HIGH-ORDER EXPANSION OF THE ENERGY EIGENVALUES OF A RELATIVISTIC COULOMB EQUATION

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Abstract

It is shown that the Herbst equation, i.e. a Coulomb potential wave equation including a free relativistic kinetic energy, presents a rather non-trivial series expansion of its eigenvalues in powers of α . In fact, in contrast to Klein-Gordon and Dirac equation, it presents not only odd powers of α but also non analytic $\ln \alpha$ terms. The first orders (α^4, α^5) are obtainable by a standard perturbation method on the Sommerfeld correction. A much more effective and systematic method is proposed to get higher orders (α^7). To appreciate the resulting expansion, we compare it to the known results coming from other approaches to relativistic bound states, namely Klein-Gordon and Dirac equations in an external field and for the two-body problem, Breit and Sucher-type equations and positronium QED result.

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1. Introduction

a) "Relativistic equations" for the bound state problem in the light of the full QED treatment

The equations with a "root square" relativistic kinetic energy, like Herbst equation¹⁾, which writes in its two-body form (equal mass case) :

$$\left(2\sqrt{\vec{p}^2 + m^2} - \frac{\alpha}{r}\right) \psi = E\psi \quad (1)$$

or its generalisation to several particles or to an arbitrary potential are now popular as a way of implementing Relativity in potential models for the two or three body problem of particle physics²⁾, or many-body problems of astrophysics³⁾. It is therefore worth trying first to discuss what one may expect from such an admittedly naïve treatment. We will mainly discuss this point for the above Herbst equation in the Coulomb potential ; comparison can be made with two corresponding well-defined problems : the two-body problem of (approximately) bound states in QED, i.e. the positronium, for which a complete although perturbative treatment is available (this point 1.a) ; the simpler external field problem (hydrogen or π -meson atoms), which has an exact solution and which should be compared to the corresponding one-body Herbst equation (dropping factor two in front of kinetic energy) (point 1.b). In fact, throughout this paper, we will restrict the effective discussion of the equation to the case of bound states in a Coulomb potential. We shall only allude to the applications of the "root square kinetic energy" type of equation to more general potentials and to the scattering problem in point c) of this introduction.

It must be stressed that the only physically correct solution to the complete problem of Relativity in particle physics is local field theory, namely in the present case QED, and the latter is the standard to which one shall compare various proposed procedures. Since QED is not exactly solvable, what is only feasible is an expansion of bound state energies in power of α . Under a general point of view, one can identify the α expansion with a non-relativistic expansion in the sense that v/c is $O(\alpha)$. Indeed, in the bound state problem, in contrast to scattering, the momenta

are small and of order $m\alpha$. The lowest order result is the Schrödinger non-relativistic binding energy. Now, a question is : which corrections to the lowest order should, and which should not, be properly termed as "relativistic" ? We may of course consider it to be the full correction at a certain order in α . But it is interesting to evaluate other popular realisations of this idea of relativity, which are obtained by emphasizing certain aspects of the full theory.

One is often tempted to identify relativity with manifest covariance. The minimal way to obtain manifest covariance is provided by the ladder B-S (Bethe-Salpeter) equation, as has often been proposed in the context of particle physics. In the case of QED, as well as of any gauge theory, manifest covariance is obtained if, in addition, the gauge condition itself is covariant. But the result is then very disappointing : ladder QED B-S equation in a covariant gauge gives the correct binding energy only at lowest order α^2 (Schrödinger equation) ; instead of the correct order α^4 corrections, it gives completely spurious $\alpha^3 \log \alpha$ terms ; inclusion of an infinite number of crossed graphs into the kernel is already necessary to get the correct first correction to Schrödinger equation of order α^4 in the fermion case and at the expense of rather complicated calculations⁴⁾. The B-S equation is tractable only in the Coulomb gauge, and one returns to perturbation around an instantaneous interaction, which gives the main effect.

The idea behind the popular appeal to the "root square" type of equation is different. One is not thinking of manifest covariance and one is working from the beginning in the Hamiltonian spirit. One has in mind the requirement that a relativistic treatment should at least include the free-particle kinetic energy expression to recover the correct zero interaction limit. One cannot object this quite reasonable demand ; nevertheless, the procedure is once more not sufficient to get the correct result even for the lowest order corrections, although it appears at least to fare better than the previous one ; as will be shown in detail later, the first correction is correct in the boson case, but in the most interesting fermion case it is already outside its scope.

A scheme which displays clearly what has been left aside and must be accounted for as additional corrections to this Herbst equation is the Hamiltonian approach of

Sucher⁵⁾. It appears that in the case of spinor electrodynamics the correct result is given by :

i) solving first a wave equation with a $\sqrt{\vec{p}^2 + m^2}$ kinetic energy and a modified Coulomb potential, affected by Λ_+ projection operators,

$$\left[2\sqrt{\vec{p}^2 + m^2} - \Lambda_+(\vec{p})\Lambda_+(-\vec{p})\frac{\alpha}{r}\Lambda_+(\vec{p})\Lambda_+(-\vec{p}) \right] \psi = E\psi \quad (2)$$

ii) adding (perturbatively) pair creation or annihilation by the Coulomb potential, and the effect of transverse photons, including in the positronium case annihilation.

It is obvious that Herbst equation does not contain the effects ii). But it also comes out that it is even not equivalent, even in perturbation, to the Sucher wave equation i) : large terms come from the expansion of Λ_+ projection operators.

At any case, it must be clear that, even if a wave equation with the relativistic free kinetic energy and a Coulomb potential (Herbst or Sucher equation) could be solved exactly or numerically, additional contributions cannot be completely expressed in a simple N-body wave equation, and they could be included only by a perturbation expansion in α . Then, one can solve the whole problem only in a series expansion, and we shall have in the end to expand also the solutions of the wave equation. It would seem therefore at first sight that solving the Herbst equation is of no real physical use and that it would be more expedient to start directly from the Schrödinger equation. Nevertheless, the expansion of the Herbst equation eigenvalues (which is the specific aim of the present article) and wave functions could still be a useful step in performing the expansion, because of the specific effects connected with this kinetic energy. And also, it could still be of use to know the properties of the wave function solutions and energy eigenvalues of the Sucher equation to proceed to the expansion beyond it (inclusion of contributions ii), wherefrom a possible interest in studying the simpler but similar Herbst equation.

b) External field problem

The above discussion, which refers to the full treatment of QED, with all its radiative corrections, may seem a little pessimistic since it is well known that there exists physically interesting situations which can be described by a much simpler apparatus than Sucher or Bethe-Salpeter formalisms. Namely, simple and exact wave equations can be written for the external field problem⁶⁾. This situation amounts to have negligible loop radiative corrections, but to include crossed graphs. Of course, we are interested in the case where the external field is a Coulomb one. The corresponding situation is obtained if one particle has a charge Ze and one sets :

$$Z \rightarrow \infty \quad \text{and} \quad \epsilon \rightarrow 0 \quad , \quad Z\epsilon^2 = \text{constant} \quad , \quad m_1 \neq m_2 \quad , \quad m_1 \rightarrow \infty \quad . \quad (3)$$

Then, the problem is governed by :

α) the Klein-Gordon equation in the spinless case,

$$\left[-\Delta + m^2 - (E + Z\alpha/r)^2 \right] \psi = 0 \quad (4)$$

β) the Dirac equation in the spin 1/2 case,

$$\left(\vec{\alpha} \cdot \vec{p} + \beta m - \frac{Z\alpha}{r} \right) \psi = E\psi \quad . \quad (5)$$

These equations can be written in a form where the comparison with Herbst equation is particularly direct, e.g. for the K-G equation⁷⁾ :

$$Eu(p) = E_p u(p) + \int d_3 \vec{q} \phi(p-q) \left[\frac{E_p + E_q}{2(E_p - E_q)^{1/2}} u(q) + \frac{E_p - E_q}{2(E_p - E_q)^{1/2}} v(q) \right] \quad (6)$$

where $E_q = \sqrt{\vec{q}^2 + m^2}$ and $\phi(q)$ is the Fourier transform of the potential. One has two independent components in the wave function obeying coupled evolution equations, of which we have written only the first one. The large component u obeys something like the Herbst equation when ϕ is the Coulomb potential ; however the potential is

modified by a momentum dependent factor ~ 1 , and there is also a contribution from the small component v (of relative order v^2/c^2 with respect to u), which is multiplied by ϕ and by a factor $O(v^2/c^2)$. It can then be shown that the lowest order correction to the Schrödinger equation is the $O(v^4/c^4)$ kinetic energy correction $-p^4/8m^3$:

$$Eu = \frac{p^2}{2m} \left(1 - \frac{p^2}{4m^2} \right) u - \frac{Z\alpha}{r} u + O(v^6/c^6) \quad . \quad (7)$$

The Herbst equation is therefore correct in this approximation of order α^4 for the spinless particle in an external Coulomb field. On the contrary, in the fermion case, it deviates already from the correct equation, the Dirac equation (eq. 5), in the $O(\alpha^4)$ terms, i.e. already at the lowest order of relativistic effects, as seen from the Foldy-Wouthuysen expansion⁸⁾ :

$$E\varphi = \left[\frac{p^2}{2m} - \frac{p^4}{8m^3} - \frac{Z\alpha}{r} + \frac{1}{4m^2} \frac{Z\alpha}{r^3} \vec{\sigma} \cdot \vec{\ell} + \frac{\pi}{2m^2} Z\alpha \delta(\vec{r}) \right] \varphi + O(v^6/c^6) \quad (8)$$

where small components have already been eliminated.

