Relativistic correction of the Coulomb interaction for energies and radii in doubly-magic nuclei

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Abstract. Effects of the relativistic correction of the Coulomb interaction on doubly-magic nuclei are discussed with Skyrme Hartree-Fock calculations. It is found that the correction to the total energy is about 2.4 MeV for $^{208}\text{Pb}$, while proton and neutron radii do not change significantly. This difference is larger than the difference of the Coulomb exchange (Fock) energy calculated with the local density (Hartree-Fock-Slater) approximation and that with the exact treatment and the neutron finite-size effect. Effects of the correction are also compared to the correction due to the vacuum polarization. It is shown that the two contributions to the total energy are comparable in light nuclei, but the latter dominates in heavy nuclei, while the contribution of the relativistic correction to the total energy is non-negligible compared to the target accuracy of the DFT calculation. Moreover, since the covariant (relativistic) density functional theory often includes effects of magnetic interaction and retardation for electromagnetic interaction, the method presented in this work enables one to make a fair comparison between the non-relativistic and the relativistic density functional calculations for electromagnetic energies.

PACS. 21.60.Jz Nuclear Density Functional Theory and extensions – 21.10.Sf Coulomb energies, analogue states

1 Introduction

Atomic nuclei are composed of protons and neutrons, which interact via the nuclear and electromagnetic (EM) interactions. Since the nuclear interaction is much stronger than the EM one, the former determines most properties of the atomic nuclei. Nevertheless, the EM interaction plays an important role when one focuses on nuclear properties related to the isospin symmetry breaking [1–10]. For more details, see reviews, e.g., Ref. [11].

The Hartree-Fock method or the density functional theory (DFT) [12–14] is a powerful method to calculate quantum many-fermion problems, including atomic nuclei. In DFT, an energy density functional (EDF), which contains information on interactions, governs the accuracy of calculation. Although the Coulomb interaction is rather simple, first-principle EDFs, even for electronic systems, have been derived approximately using in the local density approximation (LDA) [15,17], and effects of the density gradient have been included empirically or phenomenologically [18–20]. In nuclear physics, the situation is more complicated that the nuclear interaction in medium is still under discussion, and the derivation of ab initio nu-
responds to the higher-order correction of the Coulomb interaction in terms of the coupling constant $\alpha \approx 1/137$ (the fine-structure constant). Although these effects are just corrections for the Coulomb interaction, which itself is already subdominant for the nuclear total energies, it was shown that they are non-negligible compared to the desired accuracy; for instance, the proton finite-size effect, the neutron one, and the vacuum polarization contribute to the total energy of $^{208}$Pb in $\pm 8.2$ MeV, $\pm 1.2$ MeV, and $\pm 3.7$ MeV, respectively.\[40\]

Then, it is natural to consider the corrections with the same order with respect to $\alpha$; that is, the finite-light-speed correction, the self-energy, and the two-photon exchange process. Although the self-energy contributes to the energy of electrons in atoms like the vacuum polarization, while it may be weak for the energy of nucleons in atomic nuclei since the nucleon mass is heavy; the two-photon exchange may also be weak since it is also inverse proportional to the nucleon mass.\[40\] In contrast, the finite-light-speed effect does not depend on the nucleon mass, and it is known to be non-negligible in atomic structure.\[50,51\] Thus, in this work, the finite-light-speed correction to the Coulomb interaction is considered in the nuclear structure calculation in order to investigate whether its effect is small. Even if its effect is small, it is worthwhile to confirm it.

The finite-light-speed correction to the Coulomb interaction is often referred to as the relativistic correction,\[50,52,52,54\] and the Breit correction\[50,52,52,54\] is used for $\alpha \ll 1$. It is known to be non-negligible in atomic structure.\[50,51\] In atomic physics, the Breit correction dominates the vacuum polarization of the Coulomb field formed by the atomic nucleus, and thus the Breit correction should be considered once the vacuum polarization is considered. In nuclear physics, the vacuum polarization discussed in Ref.\[10\] originates from the interaction between two protons, which is different from that in atomic physics. Hence, it is interesting to compare which contribution dominates to the nuclear total energy, the Breit correction or the vacuum polarization.

Another interesting point is a comparison between the Breit correction and the correction due to the density gradient, i.e., the difference between the LDA Coulomb energy and the GGA Coulomb energy. The Breit correction had been taken into account for an exchange\[59\] or exchange-correlation\[60\] EDF in the LDA level, and was already taken into account fully for atomic DFT\[51\]. It was found in Ref.\[51\] that the Breit correction contributes to the total energies of atoms in almost the same magnitude but the opposite to the density gradient effects. In the context of nuclear physics, it was shown in Refs.\[39,61,62\] that difference between the Coulomb exchange energy calculated by the exact-Fock term or GGA and that in LDA is non-negligible in nuclear binding energies. Thus, it should be tested to what extent the Breit correction contributes to nuclear binding energies.

The covariant density functional theory (CDFT), the nuclear DFT in the relativistic scheme, is based on the covariant Lagrangian with nucleon, meson, and photon fields. Hence, effects beyond the Coulomb interaction, such as magnetic interaction and retardation, have often been considered.\[42,43,63,64\] Therefore, it is interesting to take into account the relativistic correction to the Coulomb interaction in SHF calculations to make a fair comparison with the CDFT calculations for electromagnetic energies.

The relativistic correction to the Coulomb interaction was already discussed in Refs.\[65,66\]. As discussed later, the correction used in these works is the same as the non-relativistic reduced form of the Breit correction for electronic systems.\[67,68\] The aim of this paper is modern calculation of Refs.\[65,66\]: Deriving the EDF for such corrections and performing the self-consistent calculation. I shall discuss contributions to proton and neutron radii, total energies, and single-particle energies. Note that it seems that “the Breit correction” refers the whole terms of the non-relativistic reduced form of the correction\[Eq. \eqref{eq:1}\] in the context of atomic physics, while it refers only a term of the correction in the context of nuclear physics. In order to avoid any confusion, hereinafter, I will use a term “the relativistic correction”, instead of “the Breit correction”.

