Nuclear-size effects
and a numerical approach to the Dirac equation

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Due to some current interest in this subject we have produced this note. There is no claim to anything new, except possibly to show that a direct numerical approach is quite simple and instructive. For comparison purposes we include a section on the Coulomb Klein-Gordon equation.

I. REVIEW OF DIRAC EQUATION AND PERTURBATION THEORY

The problem of a single electron in a central field is thoroughly discussed in Bjorken and Drell [1]. We also adopt some notation from [2]. The Hamiltonian

\[ H \psi = [\alpha \cdot \mathbf{p} + \beta m + V(r)]\psi = E\psi \]  

(1)

commutes with the total angular momentum

\[ J = L + S = \mathbf{r} \times \mathbf{p} + \frac{\sigma}{2}. \]

(2)

The four-component spinor \( \psi \) is constructed to be a simultaneous eigenfunction of \( H, J^2 \) and \( J_z \). It is convenient to write the general solution for a given \( j, m \) as

\[ \psi_{jm} = \begin{pmatrix} f(r) \\ \frac{r}{\kappa} \chi_{jm} \end{pmatrix}, \quad g(r) = \begin{pmatrix} -i \chi_{jm} \\ r \sigma \cdot \hat{r} \chi_{jm} \end{pmatrix}. \]

(3)

The parity \((\pm)\) refers to solutions with \( j = l \pm \frac{1}{2} \) where \( j \geq \frac{1}{2} \). The two-component spinors \( \chi^{(\pm)} \) are eigenstates of an auxiliary operator \( \hat{K} = -(1 + \sigma \cdot \mathbf{L}) \) such that \( K\chi = \kappa\chi \) with \( \kappa = \mp(j + \frac{1}{2}) \) for \( j = l \pm \frac{1}{2} \). With this notation the Dirac equation can be reduced to the following radial equations,

\[ \frac{df(r)}{dr} + \frac{\kappa}{r} f(r) - (E + m - V(r))g(r) = 0, \]
\[
\frac{dg(r)}{dr} - \frac{\kappa}{r} g(r) + (E - m - V(r)) f(r) = 0.
\] (4)

For the point charge potential \( V(r) = -\alpha/r \) the solutions are known. The energy eigenvalues are
\[
E_n = m \left[ 1 + \left( \frac{\alpha}{n - (j + \frac{1}{2}) + \sqrt{(j + \frac{1}{2})^2 - \alpha^2}} \right)^2 \right]^{-1/2}
\] (5)

where \( n \) is a positive integer and the angular momentum eigenvalues \( j \) range from \( \frac{1}{2} \) to \( j + \frac{1}{2} \leq n \). The ground-state has \( l = 0 \) which implies \( j = \frac{1}{2} \) and \( \kappa = -1 \), and \( n = 1 \) which implies the solution has zero nodes. Its energy is \( E = m \gamma \) where \( \gamma = \sqrt{1 - \alpha^2} \) and the corresponding solution is
\[
f(r) = (2m \alpha)^{3/2} \sqrt{\frac{1 + \gamma}{2 \Gamma(1 + 2 \gamma)}} (2m \alpha r)^{-\gamma - 1} e^{-\alpha r},
\]
\[
g(r) = \left( \frac{1 - \gamma}{\alpha} \right) f(r) r.
\] (6)

For this case \( \chi_{\frac{1}{2} m}^\pm \rightarrow \chi^m/\sqrt{4\pi} \) where the \( \chi^m \) is the usual up or down two-component spinor for \( m = \pm \frac{1}{2} \). Also note that there is another solution to the equations where \( f(r)/r \sim r^{-\gamma - 1} \) as \( r \rightarrow 0 \) rather than the \( r^{\gamma - 1} \) behavior in (6). But that solution is not normalizable.

