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APPENDIX A

EVALUATION OF INTEGRALS CONTAINING
CONFLUENT HYPERGEOMETRIC FUNCTIONS

The relation

$$\int_0^{\infty} z^c e^{-z} {}_1F_1(-m; c+1; z) {}_1F_1(-n; c+1; z) dz = \frac{[\Gamma(c+1)]^2 n!}{\Gamma(n+c+1)} \delta_{mn}, \quad (A1)$$

where m and n are non-negative integers; c may be any complex number; can be proven by noting that (a) the confluent hypergeometric functions ${}_1F_1(-n; c+1; z)$ are related to the generalized Laguerre polynomials $\mathfrak{L}_n^{(c)}(z)$ by the relation (38)

$$\mathfrak{L}_n^{(c)}(z) = \frac{\Gamma(n+c+1)}{n! \Gamma(c+1)} {}_1F_1(-n; c+1; z), \quad (A2)$$

and that (b) the generalized Laguerre polynomials $\mathfrak{L}_n^{(c)}(z)$ can be represented by a generating function $g(z, s)$ through the equation

$$g(z, s) = \frac{\exp(-\frac{zs}{1-s})}{(1-s)^{c+1}} = \sum_{n=0}^{\infty} \mathfrak{L}_n^{(c)}(z) s^n. \quad (A3)$$

Substitution of Eq.(A2) into Eq.(A3) gives

$$\sum_{n=0}^{\infty} \frac{\Gamma(n+c+1)}{n! \Gamma(c+1)} {}_1F_1(-n; c+1; z) s^n = \frac{\exp(-\frac{zs}{1-s})}{(1-s)^{c+1}}. \quad (A4)$$

Hence, by (a) squaring Eq.(A4), (b) multiplying throughout by $z^c e^{-z}$, and (c) integrating with respect to z from zero to infinity, we obtain

$$\begin{aligned} \sum_{m, n=0}^{\infty} \frac{\Gamma(m+c+1) \Gamma(n+c+1)}{m! n! [\Gamma(c+1)]^2} \left\{ \int_0^{\infty} z^c e^{-z} {}_1F_1(-m; c+1; z) {}_1F_1(-n; c+1; z) dz \right\} r^m s^n \\ = \int_0^{\infty} z^c \left\{ \frac{\exp\left[-\frac{(1-rs)}{(1-r)(1-s)}z\right]}{(1-r)(1-s)^{c+1}} \right\} dz. \quad (A5) \end{aligned}$$

The integral on the right hand side of Eq.(A5) can be written in terms of the gamma functions by transforming to the new variable x defined by

$$x = \frac{(1-rs)}{(1-r)(1-s)} z . \quad (A6)$$

In terms of this new variable the integral on the right hand side of Eq.(A5) becomes

$$\begin{aligned} \int_0^{\infty} z^c \frac{\exp\left[-\frac{(1-rs)}{(1-r)(1-s)}z\right]}{(1-r)(1-s)^{c+1}} dz &= \frac{1}{(1-rs)^{c+1}} \int_0^{\infty} x^c e^{-x} dx \\ &= \frac{\Gamma(c+1)}{(1-rs)^{c+1}} , \end{aligned} \quad (A7)$$

where $\Gamma(c+1)$ is the gamma function

$$\Gamma(c+1) = \int_0^{\infty} x^c e^{-x} dx ; \quad \Gamma(c+1) = c\Gamma(c) . \quad (A8)$$

Expansion of $(1-rs)^{-(c+1)}$ by Taylor series expansion yields

$$(1-rs)^{-(c+1)} = \sum_{n=0}^{\infty} \frac{\Gamma(c+n+1)}{n! \Gamma(c+1)} (rs)^n ; \quad |rs| < 1 . \quad (A9)$$

Thus Eq.(A5) becomes

$$\begin{aligned} \sum_{m,n=0}^{\infty} \frac{\Gamma(m+c+1)\Gamma(n+c+1)}{m!n! [\Gamma(c+1)]^2} \int_0^{\infty} z^c e^{-z} {}_1F_1(-m;c+1;z) {}_1F_1(-n;c+1;z) dz r^m s^n \\ = \sum_{\bar{n}=0}^{\infty} \frac{\Gamma(\bar{n}+c+1)}{\bar{n} \Gamma(c+1)} (rs)^{\bar{n}} . \end{aligned} \quad (A10)$$

Eq.(A1) is then obtained by equating the coefficients of $r^m s^n$ on the left and the right sides of Eq.(A10).

In the similar way, the integral

$$\int_0^{\infty} z^{c+q} e^{-z} {}_1F_1(-m; c+1; z) {}_1F_1(-n; c+1; z) dz \quad ; n > m, \quad (A11)$$

can be evaluated by, first, multiplying Eq.(A4) by a similar equation in which s^n is replaced by r^m , then multiplying through out by $e^{-z} z^{c+q}$ and integrating. The result is (50)

$$\begin{aligned} & \int_0^{\infty} z^{c+q} e^{-z} {}_1F_1(-m; c+1; z) {}_1F_1(-n; c+1; z) dz \\ &= (-q)_{n-m} \frac{[\Gamma(c+1)]^2 \Gamma(m+c+q+1)}{\Gamma(m+c+1) \Gamma(n+c+1)} \frac{n!}{(n-m)!} {}_3F_2 \left[\begin{matrix} -q, -q+n-m, -m \\ n-m+1, -c-q-m \end{matrix} \right], \quad (A12) \end{aligned}$$

where $(-q)_{n-m}$ is either $\frac{\Gamma(-q+n-m)}{\Gamma(-q)}$ or $(-1)^{n-m} \frac{\Gamma(q+1)}{\Gamma(q-n+m+1)}$, whichever has meaning; and ${}_3F_2$ is the generalized hypergeometric function with unit argument,

$${}_3F_2 \left[\begin{matrix} a, b, c \\ e, f \end{matrix} \right] = 1 + \frac{abc}{ef} + \frac{a(a+1)b(b+1)c(c+1)}{2!e(e+1)f(f+1)} + \dots \quad (A13)$$