c) Interest of Herbst equation

The relevance of Herbst equation can be appreciated in the light of the preceding discussion. Certainly, it is an approximate one, and it deviates from the exact result after very few orders, even in the external field problem. Nevertheless, it seems useful in various respects :

i) it allows to discuss the specific effects of including the relativistic kinetic energy term. The study of Herbst could then be of some help in preparing the discussion of the more complex Sucher equation, which is the starting point of a systematic perturbation theory of QED for bound states. The relativistic kinetic energy seems indeed to generate typical features distinguishing the wave function from the Schrödinger one, e.g. its short distance behavior. They can be discussed of course also through the K-G or Dirac equations, but Herbst equation has the advantage of being simpler and more canonical in certain respect than the former :

e.g. the kinetic energy operator is positive and the spectrum is bounded from below for sufficiently weak coupling, while the former equations have the negative-energy spectrum.

ii) it is the most straightforward quantization of the classical relativistic equation in an external field (Sommerfeld), and it is often taken as the representative of a quantum relativistic potential theory, considered per se, independently of a field theoretical derivation. This point of view is adopted by Goldberger and Watson⁹⁾. In fact, since it has the correct classical limit, it could be expected to give satisfactory results for large quantum numbers, and could be useful to take into account the kinematics of large external velocities, for instance in the scattering problem, and to handle correctly high level of excitations. It seems also useful for a qualitative discussion of systems of large numbers of relativistic particles, as encountered in astrophysics³⁾.

d) Interest of a perturbative expansion

As it has been emphasized that the correct QED solution is known only in a perturbative expansion in α , a perturbative expansion in α is also required for the equation under study in order to evaluate it by comparison to the former ; it will at the same time allow a direct comparison with other equations, in particular those quoted above : at lowest order, all the calculations converge towards the correct result given by the Schrödinger equation, but they differ after a few orders ; one could then check suggested inequalities between the respective spectra of the various wave-equations¹⁰⁾. The expansion of the kinetic energy correction could also be useful in other contexts where such corrections appear.

A series expansion of energy levels in high orders of α , as will be proposed in the third section, could be also used to test proposed analytical solutions as was done in¹¹⁾, or numerical methods of solution of the equation, and finally, if sufficiently convergent, to evaluate the result at moderate coupling or even near the critical coupling¹²⁾.

We will give first an elementary calculation based on the Rayleigh-Schrödinger perturbation method, which will give easily the first two non trivial orders, but which

becomes untractable for higher orders (section 2) ; then we present a method which allows to find very high orders, with non-analytic contributions (section 3). And finally, we will draw the conclusions from these calculations as regards the validity or degree of approximation of Herbst equation.

2. Perturbative expansion of the ground state energy in low orders in α . Wigner-Brillouin perturbation method for the Sommerfeld correction

It is tempting to use the Wigner-Brillouin (W-B) or Rayleigh-Schrödinger perturbation method around the known solutions of the Coulomb Schrödinger equation, the perturbation being the well-known "Sommerfeld" correction :

$$H' = 2 \left[\sqrt{p^2 + m^2} - m - p^2/2m \right] . \quad (9)$$

This perturbation is composed of infinitely many terms of various degree in α , commencing with α^4 , and one should gather the contributions of a given power in α , coming from the successive orders of the W-B expansion. This could in principle be done rather easily by expanding the Sommerfeld correction into powers of the momentum ; for the discrete spectrum matrix elements, one ends with integrals of powers of p^n times $(p^2 + \alpha^2)^{-4}$, which are proportional to α^m . The energy denominators could be easily handled since there one requires only the knowledge of energy with a lower accuracy.

But we encounter two limitations :

i) the Coulomb potential is singular at origin, so that the wave function decreases slowly at infinity in momentum space, and matrix elements of increasing power of p will soon diverge.

ii) it is not confining, therefore there is a continuum spectrum, which is found to contribute rather early. Calculations are easy when the free particle wave function approximates correctly the matrix element, but otherwise they become intricate.

We will proceed rather easily up to the calculation of the α^5 term, but beyond,

we shall have to recourse to a more powerful method, albeit very specific to the Coulomb potential.

At lowest order, the correction is trivial and well-known :

$$\Delta E = 2 \left\langle \sqrt{p^2 + m^2} - m - p^2/2m \right\rangle_{NR} \simeq \left\langle -\frac{2p^4}{8m^3} \right\rangle_{NR} . \quad (10)$$

We use the ground-state Coulomb wave function :

$$\varphi(p) = \frac{1}{2\pi} \frac{(m\alpha)^{5/2}}{\left[p^2 + \left(\frac{m\alpha}{2} \right)^2 \right]^2} \quad (11)$$

normalised through :

$$\int |\varphi(\vec{p})|^2 d_3\vec{p} = 1 . \quad (12)$$

The matrix element integral is convergent and trivial :

$$\Delta E = -\frac{5}{64} m\alpha^4 . \quad (13)$$

Next order is already much more complicated. Naïvely, since the next term in the expansion of $\sqrt{\vec{p}^2 + m^2}$ is $O(p^6)$, one would expects a α^6 contribution :

i) a contribution coming from the first order in the R-S expansion $\Delta E^{(1)}$:

$$\Delta E^{(1)} = \langle 0 | H' | 0 \rangle_{NR} \quad (14)$$

namely the non-relativistic average of the p^6 correction to the kinetic energy.

ii) a contribution coming from the second order in the W-B expansion $\Delta E^{(2)}$:

$$\Delta E^{(2)} = \sum_{n \neq 0} \frac{|\langle 0 | H' | n \rangle_{NR}|^2}{E_0 - E_n} \quad (15)$$

namely the one coming from the lowest order ($O(p^4)$) estimate of H' , the correction to the kinetic energy. In the discrete spectrum, the two matrix elements give $O(\alpha^8)$, to be divided by the $O(\alpha^2)$ energy denominator.

This naïve estimate immediately fails because the average of p^6 is not defined : the integral diverges linearly. It is therefore expected, as indeed found in the correct calculation, that the correction is really $O(\alpha^5)$ and not $O(\alpha^6)$. This problem is apparently present only in $\Delta E^{(1)}$ since in $\Delta E^{(2)}$ only the convergent p^4 matrix element is involved. But, as will be shown later, another divergence is present in the latter due to the sum over intermediate states.

Let us first concentrate on the calculation of $\Delta E^{(1)}$. To circumvent the divergence problem, we prevent from expanding $\sqrt{p^2 + m^2}$ and we write :

$$\begin{aligned} \left\langle 2\sqrt{p^2 + m^2} - \frac{\alpha}{r} \right\rangle_{NR} &\sim \left\langle p^2/m - \frac{\alpha}{r} \right\rangle_{NR} + \left\langle -p^4/4m^3 \right\rangle_{NR} \\ &+ 2 \left\langle \sqrt{p^2 + m^2} - m - p^2/2m + p^4/8m^3 \right\rangle_{NR} . \end{aligned} \quad (16)$$

The first two terms are exactly calculable and are respectively the α^2 and α^4 terms in the expansion. The last term can be easily estimated in its lowest order in α , α^5 , because we can now set :

$$\varphi(p) \sim \frac{1}{2\pi} \frac{(m\alpha)^{5/2}}{p^4} \quad (17)$$

factorize α^5 , and remain with an integral independent of α and converging at both ends. Apart from trivial factors, this integral is essentially ($u = p/m$) :

$$\int_0^\infty \frac{du}{u^6} \left(\sqrt{1+u^2} - 1 - u^2/2 + \frac{u^4}{8} \right) = \frac{2}{15} \quad (18)$$

whence :

$$\Delta E^{(1)} = -\frac{5m}{64}\alpha^4 + \frac{4m}{15\pi}\alpha^5 . \quad (19)$$

At this point it must be recalled that Martin and Roy have already shown that the correction is of order 5¹³).

Let us now pass to the $\Delta E^{(2)}$ contribution. As noticed before, the discrete spectrum intermediate state contribution is correctly expected to be $O(\alpha^6)$ and is therefore negligible with respect to the above contribution. But we must also consider the continuum contribution. Although p^4 still converges with one continuous spectrum wave function, we have to perform an other integral corresponding to the sum over intermediate states and the latter would once more diverge linearly. We then retain once more the Sommerfeld correction under its original unexpanded form and calculate the lowest order approximation to :

$$\Delta E_{cont}^{(2)} = -4 \int \frac{d_3 k}{E_k - E_0} \left| \left\langle \varphi_k \left| \sqrt{p^2 + m^2} - m - \frac{p^2}{2m} \right| \varphi_0 \right\rangle \right|^2 \quad (20)$$

where k is labelling the continuum wave functions. We can approximate φ_k as $\delta^3(p-k)$. Indeed, in the Born series, next orders will yield higher powers in α . The matrix element is then trivially evaluated :

$$\Delta E_{cont}^{(2)} = -4 \frac{1}{4\pi^2} (m\alpha)^5 \int \frac{d_3 \vec{k}}{E_k - E_0} \times \frac{1}{\left[k^2 + \left(\frac{m\alpha}{2} \right)^2 \right]^4} \times \left(\sqrt{k^2 + m^2} - m - k^2/2m \right)^2 \quad (21)$$

To evaluate the new integral at order α^5 , we can set $\alpha = 0$ in the integrand, since the resulting integral independent of α converges at both ends. One is then reduced to the calculation of ($v = k/m$) :

$$\int_0^\infty dv \frac{\left(\sqrt{1+v^2} - 1 - v^2/2 \right)^2}{v^8} = \frac{1}{32} \frac{31}{70} \quad (22)$$

Finally :

$$\Delta E_{cont}^{(2)} = -\frac{1}{8} \frac{31}{70} \frac{1}{\pi} m\alpha^5 \quad (23)$$