This paper is organized as follows: In Sec. 2 the theoretical framework for the relativistic correction will be shown. In Sec. 3, the relativistic correction to the total energy will be estimated analytically, and in Sec. 4 numerical results will be shown. Finally, in Sec. 5 conclusion and perspectives will be given.

## 2 Theoretical Framework

In this section, I show the theoretical framework for the relativistic correction and the DFT. Throughout this paper, an unit with $4\pi\epsilon_0 = 1$ is used and $c$ denotes the speed of light.

Quantum many-body systems can be described by using the Hamiltonian

$$H = T + V_{\text{ext}} + V_{\text{int}},$$

where $T$, $V_{\text{ext}}$, and $V_{\text{int}}$ denote the kinetic energy operator, an external potential, and an interaction, respectively. In the case of electronic systems, $V_{\text{int}}$ is identical to the EM interaction $V_{\text{EM}}$, while in the case of atomic nuclei, $V_{\text{int}}$ includes a nuclear interaction $V_{\text{nucl}}$ and the EM interaction $V_{\text{EM}}$ with $V_{\text{ext}} \equiv 0$. In most works, the Coulomb interaction between protons

$$V_{\text{Coul}}(r_j, r_k) = \frac{e^2}{r_{jk}}$$

is used for $V_{\text{EM}}$, where $r_j$ and $r_k$ are the spatial coordinates of the protons $j$ and $k$, and $r_{jk} = |r_{jk}|$. According to the quantum electrodynamics, the leading-order instantaneous interaction, in which a photon mediates between two particles with $c = \infty$, is the Coulomb interaction.
2.1 Breit correction for electronic systems

In electronic systems, the next-leading-order interaction \( (O(1/c^2)) \) in the Coulomb gauge is called the Breit correction, whose form is

\[
V_{\text{Breit}}(r_j, r_k) = -\frac{e^2}{2m_c^2c^2} \left[ \frac{\alpha_j \cdot \alpha_k}{2e^2r_{jk}} + \frac{(\alpha_j \cdot r_{jk})(\alpha_k \cdot r_{jk})}{2e^2r_{jk}^3} \right],
\]

(3)

where \( \alpha \) is a 4 \times 4 matrix defined by

\[
\alpha = \left( \begin{array}{cc}
O_2 \sigma_x & (O_2 \sigma_y) \\
(O_2 \sigma_y) & O_2 \sigma_z \\
O_2 \sigma_z & (O_2 \sigma_y) \\
(O_2 \sigma_y) & O_2 \sigma_z
\end{array} \right)
\]

(4)

with the Pauli matrices \( \sigma_x, \sigma_y, \) and \( \sigma_z \) and the 2 \times 2 zero matrix \( O_2 \). In isolated atoms, the vacuum polarization of the Coulomb field appears in higher order than the Breit correction \[58\]. The Breit correction includes the magnetic (current-current) interaction and the retardation in the non-relativistic \[57,69\]. In the Lorentz (covariant) gauge, the next-leading-order interaction corresponds to the magnetic interaction and the retardation \[65,71\].

After the Foldy-Wouthuysen–Tani transformation \[72,75\], the Breit correction [Eq. (3)] in the non-relativistic scheme is obtained as \[67,68\]

\[
\tilde{V}_{\text{Breit}}(r_j, s_j, r_k, s_k) = -\frac{\pi \hbar^2 c^2}{m_c^2} \delta (r_{jk})
\]

(5a)

\[
-\frac{e^2}{2m_c^2c^2} p_j \cdot \left( \frac{1}{r_{jk}} + \frac{r_{jk}}{r_{jk}^3} \right) \cdot p_k
\]

(5b)

\[
-8\pi \hbar^2 c^2 \delta (r_{jk}) s_j \cdot s_k
\]

(5c)

\[
-\frac{\hbar^2 e^2}{2m_c^2c^2} s_j \cdot \left( \frac{3r_{jk}r_{jk}}{r_{jk}^5} - \frac{1}{r_{jk}^3} \right) s_k
\]

(5d)

\[
+\frac{\hbar^2 e^2}{2m_c^2c^2} \frac{1}{r_{jk}^3} s_j \cdot [r_{jk} \times (2p_k - p_j)]
\]

(5e)

where \( m_c \approx 0.511 \text{ MeV}/c^2 \) is the electron mass \[76\] and \( p_j \) is the momentum of the particle \( j \). The first [Eq. (5a)] and second [Eq. (5b)] terms correspond to the Darwin term for the electron-electron Coulomb interaction, which is related to Zitterbewegung \[70\], and the retardation of the Coulomb interaction, respectively; the third and fourth terms [Eqs. (5c) and (5d)] correspond to the spin-magnetic interactions; and the fifth term [Eq. (5e)] corresponds to the electron-electron spin-orbit interaction \[60,67,68\].

Thus, in the Schrödinger scheme, if one is eager to consider the Breit correction, Eq. (5) should be considered on top of the Coulomb interaction [Eq. (2)], i.e.,

\[
V_{\text{EM}} = \frac{1}{2} \sum_{j,k} \left[ V_{\text{Coul}}(r_j, r_k) + \tilde{V}_{\text{Breit}}(r_j, s_j, r_k, s_k) \right],
\]

(6)

which will be referred to as the Coulomb-Breit interaction.

