}$$

This yields

$$E_1^k = -\frac{5}{8}\alpha^4 + \frac{64}{15\pi}\alpha^5 + \cdots \ , \tag{13}$$

$$E_1^{uu} = -\frac{16z}{\pi}\alpha^5 + \cdots \ , \tag{14}$$

$$E_1^{uv} = -\frac{2}{3\pi}\alpha^5 + \cdots \ , \tag{15}$$

with

$$z = \int_0^\infty \frac{dp}{\sqrt{\omega_p}(\sqrt{\omega_p}+1)^2(\omega_p+1)^2} \ .$$

The term of order α^4 is given correctly by Eq. (13). The next-order correction, α^5, is found in all three terms, E_1^k, E_1^{uu}, and E_1^{uv}. Yet, these α^5 corrections fail to reproduce the exact result (2), as their sum does not vanish:

$$\frac{64}{15\pi} - \frac{16z}{\pi} - \frac{2}{3\pi} \approx 0.7332 \ .$$

The reason for this discrepancy is that the α^5 corrections presented in Eqs. (13) and (14) are incomplete. One can show that the second-order (and possibly higher-order) perturbation theory corrections to the quantities E_1^k and E_1^{uu} include additional terms of order α^5, which come from the region of *finite p*. However, the corresponding corrections to E_1^{uv} are of a higher order.

Thus, the nonrelativistic Coulomb wave function appears not to be a suitable zero-order approximation to the exact solution $u(p)$ for calculating the corrections (8) and (9). We show that it is possible to remove a number of terms of $\sigma(\alpha^5)$ by redefining the zeroth-order wave function in the region of finite p. For this purpose, we may ignore the coupling between $u(p)$ and $v(p)$, as the sole contribution of order α^5 from $v(p)$ is given by the first-order correction in Eq. (15).

Let us introduce the function

$$u_0(p) = u^{(0)}\left[\frac{p}{\alpha}\right]\xi_0(p) \ , \tag{16}$$

with $\xi_0(0) = 1$. We demand that the function $u_0(p)$ should satisfy Eq. (1a) with $v(p) = 0$ for $\alpha \to 0$. In contrast to the limiting case of Eq. (4), the variable p is now held fixed. This gives

$$\xi_0(p) = \frac{(\omega_p+1)^2}{4\sqrt{\omega_p}} \ . \tag{17}$$

With the function $u(p)$ replaced by $u_0(p)$, Eqs. (8) and (9) yield

$$E_1^k=-\frac{5}{8}\alpha^4+\left[\frac{64}{15\pi}-\frac{4z_1}{\pi}\right]\alpha^5+E_2^k\ , \tag{18}$$

$$E_1^{uu}=-\frac{2z_2}{\pi}\alpha^5-\alpha^6\ln\alpha+E_2^{uu}\ , \tag{19}$$

$$E_1^{uv}=-\frac{2}{3\pi}\alpha^5+E_2^{uv}\ , \tag{20}$$

with

$$z_1=\int_0^\infty\frac{dp}{\sqrt{\omega_p}(\omega_p+1)^2}\left[\frac{2p^2}{(\sqrt{\omega_p}+1)^2(\omega_p+1)^2}+1\right]$$

and

$$z_2=\int_0^\infty\frac{dp}{(\sqrt{\omega_p}+1)^2}\left[\frac{4}{\sqrt{\omega_p}(\omega_p+1)^2}+\frac{1}{\omega_p}\right]\ .$$

A replacement of $u^{(0)}(p/\alpha)$ by $u_0(p)$ in Eq. (12) has no effect on the leading term in $v(p)$, as well as on the term of order α^5 in the energy E_1^{uv} of Eq. (15). Collecting now the α^5 terms from Eqs. (18), (19), and (20), we obtain the correct result:

$$\left[\frac{64}{15\pi}-\frac{4z_1}{\pi}\right]-\frac{2z_2}{\pi}-\frac{2}{3\pi}=0\ . \tag{21}$$

The expression $2z_1+z_2=\frac{9}{5}$ that appears in Eq. (21) can be calculated in closed form.

In order to derive the higher corrections to the energy E, we have to obtain the correction to the wave function $u_0(p)$:

$$u_1(p)=u(p)-u_0(p)\ . \tag{22}$$

The function $u_1(p)$ obeys the equation

$$(\omega_p-E)u_1(p)=\frac{\alpha}{\pi}\int_0^\infty dq\frac{q}{p}\ln\left|\frac{p+q}{p-q}\right|\frac{\omega_p+\omega_q}{2\sqrt{\omega_p\omega_q}}u_1(q)+U_1(p)+V_1(p)\ , \tag{23}$$

with

$$U_1(p)=\frac{\alpha}{\pi}\int_0^\infty dq\frac{q}{p}\ln\left|\frac{p+q}{p-q}\right|\frac{\omega_p+\omega_q}{2\sqrt{\omega_p\omega_q}}u_0(q)-(\omega_p-E)u_0(p)$$

and

$$V_1(p)=\frac{\alpha}{\pi}\int_0^\infty dq\frac{q}{p}\ln\left|\frac{p+q}{p-q}\right|\frac{\omega_p-\omega_q}{2\sqrt{\omega_p\omega_q}}v(q)\ .$$