We next consider the effect that the finite nuclear size has on the energy of the \( l = 0 \) states for any \( n \geq 1 \). Friar [2] obtained this in perturbation theory for a general nuclear charge distribution, and we summarize these results in the Appendix. He also considered various examples; here we focus on the uniformly charged sphere. Friar expresses the shift in energy due to the finite size as
\[
\Delta E = -\frac{(Z\alpha)^2 \mu}{2} \delta_B,
\] (7)

where \( \mu \) is the reduced mass \( Z \) is the nuclear charge. He then obtains
\[
\delta_B = \frac{\xi^2}{n^3} \sum_{i=0}^{2} \delta_i \xi^i + \frac{\delta \xi^2}{n^3} \Delta_R^R
\] (8)

where \( \xi = Z\alpha \mu R \), \( \delta = (Z\alpha)^2 \) and the \( \delta_i \) are
\[
\delta_0 = -\frac{4}{5}
\]
(9)
\[
\delta_1 = \frac{64}{63}
\]
(10)
\[
\delta_2 = -\frac{56954}{225225} + \frac{8}{25n} - \frac{2}{35n^2} - \frac{8}{25} \left( \psi(n) + 2\gamma + \log \left( \frac{2\xi}{n} \right) \right)
\]
(11)
\[
\Delta_R^R = \frac{4}{5} (\psi(n) + \log(2\xi/n) + 2\gamma) - \frac{4}{5n} + \frac{9}{5n^2} - \frac{45394}{17325}.
\] (12)

We shall stay in the infinite nuclear mass limit where the reduced mass \( \mu \) can be replaced by \( m \).
To get some sense of the relative size of the various perturbative contributions to $\Delta E$ we give some numerical values in Table I. We consider the electron and muon masses for $m$ and two choices of the proton charge radius $r_p$.

| perturbative order | electron (0.84) | muon (0.84) | electron (0.88) | muon (0.88) |
|--------------------|----------------|-------------|----------------|-------------|
| 1$^{st}$           | $-4.57105 \times 10^{-6}$ | $-40.408$ | $-5.01675 \times 10^{-6}$ | $-44.348$ |
| 2$^{nd}$           | $1.18951 \times 10^{-10}$ | $0.217422$ | $1.36766 \times 10^{-10}$ | $0.249985$ |
| 3$^{rd}$           | $7.33785 \times 10^{-15}$ | $0.00122601$ | $8.79555 \times 10^{-15}$ | $0.00146049$ |
| relativistic       | $-2.8115 \times 10^{-9}$ | $-0.0133812$ | $-3.07321 \times 10^{-9}$ | $-0.0145761$ |
| total correction   | $-4.57374 \times 10^{-6}$ | $-40.2027$ | $-5.01969 \times 10^{-6}$ | $-44.1112$ |

**TABLE I.** Contributions to $\Delta E$ in meV with $Z = n = 1$ and for $r_p = 0.84$ and 0.88.

We may also comment on the $r = 0$ boundary condition for the finite size charge where the potential is no longer singular. Now the two apparent $\ell = 0$ solutions behave like $f(r)/r \sim \text{constant}$ or $1/r$ respectively as $r \to 0$. Both are normalizable but the second one has another problem. As can be seen in the following section, $f(r)/r$ satisfies an equation with terms that correspond to the radial laplacian. But a laplacian acting on a $1/r$ wave function produces a $\delta$-function. This means that this apparent second solution is in fact not a solution.

**II. NUMERICAL APPROACH USING MAPLE**

We need an environment where a differential equation can be solved to high precision and where this equation can involve a piecewise defined function. Maple is such an environment, and here we will make our approach explicit by giving the Maple code.

```maple
Digits := 20:
st1 := method = ck45, abserr = 10^(-15), relerr = 10^(-15), maxfun = 100000:
```

The radius $a$ of a uniformly charged sphere in $1/\text{MeV}$ based on $r_p \approx 0.88$ fm is given.

```maple
l1 := {a = .88*sqrt(5./3.)/197.3, alpha = 1/137.035999}:
mmu := 105.65837: me := .51099894:
```