2.2 Beyond Coulomb interaction for nuclear systems

Corrections beyond the Coulomb interaction for nuclear systems were discussed several decades ago \[65,66\]. The correction was

\[
\tilde{V}_{\text{Rel}}(r_j, s_j, r_k, s_k) = -\frac{e^2}{2M^2c^2} p_j \cdot \left( \frac{1}{r_{jk}} + \frac{r_{jk}}{r_{jk}^3} \right) \cdot p_k
\]

(7a)

\[
-2\hbar \mu_\tau e_{\tau m} \frac{1}{r_{jk}^3} s_j \cdot (r_{jk} \times p_k) + \frac{2\hbar^2 e_{\tau m} e_{\tau m}}{M^2} \frac{1}{r_{jk}^3} s_j \cdot (r_{jk} \times p_j)
\]

(7b)

\[
-4\hbar \mu_\tau e_{\tau m} \frac{1}{r_{jk}^3} s_j \cdot \left( \frac{3r_{jk}r_{jk}}{r_{jk}^5} - \frac{1}{r_{jk}^3} \right) s_k
\]

(7c)

\[
-\frac{e^2}{3} \mu_\tau e_{\tau m} \frac{1}{r_{jk}^3} s_j \cdot (r_{jk} \times p_k)
\]

(7d)

\[
+e_\tau \frac{1}{M^2} \left( 2\mu_\tau - \frac{e_\tau}{2M} \right) \frac{1}{r_{jk}^3} s_k \cdot (r_{jk} \times p_k)
\]

(7e)

\[
-\frac{\hbar}{M} \left( 4\tau \mu_\tau \frac{1}{r_{jk}^3} s_j \cdot \left( \frac{3r_{jk}r_{jk}}{r_{jk}^5} - \frac{1}{r_{jk}^3} \right) s_k
\]

(7f)

\[
-\frac{e^2}{2M^2c^2} \left( 2\mu_\tau - \frac{e_\tau}{2M} \right) \frac{1}{r_{jk}^3} s_j \cdot (r_{jk} \times p_j)
\]

(7g)

where \( M \approx 389.919 \text{ MeV}/c^2 \) is the nucleon mass \[76\], \( \delta_{\tau_\pi} \) is the Kronecker delta, which is equal to 1 for \( \tau = \pi \) and 0 for \( \tau = n \), \( e_\tau \) and \( \mu_\tau \) are the charge and magnetic moment of a nucleon \( \tau \), and \( \mu_{\tau_\pi} \) is the magnetic moment of the unit of the nuclear magneton, i.e., \[76\]

\[
\mu_\tau = \frac{\tilde{\mu}_\tau}{2M},
\]

(8a)

\[
\tilde{\mu}_p = 2.79284734463,
\]

(8b)

\[
\tilde{\mu}_n = -1.91304273.
\]

(8c)

If one assumes that these two particles are electrons instead of nucleons, and accordingly, \( m_c, -e, \) and \( \mu_e \), are
factor and the magnetic moment $g_e$ one can find that Eq. (7) is identical to Eq. (5). Here, the relation between the $g$-factor and the magnetic moment $\mu_e$

$$\mu_e = \frac{eh}{4m_e} g_e$$  \hspace{1cm} (9)

and $g_e = 2$ is used, apart from the second term of Eq. (7b), in which the $g$-factor for the orbital motion of electrons $g_e = 1$ is used. In more detail, the correspondence between Eqs. (5) and (7) is shown in Table I. In the case of electronic systems, Eqs. (7e) and (7f) are cancelled out of each other.

2.3 Density functional theory for relativistic correction

In nuclear DFT, the ground-state energy is obtained by

$$E_{gs} = E_{0} + E_{\text{nucl}} \left[ \rho_{p}^{n}, \rho_{n}^{n} \right] + E_{\text{EM}} \left[ \rho_{p}^{p} \right],$$  \hspace{1cm} (10)

where $E_{0}$ is the Kohn-Sham kinetic energy, $E_{\text{nucl}}$ and $E_{\text{EM}}$ are EDFs of nuclear and EM interactions, respectively, and $\rho_{p}^{n}$ and $\rho_{n}^{n}$ are the ground-state densities of protons and neutrons. If one considers the finite charge distributions of nucleons are considered, $E_{\text{EM}}$ should depend on the ground-state charge distribution, instead of $\rho_{p}^{n}$ [40].

If one only considers the Coulomb interaction $V_{\text{EM}}$, $E_{\text{EM}}$ in LDA reads [77]

$$E_{\text{EM}} \left[ \rho \right] = E_{\text{Coul}}^{H} \left[ \rho \right] + E_{\text{Coul}}^{x} \left[ \rho \right],$$  \hspace{1cm} (11a)

$$E_{\text{Coul}}^{H} \left[ \rho \right] = \frac{e^2}{2} \int \int \frac{\rho \left( \mathbf{r} \right) \rho \left( \mathbf{r}^\prime \right)}{\left| \mathbf{r} - \mathbf{r}^\prime \right|} \, d\mathbf{r} \, d\mathbf{r}^\prime,$$  \hspace{1cm} (11b)

$$E_{\text{Coul}}^{x} \left[ \rho \right] = - \frac{3e^2}{4} \left( \frac{3}{\pi} \right)^{1/3} \int \left| \rho \left( \mathbf{r} \right) \right|^{4/3} \, d\mathbf{r},$$  \hspace{1cm} (11c)

where the density $\rho$ is the electron density $\rho_e$ for electronic systems and the proton density $\rho_p$ for electronic systems.

Recently, an EDF for the Breit correction [Eq. (5)] for electronic systems in the LDA was developed in Refs. [51] and [60]. In this paper, I consider the relativistic correction [Eq. (7)] in the nuclear DFT using the idea of such an EDF and the correspondence shown in Table I. This newly developed EDF enables one to perform the self-consistent calculation. To isolate the relativistic correction, I shall not consider the nucleon finite-size effects [5].

