Note for solution of spherical Dirac equation (DEQURK)

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1 Convention and basic formalism

We deal with the Dirac equation for spherical systems and its numerical solution in this note. First see TABLE 1 for basic conventions. In this note, I use the CGS-Gauss system of unit, and the typical units for the length and energy are of the nuclear physics, namely, fm and MeV. Note that $\hbar c \cong 197$ MeV·fm.

TABLE 1: Conventional rules in this note.

Name	Quantity	Definition
flat metric	$g^{\mu\nu} = g_{\mu\nu}$	$= diag(+,-,-,-)$
4D coordinate	$x^\mu = (x^0, x^1, x^2, x^3)$	$= (ct, x, y, z)$
	$x_\mu = (x_0, x_1, x_2, x_3)$	$= (ct, -x, -y, -z)$
4D derivative	$\partial^\mu = \frac{\partial}{\partial x_\mu}$	$= \left(\frac{\partial}{c\partial t},\ -\vec{\nabla}\right)$
	$\partial_\mu = \frac{\partial}{\partial x^\mu} = g_{\mu\nu}\partial^\nu$	$= \left(\frac{\partial}{c\partial t},\ \vec{\nabla}\right)$
4D momentum	$p^\mu = (p^0, p^1, p^2, p^3) = i\hbar\partial^\mu$	$= \left(\frac{E}{c}, \vec{p}\right)$
	$p_\mu = g_{\mu\nu}p^\nu$	$= \left(\frac{E}{c}, -\vec{p}\right)$
gamma matrices	$\gamma^\mu = \left(\gamma^0, \vec{\gamma}\right)$	$= (\beta, \beta\vec{\gamma})$
reduced derivative	$\gamma^\mu\partial_\mu = \gamma_\mu\partial^\mu$	$= \gamma^0\partial_{ct} + \vec{\gamma}\cdot\vec{\nabla}$

1.1 spin algebra

Pauli's sigma matrices read

$$\hat{s}_x \equiv \frac{\sigma_1}{2},\quad \hat{s}_y \equiv \frac{\sigma_2}{2},\quad \hat{s}_z \equiv \frac{\sigma_3}{2},\quad \text{where}\quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

These satisfy $\sigma_i\sigma_j = \delta_{ij} + i\epsilon^{ijk}\sigma_k$, and thus,

$$\begin{aligned} &\sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}, \\ &\sigma_i\sigma_j - \sigma_j\sigma_i = 2i\epsilon^{ijk}\sigma_k \Longleftrightarrow [\hat{s}_i, \hat{s}_j] = i\epsilon^{ijk}\hat{s}_k. \end{aligned} \tag{2}$$

It is also worthwhile to define $\sigma_{0,\pm 1}$:

$$\sigma_0 = \sigma_{3(z)},\quad \sigma_\pm \equiv \frac{1}{\sqrt{2}}\left(\sigma_{1(x)} \pm i\sigma_{2(y)}\right). \tag{3}$$

1.2 gamma matrices

In Dirac's representation, the (4×4) gamma matrices are defined as

$$\gamma^\mu = (\gamma^0, \vec{\gamma}) \equiv (\beta, \beta\vec{\alpha}), \tag{4}$$

where

$$\gamma^0 = \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},\quad \vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \longleftrightarrow \gamma^k = (\beta\vec{\alpha})^k = \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0 \end{pmatrix}. \tag{5}$$

Note that $\gamma_0 = \gamma^0$. The following matrices are also useful:

$$\gamma_5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix},\quad \sigma^{\mu\nu} = \frac{i}{2}\left[\gamma^\mu, \gamma^\nu\right]. \tag{6}$$

Dirac's conjugate:

$$\bar{\psi}(x) \equiv \psi^\dagger(x)\gamma^0. \tag{7}$$

Thus,

$$\bar{\psi}_a(x)\psi_b(x) = F_a^*(x)F_b(x) - G_a^*(x)G_b(x),\quad \bar{\psi}_a(x)\gamma^0\psi_b(x) = F_a^*(x)F_b(x) + G_a^*(x)G_b(x). \tag{8}$$

1.3 angular-momentum convention

Clebsch-Gordan (CG) coefficient:

$$\mathcal{C}^{(J,M)j_1,j_2}_{m_1,m_2} \equiv \langle j_1, m_1; j_2, m_2 \mid (j_1 j_2) J, M \rangle \iff |J, M\rangle = \sum_{m_1,m_2} \mathcal{C}^{(J,M)j_1,j_2}_{m_1,m_2} |j_1, m_1\rangle |j_2, m_2\rangle . \tag{9}$$

Note EQs. (3.5.14) and (3.5.17) in Edmonds's textbook [1]:

$$\mathcal{C}^{(J,M)j_2,j_1}_{m_2,m_1} = P\mathcal{C}^{(J,M)j_1,j_2}_{m_1,m_2}, \quad \mathcal{C}^{(J,-M)j_1,j_2}_{-m_1,-m_2} = P\mathcal{C}^{(J,M)j_1,j_2}_{m_1,m_2}, \tag{10}$$

where $P = (-)^{j_1+j_2-J}$. CG coefficients can be defined as REAL in any case.

The 3j symbol as in EQ. (3.7.3) in Edmonds's textbook [1]:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & -m_3 \end{pmatrix} \equiv \frac{(-)^{j_1-j_2+m_3}}{\sqrt{2j_3+1}} \mathcal{C}^{(j_3,m_3)j_1,j_2}_{m_1,m_2} = \begin{pmatrix} j_3 & j_1 & j_2 \\ -m_3 & m_1 & m_2 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & -m_3 & m_1 \end{pmatrix}. \tag{11}$$

Note that, for the 3j-symbol, an even permutation of any two columns keeps it identical, whereas an odd permutation yields the factor $(-)^{j_1+j_2+j_3}$ as in EQ. (3.7.5) in Ref. [1].