Being convinced by the two preceding calculations that the naïve power counting in α is easily misleading, we investigate carefully the higher orders in the W-B expansion $\Delta E^{(n)}$, and discover that all these orders will contain an α^5 contribution. It is coming from the case where the $n - 1$ sums over intermediate states are being done over the continuous spectrum. Since $n - 2$ among these sums over the continuous spectrum can be done trivially by using once more the plane wave approximation, it can be expressed again as a single integral :

$$\Delta E_{cont}^{(n+1)} \sim 4 \int \frac{d_3 \vec{k}}{E_k} \frac{\left(\sqrt{k^2 + m^2} - m - k^2/2m \right)^2}{k^8} \times (-1)^{n+1} \left(\frac{\sqrt{k^2 + m^2} - m - k^2/2m}{k^2/2m} \right)^n \quad (24)$$

where one has made again $\alpha = 0$ in the integrand. The sum :

$$\sum_0^\infty \Delta E_{cont}^{n+1} \quad (25)$$

can be done easily since the integrand corresponds to a geometric series, and we end with the elementary integral :

$$\int_0^\infty dv \frac{\left[\sqrt{1+v^2} - 1 - v^2/2 \right]^2}{v^8} \frac{v^2/2}{\sqrt{1+v^2} - 1} = \frac{1}{40} \quad . \quad (26)$$

Finally :

$$\Delta E_{cont} = -\frac{1}{10\pi} m \alpha^5 \quad (27)$$

and adding all the α^5 contributions

$$\Delta E = -\frac{5}{64} m \alpha^4 + \frac{1}{6\pi} m \alpha^5 \quad . \quad (28)$$

Terms with at least one sum over the discrete spectrum give a higher power. The same conclusion is checked to be true for subleading terms in the Born series of

continuum wave functions. The whole calculation is checked by the coincidence with the result of the second method.

From the results obtained, we find a difficulty in the expression proposed by authors of ¹¹⁾. The α^4 term is already different. Moreover, their expression does not satisfy the inequality :

$$E < E_0 \quad (29)$$

deduced from the operator inequality :

$$\sqrt{p^2 + m^2} < m + p^2/2m \quad (30)$$

3. Expansion in α of the $L = 0$ Eigenvalues. A new method

In this section, we obtain the expansion at small coupling constant α of the eigenvalues of the Hamiltonian

$$H = 2\sqrt{p^2 + m^2} - \frac{\alpha}{r}$$

for the $L = 0$ states, with arbitrary excitation number n , up to order α^7 included. The result is :

$$\begin{aligned} \frac{E}{2m} = & 1 - \frac{\alpha^2}{8n^2} - \frac{\alpha^4}{16n^3} \left(1 - \frac{3}{8n}\right) + \frac{\alpha^5}{12\pi n^3} \\ & - \frac{\alpha^6}{64n^3} \left\{ \frac{29}{12} + \frac{2}{\pi^2} + \frac{1}{2\pi^2} \psi''(1/2) + \log(n) - \sum_{q=1}^n \frac{1}{q} + \frac{2}{n} - \frac{5}{3n^2} + \frac{5}{16n^3} - \log\left(\frac{\alpha}{2}\right) \right\} \\ & + \frac{\alpha^7}{24\pi n^3} \left\{ \frac{307}{180} + \frac{1}{6\pi^2} + \frac{1}{4\pi^2} \psi''(1/2) + \frac{1}{8} \psi''(1/2) - \frac{1}{64\pi^2} \psi^{(4)}(1/2) \right. \\ & \left. + \log(n) - \sum_{q=1}^n \frac{1}{q} + \frac{2}{n} - \frac{11}{12n^2} - \log\left(\frac{\alpha}{2}\right) \right\} \\ & + O(\alpha^{8-\epsilon}) \end{aligned}$$

(higher powers of $\log(\alpha)$ may appear at higher orders).

We present here the main points, leaving the detailed calculations for a separate publication. In subsection 1 we derive an equation for a function related to the eigenfunction, and show how it can be used to obtain a systematic expansion by iteration. The expansion at orders 0 to 3 is done. This gives the energy up to α^5 only, as in the preceding section, in a rather complicated but systematic and safe way. Moreover, we are able to show that using analyticity properties of the wave function, one can obtain two more orders with only a little of additional calculation, which could not be obtained easily by the other method (subsection 2).

The method has the merit of being systematic, and the iteration procedure can be settled on a reasonably rigorous basis, but it is not general. Its starting point is a peculiar representation of Hilbert space of $L = 0$ states in which the Coulomb potential operator has a particularly simple form. This peculiarity was used in⁽¹¹⁾, in a trial to obtain an exact solution. Although the solution proposed by these authors turns out to be incorrect, as noticed before, we show here that this peculiarity allows at least to obtain a systematic expansion.

3.1 - Method of expansion. Energy and wave functions to order α^5

We will submit the Herbst equation to a set of successive transformations in order to get a form suitable for solution by iteration, each step giving a further term in the expansion in α of the eigenstates and associated eigenvalues. We are considering the following Hamiltonian.

$$H = 2T - \alpha V \quad , \quad T = \sqrt{p^2 + m^2} \quad , \quad V = \frac{1}{r} \quad . \quad (31)$$

The kinetic operator T and the potential operator V are defined respectively in the momentum and in the configuration representation :

$$(T\Psi)(\vec{p}) = \sqrt{\vec{p}^2 + m^2} \Psi(\vec{p}) \quad (32)$$

$$(V\Psi)(\vec{r}) = \frac{1}{|\vec{r}|} \Psi(\vec{r}) \quad . \quad (33)$$

These two standard representations of the Hilbert space of state vectors are linked by Fourier transformation, and any operator defined in one representation can be translated into the other one. For the $L = 0$ states we are considering, the three dimensional Fourier transformation reduced to the spaces $L^2([0, \infty], 4\pi r^2 dr)$ and $L^2([0, \infty], 4\pi p^2 dp)$ of the radial functions, writes :

$$\Psi(p) = \sqrt{\frac{2}{\pi}} \frac{1}{p} \int_0^\infty r dr \sin(pr) \Psi(r) \quad , \quad \Psi(r) = \sqrt{\frac{2}{\pi}} \frac{1}{r} \int_0^\infty p dp \sin(pr) \Psi(p) \quad . \quad (34)$$

The translation of V into the momentum representation is an integral operator :

$$(V\Psi)(p) = \frac{1}{\pi} \int_0^\infty dp' \frac{p'}{p} \log \frac{p+p'}{|p-p'|} \Psi(p') \quad . \quad (35)$$

Then, we consider a third representation, that we may call the analytic p -representation, linked to the configuration representation by :

$$\varphi(p) = \sqrt{2} \int_0^\infty dr \, e^{ipr} r \, \Psi(r) \quad , \quad \frac{1}{2\pi} \int_{-\infty}^\infty dp \, e^{-ipr} \varphi(p) = \sqrt{2} \, \theta(r) \, r \Psi(r) \quad . \quad (36)$$

The Hilbert space of this representation is the closed subspace $P_+ L^2(\mathbf{R}, dp)$ of $L^2(\mathbf{R}, dp)$ made up with the functions which are limit on the real axis of analytic functions in the upper complex plane. The orthogonal projector P_+ on this subspace is given by :

$$(P_+ \varphi)(p) = \frac{1}{2i\pi} \int_{-\infty}^\infty dp' \cdot \frac{\varphi(p')}{p' - p - i0} \quad . \quad (37)$$

By Fourier transformation, P_+ is just the orthogonal projection $\varphi(r) \rightarrow \theta(r) \varphi(r)$ of $L^2(\mathbf{R}, dr)$ onto its subspace $L^2([0, \infty], dr)$. Then, (36) defines a unitary transformation $\Psi \rightarrow \varphi$ from $L^2([0, \infty], 4\pi r^2 dr)$ to $P_+ L^2(\mathbf{R}, dp)$.

The interest of this analytic p -representation is that V becomes a simple integration operator :

$$(V\varphi)(p) = i \int_{-\infty}^p dp' \varphi(p') \quad . \quad (38)$$

Indeed, V^{-1} is just multiplication by r in the configuration representation, and becomes a derivation operator after a one-dimensional Fourier transformation like (36). By contrast, one sees that (34) is not just a one dimensional Fourier transformation, and this explains the more complicated expression (35) of V in p -representation. One may also consider (34) as ordinary one dimensional Fourier transformation between the functions $r \Psi(r)$ and $p \Psi(p)$ extended as odd functions to the whole real axis, but then V^{-1} is multiplication by $|r|$, not by r .

The potential energy V is now simple, but the kinetic energy T is complicated. It cannot be the multiplication by $\sqrt{p^2 + m^2}$ because this function of p is not analytic in the upper plane. Indeed T is given by :

$$(T\varphi)(p) = \sqrt{p^2 + m^2} \varphi(p) - \frac{i}{\pi} \int_{-\infty}^{\infty} dp' \frac{p'}{\sqrt{p'^2 + m^2} + \sqrt{p^2 + m^2}} \varphi(p') \quad . \quad (39)$$

Combining (38) and (39), the form of the Hamiltonian (31) in the analytic p -representation is then :

$$(H\varphi)(p) = 2\sqrt{p^2 + m^2} \varphi(p) - \frac{2i}{\pi} \int_{-\infty}^{\infty} dp' \frac{p'}{\sqrt{p'^2 + m^2} + \sqrt{p^2 + m^2}} \varphi(p') - i\alpha \int_{-\infty}^p dp' \varphi(p') \quad . \quad (40)$$

Finally, we will use a fourth representation, simply linked to the previous one by a simple change of variable :

$$p = \mathbf{p}(x) = m \frac{2x}{1 - x^2} \quad , \quad x = \mathbf{x}(p) = \frac{p}{m + \sqrt{p^2 + m^2}} \quad , \quad (41)$$

The function $p \rightarrow \mathbf{x}(p)$ is a bijection of the real axis on the interval $] -1, 1[$, and the functions in the new representation will be defined in this interval. Precisely, we take the following transformation for the functions :

$$\Psi(x) = \frac{\sqrt{2m}}{1-x^2} \varphi(\mathbf{p}(x)) , \quad \varphi(p) = \frac{\sqrt{2m}}{m + \sqrt{p^2 + m^2}} \Psi(\mathbf{x}(p)) \quad (42)$$

where the factor in front of $\varphi(\mathbf{p}(x))$ is for convenience. We have

$$\int_{-\infty}^{+\infty} dp |\varphi(p)|^2 = \int_{-1}^{+1} dx (1+x^2) |\Psi(x)|^2 ,$$

so that (42) is a unitary transformation between $L^2(\mathbf{R}, dp)$ and $L^2([-1, 1], (1+x^2)dx)$.