The Hartree and LDA exchange functionals for the Breit correction in the electronic systems [Eq. (5)] were proposed in Ref. [51] and Ref. [59], respectively. Their forms are

$$E_{\text{H, Breit}}^{H} \left[ \rho \right] = - \frac{\pi \hbar^2 e^2}{2M_e^2 c^2} \int \left| \rho \left( \mathbf{r} \right) \right|^2 \, d\mathbf{r},$$  \hspace{1cm} (12a)

$$E_{\text{H, Breit}}^{x} \left[ \rho \right] = \frac{3\pi \hbar^2 e^2}{2M_e^2 c^2} \int \left| \rho \left( \mathbf{r} \right) \right|^2 \, d\mathbf{r},$$  \hspace{1cm} (12b)

respectively, and accordingly, the total correction is

$$E_{\text{Breit}}^{\text{tot}} \left[ \rho \right] = E_{\text{Breit}}^{H} \left[ \rho \right] + E_{\text{Breit}}^{x} \left[ \rho \right],$$

$$= \frac{\pi \hbar^2 e^2}{m_e^2 c^2} \int \left| \rho \left( \mathbf{r} \right) \right|^2 \, d\mathbf{r}. \hspace{1cm} (12c)$$

The idea of the LDA is that the energy density is approximated to that of homogeneous systems; hence, Eqs. (12a) and (12b) contain only effects originating from Eqs. (5a) and (5b) [60]. In addition, due to the symmetry, Eq. (12a) does not contain the effect of the retardation [Eq. (5b)].

I shall construct an EDF for Eq. (7) in the LDA, using the knowledge of Eqs. (12a) and (12b). Because of the idea of the LDA, the EDF contains only the effect of Eqs. (7a) and (7b). Note that the spin-orbit interaction originating from the magnetic form factors of nucleons [Eqs. (7b), (7e), and (7f)] have been discussed in Refs. [7, 40, 78]; the spin-magnetic interaction [Eqs. (7e) and (7d)] has not been considered yet for the self-consistent calculation and it cannot be considered in the LDA, which is left for the future study.

Hereinafter, I will construct the LDA EDF for Eq. (7). Referring the result on Eq. (12), one can find that $E_{\text{Breit}}^{H}$ contributes both the Hartree and the exchange terms, whereas $E_{\text{Breit}}^{x}$ contributes the exchange term only.

The Hartree and the exchange EDFs of Eq. (7), respectively, read

$$E_{\text{H, Darwin}}^{H} \left[ \rho_p, \rho_n \right] = \int \left\{ \frac{C_{pp}}{2} \left| \rho_p \left( \mathbf{r} \right) \right|^2 + C_{pn} \rho_p \left( \mathbf{r} \right) \rho_n \left( \mathbf{r} \right) \right\} \, d\mathbf{r},$$

$$= \int \left\{ \frac{C_{pp}}{2} \left| \rho_p \left( \mathbf{r} \right) \right|^2 + C_{pn} \rho_p \left( \mathbf{r} \right) \rho_n \left( \mathbf{r} \right) \right\} \, d\mathbf{r},$$  \hspace{1cm} (13a)

$$E_{\text{H, Darwin}}^{x} \left[ \rho_p, \rho_n \right] = - \int \left\{ \frac{C_{pp}}{4} \left| \rho_p \left( \mathbf{r} \right) \right|^2 + \frac{C_{nn}}{4} \left| \rho_n \left( \mathbf{r} \right) \right|^2 \right\} \, d\mathbf{r},$$

$$= - \int \left\{ \frac{C_{pp}}{4} \left| \rho_p \left( \mathbf{r} \right) \right|^2 + \frac{C_{nn}}{4} \left| \rho_n \left( \mathbf{r} \right) \right|^2 \right\} \, d\mathbf{r}, \hspace{1cm} (13b)$$

where

$$C_{\tau \tau \tau} = - \frac{\pi \hbar^2 e^2}{2M^2 c^2} \left[ \delta_{\tau \tau \tau} \left( 2\tilde{\mu}_\tau - \delta_{\tau \tau} \right) + \delta_{\tau \tau} \left( 2\tilde{\mu}_\tau - \delta_{\tau \tau} \right) \right]$$

and accordingly

$$C_{pp} = - \frac{\pi \hbar^2 e^2}{M^2 c^2} \left( 2\tilde{\mu}_p - 1 \right),$$

$$C_{pn} = \frac{\pi \hbar^2 e^2}{M^2 c^2} \tilde{\mu}_n,$$

$$C_{nn} = 0.$$  \hspace{1cm} (15a)

The exchange EDF for Eq. (7a) is constructed from Eq. (12b). Equation (12b) does not include only a contribution from Eq. (5b) but also Eq. (5a). Hence, the ex-

\[1\] Effects of nucleon finite size were discussed in Refs. [11, 40].
change EDF for Eq. (5l) reads
\[
\frac{3\pi\hbar^2c^2}{2m_e^2c^2} \int [\rho(r)]^2 \, dr - \frac{1}{4} \frac{\pi\hbar^2c^2}{m_e^2c^2} \int [\rho(r)]^2 \, dr \]
\[
= \frac{5\pi\hbar^2c^2}{4m_e^2c^2} \int [\rho(r)]^2 \, dr,
\]
(16)
since the Darwin EDF for electronic systems is
\[
- \frac{1}{4} \frac{\pi\hbar^2c^2}{m_e^2c^2} \int [\rho(r)]^2 \, dr.
\]
(17)
To apply the nuclear systems, with replacing the electron mass \(m_e\) to the nucleon mass \(M\), one obtains
\[
E_{\text{retar}}^{\pi} [p_p, p_n] = \frac{5\pi\hbar^2c^2}{4M^2c^2} \int [\rho_p(r)]^2 \, dr.
\]
(18)
Combining Eqs. (13) and (18), the total EDF for the correction reads
\[
E_{\text{Rel}}^{\pi} [p_p, p_n]
\]
\[
= \int \left\{ \frac{C_{pp}}{2} \rho_p(r)^2 + C_{pn} \rho_p(r) \rho_n(r) \right\} \, dr
\]
\[
- \int \frac{C_{pp}}{4} \rho_p(r)^2 \, dr + \frac{5\pi\hbar^2c^2}{4M^2c^2} \int [\rho_p(r)]^2 \, dr
\]
\[
= \left( \frac{C_{pp}}{2} - \frac{C_{pp}}{4} + \frac{5\pi\hbar^2c^2}{4M^2c^2} \right) \int [\rho_p(r)]^2 \, dr
\]
\[
+ C_{pn} \int \rho_p(r) \rho_n(r) \, dr
\]
\[
= (3 - \bar{\mu}_p) \frac{\pi\hbar^2c^2}{2M^2c^2} \int [\rho_p(r)]^2 \, dr
\]
\[
- \bar{\mu}_n \frac{\pi\hbar^2c^2}{M^2c^2} \int \rho_p(r) \rho_n(r) \, dr
\]
(19)
\[
\approx \frac{\pi\hbar^2c^2}{M^2c^2} \int \left[ 0.1035\rho_p(r) + 1.913\rho_n(r) \right] [\rho_p(r)] \, dr.
\]
(20)
\[R_{\tau} = \left( \frac{3\sqrt{\pi}}{4\pi \rho_0} \right)^{1/3}\]
(22)
with \(N_p = Z\) and \(N_n = N\). For simplicity, the half of the saturation density of atomic nuclei \(\rho_0^p = \rho_0^n \approx 0.08\text{fm}^{-3}\) is assumed. With this density, one can estimate the Coulomb Hartree and exchange energies as [40]
\[E_{\text{Coul}}^H = \frac{3e^2}{5} \left( \frac{4\pi \rho_0^H}{3} \right)^{1/3} Z^{5/3}\]
\[\simeq 0.60z^{5/3}\text{MeV},\]
(23a)
\[E_{\text{Coul}}^\pi = \frac{3e^2}{4} \left( \frac{3\rho_0^\pi}{\pi} \right)^{1/3} Z\]
\[\simeq -0.46z\text{MeV},\]
(23b)
respectively.