We want to compare to the Friar result for the energy shift due to the finite size effect. This is his result for the $n = 1$ ground state with $Z = 1$. 
Here are these shifts for the muon and the electron in MeV.

```plaintext
> subs(m = mmu, l1, EB): q1 := evalf(%);
q1 := 0.000000044123175857857733137
> subs(m = me, l1, EB): q2 := evalf(%);
q2 := 5.0210593674052689345 × 10^{-15}
```

The following ratio then gives the residual mass dependence of these shifts beyond the trivial $m^3$ dependence.

```plaintext
> q1/q2*(me/mmu)^3;
0.99407622263401855408
```

We want to obtain this same ratio by numerically solving the Dirac equation. We consider the point charge potential,

```plaintext
> V1 := (alpha, a, r) -> -alpha/r ;
V1 := (α, a, r) ↦ −α/r
```

and the potential for the uniformly charge sphere with radius $a$.

```plaintext
> V2 := (alpha, a, r) -> piecewise(r < a, (1/2)*alpha*(r^2/a^2-3)/a, -alpha/r);
V2 := (α, a, r) ↦ \begin{cases} 
1/2 \frac{α}{a} \left( \frac{r^2}{a^2} - 3 \right) & r < a \\
- \frac{α}{r} & \text{otherwise}
\end{cases}

> plot(V2(1, 1, r), r = 0 .. 5);
```
The Dirac equation for the ground state reduces to following equations for $f(r)$ and $g(r)$ . (Maple will interpret these expressions as equations.)

> $e1:=\text{diff}(f(r), r)-f(r)/r-(E+m-V(\alpha, a, r))*g(r)$;
> 
> $e2:=\text{diff}(g(r), r)+g(r)/r+(E-m-V(\alpha, a, r))*f(r)$;

We convert these into a second order equation.

> $\text{isolate}(e1, g(r))$;
> $\text{subs}(%, e2)$;
> $\text{numer}(%)$;
> $e3:=\text{simplify}(%/r)$;

Then for the point charge the equation is

> $e4:=\text{subs}(V = V1, e3)$;

We check the exact solution and the corresponding energy.

> $f(r) = r^\sqrt{-\alpha^2+1}\exp(-m\alpha r)$, $E = m\sqrt{-\alpha^2+1}$;
> $\text{subs}(%, e4)$ : $\text{simplify}(%)$;

For the uniformly charge sphere the equation to solve is the following.
> e5 := subs(V = V2, e3):

Since Maple can handle piecewise functions there is no need to do matching across the boundary \( r = a \). So we numerically integrate this equation from the origin with boundary conditions \( f(0) = 0 \) and \( D(f)(0) = 1 \). We are not interested in the normalization of \( f(r) \). We adjust \( E \) via the shooting method to obtain the zero nodes solution with \( f(\infty) = 0 \). For the electron case:

\[
> Ee := 0.5109853341259963716:
> \]

\[
> ip := 0: ic := \{f(ip) = ip, (D(f))(ip) = 1\}:
> \]

\[
> eq := \{subs(m = me, l1, E = Ee, e5)\}:
> \]

\[
> s1 := dsolve(eq union ic, \{f(r)\}, type = numeric, st1):
> \]

\[
> odeplot(s1, [r, f(r)], ip .. 9000);
> \]

For the muon:

\[
> Emu := 105.655556781007189:
> \]

\[
> ip := 0: ic := \{f(ip) = ip, (D(f))(ip) = 1\}:
> \]

\[
> eq := \{subs(m = mmu, l1, E = Emu, e5)\}:
> \]

\[
> s1 := dsolve(eq union ic, \{f(r)\}, type = numeric, st1):
> \]

\[
> odeplot(s1, [r, f(r)], ip .. 38);
> \]
We need to compare these energies to the exact energies for the point charge case.

\[ q_3 := \text{subs}(m = \text{mmu}, l_1, m*\text{sqr}(-\alpha^2+1)) \]
\[ q_3 := 105.65555673688407403 \]

\[ q_4 := \text{subs}(m = \text{me}, l_1, m*\text{sqr}(-\alpha^2+1)) \]
\[ q_4 := 0.51098533412599135054 \]

The differences in these respective energies give the energy shifts due to the finite size effect.