Double-bar matrix element (DBME) or reduced matrix element as in EQ. (5.4.1) in Ref. [1]:

$$\begin{aligned} \left\langle j', m' \mid \hat{T}_{K,M} \mid j, m \right\rangle &= (-)^{j'-m'} \begin{pmatrix} j' & K & j \\ -m' & M & m \end{pmatrix} \left\langle j' \parallel \hat{T}_K \parallel j \right\rangle \\ &= \frac{(-)^{j'+K-j}}{\sqrt{2j'+1}} \mathcal{C}^{(j',m')K,j}_{M,m} \left\langle j' \parallel \hat{T}_K \parallel j \right\rangle = \frac{(-)^{j-m}}{\sqrt{2K+1}} \mathcal{C}^{(K,M)j',j}_{m',-m} \langle ... \rangle . \end{aligned} \tag{12}$$

1.4 Dirac spinor

Dirac spinor for the spherical system is generally given as

$$\psi_N(\boldsymbol{r}) = \psi_{nljm}(\boldsymbol{r}) = \begin{pmatrix} iF_N(\boldsymbol{r}) \\ \\ G_N(\boldsymbol{r}) \end{pmatrix} = \begin{pmatrix} if_{nlj}(r)\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \\ \\ g_{nlj}(r)\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \end{pmatrix}, \tag{13}$$

where

$$\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \equiv \sum_{v=\pm 1/2} \mathcal{C}^{(j,m)l,\frac{1}{2}}_{h,v} Y_{l,h=m-v}(\bar{\boldsymbol{r}}) \cdot \chi_v. \tag{14}$$

Of course, $\hat{s}_z \chi_{\pm\frac{1}{2}} = \pm\frac{1}{2}\chi_{\pm\frac{1}{2}}$. Note also that

$$\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) = \mathcal{Y}_{\ell jm}(\bar{\boldsymbol{r}}), \tag{15}$$

where $\ell = l \mp 1$ when $l = j \pm \frac{1}{2}$. Thus, the Dirac spinor can be reformulated as

$$\psi_{nljm}(\boldsymbol{r}) = \begin{pmatrix} if_{nlj}(r)\mathcal{Y}_{(l=j\pm 1/2)jm}(\bar{\boldsymbol{r}}) \\ g_{nlj}(r)\mathcal{Y}_{(\ell=j\mp 1/2)jm}(\bar{\boldsymbol{r}}) \end{pmatrix}. \tag{16}$$

Remember also that $(\vec{\sigma}\cdot\boldsymbol{r}/r)^2 = r^2/r^2 = 1$. For example, when the larger component has the $d_{5/2}$ ($l = 2$) character, the corresponding smaller component has the $f_{5/2}$ ($\ell = 3$) char-actor. Table 2 lists some sets of (l, ℓ).

TABLE 2: Angular quantum numbers for spherical Dirac spinors.

larger	smaller	(l, ℓ)
$s_{1/2}$	$p_{1/2}$	(0,1)
$p_{3/2}$	$d_{3/2}$	(1,2)
$p_{1/2}$	$s_{1/2}$	(1,0)
$d_{5/2}$	$f_{5/2}$	(2,3)
$d_{3/2}$	$p_{3/2}$	(2,1)

1.5 units

We assume the (1 + 3)-dimensional time and space as well as the CGS-Gauss system of units in this note. In the MKSA or CGS-Gauss system of units, except the electro-magnetic terms, the Dirac equation is given as

$$i\hbar\frac{\partial}{\partial t}\psi(t,\boldsymbol{r}) = \left[-i\hbar c\beta\vec{\gamma}\cdot\vec{\nabla} + \beta Mc^2 + W\right]\psi(t,\boldsymbol{r}), \tag{17}$$

where W is some external potential in the unit of energy (e.g., MeV). From $\beta\beta = I$ and $\gamma^\mu\partial_\mu = \beta\partial_{ct} + \vec{\gamma}\cdot\vec{\nabla}$, it is also expressed as

$$\left[i\hbar c\gamma^\mu\partial_\mu - Mc^2 - \beta W\right]\psi(t,\boldsymbol{r}) = 0. \tag{18}$$

The Lagrangian density, which works as the source of this equation, reads

$$\mathcal{L} = \bar{\psi}\left[i\hbar c\gamma^\mu\partial_\mu - Mc^2 - \beta W\right]\psi(x), \tag{19}$$

where $\bar{\psi} \equiv \psi^\dagger\beta$. Note that, because the Lagrangian $L \equiv \int d^3\boldsymbol{r}\mathcal{L}$ and Mc^2 have the dimension of energy, $\bar{\psi}\psi$ is in the unit of fm^{-3}. As coincidence, if some interaction term(s) has the form, $\mathcal{L}_{\rm I} = \bar{\psi}X\psi(x)$, then this wild-card part X must have the dimension of energy, e.g. in MeV. This knowledge may help us, for example, to infer the unit of the coupling constant.

For dimensional analysis, the action must satisfy $[S]_D = \left[\int dt \int d^3\boldsymbol{r}\mathcal{L}\right]_D = ET$, since Lagrangian (as well as Hamiltonian) keeps the dimension of energy, $\left[d^3\boldsymbol{r}\mathcal{L}\right]_D = E = ML^2T^{-2}$. Thus, Lagrangian density has $[\mathcal{L}]_D = EL^{-3}$. Note that, in the MKSA or CGS-Gauss system of units, the dimensional analysis concludes that,

$$[c^2\cdot\text{mass}]_D = [\text{energy}]_D = \left[\frac{\hbar c}{\text{length}}\right]_D = \left[\frac{\hbar}{\text{time}}\right]_D = E. \tag{20}$$

Note for "Plank's natural system of units" - In the Plank's natural system of units, one assumes that $\hbar \equiv 1$ and $c \equiv 1$. With this assumption, dimensions of mass, energy, length, and time can be related as

$$[\text{mass}]_D = [\text{energy}]_D = \left[\frac{1}{\text{length}}\right]_D = \left[\frac{1}{\text{time}}\right]_D = M^{+1}. \tag{21}$$

TABLE 3: Dimensional numbers of some quantities, $[\text{Quantity}]_D$.