### 3 Analytical Estimation

Before performing numerical many-body calculations with the relativistic correction, I estimate contribution of the correction to the total energy with a simple model and discuss the systematic behavior. As in Ref. [40], I assume hard-sphere distributions for both proton and neutron distribution \(\rho_p\) and \(\rho_n\):
\[
\rho_{\tau}(r) = \begin{cases} 
\rho_0^\tau & r \leq R_{\tau}, \\
0 & r > R_{\tau},
\end{cases}
\]
(21)
where \(R_{\tau}\) is the proton (\(\tau = p\)) or neutron (\(\tau = n\)) radius defined by
\[
\rho_0^\tau = \frac{\rho_0^\pi}{N},
\]
\[\rho_0^p, N \text{ for } R_p > R_n,
\]
(24b)

### Table 1.

| Equation | Description |
|----------|-------------|
| Eq. (7a) | Eq. (5b) | Eq. (2b) | Retardation |
| Eq. (7b) | Eq. (5c) | Eq. (2c) and (2d) | Spin-orbit interaction |
| Eq. (7c) | Eq. (5d) | Eq. (2e) | Spin-magnetic interaction (non-mutually penetrating) |
| Eq. (7d) | Eq. (5e) | Eq. (2f) | Spin-magnetic interaction (mutually penetrating) |
| Eq. (7e) | Eq. (5f) | Eq. (2g) | Darwin term |

For convenience, correspondence to Eq. (2) of Ref. [67] is also shown.
hold with $R_\leq = R_p$ for $R_p < R_n$ and $R_\geq = R_n$ for $R_p > R_n$, one, accordingly, obtains
\[
E^H_{\text{Darwin}} = \frac{C_{pp} 4\pi R_0^3}{3} \left( \frac{\rho_0^{p}}{\nu} \right)^2 + C_{pn} \frac{4\pi R_0^3}{3} \rho_0^p \rho_0^n
= -\frac{2\pi^2 \hbar^2 c^2}{3M^2 c^2} \left( (2\mu_p - 1) \left( \frac{\rho_0^{p}}{\nu} \right)^2 + 2\mu_n R_\leq \frac{\rho_0^n}{\nu} \right), \tag{25a}
\]
\[
E^X_{\text{Darwin}} = \frac{C_{pp} 4\pi R_0^3}{3} \left( \frac{\rho_0^{p}}{\nu} \right)^2
= \frac{\pi^2 \hbar^2 c^2}{3M^2 c^2} \left( 2\mu_p - 1 \right) R_0^p \left( \frac{\rho_0^{p}}{\nu} \right)^2
= \frac{\pi^2 \hbar^2 c^2}{4M^2 c^2} \left( 2\mu_p - 1 \right) \rho_0^p Z
\approx 0.018Z \text{ MeV}, \tag{25b}
\]
\[
E^{\text{retar}} = \frac{5\pi^2 \hbar^2 c^2}{3M^2 c^2} R_0^p \left( \frac{\rho_0^{p}}{\nu} \right)^2
= \frac{5\pi^2 \hbar^2 c^2}{3M^2 c^2} \rho_0^p Z
\approx 0.020Z \text{ MeV}, \tag{25c}
\]
\[
E^{\text{tot}}_{\text{Rel}} = \frac{2\pi^2 \hbar^2 c^2}{3M^2 c^2} \left[ (3 - \mu_p) R_0^p \left( \frac{\rho_0^{p}}{\nu} \right)^2 - 2\mu_n R_\leq \frac{\rho_0^n}{\nu} \right]. \tag{25d}
\]

