The Slater approximation for Coulomb exchange effects in nuclear covariant density functional theory

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The relativistic local density approximation (LDA) for the Coulomb exchange functional in nuclear systems is presented. This approximation is composed of the well-known Slater approximation in the non-relativistic scheme and the corrections due to the relativistic effects. Its validity in finite nuclei is examined by comparing with the exact treatment of the Coulomb exchange term in the relativistic Hartree-Fock-Bogoliubov theory. The relativistic effects are found to be important and the exact Coulomb exchange energies can be reproduced by the relativistic LDA within 5% demonstrated by the semi-magic Ca, Ni, Zr, Sn, and Pb isotopes from proton drip line to neutron drip line.

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The Coulomb interaction between protons is one of the most important building blocks in atomic nuclei. It is the main source of the charge symmetry-breaking in the nuclear Hamiltonian. Globally, the Coulomb interaction is the driving force for determining the \(\beta\)-stability valley away from the \(N = Z\) line. Specifically, the Coulomb interaction plays a crucial role in understanding the Coulomb displacement energies, isospin mixing, proton emission, formation barriers, \(\alpha\)-decay energy release, \(Q_a\) in superheavy elements, and more. Therefore, the nuclear density functional theory (DFT) that models the effective strong interactions has to be accompanied by an explicit functional form for the Coulomb interaction.

Generally speaking, the Coulomb interaction is the best known part of the nuclear Hamiltonian, and both its direct (Hartree) and exchange (Fock) terms can be exactly calculated at the mean-field level. However, the exchange term is very cumbersome to include due to the non-locality of the corresponding mean field, especially for the deformed nuclei. In the spirit of the DFT of Kohn and Sham, the local density approximation (LDA) has been intensively adopted in the calculations of finite nuclei since the 1970s. So far, in almost all of the non-relativistic (NR) self-consistent Hartree-Fock calculations, the Coulomb exchange energy and the corresponding single-particle potential are evaluated within a local scheme by using the so-called Slater approximation. The validity of this approximation has been discussed in the Skyrme and Gogny approaches.

During the past decades, the nuclear covariant density functional theory (CDFT) at the Hartree level, also known as the relativistic Hartree (RH) or relativistic mean-field (RMF) theory, has received much attention due to its successful description of many nuclear phenomena. The Lorentz covariant form of the theory itself guarantees the self-consistent spin-orbit potential and also puts stringent restrictions on the number of parameters in the corresponding functionals without reducing the quality of the agreement with experimental data. In order to retain the required simplicity in the RH framework, the non-local Coulomb exchange term is usually neglected. Its effects on the binding energies, radii, etc., are assumed to be absorbed into the effective meson-nucleon coupling strengths through the phenomenological fit of the model. However, this prescription of neglecting the Coulomb exchange term is not always valid, because the meson-nucleon interactions are of isospin symmetry but the Coulomb interaction is not. One example is the isospin symmetry-breaking corrections to the superallowed \(\beta\) decays, which are crucial for testing the unitarity of the Cabibbo-Kobayashi-Maskawa matrix.

Recently, the density-dependent relativistic Hartree-Fock (RHF) theory has been developed and achieved equivalent success in describing the ground- and excited-state properties as the RH theory. It has been shown that the meson exchange terms play very important roles in the nucleon effective mass splitting, symmetry energies, spin and pseudospin symmetries, shell structure and its evolutions, deformation, and spin-isospin resonances. Subsequently, a unified and self-consistent description of both RHF mean field and pairing correlations, i.e., the relativistic Hartree-Fock-Bogoliubov (RHFHB) theory, has been achieved for the exotic nuclei far from the \(\beta\)-stability valley. In the frameworks of RHF and RHFHB, for the first time, the non-local Coulomb exchange term has been taken into account exactly, which...
is crucial for understanding the isospin corrections to the superallowed $\beta$ decays \cite{18}.

With the simplicity of the local CDFT and the success in treating the Coulomb terms exactly, it is worthwhile to explore the relativistic LDA for the Coulomb exchange term, a topic less known in the nuclear physics community. The relativistic LDA may be a simple approach to implement the missing Coulomb exchange effects in the RH theory, yet keeping the merits of locality. The attempt in this direction is further supported by a recent success in folding the meson exchange terms into a local equivalent scheme \cite{22}.