The integral does not converge unless $\text{Re}(c+q+1) > 0$ and is zero if q is an integer such that $0 \leq q < n-m$. In case q is negative, it is often convenient to use the equation

$${}_3F_2 \left[\begin{matrix} -q, -q+n-m, -m \\ n-m+1, -c-q-m \end{matrix} \right] = \frac{\Gamma(c+m-q) \Gamma(c+q+1)}{\Gamma(c-q) \Gamma(c+q+m+1)} {}_3F_2 \left[\begin{matrix} q+1, q+n-m+1, -m \\ n-m+1, q-c-m+1 \end{matrix} \right]. \quad (A14)$$

As the special cases of Eq.(A12), we obtain, for $m=n$,

$$q=1 ; \int_0^{\infty} e^{-z} z^{c+1} [{}_1F_1(-n;c+1;z)]^2 dz = \frac{n! [\Gamma(c+1)]^2}{\Gamma(c+n+1)} (2n+c+1), \quad (A15)$$

$$q=0 ; \int_0^{\infty} e^{-z} z^c [{}_1F_1(-n;c+1;z)]^2 dz = \frac{n! [\Gamma(c+1)]^2}{\Gamma(c+n+1)}, \quad (A16)$$

$$q=-1; \int_0^{\infty} e^{-z} z^{c-1} [{}_1F_1(-n;c+1;z)]^2 dz = \frac{n! [\Gamma(c+1)]^2}{\Gamma(c+n+1)} \left(\frac{1}{c}\right), \quad (A17)$$

$$q=-2; \int_0^{\infty} e^{-z} z^{c-2} [{}_1F_1(-n;c+1;z)]^2 dz = \frac{n! [\Gamma(c+1)]^2}{\Gamma(c+n+1)} \left\{ \frac{2n+c+1}{(c-1)c(c+1)} \right\}. \quad (A18)$$



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APPENDIX B

NONRELATIVISTIC REDUCTION OF DIRAC HAMILTONIAN:

FOLDY-WOUTHUYSEN TRANSFORMATION

In the nonrelativistic limit where the momentum of the particle is small compared to mc , it is well-known that a spin- $\frac{1}{2}$ particle can be described by a two-component wave function in the Pauli theory. Thus, according to the requirement(4) of Section 2.4.2, in the nonrelativistic limit the Dirac theory must reduce to the Pauli theory. The purpose of this appendix is to show that in such limit these two theories are indeed equivalent.

The usual method of demonstrating the equivalence of the Dirac Dirac and Pauli theories (51) makes use of the fact that although in the Dirac theory the wave function $U(\vec{r}, t)$ is a four-component wave function, two of the four components go to zero as the momentum goes to zero, while at least one of the other two components remain finite. In the usual representation (Pauli's representation), for positive-energy eigenfunctions the last two components vanish with vanishing momentum, while for negative-energy eigenfunctions the first two components vanish with vanishing momentum. In this appendix we will consider the case of positive-energy eigenfunctions only.

By writing out the equations satisfied by the four components and solving, approximately, two of equations for the small components χ , then substituting the solutions in the remaining two equations, one obtain a pair of equations for the large components ψ which are

essentially the Pauli equation obeyed by a charged spin- $\frac{1}{2}$ particle in an electromagnetic field ;

$$i\hbar \frac{\partial}{\partial t} \varphi = \left[\frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 - \frac{q\hbar}{2mc} \vec{\sigma}^P \cdot \vec{B} + (qA_0 + mc^2) \right] \varphi . \quad (B1)$$

However, this method encounters difficulties when one wishes to go beyond the lowest order approximation - the Hamiltonian associated with the large components is no longer hermitian in the presence of external electromagnetic field because of the appearance of an imaginary electric moment of the particle.

A more general and elegant method of passing from four- to two-component wave functions in the Dirac theory was proposed in 1950 by Foldy and Wouthysen (52) who noticed that the essential reason why four components are necessary to describe a state in the Dirac theory is that in the usual representation the Dirac Hamiltonian contains "odd" operators, specifically the operator α 's, which have matrix elements connecting the upper and lower components of the wave function. Their method consists of successive canonical transformations to a new representation for the Dirac equation - the so-called Foldy-Wouthysen representation - in which the Dirac Hamiltonian is free of odd operators. Thus, in the new representation the Dirac equation is decoupled into two two-component equations : one reduces to the Pauli description in the nonrelativistic limit, the other describes the negative-energy states.

Under a canonical transformation described by

$$U'(\vec{r}, t) = \exp [iS(\vec{r}, t)] U(\vec{r}, t) , \quad (B2)$$

where $S(\vec{r}, t)$ is a hermitian transformation operator, the Dirac

equation in the usual representation is transformed to the equation

$$H'_D U'(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} U'(\vec{r}, t), \quad (B3)$$

where

$$H'_D = e^{iS(\vec{r}, t)} H_D e^{-iS(\vec{r}, t)} - i\hbar e^{iS(\vec{r}, t)} \left(\frac{\partial}{\partial t} e^{-iS(\vec{r}, t)} \right) \quad (B4)$$

is the transformed Hamiltonian which may be rewritten in the series form as

$$\begin{aligned} H'_D = & H_D + i[S, H_D] - \frac{1}{2!} [S, [S, H_D]] - \frac{i}{3!} [S, [S, [S, H_D]]] \\ & + \frac{1}{6!} [S, [S, [S, [S, H_D]]]] - \dots - \hbar \left\{ \dot{S} - \frac{i}{2!} [S, \dot{S}] \right. \\ & \left. + \frac{1}{3!} [S, [S, \dot{S}]] - \dots \right\}. \end{aligned} \quad (B5)$$

For the free particle, the complete transformation, i.e., diagonalizing the Hamiltonian, is given by the transformation operator

$$S = -\frac{i}{2}\beta \frac{\vec{\alpha} \cdot \vec{p}}{|\vec{p}|} \arctan\left(\frac{|\vec{p}|}{mc}\right). \quad (B6)$$

That is, in this case there exists a representation of the Dirac equation in which the positive-energy states and negative-energy states are separately described by two-component wave function.