In the case of $R_p < R_n$, Eqs. (25a) and (25d) read
\[
E^H_{\text{Darwin}} = -\frac{2\pi^2 \hbar^2 c^2}{3M^2 c^2} \left[ (2\mu_p - 1) \left( \frac{\rho_0^{p}}{\nu} \right)^2 + 2\mu_n \rho_0^p \rho_0^n \right] R_0^p
= -\frac{\pi^2 \hbar^2 c^2}{2M^2 c^2} \left[ (2\mu_p - 1) \rho_0^p + 2\mu_n \rho_0^n \right] Z
\approx -0.006Z \text{ MeV}, \tag{26a}
\]
\[
E^{\text{tot}}_{\text{Rel}} = \frac{2\pi^2 \hbar^2 c^2}{3M^2 c^2} \left[ (3 - \mu_p) R_0^p \left( \frac{\rho_0^{p}}{\nu} \right)^2 - 2\mu_n R_\leq \rho_0^n \rho_0^n \right]
= \frac{\pi^2 \hbar^2 c^2}{2M^2 c^2} \left[ (3 - \mu_p) \rho_0^p - 2\mu_n \rho_0^n \right] Z
\approx 0.032Z \text{ MeV}; \tag{26b}
\]
in the case of $R_p > R_n$, they read
\[
E^H_{\text{Darwin}} = -\frac{2\pi^2 \hbar^2 c^2}{3M^2 c^2} \left[ (2\mu_p - 1) \left( \frac{\rho_0^{p}}{\nu} \right)^2 + 2\mu_n R_\leq \rho_0^n \rho_0^n \right] R_0^p
= -\frac{\pi^2 \hbar^2 c^2}{2M^2 c^2} \rho_0^p \left[ (2\mu_p - 1) Z + 2\mu_n N \right]
\approx -0.037Z + 0.031N \text{ MeV}, \tag{27a}
\]
\[
E^{\text{tot}}_{\text{Rel}} = \frac{2\pi^2 \hbar^2 c^2}{3M^2 c^2} \left[ (3 - \mu_p) R_0^p \left( \frac{\rho_0^{p}}{\nu} \right)^2 - 2\mu_n R_\leq \rho_0^n \rho_0^n \right]
= \frac{\pi^2 \hbar^2 c^2}{2M^2 c^2} \rho_0^p \left[ (3 - \mu_p) Z - 2\mu_n N \right]
\approx 0.002Z + 0.031N \text{ MeV}. \tag{27b}
\]
Comparing Eqs. (23b) and (26b), one can find that the relativistic correction to the total energy $E^{\text{tot}}_{\text{Rel}}$ is 15 times smaller than the Coulomb exchange energy $E^S_{\text{Coul}}$. This means that although $E^{\text{tot}}_{\text{Rel}}$ is small compared to the other contributions, one can estimate that $E^{\text{tot}}_{\text{Rel}}$ for $^{208}$Pb may be around 2 MeV, which is a non-negligible contribution compared to the desired accuracy of $E_{\text{nuc}}$ (O(100) keV).

In atomic physics, the vacuum polarization to the Coulomb potential formed by an atomic nucleus is the next-leading order to the Breit correction, i.e., the relativistic correction of electron-electron interaction [58]. On the other hand, in nuclear structure, both the vacuum polarization and the relativistic correction are corrections to the proton-proton Coulomb interaction. Thus, it is worthwhile to compare them. In Ref. [10], the vacuum polarization was taken into account in a nuclear structure calculation using the Uehling potential [79,80]. The contribution of the vacuum polarization was estimated as
\[
E_{VP} \approx 0.0047Z^{5/3} \text{ MeV}. \tag{28}
\]

Hence, the relativistic correction and the vacuum polarization provide comparable contributions to the total energy in the light nuclei (e.g., for $Z = 20$, $E^{\text{tot}}_{\text{Rel}} \approx 0.64$ MeV and $E_{VP} \approx 0.69$ MeV) but the latter dominates in heavy nuclei (e.g., for $Z = 100$, $E^{\text{tot}}_{\text{Rel}} \approx 3.2$ MeV and $E_{VP} \approx 10$ MeV). In the next section, I shall confirm this by performing numerical calculations.

### 4 Skyrme Hartree-Fock Calculation

To calculate the ground-state density distribution and energy numerically, one needs to use a many-body calculation technique. In this paper, the Skyrme Hartree-Fock method is used.

The EDF for the correction [Eq. (19)] is implemented to the self-consistent Skyrme Hartree-Fock calculation code SKYRME_RPA [81]. In this work, doubly-magic nuclei are focused on; thus, the pairing interaction is not considered, and the spherical symmetry is assumed. The calculations are performed with a box of 15 fm with 0.1 fm mesh. The SAMi functional [82] is adopted for the nuclear EDF.

First of all, I shall mention effects to nuclear radii. Neither the proton nor the neutron radii are found to be changed more than 0.002 fm due to the relativistic correction and the vacuum polarization. Therefore, the effect of the correction on nuclear radii can be safely neglected.

Next, the ground-state energies for doubly-magic nuclei are shown in Table 2. The columns labelled “Coulomb (NR-LDA)” and “Coulomb (R-LDA)” show results with the non-relativistic Coulomb LDA [Eq. (11)] and the relativistic Coulomb LDA [Eqs. (11) and (12)], respectively. For comparison, total energies calculated with the vacuum polarization on top of the relativistic Coulomb LDA and with the non-relativistic Coulomb GGA [39] are shown in a column labelled “C. (R-LDA) & V.P.” and “Coulomb (NR-GGA)”, respectively. Both the relativistic correction and the vacuum polarization make the atomic nuclei less bound. The contribution of the former is around 0.42 MeV in $^{40}$Ca and 2.37 MeV in $^{208}$Pb. Although the relativistic correction changes $\Delta E^{\text{tot}}$ of $^{40}$Ca and $^{48}$Ni by 0.5 MeV, the mass difference is not changed.
Fig. 1. Contribution of relativistic correction and vacuum polarization to the total energies, $E_{\text{tot}}^{\text{rel}}$ and $E_{\text{VP}}$, shown as functions of proton number $Z$ in circle and square points, respectively. Empirical fits with Eqs. (29) are also shown by the solid and the dashed lines, respectively.

It was shown in Refs. [39,62] that the exact treatment or its simplified treatment called GGA of the Coulomb exchange energy makes $^{40}\text{Ca}$ bound more by around 0.32 MeV and $^{208}\text{Pb}$ by around 0.74 MeV, which can be explained as the correction of the density gradient on the LDA. Hence, the relativistic correction on the Coulomb interaction is almost comparable with or even larger than the gradient correction but opposite direction to total energies, as in the case of atoms [51]. Thus, if both contributions are considered simultaneously, even it is not obvious whether the total energy decreases or increases. Indeed, this fact was pointed out in the context of atomic physics in Ref. [51], while no first-principles relativistic Coulomb GGA functional is available, which remains an open question.