\[ q_5 := E_{\mu} - q_3 \]
\[ q_5 := 0.000000044123114970000000000 \]

\[ q_6 := E_{e} - q_4 \]
\[ q_6 := 5.02106000000000000 \times 10^{-15} \]

The ratio of these shifts can be compared to the Friar result above. The difference is in the 6th digit, which corresponds to about the accuracy we have gone.

\[ \frac{q_5}{q_6} \times (\text{me}/\text{mmu})^3 \]
\[ 0.99407472561492135455 \]

As a test of our numerical integration we can obtain \( f(r) \) for the point charge case. The point charge equation is \( e_4 \), but Maple finds this too singular to integrate from zero. Therefore we obtain a series expansion around zero and then use that to set initial conditions slightly away from zero. We use the series solution that behaves like \( r^{\sqrt{-\alpha^2+1}} \) near the origin rather than the one that behaves like \( r^{-\sqrt{-\alpha^2+1}} \).

\[ \text{Order} := 4: \]
\[ \text{dsolve}(e_4, \{f(r)\}, \text{series}) : \]
\[ \text{subs}(_\text{C1} = 0, _\text{C2} = 1, \%) : \]
\[ e_6 := \text{convert}(_\text{rhs}(%), \text{polynom}) : \]

There is no shooting needed here since we know \( E \). Using \( E = q_4 \) for the electron:

\[ \text{l2 := E = q_4: \ ip := 10^{-5}:} \]
\[ \text{subs}(m = \text{me}, l_1, l_2, e_6): \]
\[ \text{ic := \{f(ip) = subs(r = ip, \%), (D(f))(ip) = subs(r = ip, \text{diff}(\%, r))\}}: \]
\[ \text{eq := \{subs(m = me, l_1, l_2, e_4)\} :} \]
\[ \text{s1 := dsolve(eq union ic, \{f(r)\}, \text{type = numeric, st1}) :} \]
\[ \text{odeplot(s1, [[r, f(r)]]}, \]
\[ [r, \text{subs}(m = \text{me}, l_1, r^{\text{sqr}(-\alpha^2+1)}*\exp(-m*\alpha*r))], \]
\[ \text{ip .. 9000};]
We have plotted the resulting numerical \( f(r) \) along with the exact result and the agreement is excellent. The same works for the muon.

\[
\begin{align*}
12 &: E = q_3: \quad i_p := 10^{-5}; \\
& subs(m = mmu, l1, 12, e6); \\
& ic := \{f(i_p) = subs(r = i_p, \%), (D(f))(i_p) = subs(r = i_p, \text{diff}(\%, r))\}; \\
& eq := \{subs(m = mmu, l1, l2, e4)\}; \\
& s1 := dsolve(eq \cup ic, \{f(r)\}, \text{type} = \text{numeric}, \text{st1}); \\
& odeplot(s1, [[r, f(r)], [r, subs(m = mmu, l1, r^sqrt(-alpha^2+1)*exp(-m*alpha*r))]], i_p .. 38);
\end{align*}
\]

By using the point charge case as a check we could increase the accuracy of the calculations and push the result for the residual mass dependence beyond 6 digits. But already we see that Friar’s perturbative calculations are very accurate.
III. NUCLEAR-SIZE EFFECT AND THE COULOMB KLEIN-GORDON EQUATION

Due to some current misconceptions, we present an extended aside on the application of first-order perturbation theory to the nuclear-size effect within the Coulomb Klein-Gordon equation.