The new form of the potential and kinetic operators are obtained from (38) and (39) using (42) :

$$(V\Psi)(x) = 2im \frac{1}{1-x^2} \int_{-1}^x dx' \frac{1+x'^2}{1-x'^2} \Psi(x') \quad (43)$$

$$(T\Psi)(x) = m \frac{1+x^2}{1-x^2} \Psi(x) - m \frac{i}{\pi} \int_{-1}^1 dx' \frac{2x'}{1-x^2 x'^2} \frac{1+x'^2}{1-x'^2} \Psi(x') . \quad (44)$$

The eigen-equation $H\Psi = E\Psi$ then writes :

$$\begin{aligned} \frac{1+x^2}{1-x^2} \Psi(x) - \frac{i}{\pi} \int_{-1}^1 dx' \frac{2x'}{1-x^2 x'^2} \frac{1+x'^2}{1-x'^2} \Psi(x') - \frac{i\alpha}{1-x^2} \int_{-1}^x dx' \frac{1+x'^2}{1-x'^2} \Psi(x') \\ = \frac{E}{2m} \Psi(x) . \end{aligned} \quad (45)$$

The next step is to solve equation (45) for Ψ assuming that the second term in the l.h.s. of (45) is given. The heuristic motivation of doing this is the following : $\Psi(x)$ is rapidly varying near $x = 0$ when α is small, as seen in the expression of the Coulombic wave function,

$$\Psi(x) = -\frac{4}{\sqrt{\pi}} \left(\frac{\alpha}{2} \right)^{\frac{3}{2}} \frac{1-x^2}{\left[2x + i\frac{\alpha}{2}(1-x^2) \right]^2} \quad (46)$$

which corresponds to the standard configuration space wave function :

$$\Psi(x) = \frac{1}{\sqrt{\pi}} \left(\frac{m\alpha}{2} \right)^{\frac{3}{2}} \exp\left(-\frac{m\alpha r}{2}\right) .$$

But this rapid variation is not reflected in the second term where $\Psi(x)$ is smoothed out. Therefore, if we express $\Psi(x)$ in term of this smooth second term, the rapid variation of $\Psi(x)$, which complicates the problem of an expansion at $\alpha = 0$, will be entirely contained in known functions. To proceed, multiply eq. (45) by $1 - x^2$ and take the derivative with respect to x . One obtains :

$$\frac{d\Psi(x)}{dx} + \frac{2x}{\tau^2 + x^2} \Psi(x) - \frac{i\alpha}{2} \frac{1 + \tau^2}{\tau^2 + x^2} \frac{1 + x^2}{1 - x^2} \Psi(x) = \frac{-i}{4\pi} \frac{1 + \tau^2}{\tau^2 + x^2} (K\Psi)(x) \quad (47)$$

$$\begin{aligned} (K\Psi)(x) &= \int_{-1}^1 dx' K(x, x') \Psi(x') \quad , \\ K(x, x') &= -\frac{d}{dx} \frac{1 + x'^2}{1 - x'^2} \frac{4x'(1 - x^2)}{1 - x^2 x'^2} = 8xx' \frac{1 + x'^2}{(1 - x^2 x'^2)^2} \end{aligned} \quad (48)$$

where we have introduced a parameter τ linked with the eigenvalue E :

$$\cos \theta = \frac{E}{2m} = \frac{1 - \tau^2}{1 + \tau^2} \quad \tau = \operatorname{tg}(\theta/2) = \sqrt{\frac{2m - E}{2m + E}} . \quad (49)$$

Next we introduce the function $\chi(x)$ defined by the following differential equation and initial condition

$$\frac{d\chi(x)}{dx} = i\frac{\alpha}{2} \frac{1 + x^2}{1 - x^2} \frac{1 + \tau^2}{\tau^2 + x^2} \chi(x) , \quad \chi(0) = 1 \quad . \quad (50)$$

Using $\chi(x)$, equation (47) writes :

$$\frac{d}{dx} (\tau^2 + x^2) \chi(x)^{-1} \Psi(x) = -\frac{i}{4\pi} (1 + \tau^2) \chi(x)^{-1} (K\Psi)(x)$$

and integrating we obtain the seeked expression of Ψ in term of the smooth function $K\Psi$:

$$\Psi(x) = \tau^2 \frac{\chi(x)}{\tau^2 + x^2} \Psi(0) - \frac{i}{4\pi} (1 + \tau^2) \frac{\chi(x)}{\tau^2 + x^2} \int_0^x dx' \chi(x')^{-1} (K\Psi)(x') \quad . \quad (51)$$

The solution $\chi(x)$ of (50) is obtained using the decomposition

$$i\frac{\alpha}{2} \frac{1+x^2}{1-x^2} \frac{1+\tau^2}{\tau^2+x^2} = i\frac{\alpha}{2} \left(\frac{1}{1+x} + \frac{1}{1-x} \right) - \eta \left(\frac{1}{i\tau+x} + \frac{1}{i\tau-x} \right) \quad .$$

It is

$$\chi(x) = \left(\frac{1+x}{1-x} \right)^{i\alpha/2} \left(\frac{i\tau-x}{i\tau+x} \right)^\eta \quad (52)$$

where we have introduced a parameter η linked to α and E by :

$$\eta = \frac{\alpha}{2} \frac{1-\tau^2}{2\tau} = \frac{\alpha}{2(tg \theta)} \quad . \quad (53)$$

Then in (51), the rapid variation of Ψ near $x = 0$ is entirely due to the known functions $(\tau^2 + x^2)^{-1}$ and $\chi(x)$ (note that τ is of order α).

The energy E is related to η and α by :

$$\frac{E}{2m} = \frac{1}{\sqrt{1 + \frac{\alpha^2}{4\eta^2}}} \quad . \quad (54)$$

Notice that the function $\chi(x)$ has a branch point at $x = i\tau$ in the upper plane, except when η is integer. It is then tempting to think that the absence of this branch point in (51) forces η to be an integer, and equation (54) then gives the result of ¹⁾ (obtained there by more sophisticated arguments). However, this is not supported in closer inspection. We will see that η is integer only at zeroth order in α . Furthermore in subsection 2 we will obtain the condition between $K\Psi$, η and α ensuring the absence of the branch point $x = i\tau$ in (51).

Let us now take a closer look at the problem of expanding eq. (51) in α . There is the immediate difficulty that the terms in an expansion $\Psi = \Psi^{(0)} + \Psi^{(1)} + \dots$ of Ψ

are likely to be more and more singular at $x = 0$, and the integrals $K\Psi^{(p)}$ will soon become meaningless. A way out of this difficulty would be to expand Ψ in the sense of distributions, which means finding the expansion of the integral $\int \Psi(x) f(x) dx$ for any function $f(x)$ smooth at least near $x = 0$. The distribution $\Psi^{(p)}$ then keeps more information on what happens at $x = 0$ than the function defined only for $x \neq 0$, and notably $K\Psi^{(p)}$ is defined because the kernel $K(x, x')$ is smooth near $x' = 0$. But this leads us to a simpler way out, namely, derive from (51) an equation for $K\Psi$ and expand $K\Psi$.

The kernel K is such that, for any distribution φ supported in $[-1, 1]$, $(K\varphi)(x)$ is defined and smooth for $|x| < 1$. In fact $K\varphi$ is analytic with the cuts $] -\infty, -1]$ and $[1, \infty[$. Then each term $K\Psi^{(p)}$ in the expansion of $K\Psi$ is expected to have these properties.

The equation for $K\Psi$ is obtained simply by multiplying eq. (51) by K and integrating :

$$(K\Psi)(x) = \Psi(0) \tau^2 \int_{-1}^1 dx' K(x, x') \frac{\chi(x')}{\tau^2 + x'^2} - \frac{i}{4\pi} (1 + \tau^2) \int_{-1}^1 dx' K(x, x') \frac{\chi(x')}{\tau^2 + x'^2} \int_0^{x'} dx'' \chi(x'')^{-1} (K\Psi)(x'') \quad . \quad (55)$$

This will be our basic equation to be expanded. One can show that, if we insert some order $K\Psi^{(p)} = O(\alpha^{p-\varepsilon})$ in the right hand side, the double integral is $O(\alpha^{p+1-\varepsilon})$, so that the equation can indeed be used to find iteratively the expansion of $K\Psi$. The progress obtained by considering $K\Psi$ instead of directly handling the wave function Ψ can be evaluated by comparing the Coulombic expression for Ψ (46) and the one for the limit of $K\Psi$ when α goes to zero, $K\Psi^{(0)}$ which is written in equation (64) and which is seen to be quite regular. However, given $K\Psi^{(0)} \dots, K\Psi^{(p-1)}$, the obtained $K\Psi^{(p)}$ is usually still too singular at $x \rightarrow \pm 1$ for the convergence of the double integral, and the iteration stops. But this is in fact welcome because there must be some condition to determine the expansion of the energy eigenvalue E . Then along expanding $K\Psi$, we must expand the parameters in (55) $\tau = \tau^{(1)} + \tau^{(2)} + \dots$, $\eta = \eta^{(0)} + \eta^{(1)} + \dots$, and determine these other expansions at each order by the condition of absence of too singular terms in $K\Psi^{(p)}$.