In the presence of interaction, such as an external electromagnetic field, there exists no representation in which the Hamiltonian is exactly "even" but by applying successive canonical transformations one may obtain representations in which the respective Hamiltonians have an "odd" part of higher and higher order in $(1/mc^2)$. In practice, it is sufficient to get rid of the odd operators in the Hamiltonian up to terms of order

(kinetic energy/ mc^2)³ or (kinetic energy × potential energy/ m^2c^4). This will lead to a further insight in relativistic corrections entailed by the Dirac equation.

In the case where a Dirac particle is subject to interactions, the Hamiltonian operator can always be put in the form

$$H_D = \beta mc^2 + \mathcal{E} + \mathcal{O} , \quad (B7)$$

where \mathcal{E} is an even operator and \mathcal{O} is an odd operator, both of which may be explicitly time dependent. We assume that \mathcal{E} and \mathcal{O} are of no lower order in $(1/mc^2)$ than $(1/mc^2)^0$. Obviously, β commutes with all even operators and anticommutes with all odd operators in the Dirac theory, i.e.,

$$\beta \mathcal{E} = \mathcal{E} \beta , \quad \beta \mathcal{O} = -\mathcal{O} \beta . \quad (B8)$$

Moreover, the product of two even or two odd operators is an even operator whereas the product of an odd and an even operators is an odd operator.

From the examination of Eqs. (B5) and (B7), it appears that if one wants to eliminate the odd term \mathcal{O} in Eq. (B7), then the appropriate transformation operator to use is

$$S_1 = -\frac{i\beta}{2m} \mathcal{O} . \quad (B9)$$

Substituting this into Eq. (B5) and keeping the terms up to order $(1/mc^2)^3$, we obtain the transformed Hamiltonian which contains the odd terms only in order $(1/mc^2)$;

$$H_1 = \beta mc^2 + \mathcal{E}_1 + \mathcal{O}_1 , \quad (B10)$$

where

$$\mathcal{E}_1 = \mathcal{E} + \beta \left(\frac{1}{2mc^2} \mathcal{O}^2 - \frac{1}{8m^3c^6} \mathcal{O}^4 \right) - \frac{1}{8m^2c^4} ([\mathcal{O}, [\mathcal{O}, \mathcal{E}] + i\hbar \dot{\mathcal{O}}]) , \quad (\text{B11})$$

and

$$\begin{aligned} \mathcal{O}_1 = & \frac{1}{2mc^2} (\beta [\mathcal{O}, \mathcal{E}] + i\hbar \dot{\mathcal{O}}) - \frac{1}{3m^2c^4} \mathcal{O}^3 \\ & - \frac{1}{48m^3c^6} \beta [\mathcal{O}, [\mathcal{O}, [\mathcal{O}, \mathcal{E}] + i\hbar \dot{\mathcal{O}}]] . \end{aligned} \quad (\text{B12})$$

By applying a second canonical transformation

$$S_2 = - \frac{i\beta}{2mc^2} \mathcal{O}_1 \quad (\text{B13})$$

and, again, keeping the terms up to order $(1/mc^2)^3$, we obtain

$$H_2 = \beta mc^2 + \mathcal{E}_2 + \mathcal{O}_2 , \quad (\text{B14})$$

$$\mathcal{E}_2 = \mathcal{E}_1 + \frac{1}{2mc^2} \beta \mathcal{O}_1^2 , \quad (\text{B15})$$

$$\mathcal{O}_2 = \frac{1}{2mc^2} \beta ([\mathcal{O}_1, \mathcal{E}_1] + i\hbar \dot{\mathcal{O}}_1) . \quad (\text{B16})$$

The odd terms now appear in Eq.(B14) only in order $(1/mc^2)^2$.

To obtain the Hamiltonian which is free of odd terms to order $(1/mc^2)^3$ we apply another two canonical transformations generated by

$$S_3 = - \frac{i\beta}{2mc^2} \mathcal{O}_2 \quad (\text{B17})$$

and

$$S_4 = - \frac{i\beta}{2mc^2} \mathcal{O}_3 = - \frac{i\beta}{2mc^2} \left\{ \frac{\beta}{2mc^2} ([\mathcal{O}_2, \mathcal{E}_2] + i\hbar \dot{\mathcal{O}}_2) \right\} \quad (\text{B18})$$

which eliminate odd operators of order $(1/mc^2)^2$ and $(1/mc^2)^3$ respectively. We then get the required Hamiltonian

$$H_4 = \beta mc^2 + \mathcal{E}_2 = \beta mc^2 + \mathcal{E}_1 + \frac{\beta}{2mc^2} \mathcal{O}_1^2$$

or

$$H_4 = \beta mc^2 + \mathcal{E} + \beta \left(\frac{\mathcal{O}^2}{2mc^2} - \frac{\mathcal{O}^4}{8m^3c^6} \right) - \frac{1}{8m^2c^4} [\mathcal{O}, [\mathcal{O}, \mathcal{E}] + i\hbar\dot{\mathcal{O}}] - \frac{\beta}{8m^3c^6} ([\mathcal{O}, \mathcal{E}] + i\hbar\dot{\mathcal{O}})^2, \quad (B19)$$

where the terms of higher order than $(1/mc^2)^3$ have been neglect.

For the case where a Dirac particle of electric charge q interacts with an external electromagnetic field, \mathcal{E} and \mathcal{O} are

$$\mathcal{E} = qA_0 \quad \text{and} \quad \mathcal{O} = c\vec{\alpha} \cdot \left(\vec{p} - \frac{q}{c} \vec{A} \right), \quad (B20)$$

where A_0 and \vec{A} are the scalar and vector potentials of the electromagnetic field evaluated at the position of the particle.