The stationary Klein-Gordon Coulomb equation can be written as

\[ \nabla^2 + U(r) + k^2 \psi = 0 \]  

where \( k^2 = \omega^2 - m^2 \) and \( U(r) = 2\omega A_0 - A_0^2 = -\frac{2\omega\alpha}{r} - \frac{\alpha^2}{r^2} \)  

The energy eigenvalues for the Klein-Gordon Coulomb equation are

\[ \omega_{nl} = \frac{m}{\sqrt{1 + \alpha^2 (n - l + 1/2 + \sqrt{(l + 1/2)^2 - \alpha^2})^2}} \]  

A solution to the radial \( l = 0 \) equation is \( W(\lambda, \mu, \beta r)/r \) where \( W(\lambda, \mu, \beta r) \) is the Whittaker function and \( \lambda = \alpha \omega / \sqrt{m^2 - \omega^2} \), \( \mu = \sqrt{1/4 - \alpha^2} \), \( \beta = 2\sqrt{m^2 - \omega^2} \)  

We can rewrite the Klein Gordon equation as a Schrödinger-type equation with \( V(r) = -\alpha/r \)

\[ \left[ -\frac{\nabla^2}{2m} + \tilde{U}(r) \right] \psi = \epsilon \psi \]  

where \( \epsilon = \omega - m, \omega + m \approx 2m \) and \( \tilde{U}(r) = -\frac{\alpha}{r} - \frac{\alpha^2}{2mr^2} = V(r) - \frac{V^2(r)}{2m} \)  

We will now change the short-range potential to \( V_{\text{core}}(r) \) and assume it is produced by a spherical charge of radius \( a \). Thus

\[ V_{\text{core}}(r) = \frac{\alpha}{2a} \left[ \left( \frac{r}{a} \right)^2 - 3 \right] \]  

The perturbation is therefore

\[ \tilde{U}(r)_{\text{pert}} = V_{\text{core}} - \frac{V_{\text{core}}^2(r)}{2m} - V(r) + \frac{V^2(r)}{2m} \]
The first-order perturbative correction is given by

$$\Delta E_1 = N^2 \int_0^a \tilde{U}_{\text{pert}}(r)W(\lambda, \mu, \beta r)^2 \, dr \tag{21}$$

where $N$ is a normalization constant.

This integral can be done exactly but yields an extremely long expression. By expanding out the resulting Gamma functions $\Gamma(s)$, and incomplete Gamma functions $\Gamma(s, x)$, and keeping only the leading terms, an excellent approximation $\Delta E_1^a \approx \Delta E_1$ is obtained:

$$\Delta E_1^a = \frac{am^2 \alpha^4}{29400} \times \left[ 48\alpha(630 + (4807 - 1260\gamma)\alpha^2) \\
+ 49 am \left( 240 + (1201 - 480\gamma)\alpha^2 \right) \\
+ 560 \alpha^2 \log(2am\alpha)(7am(5am\alpha - 6) - 108\alpha) \right] \tag{22}$$

The dominant two terms in this expression are $\Delta E_1^a \approx 36/35 am^2 \alpha^5 + 2/5 a^2 m^3 \alpha^4$ (c.f. Dirac $2/5 a^2 m^3 \alpha^4$. Note that the first term dominates in the electron case and that the second term dominates in the muon case.)

Note that if one doesn’t assume that $\omega + m \approx 2m$, but writes

$$\tilde{U}(r)_{\text{pert}} = \frac{\omega}{m} V_{\text{core}} - \frac{V_{\text{core}}^2(r)}{2m} - \frac{\omega}{m} V(r) + \frac{V^2(r)}{2m} \tag{23}$$

one obtains an additional higher-order effect of

$$\delta \Delta E_1^a = -\frac{1}{5} a^2 \alpha^6 m^3 \tag{24}$$

i.e.

$$\Delta E_1^a = \frac{am^2 \alpha^4}{29400} \times \left[ 48\alpha(630 + (4807 - 1260\gamma)\alpha^2) \\
+ 49 am \left( 240 + (1081 - 480\gamma)\alpha^2 \right) \\
+ 560 \alpha^2 \log(2am\alpha)(7am(5am\alpha - 6) - 108\alpha) \right] \tag{25}$$