Actually we shall follow a more convenient procedure which consists in finding the values of $\tau^{(p)}$ and $\eta^{(p)}$ beforehand, and then computing $K\psi^{(p)}$ with these values. We obtain conditions possibly able to fix $\tau^{(p)}$ and $\eta^{(p)}$ from the property that $\Psi(x) \rightarrow 0$ when $x \rightarrow \pm 1$. Multiplying eq. (51) by $(\tau^2 + x^2) \chi(x)^{-1}$ and taking the limits $x \rightarrow \pm 1$, we find that $K\Psi$ must satisfy the two following conditions :

$$\frac{i}{4\pi} \int_0^{\pm 1} dx \chi(x)^{-1} (K\Psi)(x) = \frac{\tau^2}{\tau^2 + 1} \Psi(0) \quad . \quad (56)$$

Then we shall expand the conditions (56) along with eq. (55). At least up to the last order $p = 3$ we consider, it turns out that (56) gives two things, a relation between $\tau^{(p)}$ and $\eta^{(p)}$, and an integral relation to be satisfied by $K\Psi^{(p)}$. Then the part of $K\Psi^{(p)}$ proportional to $\alpha^p \log(\alpha)$ is obtained from (51), and the integral relation for this part completely fixes $\tau^{(p)}$ and $\eta^{(p)}$. Then the part of $K\Psi^{(p)}$ proportional to α^p is obtained from (51), and the integral relation for this part provides a non-trivial test of the calculation.

Curiously, in this procedure, everything is fixed though we are treating τ and η as independent functions of α in (52), (55) and (56). The fact that the obtained expansions of τ and η are in agreement with $\eta = \frac{\alpha}{2} \frac{1-\tau^2}{2\tau}$ is again a test of the calculation.

Also it may be noted that, in this first stage, no use is made of the analyticity property of Ψ .

Let us now turn to the actual expansion of (55) and (56). There is still a difficulty in the expansion on τ , because $\chi(x)$ gives rise to inverse powers of x and meaningless integrals. The main problem is the expansion of integrals of the following kind

$$A(F, f, t) = \int_{-\infty}^{\infty} dy F(y/\tau) f(y) \quad (57)$$

$$B(F, f, G, g, \tau) = \int_{-\infty}^{\infty} dy F(y/\tau) f(y) \int_0^y dy' G(y'/\tau) g(y') \quad (58)$$

where f and g are functions regular at $y = 0$ and F and G are functions regular at $y = \infty$ and at $y = -\infty$.

With these notations A and B , the equation (55) and the supplementary conditions (56) write (from now on we take the normalisation $\Psi(0) \tau^2 = 1$) :

$$(K\Psi)(x) = \frac{1}{\tau^2} A(\Phi F(\eta), h(\alpha)K(x), \tau) \quad (59)$$

$$-\frac{i}{4\pi} \frac{1+\tau^2}{\tau^2} B(F(\eta), h(\alpha)K(x), G(\eta), h(-\alpha)K\Psi, \tau) \\ \frac{i}{4\pi} A(\Phi^{-1}G_{\pm}(\eta), h(-\alpha)K\Psi, \tau) = \pm \frac{1}{\tau^2 + 1} \quad (60)$$

with

$$F(\eta, y) = \frac{1}{1+y^2} \left(\frac{y-i}{y+i} \right)^\eta, \quad (61) \\ \Phi(\eta, y) = e^{i\pi\eta sg(y)} \\ G(\eta, y) = \left(\frac{y-i}{y+i} \right)^{-\eta}, \quad G_{\pm}(\eta, y) = \theta(\pm y) G(\eta, y) \\ h(\alpha, y) = \left(\frac{1+y}{1-y} \right)^{i\alpha/2} \theta(1-|y|) \\ K(x, y) = 8xy \frac{1+y^2}{(1-x^2y^2)^2} \theta(1-|y|) \theta(1-|x|)$$

also $K\Psi(y)$ is understood to be 0 for $|y| > 1$.

One can find the series expansions of A and B in a general form. One can prove that, for f analytic at 0 and F analytic at $\pm\infty$, there is a convergent series :

$$A(F, f, \tau) = \sum_n \tau^n A_n(F, f, \tau), \quad A_n(\tau) = A_{n,0} + A_{n,1} \log(\tau) \quad .$$

Let us write respectively as $f_p(y)$ and $F_p(y)$ the terms in the expansions

$$f(y) = \sum_{p=0}^{\infty} f_p(y), \quad F(y) = \sum_{p=0}^{\infty} F_p(y)$$

of f in powers of y and of F in powers of y^{-1} . Then the coefficients $A_{n,0}(F, f)$ and $A_{n,1}(F, f)$ are given by :

$$\begin{aligned}
A_{n,0}(F, f) &= \int_{-\infty}^{\infty} dy \left[F(y) - \sum_{p < n} F_p(y) - \theta(|y| - 1) F_n(y) \right] f_{n-1}(y) \\
&+ \int_{-\infty}^{\infty} dy F_n(y) \left[f(y) - \sum_{p < n} f_{p-1}(y) - \theta(1 - |y|) f_{n-1}(y) \right] \\
A_{n,1}(F, f) &= -(F_{n,+} - F_{n,-}) f_{n-1}
\end{aligned} \tag{62}$$

with $F_{n,\pm}$ defined by $F_n(y) = F_{n,\pm} y^{-n}$ ($y \gtrless 0$).

We have also a convergent series for B :

$$B(F, f, G, g, \tau) = \sum_n \tau^n B_n(F, f, G, g, \tau), \quad B_n(\tau) = B_{n,0} + B_{n,1} \log(\tau)$$

with more complicated coefficients ! Let us define analogously :

$$g(y) = \sum_{p=0}^{\infty} g_p(y) \quad , \quad G(y) = \sum_{p=0}^{\infty} G_p(y) \quad .$$

Then :

$$\begin{aligned}
B_{n,0}(F, f, G, g) &= \sum_{p+q=n} \left\{ \int_{-\infty}^{\infty} dy \int_0^y dy' f_{p-1}(y) g_{q-1}(y') \left\{ \left[F(y) - \sum_{r \leq p} F_r(y) \right] G(y') \right. \right. \\
&\quad \left. \left. - \sum_{r > p} F_r(y) \left[\sum_{s < n-r} G_s(y') + \theta(|y'| - 1) G_{n-r}(y') \right] \right\} \right. \\
&\quad \left. + \int_{-\infty}^{\infty} dy \int_0^y dy' \left\{ f(y) \left[g(y') - \sum_{s \leq q} g_{s-1}(y') \right] \right. \right. \\
&\quad \left. \left. - \sum_{s > q} g_{s-1}(y') \left[\sum_{r < n-s} f_{r-1}(y) + \theta(1 - |y'|) f_{n-s-1}(y) \right] \right\} F_p(y) G_q(y') \right. \\
&\quad \left. - \sum_{r < p} \int_{-\infty}^{\infty} dy \int_y^{sg(y)\infty} dy' f_{p-1}(y) g_{q-1}(y') F_r(y) \left[G(y') - \sum_{s < n-r} G_s(y') - \theta(|y'| - 1) G_{n-r}(y') \right] \right. \\
&\quad \left. - \sum_{s < q} \int_{-\infty}^{\infty} dy \int_y^{sg(y)\infty} dy' g_{s-1}(y') \left[f(y) - \sum_{r < n-s} f_{r-1}(y) - \theta(1 - |y'|) f_{n-s-1}(y) \right] F_p(y) G_q(y') \right. \\
&\quad \left. + \int_{-\infty}^{\infty} dy \int_0^{sg(y)\infty} dy' \left[f(y) - \sum_{r < p} f_{r-1}(y) - \theta(|y'| - |y|) f_{p-1}(y) \right] F_p(y) g_{q-1}(y') \right\}
\end{aligned} \tag{63}$$

$$\left[G(y') - \sum_{s < q} G_s(y') - \theta(|y'| - |y|) G_q(y') \right] \Bigg\}$$

$$B_{n,1}(F, f, G, g) = - \sum_{p+q=n} \left\{ f_{p-1} F_p \int_{-\infty}^{\infty} dy \, g_{q-1}(y) \left[G(y) - \sum_{s < q} G_s(y) - \theta(|y| - 1) G_q(y) \right] \right. \\ \left. + g_{q-1} G_q \int_{-\infty}^{\infty} dy \left[f(y) - \sum_{r < p} f_{r-1}(y) - \theta(1 - |y|) f_{p-1}(y) \right] F_p(y) \right\} .$$

Contrary to $A(F, f, \tau)$, these formulae for $B(F, f, G, g, \tau)$ assume F and G analytic at ∞ (with the same expansion at $+\infty$ and $-\infty$). In the general case, $\log^2(\tau)$ terms appear.

With (62), (63), (59), (60) and (61), we have now all the ingredients for the expansion.

We can verify that the double integral in (55) produces the next order in α from a given order of $K\Psi$. This means that $B_2(F(\eta), \eta(\alpha)K(x), G(\eta), h(-\alpha)K\Psi, \tau)$ vanishes with α . Indeed for $\alpha = 0$, it is given by

$$B_2(F(\eta), K(x), G(\eta), K\Psi, \tau) = \int_{-\infty}^{\infty} dy \, y^{-2} K(x, y) \int_0^y dy' K\Psi(y') = 0 .$$

The vanishing is due to the fact that $K(x, y)$ and $K\Psi(y)$ are odd functions of y .