Thus

$$\begin{aligned} \mathcal{O}^2 &= c^2 \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 - \hbar c q \vec{\sigma}^D \cdot \vec{B}; \quad \vec{B} = \nabla \times \vec{A} = \text{magnetic field}, \\ \mathcal{O}^4 &= c^4 \left(\vec{p} - \frac{q}{c} \vec{A} \right)^4 - \hbar c^3 q \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 (\vec{\sigma}^D \cdot \vec{B}) - \hbar c^3 q (\vec{\sigma}^D \cdot \vec{B}) \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 \\ &\quad + \hbar^2 c^2 q^2 |\vec{B}|^2 \\ &= c^4 \left(\vec{p} - \frac{q}{c} \vec{A} \right)^4 - \hbar c^3 q \cdot 2 (\vec{\sigma}^D \cdot \vec{B}) \left(\vec{p} - \frac{q}{c} \vec{A} \right) - \hbar^2 \text{div} [\text{grad}(\vec{\sigma}^D \cdot \vec{B})] \\ &\quad - 2i\hbar [\text{grad}(\vec{\sigma}^D \cdot \vec{B})] \cdot \left(\vec{p} - \frac{q}{c} \vec{A} \right) + \hbar^2 c^2 q^2 |\vec{B}|^2, \\ [\mathcal{O}, \mathcal{E}] + i\hbar\dot{\mathcal{O}} &= i\hbar c q \vec{\alpha} \cdot \left(-\text{grad} A_0 - \frac{\dot{\vec{A}}}{c} \right) = i\hbar c q \vec{\alpha} \cdot \vec{E}, \\ \vec{E} &= -\text{grad} A_0 - \frac{\dot{\vec{A}}}{c} = \text{electric field}, \\ ([\mathcal{O}, \mathcal{E}] + i\hbar\dot{\mathcal{O}})^2 &= -\hbar^2 c^2 q^2 |\vec{E}|^2, \\ [\mathcal{O}, [\mathcal{O}, \mathcal{E}] + i\hbar\dot{\mathcal{O}}] &= \hbar^2 c^2 q \text{div} \vec{E} + i\hbar^2 c^2 q \vec{\sigma}^D \cdot \text{curl} \vec{E} \\ &\quad + 2\hbar c^2 q \vec{\sigma}^D \cdot \vec{E} \times \left(\vec{p} - \frac{q}{c} \vec{A} \right). \end{aligned}$$

Collect everything together and keep terms only through order (kinetic energy/mc²)³ and (kinetic energy potential energy/m²c⁴), we obtain

$$\begin{aligned}
 H_4 = & \beta \left[mc^2 + \frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 - \frac{p^4}{8m^3 c^2} \right] + qA_0 - \frac{q\hbar\beta}{2mc} (\vec{\sigma}^D \cdot \vec{B}) \\
 & - \frac{q\hbar}{4m^2 c^2} \vec{\sigma}^D \cdot \vec{E} \times \left(\vec{p} - \frac{q}{c} \vec{A} \right) - \frac{iq\hbar^2}{8m^2 c^2} \vec{\sigma}^D \cdot \text{curl } \vec{E} \\
 & - \frac{q\hbar^2}{8m^2 c^2} \text{div } \vec{E} \quad (B21)
 \end{aligned}$$

Since the Hamiltonian in Eq.(B21) is free of odd operators, its eigenfunctions are two-component functions corresponding to positive and negative energies. For positive energies β and $\vec{\sigma}^D$ should be set equal to I and $\vec{\sigma}^P$ respectively. We then get the reduced Hamiltonian

$$\begin{aligned}
 H^{\text{red}} = & mc^2 + \frac{1}{2m} \left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 - \frac{p^4}{8m^3 c^2} + qA_0 - \frac{q\hbar}{2mc} \vec{\sigma}^P \cdot \vec{B} \\
 & - \frac{q\hbar}{4m^2 c^2} \vec{\sigma}^P \cdot \vec{E} \times \left(\vec{p} - \frac{q}{c} \vec{A} \right) - \frac{iq\hbar^2}{8m^2 c^2} \vec{\sigma}^P \cdot \text{curl } \vec{E} \\
 & - \frac{q\hbar^2}{8m^2 c^2} \text{div } \vec{E} \quad (B22)
 \end{aligned}$$

which will be recognized as essentially the Pauli Hamiltonian for a nonrelativistic particle of spin- $\frac{1}{2}$ interacting with an external electromagnetic field.

The individual terms in Eq.(B22) have a direct physical interpretation. the terms in the first bracket give the series expansion of

$$c\sqrt{\left[\left(\vec{p} - \frac{q}{c} \vec{A} \right)^2 - m^2 c^2 \right]}$$

to the desired order, showing the relativistic mass increase.

The second and third terms are, respectively, the electrostatic and

the magnetic dipole potential energies. The following two terms which taken together are hermitian comprise the spin-orbit coupling interaction. Finally, the last term, the so-called Darwin term, is a well-known correction to the Pauli theory arising from the Dirac theory. It corresponds to a correction to the direct point charge interaction due to the fact that in the Dirac theory the particle is not concentrated at a point but is spread out over a volume with a radius whose magnitude is roughly \hbar/mc - the phenomena which is known as Zitterbewegung.

For an electron in a static Coulomb potential, i.e., the three dimensional hydrogen atom problem, we have

- (a) the electrostatic potential energy

$$qA_0 = -\frac{Ze^2}{r},$$

- (b) the magnetic dipole potential energy

$$-\frac{q\hbar}{2mc} \vec{\sigma}^P \cdot \vec{B} = 0,$$

- (c) the spin-orbit interaction energy ($\text{curl } \vec{E} = 0$)

$$-\frac{q\hbar}{4m^2c^2} \vec{\sigma}^P \cdot \vec{E} \times \vec{p} = \frac{Ze^2\hbar}{4m^2c^2} \frac{\vec{\sigma}^P \cdot \vec{L}}{r^3},$$

- and (d) the Darwin term

$$-\frac{q\hbar^2}{8m^2c^2} \text{div } \vec{E} = -\frac{Ze^2\hbar^2\pi}{2m^2c^2} \delta(\vec{r}).$$

Thus, the reduced Hamiltonian is

$$H^{\text{red}} = mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} - \frac{Ze^2}{r} + \frac{Ze^2\hbar}{4m^2c^2} \frac{\vec{\sigma}^P \cdot \vec{L}}{r^3} - \frac{Ze^2\hbar^2\pi}{2m^2c^2} \delta(\vec{r}). \quad (\text{B23})$$

The last term, the Darwin term, gives a relativistic shift to S-levels.