I also compare the relativistic correction and the vacuum polarization. The vacuum polarization also makes the atomic nuclei less bound, and contribution to the total energy is approximately 0.4 MeV in $^{40}\text{Ca}$ and 3.7 MeV in $^{208}\text{Pb}$. Thus, as discussed in Sec. 3, the vacuum polarization gives a comparable contribution to the total energy to the relativistic correction in light nuclei, but it contributes more in heavy nuclei.

The systematic behavior of the relativistic correction and the vacuum polarization shall be discussed next. The contributions of the relativistic correction and the vacuum polarization can be seen as the difference of the second and the third columns and the third and the fourth columns in Table 2 respectively. The proton number $Z$ dependence of these contributions are shown in Fig. 1. These energies are fitted with $E = aZ^b$, where $a$ and $b$ are adjustable parameters. The results are

$$E_{\text{tot}}^{\text{rel}} \simeq 0.01660Z^{1.12} \text{ MeV},$$

$$E_{\text{VP}} \simeq 0.00398Z^{1.55} \text{ MeV},$$

which are consistent to Eqs. (26b) and (28).

The breakdown of the relativistic correction [Eq. (19)] is shown in Table 3. The columns labelled $E_{\text{Darwin}}^H$, and $E_{\text{retar}}^x$ are Darwin Hartree energy [Eq. (13a)], Darwin exchange one [Eq. (13b)], retardation exchange one [Eq. (18)], respectively. As shown, in $N \leq Z$ nuclei, $E_{\text{Darwin}}^H < 0$ holds, while in $N > Z$ nuclei, $E_{\text{Darwin}}^H > 0$ holds. The Darwin Hartree energy reads

$$E_{\text{Darwin}}^H = -\pi \hbar^2 c^2 \iint \left\{ \frac{2\tilde{\rho}_p - \rho_p}{2} \rho_p (r) + \tilde{\rho}_p \rho_p (r) \right\} \rho_p (r) \, dr$$

$$\approx -\pi \hbar^2 c^2 \iint \left\{ 2.292\tilde{\rho}_p (r) - 1.913\rho_p (r) \right\} \rho_p (r) \, dr; \quad (30)$$

hence, $[2.292\rho_p (r) - 1.913\rho_p (r)]$ determines the sign of $E_{\text{Darwin}}^H$. In $N \leq Z$ nuclei, $\rho_p (r) > \rho_p (r)$ holds and, accordingly, it is negative (i.e., $E_{\text{Darwin}}^H > 0$), whereas, in $N < Z$ nuclei, $\rho_p (r) < \rho_p (r)$ holds and accordingly, it can be positive (i.e., $E_{\text{Darwin}}^H < 0$) in contrast to Eq. (25a). The Darwin and retardation exchange energies are also fitted with $E = aZ^b$, where the results are

$$E_{\text{Darwin}}^x \simeq 0.01312Z^{0.97} \text{ MeV},$$

$$E_{\text{retar}}^x \simeq 0.01431Z^{0.97} \text{ MeV},$$

which are consistent to Eqs. (25b) and (25c).

The exchange contribution to the EM energy shall be further discussed. The ratio of the Coulomb or relativistic Coulomb exchange energy to the exact Coulomb exchange energy

$$\frac{\Delta E_x}{E_{\text{exact}}} = \frac{E_{\text{Coul}}^x - E_{\text{exact}}^x}{E_{\text{exact}}^x}$$

is shown in Fig. 2. Here, the exact Coulomb exchange energy is calculated by using the modified GGA-PBE functional with $\lambda = 1.25$, which reproduces the exact Coulomb exchange energy less than 500 keV error [39]. The non-relativistic and relativistic Coulomb LDA exchange energies are calculated by using $E_{\text{Coul}}^x$ [Eq. (11c)] and $E_{\text{Coul}}^x + E_{\text{Darwin}}^x + E_{\text{retar}}^x$ [Eqs. (13b) and (18)], respectively. It is seen that the absolute value of the relative change $|\Delta E_x|$ for the difference between the exact and LDA non-relativistic Coulomb exchange energy gets smaller as $A$ increases in light nuclei and reaches almost constant $\Delta E_x \approx -3\%$ in heavy nuclei ($A \gtrsim 100$). The absolute value of the relative change $|\Delta E_x|$ for the difference between the non-relativistic and relativistic LDA Coulomb exchange energy behaves similarly, while its value is larger and reaches almost constant $\Delta E_x \approx -9\%$ in heavy nuclei. The Darwin contribution and the retardation one are almost the same size.

This difference has been studied in the relativistic (covariant) density functional theory [63,64]. The exact Coulomb exchange energy in this paper corresponds to Eq. (4) in Ref. [64] which does not seem to include the relativistic correction. They also show that difference between the non-relativistic and relativistic LDA exchange energies is approximately 1 MeV. With considering such difference, $E_{\text{Coul}}^x + E_{\text{Darwin}}^x$ calculated in this work is almost consistent qualitatively with, but almost twice of Figs. 1 and 4 of Ref. [64], because Ref. [64] does not
Coulomb LDA \[Eqs. (11) and (19)\], respectively. For comparison, total energies calculated with the vacuum polarization on top of the relativistic Coulomb LDA and with the non-relativistic Coulomb GGA are shown in a column labelled “C. (R-LDA) & V.P.” and “Coulomb (NR-GGA)”, respectively.