Quantity	In MKSA or CGS-Gauss	In Plank's natural
mass	M	M^{+1}
time and length	T and L	M^{-1}
energy	$E = ML^2T^{-2}$	M^{+1}
$\mathcal{L}$ or $\mathcal{H}$	EL^{-3}	M^{+4}
$\bar{\psi}\psi(x)$	L^{-3}	M^{+3}
$\phi^2(x)$ (scalar boson)	$E^{-1}L^{-3}$	M^{+2}
$A^\mu A_\mu(x)$ (vector boson)	$E^{-1}L^{-3}$	M^{+2}

2 Dirac equation with spherical potential(s)

We discuss the spherical Dirac equation in the following form:

$$i\hbar c\frac{\partial}{\partial(ct)}\psi(t,\boldsymbol{r}) = \left[-i\hbar c\beta\vec{\gamma}\cdot\vec{\nabla} + \beta Mc^2 + \beta S(r) + W(r)\right]\psi(t,\boldsymbol{r}), \tag{22}$$

where $S(r)$ and $W(r)$ are the spherical, scalar and vector potentials, respectively, given in the unit of energy (e.g., MeV). From $\beta\beta = I$ and $\gamma^\mu\partial_\mu = \beta\partial_{ct} + \vec{\gamma}\cdot\vec{\nabla}$, it is also expressed as

$$\left[i\hbar c\gamma^\mu\partial_\mu - Mc^2 - S(r) - \beta W(r)\right]\psi(t,\boldsymbol{r}) = 0. \tag{23}$$

The Lagrangian density, which works as the source of this equation, reads

$$\mathcal{L} = \bar{\psi}\left[i\hbar c\gamma^\mu\partial_\mu - Mc^2 - S(r) - \beta W(r)\right]\psi(x), \tag{24}$$

where $\bar{\psi} \equiv \psi^\dagger \beta$. Note that, in the meson-exchange model for atomic nuclei, the potential terms are obtained from the sigma and omega meson fields. That is, $S(r) = g_\sigma \sigma(r)$ and $W(r) = g_\omega \omega(r)$ with $\omega_\mu = \delta_{\mu 0}\omega(r)$, respectively. In numerical calculations, these meson fields need to be solved self-consistently to the fermion field. In the following, however, these potentials are given as the external input parameters.

2.1 large and small components

For the time-independent solution of EQ. (22), that is, $i\hbar\partial_t \psi = E_N \psi$, the Dirac equation reads

$$\left[-i\hbar c\beta\vec{\gamma}\cdot\vec{\nabla} + \beta Mc^2 + \beta S(r) + W(r)\right]\psi_N(t,\boldsymbol{r}) = E_N \psi_N(t,\boldsymbol{r}). \tag{25}$$

Dirac spinor for the spherical system is generally given as in EQ. (13). In addition, we use $f_{nlj}(r) = a_{nlj}(r)/r$ and $g_{nlj}(r) = b_{nlj}(r)/r$ in the following sections. Therefore,

$$\psi_N(\boldsymbol{r}) = \psi_{nljm}(\boldsymbol{r}) = \begin{pmatrix} iF_N(\boldsymbol{r}) \\ \\ G_N(\boldsymbol{r}) \end{pmatrix} = \begin{pmatrix} i\frac{a_{nlj}(r)}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \\ \\ \frac{b_{nlj}(r)}{r}\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \end{pmatrix}, \tag{26}$$

where

$$\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \equiv \sum_{v=\pm 1/2} \mathcal{C}_{h,v}^{(j,m)l,\frac{1}{2}} Y_{l,h=m-v}(\bar{\boldsymbol{r}})\cdot\chi_v, \quad \text{with} \quad \hat{s}_z\chi_{\pm\frac{1}{2}} = \pm\frac{1}{2}\chi_{\pm\frac{1}{2}}. \tag{27}$$

Remember that $\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) = \mathcal{Y}_{\ell jm}(\bar{\boldsymbol{r}})$, where $\ell = l \mp 1$ when $l = j \pm \frac{1}{2}$.

By using this ansatz EQ. (26), the EQ. (25) is transformed as

$$\begin{aligned} -i\hbar c\vec{\sigma}\cdot\vec{\nabla}G_N(\boldsymbol{r}) + \left[Mc^2 + S(r) + W(r)\right]iF_N(\boldsymbol{r}) &= E_N iF_N(\boldsymbol{r}), \\ -i\hbar c\vec{\sigma}\cdot\vec{\nabla}iF_N(\boldsymbol{r}) + \left[-Mc^2 - S(r) + W(r)\right]G_N(\boldsymbol{r}) &= E_N G_N(\boldsymbol{r}). \end{aligned} \tag{28}$$

Before going to the further calculations, now we focus on the $\vec{\sigma}\cdot\vec{\nabla}$ term. By using,

$$\left(\vec{\sigma}\cdot\vec{A}\right)\left(\vec{\sigma}\cdot\vec{B}\right) = \vec{A}\cdot\vec{B} + i\vec{\sigma}\cdot\left(\vec{A}\times\vec{B}\right) , \tag{29}$$

then the operator $\vec{\sigma}\cdot\vec{\nabla}$ becomes

$$\begin{aligned} \vec{\sigma}\cdot\vec{\nabla} &= \frac{(\vec{\sigma}\cdot\vec{r})^2}{r^2}\vec{\sigma}\cdot\vec{\nabla} = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}(\vec{\sigma}\cdot\vec{r})(\vec{\sigma}\cdot\vec{\nabla}) \\ &= \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left[\vec{r}\cdot\vec{\nabla} + i\vec{\sigma}\cdot(\vec{r}\times\vec{\nabla})\right] \\ &= \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left[\vec{r}\cdot\vec{\nabla} - \vec{\sigma}\cdot\vec{L}/\hbar\right] = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left[r\frac{d}{dr} - \frac{2\vec{S}\cdot\vec{L}}{\hbar^2}\right], \end{aligned} \tag{30}$$

where we have used $\vec{\sigma} = 2\vec{S}/\hbar$, $i\vec{\nabla} = -\vec{p}/\hbar$, and $\vec{L} = \vec{r}\times\vec{p}$. Namely, the spin-orbit coupling is naturally concluded from "kinetic term" in the Dirac formalism. If the gap of potentials, $S(r) - W(r)$, is constant, this spin-orbit term vanishes, as we see in the following.