Appendix A: Nuclear-size corrections for a general charge distribution

Friar[2] finds

$$\Delta E_n = \frac{2\pi}{3} |\phi_n(0)|^2 Z\alpha \left( \langle r^2 \rangle - \frac{Z\alpha\mu}{2} \langle r^3 \rangle_{(2)} + (Z\alpha)^2 F_{\text{REL}} + (Z\alpha\mu)^2 F_{\text{NR}} \right) \tag{A1}$$

where

$$\langle r^p \rangle_{(2)} = \int d^3 s \, d^3 r \, \rho(r)\rho(s)|\mathbf{r} - \mathbf{s}|^p \tag{A2}$$
\[ F_{\text{REL}} = -\langle r^2 \rangle (\log(\beta r)) + \psi(n) + 2\gamma - 2 - \frac{\langle r^3 \rangle (1/r)}{3} + I_2^{\text{REL}} + I_3^{\text{REL}} \]  

(A3)

\[ F_{\text{NR}} = \frac{\langle r^4 \rangle}{10} + \frac{2}{3} \langle r^2 \rangle \langle r^2 \log(\beta r) \rangle + \frac{2}{3} \langle r^2 \rangle^2 (\psi(1) + 2\gamma - \frac{7}{3}) + \langle r^3 \rangle + \langle r^5 \rangle (1/r) + I_2^{\text{NR}} + I_3^{\text{NR}} \]  

(A4)

\[ I_2 = \int d^3 s \rho(s) \int d^3 t \rho(t) J^{(2)}(s, t) \Theta(s-t) \]  

(A5)

\[ I_3 = \int d^3 u \rho(u) \int d^3 t \rho(t) \int d^3 s \rho(s) J^{(3)}(s, t, u) \Theta(u-t) \Theta(t-s) + \text{sym.} \]  

(A6)

\[ J^{(2)}_{\text{REL}}(s, t) = -(t^2 + s^2) \ln(s/t) - \frac{t^3}{3s} + \frac{s^3 - t^2}{3} \]  

(A7)

\[ J^{(3)}_{\text{REL}}(s, t, u) = -\frac{s^2}{3} \ln(s/t) - \frac{s^4}{45tu} + \frac{s^3}{9} \left( \frac{1}{u} + \frac{1}{t} \right) + \frac{s^2 t^2}{36u^2} - \frac{2s^2 t}{9u} + \frac{s^2}{9} \]  

(A8)

\[ J^{(2)}_{\text{NR}}(s, t) = \frac{t^5}{9s} - \frac{s^5}{9t} + t^3s - s^3t + \frac{(s^4 - t^4)}{2} + \frac{2s^2 t^2}{3} \ln(s/t) \]  

(A9)

\[ J^{(3)}_{\text{NR}}(s, t, u) = \frac{2s^2 t u}{3} + \frac{s^4 u}{15t} - \frac{s^3 u}{3} + \frac{2s^2 t^3}{27u} + \frac{s^4 t}{15u} + \frac{8s^6}{945tu} - \frac{s^5}{27u} - \frac{2s^2 t^2 \ln(t/u)}{9} + \frac{2s^2 t^2}{27} - \frac{s^4 t}{3} - \frac{s^5}{27t} + \frac{s^4}{6} \]  

(A10)

\[ |\phi_n(0)|^2 \equiv (Z\alpha \mu)^3 / \pi n^3, \beta = 2Z\alpha \mu / n, \psi(n) \text{ is the digamma function and } \gamma \text{ is Euler's constant.} \]

For completeness we give the correction due to recoil when keeping a finite nuclear mass.

\[ \Delta E_R = -\frac{(Z\alpha)^4 \mu^2}{8m_N} - \frac{(Z\alpha)^5 \mu^3}{8m_N} \langle r \rangle_{(2)} + \Delta E_{RB}^{\text{non-B}}. \]  

(A11)

\[ \langle r \rangle_{(2)} = \frac{36}{35} R \text{ for the uniform sphere. } \Delta E_{RB}^{\text{non-B}}, \text{ the "non-Breit" finite size correction of order } (Z\alpha)^5, \text{ is expected to be small.} \]

[1] J. D. Bjorken and S. D. Drell, “Relativistic quantum mechanics,” McGraw-Hill, New York, 1964, ISBN-0070054932.

[2] J. L. Friar, Annals Phys. 122, 151 (1979).