As $\alpha\to 0$, the inhomogeneous terms $U_1(p)$ and $V_1(p)$ can be written, after some manipulations, as

$$U_1(p)\approx\frac{A\alpha^5}{8\pi p\sqrt{\omega_p}}\int_0^\infty\frac{dq}{q}\ln\left|\frac{p+q}{p-q}\right|\times\frac{(\omega_p+\omega_q)(\omega_q-1)+4\omega_q}{\omega_q(\omega_q+1)} \tag{24}$$

and

$$V_1(p)\approx-\frac{A\alpha^5}{8\pi p\sqrt{\omega_p}}\int_0^\infty\frac{dq}{q}\ln\left|\frac{p+q}{p-q}\right|\times\frac{(\omega_p-\omega_q)(\omega_q-1)}{\omega_q(\omega_q+1)}\ . \tag{25}$$

Furthermore, we write

$$U_1(p)+V_1(p)\approx\frac{A\alpha^5}{4\pi p\sqrt{\omega_p}}\int_0^\infty\frac{dq}{q}\ln\left|\frac{p+1}{p-q}\right|=\frac{A\pi\alpha^5}{8p\sqrt{\omega_p}}\ . \tag{26}$$

Let us represent the function $u_1(p)$ for $\alpha\to 0$ at a fixed p as

$$u_1(p)\approx u^{(0)}(p/\alpha)\xi_1(p)\ . \tag{27}$$

The function $\xi_1(p)$, as obtained from solving Eq. (23) with the inhomogeneous term from Eq. (26) for $\alpha\to 0$, reads

$$\xi_1(p)=\frac{\pi}{8}\frac{\omega_p+1}{\sqrt{\omega_p}}p\alpha\ . \tag{28}$$

The resulting expansion of the solution $u(p)$ takes the form

$$u(p)=\frac{A\alpha^4}{(p^2+\alpha^2)^2}\left[\frac{(\omega_p+1)^2}{4\sqrt{\omega_p}}+\frac{\pi}{8}\frac{\omega_p+1}{\sqrt{\omega_p}}p\alpha+\cdots\right]\ ,\quad \alpha\to 0\ . \tag{29}$$

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

$$\begin{aligned}E_2^k&=N^{-1}\int d^3pu(0)\left[\frac{p}{\alpha}\right]\left[\omega_p-1-\frac{p^2}{2}\right]u_1(p)+\cdots\\&=-\frac{\pi^2}{4}A^2\alpha^9\int_0^\infty\frac{p^7dp}{(p^2+\alpha^2)^4\sqrt{\omega_p}(\omega_p+1)}+\cdots\\&=\alpha^6\ln\alpha+O(\alpha^6)\end{aligned} \tag{30}$$

and

$$E_2^{uu}=O(\alpha^6)\ , \tag{31}$$

$$E_2^{uv}=O(\alpha^6)\ . \tag{32}$$

Inspection of the corrections shows that the $\alpha^6\ln\alpha$ terms given by Eqs. (19) and (30) cancel each other, quite in accord with the absence of such a term in the expansion (2). The term $-\alpha^6\ln\alpha$ in Eq. (19) is apparently independent of the coupling between the functions $u(p)$ and $v(p)$. Its counterpart from Eq. (30) seems, at first sight, to be dependent on this coupling, since the correction $u_1(p)$ depends on the inhomogeneous term $V_1(p)$ determined by $v(p)$. However, a closer inspection shows that this is not the case. Equation (30) reveals that the term $\alpha^6\ln\alpha$ is governed by the behavior of the function $u_1(p)$ at small momenta. This, in turn, is determined by the $1/p$ dependence in the inhomogeneous term (26). It is readily seen from Eqs. (24) and (25) that this growth comes from the first term only, $v_1(p)\approx p^{-1}$ as $p\to 0$, $V_1(0)=\text{const}<\infty$, and is v independent. Correspondingly, the term $\alpha^6\ln\alpha$ in Eq. (30) is independent of the particle-antiparticle interaction.