This follows since in the present approximation it is proper to use nonrelativistic wave functions for which only S-states have non-vanishing values at the origin.

Foldy-Wouthuysen Transformation for the Two Dimensional Hydrogen Atom : In the case of the two dimensional hydrogen atom, the Dirac Hamiltonian in the usual representation is

$$\begin{aligned} H_D &= \beta mc^2 + c\alpha_x p_x + c\alpha_y p_y - \frac{Ze^2}{\rho} ; \rho = \sqrt{(x^2+y^2)} \\ &= \beta mc^2 + \mathcal{O} + \mathcal{E} . \end{aligned} \quad (B24)$$

where now

$$\mathcal{O} = c\alpha_x p_x + c\alpha_y p_y \quad \text{and} \quad \mathcal{E} = -\frac{Ze^2}{\rho} . \quad (B25)$$

A straightforward calculation gives

$$H_H = \beta mc^2 + \frac{1}{2m}(p_x^2+p_y^2) + \frac{1}{8m^3 c^2}(p_x^2+p_y^2)^2 - \frac{Ze^2}{\rho} + \frac{Ze^2 \hbar}{4m^2 c^2 \rho^3} 6_z^D L_z - \frac{Ze^2 \hbar^2}{8m^2 c^2 \rho^3} . \quad (B26)$$

Thus, the reduced Hamiltonian is

$$H^{\text{red}} = mc^2 + \frac{1}{2m}(p_x^2+p_y^2) + \frac{1}{8m^3 c^2}(p_x^2+p_y^2)^2 - \frac{Ze^2}{\rho} + \frac{Ze^2 \hbar}{4m^2 c^2 \rho^3} 6_z^D L_z - \frac{Ze^2 \hbar^2}{8m^2 c^2 \rho^3} , \quad (B27)$$

where the third term is the first relativistic correction to the kinetic energy; the fifth term is just the spin-orbit coupling energy ; and the last term is the two dimensional analog of the three three dimensional Darwin term.

APPENDIX C

PROGRAM TO CALCULATE THE CONSTANT COEFFICIENTS OF THE NORMALIZED RELATIVISTIC RADIAL FUNCTIONS.

The following program was used to evaluate the constant coefficients of the terms

$$\left(\frac{\rho}{a_0}\right)^{J+\gamma_k-1/2} \exp(-\lambda_{nk} a_0 \left(\frac{\rho}{a_0}\right)), \quad J = 0, 1, 2, \dots, \bar{n},$$

for $a_0 R_{nk}^1 \left(\frac{\rho}{a_0}\right)$ and $a_0 R_{nk}^4 \left(\frac{\rho}{a_0}\right)$, which are, according to Eqs.(4.168) - (4.170),

$$\left\{ \frac{\Gamma(\bar{n}+2\gamma_k+1)}{N_{nk}(N_{nk}-k)[\Gamma(2\gamma_k+1)]^2 \bar{n}!} \right\}^{1/2} (a_0 \lambda_{nk}) (2a_0 \lambda_{nk})^{\gamma_k-1/2} (1 \pm \epsilon_{nk})^{1/2}$$

$$\times \begin{cases} \pm(N_{nk}-k) - \bar{n} & ; \text{ for } J = 0 \\ \frac{(-2a_0 \lambda_{nk})^J}{\left[\prod_{I=1}^J (2\gamma_k+I) \right]} \binom{\bar{n}}{J} \left[\pm(N_{nk}-k) - (\bar{n}-J) \right] & ; \text{ for } J \neq 0 \end{cases}$$

where the upper and lower signs stand for the large and small components, respectively.

The variables and parameters used in the program are related to those used in Chapter IV as follow :

$$BR\# = a_0 \text{ (Bohr's radius)}$$

$$ME\# = m \text{ (electron rest mass)}$$

$$FSC\# = \alpha \text{ (Sommerfeld's fine structure constant)}$$

$$VL\# = c \text{ (speed of light in vacuum)}$$

$$HB\# = \hbar = \frac{h}{2\pi}, \quad h = \text{Planck's constant}$$

$$X = (\rho/a_0)$$

$$N = \bar{n}$$

$$Z = \text{atomic number}$$

$$NF = \bar{n}!$$

$$A\# = \gamma_k = \sqrt{(k^2 - (Z\alpha)^2)}$$

$$GB\# = \Gamma(2\gamma_k + 1)$$

$$C\# = \gamma_k - \frac{1}{2}$$

$$GD\# = \Gamma(\bar{n} + 2\gamma_k + 1)$$

$$F\# = N_{nk}$$

$$E\# = \epsilon_{nk}$$

$$E1\# = \sqrt{(1 + \epsilon_{nk})}$$

$$E2\# = \sqrt{(1 - \epsilon_{nk})}$$

$$E3\# = \sqrt{(1 - (\epsilon_{nk})^2)}$$

$$H\# = \lambda_{nk}$$

$$I\# = a_0 \lambda_{nk}$$

$$J\# = (2a_0 \lambda_{nk})^{\gamma_k - \frac{1}{2}}$$

$$RCN\# = c_{nk} \quad (\text{radial normalization constant})$$

$$P\# = \left\{ \frac{\Gamma(\bar{n} + 2\gamma_k + 1)}{N_{nk} (N_{nk} - k) [\Gamma(2\gamma_k + 1)]^{2\bar{n}}} \right\}^{\frac{1}{2}} (a_0 \lambda_{nk}) (2a_0 \lambda_{nk})^{\gamma_k - \frac{1}{2}} (1 \pm \epsilon_{nk})^{\frac{1}{2}}$$