2.2 spin-orbit coupling and Darwin term

Before going to the numerical solution, we check several characters of the Dirac equation. From EQ. (28),

$$G_N(\boldsymbol{r}) = \frac{-i\hbar c}{E_N + Mc^2 + S(r) - W(r)}\vec{\sigma}\cdot\vec{\nabla}iF_N(\boldsymbol{r}). \tag{31}$$

Thus, the corresponding large component reads

$$-(\hbar c)^2\vec{\sigma}\cdot\vec{\nabla}\frac{\vec{\sigma}\cdot\nabla i\vec{F_N}(\boldsymbol{r})}{E_N + Mc^2 + S(r) - W(r)} + \left[Mc^2 + S(r) + W(r)\right]iF_N(\boldsymbol{r}) = E_N iF_N(\boldsymbol{r}). \tag{32}$$

We use $\epsilon_N(r) \equiv E_N + Mc^2 + S(r) - W(r)$ and $iF_N \longrightarrow F_N$ in the following. Since $(\vec{\sigma}\cdot\vec{\nabla})^2 = \nabla^2$, it becomes

$$\begin{aligned} -\frac{(\hbar c)^2}{\epsilon_N(r)}\nabla^2 F_N(\boldsymbol{r}) - (\hbar c)^2\left(\vec{\sigma}\cdot\vec{\nabla}\frac{1}{\epsilon_N(r)}\right)\left(\vec{\sigma}\cdot\vec{\nabla}F_N(\boldsymbol{r})\right) & \\ + \left[Mc^2 + S(r) + W(r)\right]F_N(\boldsymbol{r}) &= E_N F_N(\boldsymbol{r}). \end{aligned} \tag{33}$$

Next, for the second term, please notice that

$$\left(\vec{\sigma}\cdot\vec{\nabla}\frac{1}{\epsilon_N(r)}\right) = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left[r\frac{d\epsilon_N^{-1}(r)}{dr} - \left(\vec{\sigma}\cdot\vec{L}\frac{1}{\epsilon_N(r)}\right)\right] = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left[r\frac{d\epsilon_N^{-1}(r)}{dr} - 0\right],$$
$$\left(\vec{\sigma}\cdot\vec{\nabla}F_N(\boldsymbol{r})\right) = \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\left[r\frac{d}{dr} - \frac{2\vec{S}\cdot\vec{L}}{\hbar^2}\right]F_N(\boldsymbol{r}). \tag{34}$$

Thus, by using $(\vec{\sigma}\cdot\vec{r})^2/r^4 = 1/r^2$, the EQ. (33) is transformed as

$$\begin{aligned}
-\frac{(\hbar c)^2}{\epsilon_N(r)}\nabla^2 F_N(\boldsymbol{r}) - \frac{(\hbar c)^2}{r^2}\left[r\frac{d\epsilon_N^{-1}(r)}{dr}\right]\left[r\frac{d}{dr} - \frac{2\vec{S}\cdot\vec{L}}{\hbar^2}\right]F_N(\boldsymbol{r}) & \\
+\left[Mc^2 + S(r) + W(r)\right]F_N(\boldsymbol{r}) &= E_N F_N(\boldsymbol{r}), \\
\Longrightarrow \Bigg[-\frac{(\hbar c)^2}{\epsilon_N(r)}\nabla^2 - (\hbar c)^2\frac{(-)\epsilon'_N(r)}{\epsilon_N^2(r)}\frac{d}{dr} + \frac{(\hbar c)^2}{r}\frac{(-)\epsilon'_N(r)}{\epsilon_N^2(r)}\frac{2\vec{S}\cdot\vec{L}}{\hbar^2} & \\
+S(r) + W(r)\Bigg]F_N(\boldsymbol{r}) &= (E_N - Mc^2)F_N(\boldsymbol{r}),
\end{aligned} \tag{35}$$

where the 1st term in the LHS corresponds to the kinetic energy, the 2nd term is so-called Darwin term, and the 3rd term indicates the spin-orbit coupling. These Darwin and spin-orbit terms can be naturally concluded from the Dirac equation, whereas those were just introduced as "phenomenology" in the Schroedinger equation.

It is convenient to find that,

- the total potential is given as $S(r) + W(r)$, whereas,
- the spin-orbit and Darwin terms depend on the $\epsilon'_N(r) = S'(r) - W'(r)$.