### Table 2. Ground-state energies calculated with the SAMi functional \[82\] shown in MeV. The columns labelled “Coulomb (NR-LDA)” and “Coulomb (R-LDA)” show results calculated with the non-relativistic Coulomb LDA \[Eq. (11)\] and the relativistic Coulomb LDA \[Eqs. (11) and (19)\], respectively. For comparison, total energies calculated with the vacuum polarization on top of the relativistic Coulomb LDA and with the non-relativistic Coulomb GGA are shown in a column labelled “C. (R-LDA) & V.P.” and “Coulomb (NR-GGA)”, respectively.

| Nuclei | Coulomb (NR-LDA) | Coulomb (R-LDA) | C. (R-LDA) & V.P. | Coulomb (NR-GGA) |
|--------|------------------|-----------------|-------------------|------------------|
| He     | −27.5263         | −27.5001        | −27.4918          | −27.6011         |
| 16O    | −130.4800        | −130.3340       | −130.2444         | −130.6630        |
| 40Ca   | −347.0848        | −346.6639       | −346.2544         | −347.4045        |
| 48Ca   | −415.6148        | −415.1194       | −414.7093         | −415.9293        |
| 48Ni   | −352.6388        | −352.1357       | −351.4160         | −353.0443        |
| 100Sn  | −811.6641        | −810.4970       | −808.6876         | −812.2390        |
| 132Sn  | −1103.0881       | −1101.6342      | −1099.9484        | −1103.6397       |
| 208Pb  | −1636.6149       | −1634.2456      | −1630.5350        | −1637.3582       |
| 310126 | −2131.4146       | −2127.8446      | −2120.5577        | −2132.3711       |

### Table 3. Breakdown of the relativistic correction \[Eq. (19)\] shown in MeV. The columns labelled $E_{\text{Darwin}}^H$, $E_{\text{Darwin}}^\text{retar}$, and $E_{\text{total}}^\text{retar}$ are Darwin Hartree energy \[Eq. (13a)\], Darwin exchange energy \[Eq. (13b)\], and retardation exchange energy \[Eq. (18)\], respectively.

| Nuclei | $E_{\text{Darwin}}^H$ | $E_{\text{Darwin}}^\text{retar}$ | $E_{\text{total}}^\text{retar}$ |
|--------|-----------------------|-----------------------------------|----------------------------------|
| 4He    | −0.0048               | +0.0148                           | +0.0162                          |
| 16O    | −0.0256               | +0.0821                           | +0.0895                          |
| 40Ca   | −0.0704               | +0.2349                           | +0.2562                          |
| 48Ca   | +0.0379               | +0.2230                           | +0.2432                          |
| 48Ni   | −0.2429               | +0.3568                           | +0.3890                          |
| 100Sn  | −0.1869               | +0.6475                           | +0.7060                          |
| 132Sn  | +0.3026               | +0.5305                           | +0.6002                          |
| 208Pb  | +0.4221               | +0.9311                           | +1.0153                          |
| 310126 | +0.5492               | +1.4445                           | +1.5750                          |

Lastly, a change of the single-particle energies is discussed, for which $^{208}\text{Pb}$ is taken as an example. The single-particle energies calculated with the non-relativistic and relativistic Coulomb LDA are shown in Table 3. For comparison, those calculated with the vacuum polarization on top of the relativistic LDA are shown. It is seen that the proton single-particle energies change by about 0.04 MeV in inner shells while 0.01 MeV in outer shells, due to the relativistic correction. In contrast, the change due to the vacuum polarization does not depend on orbitals strongly, and its value is about 0.1 MeV. This difference is due to the nature of interaction: the relativistic correction is the point-coupling interaction, while the vacuum polarization is finite range. Since the Darwin Hartree term contributes to the neutron mean-field potential (see Eq. (20)), the neutron single-particle energies change by about 0.04 MeV in inner shells while 0.01 MeV in outer shells, due to the relativistic correction. In contrast, the vacuum polarization changes neutron single-particle energies only by less than 0.01 MeV.

### 5 Conclusion and Perspectives

In this paper, the relativistic correction of the Coulomb interaction was introduced in Skyrme Hartree-Fock calculations using the local density approximation (LDA). The correction contains the Darwin term, the retardation, the spin-orbit interaction, and the spin-magnetic interaction, while only the first and second terms were considered in this paper because of the LDA.

It was found that the relativistic correction makes $^{40}\text{Ca}$ less bound by 0.4 MeV and $^{208}\text{Pb}$ by 2.4 MeV, which are comparable with or even larger than the difference between the exact Coulomb exchange (exact-Fock), or its simplified treatment called the generalized gradient approximation (GGA), and the LDA (Hartree-Fock-Slater approximation) Coulomb exchange energies $^{38,39,61,62}$, but with the opposite sign. Thus, once both the exact treatment and the relativistic correction are considered at the same time, even the sign of the total correction is not obvious, as was pointed out also in the context of atomic...
physicists\cite{51}. In addition, since the desired accuracy of the nuclear EDF is 100 keV order, the relativistic correction is often non-negligible, as well as the correction due to the density gradient.

The correction was also compared with the vacuum polarization. Since the proton-number dependence of the vacuum polarization is stronger than that of the relativistic correction, these two contributions to the total energy are comparable in light nuclei, but the former dominates in heavy nuclei. This behavior is in contrast to atoms, in which the vacuum polarization is sub-dominant to the Breit correction\cite{58}. Although the contribution of vacuum polarization to the total energy is usually tiny, it is non-negligible to discuss mirror nuclei mass difference or the isobaric analog energy\cite{10,11}, whereas the relativistic correction does not contribute to such properties.

In relativistic Hartree-Fock calculation, the current-current Hartree interaction is often considered, and the relativistic correction is also considered to the Fock term exactly or by using LDA. In this work, the relativistic correction is consistently considered in the Hartree-Fock-Slater approximation. The magnetic (current-current) interaction and the retardation appear in the next-leading order of the electromagnetic interaction in the Lorenz gauge, which corresponds to the Breit correction in the Coulomb gauge\cite{69}. Hence, the difference between them is which gauge is introduced in quantum electrodynamics calculation\cite{69,71}. Thus, it can be concluded that by introducing the relativistic correction to non-relativistic Hartree-Fock calculations as proposed in this work, one can directly compare electromagnetic energies obtained by non-relativistic and relativistic calculations.

In this calculation, the spin-orbit and spin-magnetic interactions were not considered. The former has been discussed in Refs.\cite{4,78}, while the latter has not been considered in the self-consistent calculation. Consideration of the latter is left for a future task. The relativistic Coulomb GGA functional is indispensable to achieve more accurate calculation in both atomic and nuclear structure calculations, which remains as a future perspective.

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