The notations for the expansion coefficients will be

$$\eta = \eta^{(0)} + \eta^{(1)} + \dots , \quad \tau = \tau^{(1)} + \tau^{(2)} + \dots$$

$$K\Psi = (K\Psi)^{(0)} + (K\Psi)^{(1)} + \dots$$

where $\eta^{(q)}$, $\tau^{(q)}$, $(K\Psi)^{(q)}$ are proportional to α^q up to logarithms. After some calculations, the following results are obtained.

At order 0, we find :

$$\eta^{(0)} = n \geq 1 , (K\Psi)^{(0)}(x) = -8 i \pi (-1)^n x \theta(1 - |x|) . \quad (64)$$

At order 1, we have :

$$\eta^{(1)} = 0 \quad , \quad \tau^{(1)} = \frac{\alpha}{4n} \quad , \quad (65)$$

$$\int_0^x dx' (K\Psi)^{(1)}(x') = 4 i \alpha (-1)^n (1-x^2) \left(\frac{1+x^2}{2x} \log \frac{1+x}{1-x} - 1 \right) \quad .$$

At order 2, we have :

$$\eta^{(2)} = -\frac{\alpha^2}{4} \quad , \quad \tau^{(2)} = 0 \quad (66)$$

$$\begin{aligned} (-1)^n \int_0^x dx' (K\Psi)^{(2)}(x') &= i \frac{1}{\pi} \alpha^2 (1+x^2) \int_{-1}^1 dy \log(1-x^2 y^2) \frac{1}{y} \log \frac{1+y}{1-y} \\ &+ i \frac{1}{\pi} \alpha^2 (1-x^2) \left(\frac{(1+x^2)^2}{4x^2} \log^2 \frac{1+x}{1-x} - \frac{1+x^2}{x} \log \frac{1+x}{1-x} + 1 \right) - i \pi \frac{\alpha^2}{4n^2} (n^2+1) (1-x^2) x^2 \\ &+ \left\{ i \pi \frac{\alpha^2}{4n^2} [Z(n)+1] - i \frac{1}{\pi} \frac{\alpha^2}{2} \Psi''(1/2) + i \pi \alpha^2 \log \left(\frac{\alpha}{4n} \right) \right\} x^2 \quad . \end{aligned}$$

We have introduced a notation $Z(n)$ for a quantity that will appear several times :

$$Z(n) = -6n^2 - (2n-1) [1 - (-1)^n] + 4n^2 \sum_{q=1}^n \frac{1 - (-1)^q}{q} \quad . \quad (67)$$

At order 3, the calculations become very lengthy, but we are still able to obtain :

$$\eta^{(3)} = \frac{\alpha^3}{3\pi} \quad , \quad \tau^{(3)} = \frac{\alpha^3}{16n^2} - \frac{\alpha^3}{64n^3} \quad , \quad (68)$$

which gives the energy to order α^5 (see below) and the corresponding term of the expansion of $(-1)^n \int_0^x dx' (K\Psi)(x')$, which will be used in the next subsection to obtain further terms in the expansion of η and τ in a rather economical way :

$$\begin{aligned} (-1)^n \int_0^x dx' (K\psi)^{(3)}(x') &= \\ &-i \frac{1}{\pi^2} \frac{\alpha^3}{2} (1+x^2) x^2 \int_{-1}^1 dy \int_y^{sg(y)} dy' \frac{y}{1-x^2 y^2} \frac{(1+y'^2)^2}{1-y'^2} \times \end{aligned}$$

$$\begin{aligned}
& \times \int_{-1}^1 dy'' \left[y'^{-2} \log(1 - y'^2 y''^2) - \log(1 - y''^2) \right] \frac{1}{y''} \log \frac{1 + y''}{1 - y''} \\
& + i \frac{1}{\pi^2} \frac{\alpha^3}{3} (1 + x^2) \int_{-1}^1 dy' \log(1 - x^2 y'^2) \log \frac{1 + y'}{1 - y'} y'^{-1} \\
& + i \frac{\alpha^3}{2} (1 + x^2) \int_{-1}^1 dy \frac{\log(|y|)}{1 - y^2} \log(1 - x^2 y^2) - i \frac{\alpha^3}{2} x^2 (1 + x^2) \int_{-1}^1 dy \frac{\log(|y|)}{1 - x^2 y^2} \\
& - i \frac{1}{\pi^2} \frac{\alpha^3}{24} \Psi^{(4)}(1/2) x^2 \\
& - i \frac{1}{\pi^2} \frac{\alpha^3}{6} \Psi''(1/2) \left[(1 + x^2) \log(1 - x^2) + \frac{1 + 3x^2}{2x^2} \left(\frac{1 + x^2}{2x} \log \frac{1 + x}{1 - x} - 1 \right) - \frac{2}{3} - \frac{20}{3} x^2 - 2\pi^2 x^2 \right] \\
& - i \frac{\alpha^3}{4n^2} \left[Z(n) + 4n^2 \log\left(\frac{\alpha}{4n}\right) \right] \left[(1 - x^2) \left(\frac{1 + x^2}{2x} \log \frac{1 + x}{1 - x} - 1 \right) + \frac{4x^2}{3} \right] \\
& + i \frac{1}{\pi^2} \frac{\alpha^3}{6} (1 - x^2) \left[\frac{1 + 10x^2 + x^4}{4x^2} \frac{1 + x^2}{3x} \log^3 \frac{1 + x}{1 - x} - \frac{(1 + x^2)^2}{2x^2} \log^2 \frac{1 + x}{1 - x} + \frac{1 + x^2}{x} \log \frac{1 + x}{1 - x} - \frac{2}{3} \right] \\
& - i \frac{\alpha^3}{12n^2} (1 - x^2) \left[\frac{1 + x^2 + 4x^4}{x^2} \left(\frac{1 + x^2}{2x} \log \frac{1 + x}{1 - x} - 1 \right) - \frac{4}{3} \right] \\
& - i \frac{\alpha^3}{3} \left[(1 + x^2) \log(1 - x^2) + \frac{1 + x^2}{x} \log \frac{1 + x}{1 - x} - 2 \right] \\
& - i \frac{\alpha^3}{9} (1 - x^2) \left[\frac{2 - 22x^2 + 5x^4}{4x^2} \left(\frac{1 + x^2}{2x} \log \frac{1 + x}{1 - x} - 1 \right) - \frac{2}{3} \right] \\
& - i \frac{11\alpha^3}{9} x^2 .
\end{aligned}$$

We have obtained expansions of η and τ :

$$\eta = n - \frac{\alpha^2}{4} + \frac{\alpha^3}{3\pi} + \dots$$

$$\tau = \frac{\alpha}{4n} + \frac{\alpha^3}{16n^2} - \frac{\alpha^3}{64n^3} + \dots$$

These expansions are in agreement with the relation $\eta = \frac{\alpha}{2} \frac{1-\tau^2}{2\tau}$ between η and τ , but have been obtained independently and this gives a hint that everything works correctly.

This expansion of η gives the best result so far concerning the energy :

$$\frac{E}{2m} = \left(1 + \frac{\alpha^2}{4\eta^2}\right)^{-1/2} = 1 - \frac{\alpha^2}{8n^2} - \frac{\alpha^4}{16n^3} \left(1 - \frac{3}{8n}\right) + \frac{\alpha^5}{12n\pi} + \dots$$

This is rather meager compared to our effort, but we shall see now that, using the expansion obtained on the wave function, we get the expansions of η and of the energy with two more terms.

3.2 - Further expansion of the energy using analyticity.

Energy to order α^7

Up to now, we have not used the analyticity properties of $\Psi(x)$. This is what we will do now. Let us consider the equation for $\Psi(x)$:

$$\Psi(x) = \frac{\chi(x)}{\tau^2 + x^2} - \frac{i}{4\pi} (1 + \tau^2) \frac{\chi(x)}{\tau^2 + x^2} \int_0^x dx' \chi(x')^{-1} (K\Psi)(x')$$

with

$$K(x, x') = 8xx' \frac{1 + x'^2}{(1 - x^2x'^2)^2} \quad , \quad \chi(x) = \left(\frac{1+x}{1-x}\right)^{i\alpha/2} \left(\frac{i\tau - x}{i\tau + x}\right)^\eta \quad ,$$

the function $\Psi(x)$ in the left side must be analytic in the upper half plane. However in the right side, the function $\chi(x)$ has a branch point $x = i\tau$ (except if η is integer, but we have seen that η is integer only in lowest order in α). The function $(K\Psi)(x)$ is analytic in the plane with the cuts $]-\infty, -1]$ and $[1, \infty[$, due to the properties of the kernel K and without any analyticity condition on Ψ . In order that the singularity of $\chi(x)$ in the upper half-plane does not generate a singularity of $\Psi(x)$, one can show by

contour deformation that the function $(K\Psi)(x)$ (and the parameters α, η, τ) must satisfy the following condition :

$$1 - e^{-2i\pi\eta} = \frac{i}{4\pi} (1 + \tau^2) \int_{\gamma_\tau} dx \chi(x)^{-1} (K\Psi)(x) \quad (69)$$

where γ_τ is a loop starting at $x = 0$, encircling $x = i\tau$, and returning at $x = 0$. This is the equation which will allow us to get further terms with rather little additional calculations.