Thus, even though the total potential is zero or very small, it does not guarantee the free condition for fermions. Remember also that, for the spin-orbit coupling term,

$$2\vec{S}\cdot\vec{L}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) = \hbar^2 K_{lj}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}), \tag{36}$$

where

$$\begin{aligned}
K_{lj} = j(j+1) - l(l+1) - \frac{3}{4} &= l, \quad \text{when} \;\; j = l + \frac{1}{2}, \\
&= -l-1, \quad \text{when} \;\; j = l - \frac{1}{2}.
\end{aligned} \tag{37}$$

It is also convenient to note that,

$$\begin{aligned}
2\vec{S}\cdot\vec{L}\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) &= 2\vec{S}\cdot\vec{L}\mathcal{Y}_{\ell,jm}(\bar{\boldsymbol{r}}), \quad \text{with } \ell = l\pm 1 \text{ for } j = l \pm \frac{1}{2}, \\
&= \hbar^2 Q_{lj}\mathcal{Y}_{\ell,jm}(\bar{\boldsymbol{r}}),
\end{aligned} \tag{38}$$

where

$$\begin{aligned}
Q_{lj} = j(j+1) - \ell(\ell+1) - \frac{3}{4} &= -l-2, \quad \text{when} \;\; j = l + \frac{1}{2}, \\
&= l-1, \quad \text{when} \;\; j = l - \frac{1}{2}.
\end{aligned} \tag{39}$$

2.3 reduction from Dirac to Schroedinger equations

The correspondence between the EQ. (35) and the Schroedinger equation is obtained as follows. First (i) we assume $S(r) = 0$, namely, only the vector-type potential is finite. Notice that, e.g. the Coulomb potential mediated by the photon (vector-gauge field) is consistent to this assumption. Then (ii) in the non-relativistic limit, $E_N - W(r) \cong Mc^2$, and thus, $\epsilon_N(r) \cong 2Mc^2$. Note also that $\epsilon'_N(r) = -W'(r)$. Therefore, the EQ. (35) is approximated as

$$\left[-\frac{\hbar^2}{2M}\nabla^2 - (\hbar c)^2\frac{W'(r)}{4M^2c^4}\frac{d}{dr} + \frac{(\hbar c)^2}{r}\frac{W'(r)}{4M^2c^4}\frac{2\vec{S}\cdot\vec{L}}{\hbar^2} + W(r)\right]F_N(\boldsymbol{r}) = (E_N - Mc^2)F_N(\boldsymbol{r}). \tag{40}$$

The 1st and 4th terms are well-known kinetic and potential terms in the Schroedinger equation, respectively.

2.4 solution of free Dirac equation

For $E = +\sqrt{c^2\vec{p}^2 + c^4M^2} > 0$ without external potentials, there are two solutions with $p_0 = +E$ and $p_0 = -E$:

$$\begin{aligned}
\psi_{[+E,\ +\vec{p},\ +s]}(x) &= \exp\left[-i\frac{p^\mu x_\mu}{\hbar}\right]\sqrt{\frac{E+M}{2E}}\begin{pmatrix} 1 \\ \frac{\vec{\sigma}\cdot\vec{p}}{M+E} \end{pmatrix}\chi_{+s}\ , \\
\psi_{[-E,\ -\vec{p},\ -s]}(x) &= \exp\left[+i\frac{p^\mu x_\mu}{\hbar}\right]\sqrt{\frac{E+M}{2E}}\begin{pmatrix} \frac{\vec{\sigma}\cdot\vec{p}}{M+E} \\ 1 \end{pmatrix}\chi_{-s}\ .
\end{aligned} \tag{41}$$

3 Numerical solution of spherical Dirac equation

Our goal in this section is to summarize necessary points for the numerical solution of spherical Dirac equation. We start again from EQ. (28):

$$\begin{aligned}
-i\hbar c\vec{\sigma}\cdot\vec{\nabla}G_N(\boldsymbol{r}) + \left[Mc^2 + S(r) + W(r)\right]iF_N(\boldsymbol{r}) &= E_N iF_N(\boldsymbol{r}), \\
-i\hbar c\vec{\sigma}\cdot\vec{\nabla}iF_N(\boldsymbol{r}) + \left[-Mc^2 - S(r) + W(r)\right]G_N(\boldsymbol{r}) &= E_N G_N(\boldsymbol{r}).
\end{aligned} \tag{42}$$

Notice that, from EQ.(30),

$$\vec{\sigma}\cdot\vec{\nabla} = \frac{(\vec{\sigma}\cdot\vec{r})^2}{r^2}\vec{\sigma}\cdot\vec{\nabla} = \frac{\vec{\sigma}\cdot\boldsymbol{r}}{r^2}\left[\vec{r}\cdot\vec{\nabla} - \vec{\sigma}\cdot\vec{L}/\hbar\right] = \frac{\vec{\sigma}\cdot\boldsymbol{r}}{r^2}\left[r\frac{d}{dr} - \frac{2\vec{S}\cdot\vec{L}}{\hbar^2}\right], \tag{43}$$

where we have used $\vec{\sigma} = 2\vec{S}/\hbar$, $i\vec{\nabla} = -\vec{p}/\hbar$, and $\vec{L} = \vec{r}\times\vec{p}$. Using the label K_{lj} and Q_{lj}, which are determined as $2\vec{S}\cdot\vec{L}\mathcal{Y}_{ljm} = \hbar^2 K_{lj}\mathcal{Y}_{ljm}$ and $2\vec{S}\cdot\vec{L}\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm} = \hbar^2 Q_{lj}\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}$, one finds that

$$\begin{aligned}
\vec{\sigma}\cdot\vec{\nabla}iF_N(\boldsymbol{r}) &= \vec{\sigma}\cdot\vec{\nabla}iF_{nlj}(r)\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) = \frac{\vec{\sigma}\cdot\boldsymbol{r}}{r^2}i\left[r\frac{dF_{nlj}(r)}{dr} - K_{lj}F_{nlj}(r)\right]\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}), \\
&= i\left[\frac{dF_{nlj}(r)}{dr} - \frac{K_{lj}}{r}F_{nlj}(r)\right]\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}),
\end{aligned} \tag{44}$$

and

$$\begin{aligned}
\vec{\sigma}\cdot\vec{\nabla}G_N(\boldsymbol{r}) &= \vec{\sigma}\cdot\vec{\nabla}G_{nlj}(r)\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) = \frac{\vec{\sigma}\cdot\boldsymbol{r}}{r^2}\left[r\frac{dG_{nlj}(r)}{dr} - Q_{lj}G_{nlj}(r)\right]\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) \\
&= \left[\frac{dG_{nlj}(r)}{dr} - \frac{Q_{lj}}{r}G_{nlj}(r)\right]\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}).
\end{aligned} \tag{45}$$