The relativistic LDA has been explored for electronic systems in past decades. The extension of the Hohenberg and Kohn theorem \cite{35} to relativistic systems was first formulated in Ref. \cite{36} by utilizing a quantum electrodynamics (QED)-based Hamiltonian with the four-current. Within the no-sea approximation, which is also called no-pair approximation in atomic physics \cite{39}, the total energy of the system can be expressed as a functional with respect to the four-current $j^\mu (r) = (\rho (r), \mathbf{J} (r))$ \cite{37, 38}, instead of only $\rho (r)$ in the NR case. In complete analogy with the NR case, the relativistic LDA for the Coulomb exchange energy functional $E_{\text{Cex}}^{\text{RLDA}} [j^\mu (r)]$ is constructed by using the model of relativistic homogeneous electron gas. As the space-like component $\mathbf{J}$ vanishes in the homogeneous systems, the full $j^\mu$-dependence of the exact exchange energy functional is reduced to a pure density-dependence in the relativistic LDA. The relativistic corrections, i.e., the differences between $E_{\text{Cex}}^{\text{RLDA}} [\rho (r)]$ and $E_{\text{Cex}}^{\text{NR}} [\rho (r)]$, are shown to be substantial, see Ref. \cite{22} for details.

In this Rapid Communication, the relativistic LDA for the Coulomb interaction in nuclear physics will be presented. The main focus will be its validity by comparing with the exact RHFB results and the relativistic corrections to the traditional Slater approximation.

Before introducing the relativistic LDA, it is illuminating to briefly recall the Coulomb energies and the corresponding LDA for the exchange term in the NR systems.

In the non-relativistic scheme, the proton density distribution in nuclei reads

$$\rho_p (r) = \sum_i v_i^2 \psi_i^*(r) \psi_i (r),$$  

(1)

with the single-particle wave functions $\psi_i (r)$ and occupation probabilities $v_i^2$. The direct term of Coulomb energy is simply a functional of $\rho_p (r)$, i.e.,

$$E_{\text{Cdir}} = \frac{e^2}{2} \int d^3 r d^3 r' \frac{\rho_p (r) \rho_p (r')}{|r - r'|},$$  

(2)

and the corresponding Hartree potential for protons reads

$$V_{\text{Cdir}} (r) = \frac{\delta E_{\text{Cdir}} [\rho_p (r)]}{\delta \rho_p (r)} = \frac{e^2}{2} \int d^3 r \rho_p (r') \frac{\rho_p (r')}{|r - r'|},$$  

(3)

In contrast, the exchange term of Coulomb energy,

$$E_{\text{Cex}} = -\frac{e^2}{2} \sum_{ij} v_i^2 v_j^2 \int d^3 r d^3 r' \frac{\psi_i^* (r) \psi_j^* (r') \psi_j (r')}{|r - r'|},$$  

(4)

leads to non-local single-particle potentials and thus is more complicated to calculate.

In the spirit of the LDA, the exchange energy density of an inhomogeneous system with density $\rho (r)$ is locally approximated by the exchange energy density of a homogeneous system with density $n = \rho (r)$. In the homogeneous nuclear matter, the single-particle wave functions are the plane-wave solutions of the Schrödinger equation, so that the Coulomb exchange energy shown in Eq. \cite{41} per unit volume can be calculated analytically as

$$e_{\text{Cex}} = -\frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} e^2 n_p^{4/3},$$  

(5)

where $n_p$ is the proton density. Therefore, by using the LDA, the Coulomb exchange energy in finite nuclei is determined as

$$E_{\text{Cex}}^{\text{LDA}} = -\frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} e^2 \int d^3 r \rho_p^{4/3} (r).$$  

(6)

This is the well-known Slater approximation \cite{40} widely used in the non-relativistic DFT. The corresponding single-particle potential for protons reads

$$V_{\text{Cex}}^{\text{LDA}} (r) = -\frac{\delta E_{\text{Cex}}^{\text{LDA}} [\rho_p (r)]}{\delta \rho_p (r)} = -\left( \frac{3}{\pi} \right)^{1/3} e^2 \rho_p^{1/3} (r).$$  

(7)

In the relativistic scheme, the variables of the energy functional include not only the density distributions but also the currents. The proton density distribution and currents read

$$\rho_p (r) = \sum_i v_i^2 \bar{\psi}_i (r) \gamma^0 \psi_i (r),$$  

(8a)

$$\mathbf{j}_p (r) = \sum_i v_i^2 \bar{\psi}_i (r) \gamma \psi_i (r),$$  

(8b)

respectively. It should be emphasized that the summations over $i$ include only the particles in the Fermi sea, i.e., the no-sea approximation, which is the so-called no-pair approximation in atomic physics \cite{39}.