In this formula, the function $\chi(x)$ is as defined only in the part of γ_τ between the beginning $x = 0$ and the intersection with the cut $[i\tau, i\infty[$, and is defined further on by analytic continuation along γ_τ . To obtain a more explicit formula, notice that, for $x > 0$, and therefore at the beginning of γ_τ , we have

$$\chi(x)^{-1} = e^{-i\pi\eta} G(\eta, x/\tau) h(-\alpha, x) \quad .$$

Furthermore $G(\eta, x/\tau)$ is analytic with the cut $[-i\tau, i\tau]$ so that γ_τ is included in the analyticity domain of $G(\eta, x/\tau)$ (with the understanding that γ_τ begins at $x = 0_+$ and ends at $x = 0_-$). Then, this gives an expression for $\chi(x)^{-1}$ under the integral valid on all γ_τ and, with a further rescaling of the integration variable, our condition for the analyticity of Ψ writes

$$8\pi \sin(\pi\eta) = (1 + \tau^2) \tau \int_{\gamma_1} dx G(\eta, x) h(-\alpha, \tau x) (K\Psi)(\tau x) \quad . \quad (70)$$

Now, this equation is suitable to obtain an expansion of the energy from an expansion of $K\Psi$. Indeed, if $K\Psi$ and η are known up to some order α^p , then the right hand side and therefore η are obtained up to α^{p+2} (since $(K\Psi)(0) = 0$), and the energy is obtained up to α^{p+4} . Having obtained $K\Psi$ up to α^3 , equation (70) allows us to obtain the energy up to α^7 .

Next we must expand equation (70), but this presents no difficulty. Since $h(-\alpha, x)$ and $(K\Psi)(x)$ are analytic in the unit disk which includes γ_τ , we may use the expansions

$$h(-\alpha, x) = \sum_{p \geq 0} h(-\alpha)_p x^p \quad , \quad (K\Psi)(x) = \sum_{p \geq 1} (K\Psi)_p x^p \quad .$$

The resulting expansion of $h(-\alpha, \tau x)(K\Psi)(\tau x)$ has radius of convergence $R = \tau^{-1}$, and can be exchanged with the integral, giving a convergent series :

$$-4 i \sin(\pi\eta) = \left(1 + \tau^2\right) \sum_{p \geq 1} A(\eta, p) \left[\sum_{q=1}^p h(-\alpha)_{p-q} (K\Psi)_q \right] \tau^{p+1}$$

$$\text{with } A(\eta, p) = \frac{1}{2i\pi} \int_{\gamma_1} dx G(\eta, x) x^p \quad .$$

To the required order, and using that $\tau = O(\alpha)$ and that $K\Psi$ is an odd function, this is :

$$\begin{aligned} -4 i \sin(\pi\eta) &= \left(1 + \tau^2\right) A(\eta, 1) (K\Psi)_1 \tau^2 - i \alpha A(\eta, 2) (K\Psi)_1 \tau^3 \\ &\quad + A(\eta, 3) (K\Psi)_3 \tau^4 + O(\alpha^6) \quad . \end{aligned} \quad (71)$$

To compute the integral $A(\eta, p)$ we have the difficulty that $G(\eta, x)$ is too singular at $x = i$ to allow shrinking γ_1 to $[0, i]$. We can replace the path γ_1 by a loop γ'_1 starting at $x = 0_+$ and returning at $x = 0_-$ after encircling clockwise the other branch point $x = -i$ where $G(\eta, x)$ is integrable, plus an anticlockwise loop γ around the cut $[-i, i]$. We can shrink γ'_1 to $[0, -i]$ and deform γ into a circle of arbitrary large radius R . The result is :

$$\begin{aligned} A(\eta, p) &= \frac{1}{2\pi} \int_0^{2\pi} d\theta R^{p+1} e^{i(p+1)\theta} G(\eta, R e^{i\theta}) \\ &\quad - \frac{(-i)^p}{2\pi} \int_0^1 dy y^p [G(\eta, -iy + 0) - G(\eta, -iy - 0)] \\ &= G_{p+1}(\eta) + \frac{1}{\pi} \sin(\pi\eta) B(\eta, p) \end{aligned}$$

with $G_p(\eta)$ defined by :

$$G(\eta, x) = \sum_{p=0}^{\infty} G_p(\eta) x^{-p} \quad .$$

$$\text{and } B(\eta, p) = (-i)^{p+1} \int_0^1 dy y^p \left(\frac{1+y}{1-y} \right)^{-\eta} .$$

We find :

$$\begin{aligned}
B(n, p) &= (-1)^n \int_0^{-i} dx \, x^p G(n, x) \\
&= (-1)^n \left\{ \sum_{q=1}^{p+1} \frac{(-i)^q}{q} G_{p-q+1}(n) + \sum_{q=1}^n \frac{(-1)^q}{q} G_{p+1}(n-q) + G_{p+1}(n) \log(2) \right\} \\
B(n, 1) &= (-1)^n \left\{ \frac{1}{2} (2n-1) (-1)^n - 2n^2 \left[\log(2) + \sum_{q=1}^n \frac{(-1)^q}{q} \right] \right\} .
\end{aligned}$$

We are now ready to obtain the expansion of η from formula (71) starting with $\eta^{(0)} = n$ (integer > 0) already known at order 0. In fact, we already know also $\eta^{(1)}$, $\eta^{(2)}$ and $\eta^{(3)}$, but it is useful to verify that they are recovered from formula (71), because this amounts to verify the analyticity of Ψ that was not used in the calculation of the expansion of $K\Psi$.

The expansion of τ is obtained along with the one of η using :

$$\tau = \frac{\frac{\alpha}{2\eta}}{1 + \sqrt{1 + \frac{\alpha^2}{4\eta^2}}} = \frac{\alpha}{4\eta} - \frac{\alpha^3}{64\eta^3} + O(\alpha^5) \quad . \quad (72)$$

The terms in the expansion of $(K\Psi)_1$ and $(K\Psi)_3$ that we use are the followings :

$$\begin{aligned}
(-1)^n (K\Psi)_1^{(0)} &= -8 \, i\pi \, , \quad (-1)^n (K\Psi)_3^{(0)} = 0 \\
(-1)^n (K\Psi)_1^{(1)} &= i \frac{32\alpha}{3} \, , \quad (-1)^n (K\Psi)_3^{(1)} = -i \frac{64\alpha}{5} \\
(-1)^n (K\Psi)_1^{(2)} &= -i \frac{1}{\pi} \alpha^2 \Psi''(1/2) + i \pi \frac{\alpha^2}{2n^2} \left[Z(n) + 4n^2 \log\left(\frac{\alpha}{4n}\right) \right] - 4 \, i \frac{1}{\pi} \alpha^2 - i \, \pi \frac{\alpha^2}{2} \\
(-1)^n (K\Psi)_1^{(3)} &= -i \frac{1}{\pi^2} \frac{\alpha^3}{12} \Psi^{(4)}(1/2) + i \frac{1}{\pi^2} \frac{2\alpha^3}{3} \Psi''(1/2) (2 + \pi^2) \\
&\quad - i \frac{4\alpha^3}{3n^2} \left[Z(n) + 4n^2 \log\left(\frac{\alpha}{4n}\right) \right] + i \frac{1}{\pi^2} \frac{8\alpha^3}{9} - i \frac{14\alpha^3}{45n^2} - i \frac{128\alpha^3}{135} \quad .
\end{aligned}$$

Now, we can proceed from (71) and (72).

Order 0 : $\eta^{(0)} = n$

Order 1 : $\tau^{(1)} = \frac{\alpha}{4\eta^{(0)}} = \frac{\alpha}{4n}$
 $-4 \, i\pi \cos\left(\pi\eta^{(0)}\right) \eta^{(1)} = 0 \quad \implies \quad \eta^{(1)} = 0$

Order 2 : $\tau^{(2)} = 0$

$$-4 i \pi (-1)^n \eta^{(2)} = G_2(n) (K\Psi)_1^{(0)} \left(\tau^{(1)} \right)^2 = 16 i \pi n^2 (-1)^n \frac{\alpha^2}{16n^2} \implies \eta^{(2)} = -\frac{\alpha^2}{4}$$

Order 3 : $\tau^{(3)} = -\frac{\alpha}{4n} \frac{\eta^{(2)}}{n} - \frac{\alpha^3}{64n^3} = \frac{\alpha^3}{16n^2} - \frac{\alpha^3}{64n^3}$

$$-4 i \pi (-1)^n \eta^{(3)} = G_2(n) (K\Psi)_1^{(1)} \left(\tau^{(1)} \right)^2 = -2n^2 \frac{32}{3} i \alpha (-1)^n \frac{\alpha^2}{16n^2} \implies \eta^{(3)} = \frac{\alpha^3}{3\pi}$$

Order 4 : $\tau^{(4)} = -\frac{\alpha}{4n} \frac{\eta^{(3)}}{n} = -\frac{\alpha^4}{12\pi n^2}$

$$\begin{aligned} -4 i \pi (-1)^n \eta^{(4)} &= G_2(n) (K\Psi)_1^{(2)} \left(\tau^{(1)} \right)^2 \\ &\quad + 2G_2(n) (K\Psi)_1^{(0)} \tau^{(1)} \tau^{(3)} \\ &\quad + [G_2'(n) + (-1)^n B(n, 1)] \eta^{(2)} (K\Psi)_1^{(0)} \left(\tau^{(1)} \right)^2 \\ &\quad + G_2(n) (K\Psi)_1^{(0)} \left(\tau^{(1)} \right)^4 \\ &\quad - i \alpha G_3(n) (K\Psi)_1^{(0)} \left(\tau^{(1)} \right)^3 + G_4(n) (K\Psi)_3^{(0)} \left(\tau^{(1)} \right)^4 \end{aligned}$$

$$\eta^{(4)} = -\frac{\alpha^4}{16} \left\{ \frac{29}{12} + \frac{2}{\pi^2} + \frac{1}{2\pi^2} \Psi''(1/2) + \log(n) - \sum_{q=1}^n \frac{1}{q} + \frac{1}{2n} - \frac{1}{6n^2} - \log\left(\frac{\alpha}{2}\right) \right\}$$