Therefore, EQ. (42) is transformed as

$$\begin{aligned}
-i\hbar c\left[\frac{dG_{nlj}(r)}{dr} - \frac{Q_{lj}}{r}G_{nlj}(r)\right]\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) &= \left[E_N - W(r) - S(r) - Mc^2\right]iF_{nlj}(r)\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}), \\
-i\hbar c\cdot i\left[\frac{dF_{nlj}(r)}{dr} - \frac{K_{lj}}{r}F_{nlj}(r)\right]\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}) &= \left[E_N - W(r) + S(r) + Mc^2\right] \\
&\qquad G_{nlj}(r)\frac{\vec{\sigma}\cdot\boldsymbol{r}}{r}\mathcal{Y}_{ljm}(\bar{\boldsymbol{r}}).
\end{aligned} \tag{46}$$

Thus,

$$\begin{aligned}
\frac{dF_{nlj}}{dr} &= \frac{K_{lj}}{r}F_{nlj}(r) + \frac{Mc^2 + S(r) + E_N - W(r)}{\hbar c}G_{nlj}(r), \\
\frac{dG_{nlj}}{dr} &= \frac{Mc^2 + S(r) - E_N + W(r)}{\hbar c}F_{nlj}(r) + \frac{Q_{lj}}{r}G_{nlj}(r).
\end{aligned} \tag{47}$$

For another representation with $F_{nlj}(r) \equiv \frac{a_{nlj}(r)}{r}$ and $G_{nlj}(r) \equiv \frac{b_{nlj}(r)}{r}$, these equations change as

$$\begin{aligned}
\frac{da_{nlj}}{dr} &= \frac{K_{lj}+1}{r}a_{nlj}(r) + \frac{Mc^2 + S(r) + E_N - W(r)}{\hbar c}b_{nlj}(r), \\
\frac{db_{nlj}}{dr} &= \frac{Mc^2 + S(r) - E_N + W(r)}{\hbar c}a_{nlj}(r) + \frac{Q_{lj}+1}{r}b_{nlj}(r).
\end{aligned} \tag{48}$$

Here, one can use a trick: $K_{lj}+1=-Q_{lj}-1$ for whatever $j=l\pm 1/2$. Thus, by using

$$\begin{aligned} \kappa_{lj} \equiv K_{lj}+1 = -Q_{lj}-1 &= l+1 \ \text{ for } \ j=l+1/2, \\ &= -l \ \text{ for } \ j=l-1/2, \end{aligned} \tag{49}$$

then one finally gets

$$\begin{aligned} \frac{da_{nlj}}{dr} &= \frac{\kappa_{lj}}{r}a_{nlj}(r) + \frac{Mc^2+S(r)+E_N-W(r)}{\hbar c}b_{nlj}(r), \\ \frac{db_{nlj}}{dr} &= \frac{Mc^2+S(r)-E_N+W(r)}{\hbar c}a_{nlj}(r) + \frac{-\kappa_{lj}}{r}b_{nlj}(r). \end{aligned} \tag{50}$$

In the following, we introduce the new symbols as

$$s(r) \equiv Mc^2+S(r), \qquad v(r) \equiv E_N - W(r), \qquad \epsilon_N(r) \equiv s(r)+v(r).$$

Then the last equations for $\{a_{nlj}(r), b_{nlj}(r)\}$ read

$$\frac{d}{dr}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \frac{\kappa}{r} & \frac{s+v}{\hbar c} \\ \frac{s-v}{\hbar c} & \frac{-\kappa}{r} \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}. \tag{51}$$

Since this EQ. (51) is simply the single-derivative matrix equation, the 4th-order Runge-Kutta (RK4) method can be utilized to obtain the numerical solutions of $a_{nlj}(r)$ and $b_{nlj}(r)$ [2]. Here we summarize TIPs for numerical implementation:

- Physical input parameters necessary: (i) mass and energy (Mc^2, E_N); (ii) quantum numbers of interest $N=(n,l,j)$; (iii) scalar and vector potentials $S(r)$ and $W(r)$; physical constants.
- Numerical parameters necessary: (i) cutoff maximum and minimum energies; (ii) radial mesh parameters $(dr, R_{\max})$.
- For finding the eigenenergy E_N of the bound state, as one example, one should employ the iteration combined with the node-counting technique. Namely, the RK4 solution for the fixed set of (n,l,j) is repeated by elaborating the input E_{nlj} until when the results are expected as converged.
- For the starting values of $f_{nlj}(r)$ and $g_{nlj}(r)$ necessary to use the RK4 method, one can refer to their asymptotic forms at $r\cong 0$, which are given in the following sections.

3.1 large component $a(r)$

First, we eliminate $b(r)$:

$$\begin{aligned} b(r) &= \frac{\hbar c}{\epsilon_N(r)}\left(a'(r)-\frac{\kappa}{r}a(r)\right), \\ b'(r) &= \hbar c\left\{(-)\frac{\epsilon_N'}{\epsilon_N^2}\left(a'(r)-\frac{\kappa}{r}a(r)\right)+\frac{1}{\epsilon_N}\left(a''(r)-\frac{\kappa}{r}a'(r)+\frac{\kappa}{r^2}a(r)\right)\right\} \\ &= (\text{from EOM...}) = \frac{s(r)-v(r)}{\hbar c}a(r) - \frac{\kappa}{r}\frac{\hbar c}{\epsilon_N}\left(a'(r)-\frac{\kappa}{r}a(r)\right). \end{aligned} \tag{52}$$