$$Q\# = \left\{ \begin{array}{l} 1; \text{ for } J = 0 \\ \prod_{I=1}^J (2\gamma_k + I); \text{ for } J \neq 0 \end{array} \right.$$

$$\begin{matrix} \text{CLJ\#} \\ \text{CSJ\#} \end{matrix} = \begin{cases} [\pm(N_{nk}^{-k}) - \bar{n}] ; \text{ for } J = 0 \\ (-2)^J \binom{\bar{n}}{J} [\pm(N_{nk}^{-k}) - (\bar{n} - J)] ; \text{ for } J \neq 0 \end{cases}$$

$$\begin{matrix} \text{NCLJ\#} \\ \text{NCSJ\#} \end{matrix} = \text{CFJ\#} \times \begin{cases} \text{P\#} \times \text{CLJ\#} \\ \text{Q\#} \times \text{CSJ\#} \end{cases}$$

$$= \text{coefficient of the term } \left(\frac{\rho}{a_0}\right)^{J+\gamma_k-\frac{1}{2}} \exp(-a_0 \lambda_{nk} \left(\frac{\rho}{a_0}\right))$$

$$\text{for } \begin{cases} a_0 R_{nk}^1(\rho/a_0) \\ a_0 R_{nk}^4(\rho/a_0) \end{cases}$$



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```

10 REM PROGRAM TO FIND THE NORMALIZED RADIAL FUNCTIONS
20 REM OF THE 2-DIMENSIONAL RELATIVISTIC H-LIKE ATOMS
30 REM THE LARGE COMPONENT OF THE RADIAL WAVE FUNCTION IS
40 REM  $RL(N,K,X) = ((X^C\#) * EXP(-I\# * X) * \sum_{J=0}^N \text{OF}(NCLJ\# * (X^J))) / BR$ 
50 REM THE SMALL COMPONENT OF THE RADIAL WAVE FUNCTION IS
60 REM  $RS(N,K,X) = ((X^C\#) * EXP(-I\# * X) * \sum_{J=0}^N \text{OF}(NCSJ\# * (X^J))) / BR$ 
70 REM X=RADIAL DISTANCE / BOHR RADIUS (BR=0.52917706D-10 m)
80 REM ELECTRON REST MASS = 0.9109534D-30 kg
90 REM SPEED OF LIGHT IN VACUUM = 2.99792458D8 m/s
100 REM FINE STRUCTURE CONSTANT = 7.2973506D-3
110 REM (PLANCK CONSTANT/2*PI) = 1.0545887D-34 J*s
120 REM THIS PROGRAM CALCULATE THE CONSTANT FACTORS OF
130 REM BR*RL(N,K,X) AND BR*RS(N,K,X):NCLJ# & NCSJ#:
200 M=1
210 LPRINT "DATA SET NUMBER ";M
220 PRINT "ENTER DATA (N,K,Z)":INPUT N,K,Z
230 LPRINT "N=";N;"K=";K;"Z=";Z
240 REM CHANGE ANY VARIABLES
250 PRINT "ANY ALTERATIONS (Y/N)"
260 INPUT A$
270 IF A$ <> "Y" AND A$ <> "N" THEN GOTO 250
280 IF A$ = "N" THEN GOTO 320
290 PRINT "NEW VALUE OF N,K,Z":INPUT N,K,Z
300 GOTO 250
310 REM MENU OF OPERATIONS
320 PRINT "TO PERFORM CALCULATION, TYPE 1"
330 PRINT "TO ENTER ANOTHER DATA SET, TYPE 2"
340 PRINT "TO END PROGRAM, TYPE 3"
350 INPUT Q$
360 IF Q$="1" THEN GOSUB 400: GOTO 320
370 IF Q$="2" THEN M=M+1: GOTO 210
380 IF Q$="3" THEN GOTO 1050
390 GOTO 320
400 REM CALCULATE THE CONSTANT FACTORS OF 2-D.RELA. WAVE FNS.
410 Y=N
420 GOSUB 1100
430 NF=YF
440 FSC#=7.2973506000000001D-03
450 A1#=((K*K)-(Z*Z*FSC#*FSC#))
460 T#=A1#
470 GOSUB 1200
480 A#=SRT#
490 B#=(2*A#)+1
500 XT#=B#
510 GOSUB 1350
520 GB#=GAM#
530 C#=A#-.5
540 D#=N+B#
550 XT#=D#
560 GOSUB 1350
570 GD#=GAM#
580 F1#=((N*N)+(2*N*A#)+(K*K))
590 T#=F1#
600 GOSUB 1200
610 F#=SRT#
620 R#=GB#*GB#/GD#
630 G1#=NF*F#*(F#-K)*R#
640 T#=G1#
650 GOSUB 1200
660 G#=SRT#

```