The higher corrections, of order α^6, are present in all three terms, E_2^k, E_2^{uu}, and E_2^{uv}. Note that E_2^k includes a special term of order α^6 coming from the expansion of the overlap integral (11). Estimates of the behavior of the correction to $u^{(0)}(x)$ at large x show that $N=1+O(\alpha^2)$ for $\alpha\to 0$. We do not present the calculation of the complete α^6 correction to the energy E in the FV representation, but show that it depends on the v-v interaction. Indeed, the correction $\Delta v(p)$ associated with the v-v interaction to the leading term in the function $v(p)$ given by Eq. (12) reads

$$\Delta v(p)=-\frac{1}{\omega_p+E}\frac{\alpha}{\pi}\int_0^\infty dq\frac{q}{p}\ln\left|\frac{p+1}{p-q}\right|\frac{\omega_p+\omega_q}{2\sqrt{\omega_p\omega_q}}v(q)\ . \tag{33}$$

This correction generates the following contribution E^{vv} to the energy correction E_2^u:

$$\begin{aligned}E^{vv}&=N^{-1}\int d^3pu^{(0)}\left[\frac{p}{\alpha}\right]\left[-\frac{\alpha}{\pi}\right]\\&\quad\times\int_0^\infty dq\frac{q}{p}\ln\left|\frac{p+q}{p-q}\right|\frac{\omega_p-\omega_q}{2\sqrt{\omega_p\omega_q}}\Delta v(q)\\&\approx\frac{\alpha^6}{\pi}\int_0^\infty\frac{dqq^2f(q)}{\sqrt{\omega_q}(\omega_q+1)},\quad \alpha\to 0\ ,\end{aligned}\tag{34}$$

where

$$f(p)=\frac{1}{\sqrt{\omega_p}(\omega_p+1)}\frac{1}{\pi}\int_0^\infty dq\frac{q}{p}\ln\left|\frac{p+q}{p-q}\right|\frac{\omega_p+\omega_q}{\omega_q(\omega_q+1)^2}\ .$$

Therefore we conclude that in order to obtain the spectrum correctly including the α^6 part it is not sufficient to treat Eq. (1b) in the lowest order in α.

III. CONCLUSION

We have demonstrated in the FV representation of the Klein-Gordon-Coulomb problem that the expansion of the particle energy for small α can be represented as

$$E=E^{uu}+E^{uv}\ , \tag{35}$$

with

$$E^{uu}=1-\alpha^2/2-\tfrac{5}{8}\alpha^4+a\alpha^5+b\alpha^6\ln\alpha+c\alpha^6+\cdots \tag{36}$$

and

$$E^{uv}=d\alpha^5+e\alpha^6+\cdots\ . \tag{37}$$

Here we imply that the energy E^{uu} depends only on the particle-particle interaction and that the other part, E^{uv}, represents the connection to the antiparticle sector. Solving the equation for the particles only $[v(p)=0]$ gives the correct energy E up to order α^4 inclusively. 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 to determine d. To reproduce the energy up to α^6, the first-order account of the interaction between antiparticles is necessary as it enters in the coefficient e. For Eqs. (1) the following relations are valid: $a+d=0$ and $b=0$. This result cannot be obtained easily from the zeroth-order nonrelativistic Coulomb wave function. Instead one has to make use of an appropriate zeroth-order solution to the integral equation for $u(p)$ given by $u_0(p)$ from Eq. (16). Furthermore we note that the second term in the square brackets in (29) is required to obtain a perfect cancellation between the $\alpha^6\ln\alpha$ contributions arising in Eqs. (19) and (30) resulting in $b=0$ in (36).

Since the Klein-Gordon equation in the Feshbach-Villars representation is a typical example of few-particle relativistic equations, we believe that the results obtained here can be generalized to other systems, such as the Dirac-Coulomb problem and few-body relativistic quasipotential equations [3–11]. We remark that, in the positronium problem, quasipotential approaches that ignore the virtual pair contribution also fail to obtain the correct $O(\alpha^5)$ dependence of the ground-state energy [11]. It is possible to correct this discrepancy with a wave-function expansion such as Eq. (29) presented in this paper.

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[1] H. Feshbach and F. Villars, Rev. Mod. Phys. **30**, 24 (1985).
[2] I. Guiasu and R. Koniuk, Can. J. Phys. **71**, 360 (1993).
[3] W. Dykshoorn and R. Koniuk, Phys. Rev. A **41**, 64 (1990); J. W. Darewych and M. Horbatsch, J. Phys. B **23**, 337 (1990).
[4] L. Xiao, J. W. Darewych, and M. Horbatsch, Phys. Rev. A **42**, 69 (1990).
[5] T. Zhang and R. Koniuk, Phys. Rev. D **43**, 1688 (1991).
[6] J. R. Spence and J. P. Vary, Phys. Lett. B **254**, 1 (1991).
[7] B. A. Arbuzov, E. E. Boos, V. I. Savrin, and S. A. Shichanin, Phys. Lett. B **240**, 477 (1990).
[8] V. G. Kadyshevsky, Nucl. Phys. B **6**, 125 (1968).
[9] E. E. Salpeter, Phys. Rev. **87**, 328 (1957).
[10] A. Klein and R. M. Dreizler, Phys. Rev. A **45**, 4340 (1992).
[11] G. Hardekopf and J. Sucher, Phys. Rev. A **30**, 703 (1984); **31**, 2020 (1985), and references therein.