By some calculations,

$$\begin{aligned} &\Longrightarrow \ a''(r)-\frac{\kappa}{r}a'(r)+\frac{\kappa}{r^2}a(r)-\frac{\epsilon_N'}{\epsilon_N(r)}\left(a'(r)-\frac{\kappa}{r}a(r)\right) = \frac{s^2-v^2}{(\hbar c)^2}a(r)-\frac{\kappa}{r}\left(a'(r)-\frac{\kappa}{r}a(r)\right) \\ &\Longrightarrow \ a''(r)-\frac{\epsilon_N'}{\epsilon_N}a'(r)+\left(\frac{\kappa}{r^2}+\frac{\epsilon_N'(r)}{\epsilon_N(r)}\cdot\frac{\kappa}{r}-\frac{s^2-v^2}{(\hbar c)^2}-\frac{\kappa^2}{r^2}\right)a(r)=0 \\ &\qquad a''(r)-\frac{\epsilon_N'}{\epsilon_N}a'(r)+\left(-\frac{l(l+1)}{r^2}+\frac{\epsilon_N'}{\epsilon_N}\cdot\frac{\kappa}{r}-\frac{s^2-v^2}{(\hbar c)^2}\right)a(r)=0, \end{aligned} \tag{53}$$

where we have used $\kappa_{lj}(\kappa_{lj}-1)=l(l+1)$ for whatever $j=l\pm 1/2$. Or equivalently,

$$\begin{aligned} &-\frac{(\hbar c)^2}{\epsilon_N(r)}a''(r)+\frac{(\hbar c)^2\epsilon_N'(r)}{\epsilon_N^2(r)}a'(r)+\left[\frac{(\hbar c)^2}{\epsilon_N(r)}\frac{l(l+1)}{r^2}-\frac{(\hbar c)^2\epsilon_N'(r)}{\epsilon_N^2(r)}\frac{\kappa}{r}+s(r)-v(r)\right]a(r)=0, \\ &\left\{-\frac{(\hbar c)^2}{\epsilon_N(r)}\frac{d^2}{dr^2}+\frac{(\hbar c)^2\epsilon_N'(r)}{\epsilon_N^2(r)}\frac{d}{dr}+\left[\frac{(\hbar c)^2}{\epsilon_N(r)}\frac{l(l+1)}{r^2}-\frac{(\hbar c)^2\epsilon_N'(r)}{\epsilon_N^2(r)}\frac{\kappa}{r}+S(r)+W(r)\right]\right\}a(r) \\ &= \left(E_N-Mc^2\right)a(r). \end{aligned} \tag{54}$$

Then, in the non-relativistic limit, this equation becomes the Schroedinger equation with the potential $S(r)+W(r)$.

3.2 small component $b(r)$

Next we focus on $b_{nlj}(r)$. By introducing $\zeta_N \equiv s(r) - v(r) = Mc^2 + S(r) - E_N + W(r)$,

$$\begin{aligned} a(r) &= \frac{\hbar c}{\zeta_N(r)} \left(b'(r) + \frac{\kappa}{r} b(r) \right), \\ a'(r) &= \hbar c \left\{ (-) \frac{\zeta_N'}{\zeta_N^2} \left(b'(r) + \frac{\kappa}{r} b(r) \right) + \frac{1}{\zeta_N(r)} \left(b''(r) + \frac{\kappa}{r} b'(r) - \frac{\kappa}{r^2} b(r) \right) \right\} \\ &= (\text{from EOM...}) = \frac{\kappa}{r} \frac{\hbar c}{\zeta_N(r)} \left(b'(r) + \frac{\kappa}{r} b(r) \right) + \frac{s(r)+v(r)}{\hbar c} b(r) \end{aligned} \tag{55}$$

By some calculations,

$$\begin{aligned} &\Longrightarrow \quad b''(r) + \frac{\kappa}{r} b'(r) - \frac{\kappa}{r^2} b(r) - \frac{\zeta_N'}{\zeta_N} \left(b'(r) + \frac{\kappa}{r} b(r) \right) = \frac{\kappa}{r} \left(b'(r) + \frac{\kappa}{r} b(r) \right) + \frac{s^2 - v^2}{(\hbar c)^2} b(r) \\ &\Longrightarrow \quad b''(r) - \frac{\zeta_N'}{\zeta_N} b'(r) + \left(-\frac{\kappa(\kappa+1)}{r^2} - \frac{\zeta_N'}{\zeta_N} \cdot \frac{\kappa}{r} - \frac{s^2 - v^2}{(\hbar c)^2} \right) b(r) = 0. \end{aligned} \tag{56}$$

By dividing this equation by $-\epsilon_N(r)/(\hbar c)^2$, where $\epsilon_N(r) = s(r) + v(r)$, one finds

$$\begin{aligned} &\left\{ -\frac{(\hbar c)^2}{\epsilon_N(r)} \frac{d^2}{dr^2} + \frac{(\hbar c)^2 \zeta_N'(r)}{\epsilon_N(r)\zeta_N(r)} \frac{d}{dr} + \left[\frac{(\hbar c)^2}{\epsilon_N(r)} \frac{\kappa(\kappa+1)}{r^2} - \frac{(\hbar c)^2 \epsilon_N'(r)}{\epsilon_N(r)\zeta_N(r)} \frac{\kappa}{r} + S(r) + W(r) \right] \right\} b(r) \\ &= \left(E_N - Mc^2 \right) b(r). \end{aligned} \tag{57}$$

3.3 asymptotic form at $r \cong 0$ with $W'(r) = S'(r) = 0$

Within this assumption, the EQ. (53) is approximated as

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - C(r) \right] a_{nlj}(r) \cong 0, \quad C(r) \equiv \frac{s^2(r) - v^2(r)}{(\hbar c)^2}, \quad \frac{d}{dr} C(r \cong 0) = 0. \tag{58}$$