```

670 E#=(N+A#)/F#
680 T#=1+E#
690 GOSUB 1200
700 E1#=SRT#
710 T#=1-E#
720 GOSUB 1200
730 E2#=SRT#
740 T#=1-(E#*E#)
750 GOSUB 1200
760 E3#=SRT#
770 ME#=9.1095340000000003D-31
780 VL#=299792458#
790 HB#=1.0545887D-34
800 H#=(ME#*VL#*E3#)/HB#
810 BR#=5.2917705999999999D-11
820 I#=BR#*H#
830 GOTO 4500
840 L#=I#*J#
850 P#=(L#*E1#)/G#
860 Q#=(L#*E2#)/G#
870 T#=2
880 GOSUB 1200
890 SR2#=SRT#
900 RCN#=H#/(SR2#*G#)
910 LPRINT "A=";A#;TAB(40);"B=";B#
920 LPRINT "C=";C#;TAB(40);"D=";D#
930 LPRINT "F=";F#;TAB(40);"H=";H#
940 LPRINT "I=";I#;TAB(40);"C1=";C#+1
950 LPRINT "ENERGY/REST MASS =" ;E#
960 LPRINT "RADIAL NORMALIZATION FACTOR =" ;RCN#
970 FOR J=0 TO N
980 GOSUB 3850
990 GOSUB 4000
1000 NCLJ#=P#*CFJ#*CLJ#
1010 NCSJ#=Q#*CFJ#*CSJ#
1020 LPRINT "J=";J;TAB(10);"NCLJ#=";NCLJ#;TAB(40);"NCSJ#=";NCSJ#
1025 LPRINT;TAB(10);"1+C#+J=";1+C#+J
1030 NEXT J
1035 LPRINT "-----"
-----
1040 RETURN
1050 END
1100 REM CALCULATE Y!=YF
1110 YF=1
1120 IF Y=0 THEN GOTO 1160
1130 FOR I=1 TO Y
1140 YF=YF*I
1150 NEXT I
1160 RETURN
1200 REM CALCULATE THE SQUARE ROOT OF T#;SRT#
1210 REM BY NEWTON'S METHOD WITH ACCURACY 1D-17
1220 AC#=1D-17
1230 XO#=1
1240 XN#=((T#/XO#)+XO#)/2
1250 IF ABS(XN#-XO#)>AC# THEN XO#=XN#:GOTO 1240
1260 SRT#=XN#
1270 RETURN

```

```

1350 REM CALCULATE THE GAMMA FUNCTIONS, GAM#(XT#), BY USING
1360 REM THE FIVE POINTS AITKEN'S ITERATION METHOD
1370 DEF FNU#(X#,X0#,XN#,YN#)=(Y0#*(XN#-X#)-YN#*(X0#-X#))/(XN#-X0#)
1380 DEF FNV#(X#,X0#,X1#,XN#,YN#)=(FNU#(X#,X0#,X1#,Y1#)*(XN#-X#)-
FNU#(X#,X0#,XN#,YN#)*(X1#-X#))/(XN#-X1#)
1390 DEF FNW#(X#,X0#,X1#,X2#,XN#,YN#)=(FNV#(X#,X0#,X1#,X2#,Y2#)*(XN#-X#)-
FNV#(X#,X0#,X1#,XN#,YN#)*(X2#-X#))/(XN#-X2#)
)
1400 DEF FNY#(X#,X0#,X1#,X2#,X3#,XN#,YN#)=(FNW#(X#,X0#,X1#,X2#,X3#,Y3#)*
(XN#-X#)-FNW#(X#,X0#,X1#,X2#,XN#,YN#)*(X3#-
X#))/(XN#-X3#)
1410 REM GAM#(XT#)=MF#*GAM#(X#)
1440 X#=-XT#-INT(XT#-1)
1450 REM CALCULATE MF#
1460 IF XT#<0 THEN GOSUB 3750:GOTO 1550
1470 IF XT#>0 AND XT#<1 THEN MF#=(1/XT#):GOTO 1550
1480 MF#=1
1490 IF XT#=>1! AND XT#<=2! THEN GOTO 1550
1500 REM CALCULATE MF# FOR XT#>2
1510 FOR I=1 TO INT(XT#-1)
1520 MI#=(XT#-I)
1530 MF#*=MF#*MI#
1540 NEXT I
1550 REM SPECIFICATION OF THE FIVE POINTS :
1900 IF X#=>1.68 AND X#<1.7 THEN GOTO 3080
1930 IF X#=>1.74 AND X#<1.76 THEN GOTO 3170
2000 IF X#=>1.88 AND X#<1.9 THEN GOTO 3380
2010 IF X#=>1.9 AND X#<1.92 THEN GOTO 3410
2020 IF X#=>1.92 AND X#<1.94 THEN GOTO 3440
2030 IF X#=>1.94 AND X#<1.96 THEN GOTO 3470
2040 IF X#=>1.96 AND X#<1.98 THEN GOTO 3500
2050 IF X#=>1.98 AND X#<=2! THEN GOTO 3530
3080 X0#=1.68 :X1#=1.685:X2#=1.69 :X3#=1.695 :X4#=1.7
3090 Y0#=.9050010302000002# :Y1#=.9058818996000001# :Y2#=.9067818180000001#
3100 Y3#=.9077007850000001# :Y4#=.9086387329000001# :GOTO 3600
3170 X0#=1.74 :X1#=1.745 :X2#=1.75 :X3#=1.755 :X4#=1.76
3180 Y0#=.9168260252000002# :Y1#=.9179347950000001# :Y2#=.9190625268#
3190 Y3#=.9202092224000002# :Y4#=.9213748846000002# :GOTO 3600
3380 X0#=1.88 :X1#=1.885 :X2#=1.89 :X3#=1.895 :X4#=1.9
3390 Y0#=.9550708530000001# :Y1#=.9567153398# :Y2#=.9583793077000001#
3400 Y3#=.9600627927000002# :Y4#=.9617658391000001# :GOTO 3600
3410 X0#=1.9 :X1#=1.905 :X2#=1.91 :X3#=1.915 :X4#=1.92
3420 Y0#=.9617658319000001# :Y1#=.9634884632000001# :Y2#=.9652307261000001#
3430 Y3#=.9669926608000001# :Y4#=.9687743090000001# :GOTO 3600
3440 X0#=1.92 :X1#=1.925 :X2#=1.93 :X3#=1.935 :X4#=1.94
3450 Y0#=.9687743090000001# :Y1#=.9705757134000002# :Y2#=.9723969178#
3460 Y3#=.9742379672000001# :Y4#=.9770989075000001# :GOTO 3600
3470 X0#=1.94 :X1#=1.945 :X2#=1.95 :X3#=1.955 :X4#=1.96
3480 Y0#=.9760989075000001# :Y1#=.9779797861000001# :Y2#=.9798806513000001#
3490 Y3#=.9818015524000001# :Y4#=.9837425404000001# :GOTO 3600
3500 X0#=1.96 :X1#=1.965 :X2#=1.97 :X3#=1.975 :X4#=1.98
3510 Y0#=.9837425404000001# :Y1#=.9857036664000001# :Y2#=.9876649838000002#
3520 Y3#=.9896865462000001# :Y4#=.9917084087000001# :GOTO 3600
3530 X0#=1.98 :X1#=1.985 :X2#=1.99 :X3#=1.995 :X4#=2!
3540 Y0#=.9917084087000001# :Y1#=.9937506274# :Y2#=.9958132598#
3550 Y3#=.9978963643# :Y4#=1# :GOTO 3600

```