Order 5 : $\tau^{(5)}$ unused

$$\begin{aligned} -4 i \pi (-1)^n \eta^{(5)} &= G_2(n) (K\Psi)_1^{(3)} \left(\tau^{(1)} \right)^2 \\ &\quad + 2G_2(n) (K\Psi)_1^{(1)} \tau^{(1)} \tau^{(3)} \\ &\quad + 2G_2(n) (K\Psi)_1^{(0)} \tau^{(1)} \tau^{(4)} \\ &\quad + [G_2'(n) + (-1)^n B(n, 1)] \eta^{(2)} (K\Psi)_1^{(1)} \left(\tau^{(1)} \right)^2 \\ &\quad + [G_2'(n) + (-1)^n B(n, 1)] \eta^{(3)} (K\Psi)_1^{(0)} \left(\tau^{(1)} \right)^2 \\ &\quad + G_2(n) (K\Psi)_1^{(1)} \left(\tau^{(1)} \right)^4 \\ &\quad - i \alpha G_3(n) (K\Psi)_1^{(1)} \left(\tau^{(1)} \right)^3 + G_4(n) (K\Psi)_3^{(1)} \left(\tau^{(1)} \right)^4 \end{aligned}$$

$$\begin{aligned} \eta^{(5)} &= \frac{\alpha^5}{6\pi} \left\{ \frac{307}{180} + \frac{1}{6\pi^2} + \frac{1}{4\pi^2} \Psi''(1/2) + \frac{1}{8} \Psi''(1/2) - \frac{1}{64\pi^2} \Psi^{(4)}(1/2) \right. \\ &\quad \left. + \log(n) - \sum_{q=1}^n \frac{1}{q} + \frac{1}{2n} - \frac{1}{6n^2} - \log\left(\frac{\alpha}{2}\right) \right\} . \end{aligned}$$

Finally, the expansion of E is obtained from the expansion of η :

$$\begin{aligned} \frac{E}{2m} &= \left(1 + \frac{\alpha^2}{4\eta^2} \right)^{-1/2} = 1 - \frac{\alpha^2}{8\eta^2} + \frac{3\alpha^4}{128\eta^4} - \frac{5\alpha^6}{1024\eta^6} + O(\alpha^8) \\ &= 1 - \frac{\alpha^2}{8n^2} + \left[\frac{\alpha^2}{4n^3} \eta^{(2)} + \frac{3\alpha^4}{128n^4} \right] + \frac{\alpha^2}{4n^3} \eta^{(3)} \end{aligned}$$

$$\begin{aligned}
& + \left[\frac{\alpha^2}{4n^3} \eta^{(4)} - \frac{3\alpha^2}{8n^4} (\eta^{(2)})^2 - \frac{3\alpha^4}{32n^5} \eta^{(2)} - \frac{5\alpha^6}{1024n^6} \right] \\
& + \left[\frac{\alpha^2}{4n^3} \eta^{(5)} - \frac{3\alpha^2}{4n^4} \eta^{(2)} \eta^{(3)} - \frac{3\alpha^4}{32n^5} \eta^{(3)} \right] + O\left(\alpha^8 \log\left(\frac{1}{\alpha}\right)\right) + O\left(\alpha^2 \eta^{(6)}\right)
\end{aligned}$$

$$\begin{aligned}
\frac{E}{2m} &= 1 - \frac{\alpha^2}{8n^2} - \frac{\alpha^4}{16n^3} \left(1 - \frac{3}{8n}\right) + \frac{\alpha^5}{12\pi n^3} \\
& - \frac{\alpha^6}{64n^3} \left\{ \frac{29}{12} + \frac{2}{\pi^2} + \frac{1}{2\pi^2} \Psi''(1/2) + \log(n) - \sum_{q=1}^n \frac{1}{q} + \frac{2}{n} - \frac{5}{3n^2} + \frac{5}{16n^3} - \log\left(\frac{\alpha}{2}\right) \right\} \\
& + \frac{\alpha^7}{24\pi n^3} \left\{ \frac{307}{180} + \frac{1}{6\pi^2} + \frac{1}{4\pi^2} \Psi''(1/2) + \frac{1}{8} \Psi''(1/2) - \frac{1}{64\pi^2} \Psi^{(4)}(1/2) \right. \\
& \quad \left. + \log(n) - \sum_{q=1}^n \frac{1}{q} + \frac{2}{n} - \frac{11}{12n^2} - \log\left(\frac{\alpha}{2}\right) \right\} \\
& + O\left(\alpha^8 \log\left(\frac{1}{\alpha}\right)\right) + O\left(\alpha^2 \eta^{(6)}\right) . \tag{73}
\end{aligned}$$

4. Comparison with other bound state equations and with the full positronium result

In conclusion of these calculations, we can return in a more quantitative manner to the comparison and evaluation of the perturbative series in α for various proposed equations, which we began in the introduction. Namely, we will compare our results with the Klein-Gordon and Dirac equations in an external field and, for the two-body problem, with the full QED positronium results and with Breit and Sucher-type equations.

For definiteness, we shall give results for the ground state : $L = 0$, $S = 0$, and no radial excitation : $n = 1$. Of course, all equations and procedures give the Schrödinger binding energy in the weak binding limit and we shall give therefore only $\Delta E \equiv E - E$ (Schrödinger). We will proceed by first considering the simpler external field problem.

i) External field

In this case, the comparison should be made with the one-body version of Herbst equation, for which our results translate into :

$$\Delta E = -\frac{5}{8} m\alpha^4 + \frac{8}{3\pi} m\alpha^5 - m\alpha^6 \ln \alpha^{-1} + \dots \quad (74)$$

In comparison, K-G equation in a Coulomb field gives¹⁴⁾

$$\Delta E = -\frac{5}{8} m\alpha^4 - \frac{21}{16} m\alpha^6 + \dots \quad (75)$$

Therefore, as announced, the first corrections to Schrödinger deduced from Herbst are correct for a scalar particle in an external field. In addition, one sees that for sufficiently small α , the Herbst energy level is above the K-G one : this is in accord with an inequality established by Martin and Roy¹⁰⁾.

On the other hand, the Dirac equation result writes¹⁵⁾ :

$$\Delta E = -\frac{1}{8} m\alpha^4 - \frac{1}{16} m\alpha^6 \quad (76)$$

Therefore, in this latter case, the Herbst equation is already completely incorrect for the first correction. This is due to the well-known Darwin term, which is of the same order as the kinetic energy correction. It contributes with opposite sign (+). The Herbst energy is this time below the correct result. For excited levels with $\ell \neq 0$, one would also miss the spin-orbit effect, which is of the same order. A general remark is that the series expansion of Herbst equation does not preserve the simple analytic behavior of Klein-Gordon and Dirac equation, which had only even integer powers.

ii) Two-body problem

Our result for Herbst equation is

$$\Delta E = -\frac{5}{64} m\alpha^4 + \frac{m\alpha^5}{6\pi} - \frac{m\alpha^6}{32} \ln \alpha^{-1} + O(\alpha^6) \quad (77)$$

We will compare it only with fermion calculations.

This is to be compared with the full QED result for parapositronium¹⁶⁾

$$\Delta E = -\frac{21}{64}m\alpha^4 + 0 \left(m\alpha^5 \ln \alpha^{-1} \right) \quad . \quad (78)$$

Not surprisingly in view of the external field results there is failure at the lowest order of relativistic corrections. Let us make precise the origin of the discrepancy, i.e., what are the $m\alpha^4$ terms missing in Herbst equation. In the systematic expansion method of Sucher, it appears that one should first solve the Sucher equation (2) and then add perturbatively Coulomb pair contributions and transverse photon contributions.

Let us then write first the result of Sucher equation with Coulomb interaction¹⁷⁾ :

$$\Delta E = \frac{3}{64} m\alpha^4 - \frac{1}{8\pi} \left(\frac{\pi}{2} + \frac{5}{3} \right) m\alpha^5 + 0 \left(m\alpha^6 \ln \alpha^{-1} \right) \quad . \quad (79)$$

We make a minor correction to Hardekopf-Sucher paper by reestablishing a factor $1/\pi$ in α^5 terms, which is obviously lacking in their eq. (4.1).

This result is already completely different from Herbst one, and already at order α^4 . The origin is in the Λ_+ projectors which produce an effect analogous to Darwin correction. It is to be noted that, in contrast to the kinetic energy correction, these effects are purely quantum effects.

The exchange of transverse photons adds further $m\alpha^4$ terms :

$$\Delta E_T = -3/8 m \alpha^4 \quad . \quad (80)$$

Annihilation is in principle of order α^4 , but it happens to vanish for the parapositronium $S = 0$ at this order (in contrast to the orthopositronium $S = 1$). All other effects are found to be of order α^5 at least. An equation which gives the correct α^4 terms (except for the possible annihilation) is the one obtained by adding to the Coulomb interaction the Breit interaction in the equation of Sucher (with Λ_+ projectors¹⁷⁾. (Let us recall that the Breit equation, without Λ_+ projectors, would give spurious α^4 terms¹⁸⁾).

5. Conclusion

Herbst equation cannot be considered as a realistic equation for detailed knowledge of the spectrum of electromagnetically-bound fermions. This is for partly obvious reasons : it ignores of course spin and annihilation effects and these happen to generate large terms, comparable with the ones coming from the relativistic kinetic energy correction. The presence of the Darwin correction should be stressed since, although spin-independent, it comes from the presence of spin.

Nevertheless it may be useful because it presents problems which will probably be present in more realistic equations like Sucher equation : non-analytic series expansion as detailed in the present article, critical behavior at some α , and peculiar short distance behavior of the wave-function as we will analyse in next articles. The equation may even be of direct physical interest in other situations, like in astrophysics, where the relativistic kinetic energy could be the major feature.

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