Correspondingly, the direct term of Coulomb energy reads

$$E_{\text{Cdir}}^{\text{R}} = \frac{e^2}{2} \int d^3 r d^3 r' \frac{j^\mu_p (r) j_{\mu}^\nu (r')}{|r - r'|},$$

(9)

$$= \frac{e^2}{2} \int d^3 r d^3 r' \left[ \frac{\rho_p (r) \rho_p (r')}{|r - r'|} - \frac{\mathbf{j}_p (r) \cdot \mathbf{j}_p (r')}{|r - r'|} \right],$$

where the first and second terms are the contributions from the time-like and space-like components of the
Coulomb field, respectively. They are called Coulomb and transverse contributions in Ref. [39]. For the systems with time-reversal symmetry, the contribution from the space-like component vanishes. Then, Eq. (4) has the same structure as Eq. (2).

On the other hand, the exchange term of Coulomb energy is [39]
\[ E_{Cex}^{RLDA} = -\frac{e^2}{2} \sum_{i<j} v_i^2 v_j^2 \int d^3r \int d^3r' |\varphi_i(r)\varphi_j(r')\gamma_\mu \varphi_i(r')|, \]
where \( \varphi_i \) are the single-particle energies.

In the relativistic homogeneous nuclear matter, the single-particle wave functions are the plane-wave solutions of the Dirac equation. As a result, the time-like component \( \bar{e}_{Cex}^{RLDA} \) and space-like component \( \bar{e}_{Cex} \) of the Coulomb exchange energy shown in Eq. (5) per unit volume can be, respectively, expressed as [38, 39]
\[ \bar{e}_{Cex}^{RLDA} = e_{Cex} \Phi(\beta) \quad \text{and} \quad \bar{e}_{Cex} = e_{Cex} \bar{\Phi}(\beta), \]
by the NR one \( e_{Cex} \) in Eq. (5) together with
\[ \Phi(\beta) = \frac{5}{6} + \frac{1}{3\beta^2} + \frac{2\eta}{3\beta^3} \ln \beta - \frac{2\eta^4}{3\beta^4} \ln \eta \]
\[ -\left( \frac{\eta}{\beta^2} - \frac{\eta}{3\beta^2} \right)^2 \]
\[ + 1 - \frac{1}{9} \beta^2 + \frac{13}{180} \beta^4 + \cdots \]
\[ (12a) \]
\[ \bar{\Phi}(\beta) = \frac{1}{6} - \frac{1}{3\beta^2} + \frac{2\eta}{3\beta^3} \ln \beta + \frac{2\eta^4}{3\beta^4} \ln \eta \]
\[ - \left( \frac{\eta}{\beta^2} - \frac{\eta}{3\beta^2} \right)^2 \]
\[ = -\frac{5}{9} \beta^2 + \frac{59}{180} \beta^4 + \cdots, \]
\[ (12b) \]
where \( \beta = (3\pi^2 n_p)^{1/3}/M \), \( \eta = \sqrt{1 + \beta^2} \), and \( M \) is the proton mass. The details can be found in Ref. [39] and the references therein.

From Eqs. (11) and (12), the relativistic results are identical to the NR counterparts at the zero density limit. The relativistic corrections to the Coulomb exchange energy increase with the density. For the symmetric nuclear matter, \( n_p \approx 0.08 \text{ fm}^{-3} \) at the saturation density, one has \( \beta \sim 0.28, \beta^2 \sim 0.078, \) and \( \beta^4 \sim 0.006 \). Therefore, the relativistic corrections to the Coulomb exchange energy are expected to be substantial in nuclear systems, and the contributions from \( \beta^4 \) and higher-order terms can be neglected. Accordingly, the relativistic effect from the space-like component is 5 times that from the time-like component, as shown in Eq. (12).