```

3600 U1#=FNU#(X#,XO#,X1#,Y1#)
3610 U2#=FNU#(X#,XO#,X2#,Y2#)
3620 U3#=FNU#(X#,XO#,X3#,Y3#)
3630 U4#=FNU#(X#,XO#,X4#,Y4#)
3640 V2#=FNV#(X#,XO#,X1#,X2#,Y2#)
3650 V3#=FNV#(X#,XO#,X1#,X3#,Y3#)
3660 V4#=FNV#(X#,XO#,X1#,X4#,Y4#)
3670 W3#=FNW#(X#,XO#,X1#,X2#,X3#,Y3#)
3680 W4#=FNW#(X#,XO#,X1#,X2#,X4#,Y4#)
3690 FY4#=FNY#(X#,XO#,X1#,X2#,X3#,X4#,Y4#)
3730 GAM#=-MF**FY4#
3740 RETURN
3750 REM CALCULATE MF# FOR XT#<0
3760 S#=-XT#
3770 FOR I=1 TO ABS(INT(XT#))
3780 SI#=(XT#+I)
3790 S#=-S**SI#
3800 NEXT I
3810 MF#=(1/S#)
3820 RETURN
3850 REM CALCULATE CFJ#
3860 IJ#=1
3870 BJ#=1
3880 IF J=0 THEN GOTO 3970
3890 FOR I=0 TO (J-1)
3900 BI#=(B#+I)
3910 BJ#=BJ**BI#
3920 NEXT I
3930 REM IJ#=I#^J
3940 FOR MO=1 TO J
3950 IJ#=IJ**I#
3960 NEXT MO
3970 CFJ#=IJ#/BJ#
3980 RETURN
4000 REM CALCULATE CLJ# & CSJ#
4010 NJ=N-J
4020 Y=J
4030 GOSUB 1100
4040 JF=YF
4050 Y=NJ
4060 GOSUB 1100
4070 NJF=YF
4080 CLJ#=((F#-K)-NJ)*((-2)^J)*NF)/(JF*NJF)
4090 CSJ#=-((F#-K)+NJ)*((-2)^J)*NF)/(JF*NJF)
4100 RETURN
4120 REM CALCULATE X#^P-XP#
4130 XP#=1
4140 IF P=0 THEN GOTO 4180
4150 FOR K1=1 TO P
4160 XP#=-XP**X#
4170 NEXT K1
4180 RETURN

```

```

4200 REM PROGRAM TO CALCULATE THE NATURAL LOGARITHM OF W#:NLW#
4210 REM NLW# = (2*W1#) + 2*(W1#^3)/3 + 2*(W1#^5)/5 + ....
4220 W1#=(W#-1)/(W#+1)
4230 NLW#=2*W1#
4240 J1=3
4250 X#=W1#:P=J1
4260 GOSUB 4120
4270 W1J#=(2*XP#)/P
4280 NLW#=NLW#+W1J#
4290 IF ABS(W1J#)>1D-17 THEN J1=J1+2:GOTO 4250
4300 RETURN
4350 REM PROGRAM TO CALCULATE EXP(Z#)=EXZ# FOR 0<Z#<1
4360 REM EXZ# = 1 + Z# + (Z#^2)/2! + (Z#^3)/3! + ....
4370 EXZ#=1
4380 L=1
4390 X#=Z#:P=L
4400 GOSUB 4120
4410 ZL#=XP#
4420 Y=L
4430 GOSUB 1100
4440 LF=YF
4450 ZLF#=ZL#/LF
4460 EXZ#=EXZ#+ZLF#
4470 IF ZLF#>1D-17 THEN L=L+1:GOTO 4390
4480 RETURN
4500 REM PROGRAM TO CALCULATE J#=(2*I#)^C#
4510 REM Z1#= LN(J#)=C#* LN(2*I#)=C#*((M1+1)*LN(2)+ LN(I1#))=C#*(Z2#+NLI1#)
4520 REM WHERE I#=(2^M1)*I1# AND 0.5<I1#<2.0
4530 REM M1=-FOR I#<0 &M1=+FOR I#>0
4540 REM CALAULATE I1# & M1
4550 M1=0
4560 I2=2^M1
4570 IF I#<1 THEN I1#=I#*I2:GOTO 4590
4580 I1#=I#/I2
4590 IF I1#<.5 OR I1#>2 THEN M1=M1+1:GOTO 4560
4600 REM NLJ#= LN(J#)
4610 NL2#=.6931471805599453#
4620 IF I#<1 THEN Z2#=(-M1+1)*NL2# :GOTO 4640
4630 Z2#=(M1+1)*NL2#
4640 W#=I1#
4650 GOSUB 4200
4660 NLI1#=NLW#
4670 Z1#=C#*(Z2#+NLI1#)
4680 REM FOR Z1#>0:J#=EXP(Z1#)=EXP(Z#)*EXP(INT(Z1#))
4690 REM FOR Z1#<0:J#=EXP(Z1#)=EXP(Z#)/EXP(ABS(INT(Z1#)))
4700 Z#=Z1#-INT(Z1#)
4710 REM Z# IS ALWAYS A POSITIVE NUMBER <1
4720 GOSUB 4350
4730 EX#=2.718281828459045#
4740 X#=EX#
4750 IF Z1#<0 THEN P=ABS(INT(Z1#)):GOTO 4770
4760 P=INT(Z1#)
4770 GOSUB 4120
4780 IF Z1#<0 THEN J#=EXZ#/XP# :GOTO 840
4790 J#=XP#*EXZ#
4800 GOTO 840

```

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