(i) Because this equation keeps the same for $r \longrightarrow -r$, the asymptotic form must be $a(r) \cong \sum_n r^{2n+1}$ or $\cong \sum_n r^{2n}$, in its expanded form. (ii) By considering the special case with $S(r) = W(r) \equiv 0$, namely $C(r) = const.$, the possible form can be limited as $a(r) \cong r^{l+1} + \mathcal{O}(r^{l+3})$. (iii) Assuming $a(r) \cong r^{l+1} + \chi C(r) r^{l+3} + \mathcal{O}(r^{l+5})$, the factor χ must satisfy that,

$$0 \cdot \frac{r^{l+1}}{r^2} + \frac{r^{l+3}}{r^2} \left\{ \chi(l+3)(l+2) - \chi(l+1)l - 1 \right\} C(r) + \mathcal{O}(r^{l+5-2}) \cong 0 \longrightarrow \chi = \frac{1}{4l+6}. \tag{59}$$

Therefore, without the normalization,

$$a_{nlj}(r \cong 0) = r^{l+1} + \frac{C(r)}{4l+6} r^{l+3} + \mathcal{O}(r^{l+5}). \tag{60}$$

The corresponding $b_{nlj}(r)$ can be computed from the Dirac equation:

$$b_{nlj}(r \cong 0) = \frac{\hbar c}{s(r) + v(r)} \left[\frac{da_{nlj}}{dr} - \frac{\kappa_{lj}}{r} a_{nlj}(r) \right]. \tag{61}$$

4 Sample calculation

For the benchmark of programme DEQURK to solve the spherical Dirac equation with RK4 method, we present the sample calculations for the single-proton energies in the ^{100}Sn nucleus.

- In FIG. 1, the scalar and vector potentials utilized for this p+^{100}Sn system are displayed. Notice that the vector potential $W(r)$ includes the Coulomb barrier in addition to the attractive-nuclear potential. These potentials are obtained by fitting them to the self-consistent mean-field results from Relativistic Hartree-Bogoliubov (RHB) calculations with the DD-PC1 parameters [3].

- In FIG. 2, the Dirac-spinor functions, $f_{nlj}(r) = a_{nlj}(r)/r$ and $g_{nlj}(r) = b_{nlj}(r)/r$, are presented for $1s_{1/2}$, $2s_{1/2}$, $1p_{3/2}$, and $2s_{3/2}$ orbits of protons. Each state is normalized as $\int \bar{\psi}(\boldsymbol{r})\psi(\boldsymbol{r}) d\boldsymbol{r} = 1$. Notice that the smaller component $g_{nlj}(r)$ is indeed minor compared to the larger component $f_{nlj}(r)$.

- In TABLE 4, the single-proton energies of protons are summarized. The DEQURK method approximately reproduces these energies obtained from RHB with DD-PC1 Lagrangian. The small deviation is due to the fitting errors in potentials.

TABLE 4: Single-particle energies for protons in ^{100}Sn. The unit is MeV. The scalar and vector potentials are plotted in FIG. 1. The corresponding results from RHB with DD-PC1 are also presented [3, 4].

Orbit	DEQURK (Runge-Kutta)	RHB with DD-PC1
$1s_{1/2}$	-48.888	-47.985
$2s_{1/2}$	-20.653	-19.528
$1p_{3/2}$	-39.562	-38.346
$2p_{3/2}$	-6.981	-6.767
$1p_{1/2}$	-38.354	-37.240
$2p_{1/2}$	-5.781	-5.300
$1d_{5/2}$	-28.429	-26.976
$1d_{3/2}$	-25.306	-23.975
$1f_{7/2}$	-16.386	-14.987
$1f_{5/2}$	-10.957	-9.553

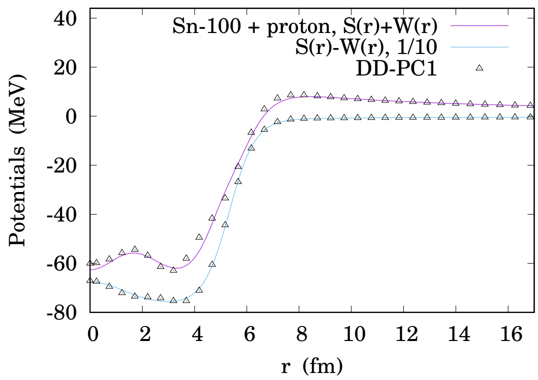

FIG. 1: The scalar and vector potentials used for p+^{100}Sn system. The corresponding results obtained from RHB calculation with DD-PC1 Lagrangian are also plotted [3].

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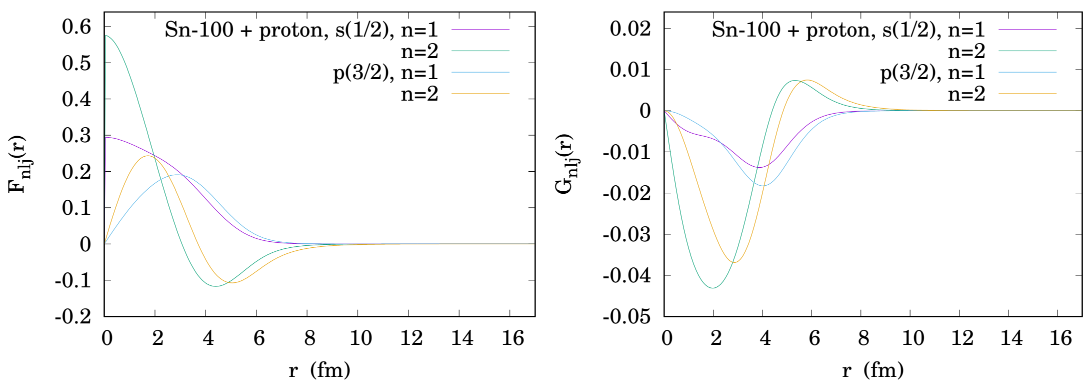

FIG. 2: The Dirac-spinor functions, $F_N(r) = a_{nlj}(r)/r$ and $G_N(r) = b_{nlj}(r)/r$, obtained with DEQURK for $1s_{1/2}$, $2s_{1/2}$, $1p_{3/2}$, and $2s_{3/2}$ orbits of protons.