From Eq. (11), up to the order of \( \beta^2 \), the Coulomb exchange energy in the relativistic LDA is
\[ E_{Cex}^{RLDA} = -\frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} e^2 \int d^3r \rho_p^{1/3} \left[ 1 - \frac{2}{3} \frac{(3\pi^2 \rho_p)^{2/3}}{M^2} \right]. \]
(13)

\[ \Delta E_{Cex} = \frac{E_{Cex}^{RLDA} - E_{Cex}^{exact}}{E_{Cex}^{exact}}. \]

FIG. 1: (Color online) Coulomb exchange energies in Pb isotopes calculated by RHF theory [32] with PKA1 [21]. The results obtained with the same proton density distributions \( \rho_p(r) \) but within the relativistic and non-relativistic (NR) local density approximations (LDA) and their relative deviations from the exact results are shown in the upper and lower panels, respectively. The corresponding results calculated by Eq. (4), the exact formula for the NR case, are also shown for comparison.

The corresponding contribution to the single-particle potential for protons reads
\[ V_{Cex}^{RLDA}(r) = - \left( \frac{3}{\pi} \right)^{1/3} e^2 \rho_p^{1/3}(r) + \left( \frac{3\pi}{M^2} \right) e^2 \rho_p(r). \]
(14)

In the following, the properties of finite nuclei are calculated in the density-dependent RHF theory [32] with PKA1 [21] and D1S [10] effective interactions for the particle-hole and particle-particle channels, respectively. The RHF equations are solved on a Dirac Woods-Saxon basis [11] within a spherical box of radius \( R_{\text{max}} = 20 \text{ fm} \), and the numbers of positive and negative energy levels for each \((l,j)\)-state are fixed to \( N_F = 28 \) and \( N_D = 12 \), respectively.

In the standard RHF calculations, the Coulomb exchange energy and the corresponding non-local single-particle potential are calculated exactly. They are labeled with the superscript “exact”. The corresponding results obtained by using the relativistic LDA shown in Eqs. (13) and (14) are labeled with the superscript RLDA. In order to quantitatively investigate the relativistic corrections in Eq. (11), the results of the non-relativistic LDA shown in Eqs. (6) and (7) labeled with the superscript NRLDA are also presented for comparison. The relative deviations of the approximate Coulomb exchange energies from the RHF results are defined as
In order to exclude the effects due to self-consistency, one-step calculations have been performed to investigate the effects of the LDA approximation on Coulomb exchange energies, i.e., $E_{Cex}^{RLDA}$ and $E_{Cex}^{NRLDA}$ are respectively obtained with the relativistic and NR LDA by the same converged proton density distributions $\rho_p(r)$ given by the self-consistent RHFB calculations. By taking the even-even Pb isotopes from proton drip line to neutron drip line as examples, the Coulomb exchange energies $E_{Cex}$ are shown as a function of mass number $A$ in the upper panel of Fig. 1. The corresponding relative deviations $\Delta E_{Cex}$ defined in Eq. (15) are shown in the lower panel. The results calculated by using Eq. (4), the exact formula for the NR case, are also shown for comparison. In addition, the proton density distributions $\rho_p(r)$ in the nuclei $^{188}$Pb, $^{208}$Pb, $^{228}$Pb, and $^{248}$Pb are illustrated in Fig. 2.

In general, the magnitudes of the Coulomb exchange energies $E_{Cex}$ decrease with increasing mass number, i.e., with increasing size. For each nucleus, the magnitude of $E_{Cex}$ is overestimated by the NR LDA or the traditional Slater approximation, and substantially improved when the relativistic corrections are taken into account. From the relative deviations (see the lower panel of Fig. 1), the relativistic correction improvements range from 4.5% in $^{182}$Pb to 3.5% in $^{200}$Pb. The isotopic dependence of the relativistic effect in Eq. (13) is related to the proton density distributions. As shown in the insert of Fig. 2, it is clear that the relevant $r^2\rho_p^2(r)$ distribution much decreases and becomes slightly narrower close to the surface region with the neutron number, which results in a smaller relativistic correction. Accordingly, the relative deviations $\Delta E_{Cex}$ due to the relativistic LDA decrease from 3.6% in $^{182}$Pb to 1.7% in $^{200}$Pb. As shown in Fig. 2 in the heavy nuclei, the inner proton density is almost flat that forms a near uniform density region, and the tail part of density varies slowly. These are the reasons why the LDA works well.

In order to investigate the effects due to the self-consistency, the self-consistent RLDA calculations have been performed. In Fig. 3 the proton single-particle energy shifts $\varepsilon_p^{RLDA} - \varepsilon_p^{exact}$ in $^{208}$Pb are shown as a function of the single-particle energy $\varepsilon_p^{exact}$. It is seen that, in the relativistic LDA, the occupied and unoccupied proton states are pushed up and down, respectively. The energy shifts are around +400 keV for the deeply bound states, +100 keV for the states near the Fermi surface, and −200 keV for the unoccupied bound states. A very similar shifting behavior was shown in Ref. [9] in the NR Skyrme Hartree-Fock framework. As the occupied states are pushed up due to the RLDA, the total kinetic energy of protons increases by 2.73 MeV, which is completely canceled out by the self-consistent effects of the neutron kinetic (−2.12 MeV), mesons (−1.18 MeV), and Coulomb direct (+0.58 MeV) energies. The same kind of self-consistent cancellation between the kinetic energy and other channels was also noted in Ref. [9]. As a result, the total energy difference between the RLDA and RHFB calculations, −0.97 MeV, is mainly due to the difference in the Coulomb exchange energies, −0.99 MeV.
In Fig. 1, we show the systematics of calculated results using the self-consistent relativistic LDA for the semi-magic Ca, Ni, Zr, Sn, and Pb isotopes from proton drip line to neutron drip line. The traditional doubly magic nuclei are marked by the open symbols. Comparing with the exact Coulomb exchange energies calculated in RHFB, it is found that the relative deviations $\Delta E_{\text{Cex}}$ introduced by the relativistic LDA are less than 5% for all these five semi-magic isotopes. In addition, from the differences between the solid and dashed lines, the relativistic corrections to the LDA are found to play substantial roles in improving the results by 3~5%.

Therefore, one can conclude that the relativistic version of LDA shown in Eqs. (3) and (4) for the Coulomb exchange term in nuclear CDFT is very robust and promising. In particular, the relativistic corrections to the traditional Slater approximation shown in Eqs. (1) and (2) are very important.

Another good test for the RLDA is the Coulomb Displacement Energies (CDE) of mirror nuclei. As one of the clearest cases [42], it is found that the experimental mirror binding energy difference $E_B(^{17}\text{O}) - E_B(^{17}\text{F}) = 3.54$ MeV [43] can be well reproduced by the RHFB calculation, 3.47 MeV, with blocking for the odd nucleon [42], while 3.33 MeV by the RLDA calculation. Another representative case is the pair of $^{48}\text{Ni}$ and $^{48}\text{Ca}$ [44]. For this case, the mirror binding energy difference $E_B(^{48}\text{Ni}) - E_B(^{48}\text{Ca})$ obtained by the RHFB and RLDA calculations are almost identical, which are 63.44 and 63.38 MeV, respectively. Nevertheless, the experimental value 66.95(53) MeV [45] is underestimated to some extent, because the charge-symmetry breaking interactions, which are found important for CDE [44, 45], are not included.

In summary, the relativistic LDA for the Coulomb exchange functional in nuclear systems is presented. This approximation is composed of the well-known Slater approximation in the NR scheme and the corrections due to the relativistic effects. The validity of the relativistic LDA in finite nuclei calculations is examined by comparing with the results of the RHFB theory, where the non-local Coulomb exchange term is treated exactly. It is found that the relative deviations of the Coulomb exchange energies in the self-consistent RLDA calculations are in general less than 5% for semi-magic Ca, Ni, Zr, Sn, and Pb isotopes from proton drip line to neutron drip line. For the proton single-particle energy shifts, the relativistic LDA pushes the occupied and unoccupied states upward and downward, respectively, which is in agreement with the previous NR Hartree-Fock calculations. Finally, it is also worthwhile to emphasize that the relativistic corrections to the LDA are found to play substantial roles in improving the agreement with the exact results by 3~5%. This study opens a new door for implementing the Coulomb exchange effects in the RH theory yet keeping its merits of locality in the future.

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