Nuclear effective charge factor originating from covariant density functional theory

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Abstract

Guiding by the relativistic local density approximation, we explore a phenomenological formula for the coupling strength of Coulomb field to take into account the Coulomb exchange term effectively in the relativistic Hartree approximation. Its validity in finite nuclei is examined by comparing with the exact treatment of the Coulomb exchange energies in the relativistic Hartree-Fock-Bogoliubov approach. It is found that the exact Coulomb exchange energies can be reproduced by employing the phenomenological formula with the relative deviations less than 1% for semi-magic Ca, Ni, Sn, and Pb isotopes. Furthermore, we check the applicability of the phenomenological formula for the effective interactions in the relativistic Hartree approach by investigating the binding energy differences of mirror nuclei.

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As one of the most significant building blocks in nuclei, the Coulomb interaction between protons in nuclei plays an important role in understanding many nuclear phenomena, such as the Coulomb displacement energies, isospin mixing, proton emission, and fission barriers. It therefore requires an efficient and precise treatment of the Coulomb effects for the reliable description of nuclear structure properties [1–3].

During the past years, the density functional theory (DFT) with the Lorentz symmetry, namely, the covariant density functional theory (CDFT), has received wide attention due to many successes achieved in describing lots of nuclear phenomena [2, 3] as well as its successful applications in the astrophysics [4–10]. Specifically, there exist two widely used approaches in the CDFT framework: the relativistic Hartree (RH) [2, 3, 11] and relativistic Hartree-Fock (RHF) approaches [12, 13]. The former one is usually known as the relativistic mean field (RMF) model.

Compared with simple direct (Hartree) term, the Coulomb exchange (Fock) term is very cumbersome and time-consuming in the practical calculations due to the non-locality commonly existing in the Fock mean field. To keep the consistent with the approach itself and retain the simplicity of the theory, the non-local Coulomb exchange term is usually neglected in the RH framework. Its effects, in principle, can be taken into account partially by the parametrization of the effective coupling strengths of the model. In the recent years, the RHF approach has been well developed with substantial improvements in the self-consistent descriptions of nuclear shell structure and the evolution, the restoration of relativistic symmetry, exotic nuclei, the low-energy excitation mode, etc. [13–20]. Additionally it is also found from the RHF approach that the prescription of neglecting the Coulomb exchange term in RH approach is not always valid. 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 [21]. It is therefore desirable for the RH approach to get the Coulomb exchange effects involved efficiently with satisfied accuracy.

In the non-relativistic framework, the Coulomb exchange term is usually evaluated within the local density approximation (LDA), which is the well-known Slater approximation [22]. The validity of this approximation has been investigated in the Skyrme [23, 24] or Gogny [25] approaches. The relativistic local density approximation (RLDA) for the Coulomb exchange functional in nuclear systems, which is the Slater approximation with relativistic corrections, has been developed recently [27]. It is found that the relativistic corrections can remarkably...
improve the description of the exact Coulomb exchange energies in the relativistic Hartree-Fock-Bogoliubov (RHFB) approach and the relative deviations are less than 5% for semi-magic isotopes. However, there still exist some systematic deviations between the self-consistent RLDA calculations and the exact values for heavy nuclei, such as Sn and Pb isotopes.

Within the RH approach, the meson-nucleon coupling strengths are parameterized to obtain appropriate quantitative description of nuclear structure properties and consequently part of the effects beyond Hartree and no-sea approximation can be taken into account effectively. Following this spirit, we will explore a phenomenological formula for the coupling strength of Coulomb field to include the Coulomb exchange term effectively in the RH approximation. In this work, we first explore the form of this phenomenological formula guiding by the RLDA, and then examine its validity by comparing with the exact treatment of the Coulomb exchange term in the RHFB approach [17]. Furthermore, we employ this formula to investigate the binding energy differences of mirror nuclei and check its validity in the RH approach, with the effective interactions NL3 [28], PKDD [29], and DD-ME2 [30].

In the RHF framework, the Coulomb energy $E_C$ for the nuclear system with time-reversal symmetry consists of the direct term $E_{C_{\text{dir}}}$ and the exchange one $E_{C_{\text{ex}}}$:

$$E_{C_{\text{dir}}} = \frac{e^2}{2} \int d^3r d^3r' \rho_p(r)\rho_p(r') \frac{\rho_p(r)\rho_p(r')}{|r - r'|},$$  \hspace{1cm} (1)

$$E_{C_{\text{ex}}} = -\frac{e^2}{2} \sum_{ij} v_i^2 v_j^2 \int d^3r d^3r' \cos(|\varepsilon_i - \varepsilon_j||r - r'|) \frac{|r - r'|}{|r - r'|} \times \bar{\psi}_i(r)\gamma^\mu \psi_j(r)\bar{\psi}_j(r')\gamma^\mu \psi_i(r'),$$  \hspace{1cm} (2)

where $\rho_p(r)$, $\varepsilon_i$, $v_i^2$ and $\psi_i$ denote the proton density, the single-particle energy, occupation probability, and wave function, respectively [27]. By introducing the effective charge factor

$$\eta = \sqrt{1 + \frac{E_{C_{\text{ex}}}}{E_{C_{\text{dir}}}}},$$  \hspace{1cm} (3)

the Coulomb energy $E_C$ can be expressed as

$$E_C = \eta^2 E_{C_{\text{dir}}} = \frac{(\eta e)^2}{2} \int d^3r d^3r' \rho_p(r)\rho_p(r') \frac{\rho_p(r)\rho_p(r')}{|r - r'|}.$$  \hspace{1cm} (4)

Then the $E_{C_{\text{ex}}}$ can be taken into account effectively in the Hartree approximation by merely changing $e$ to $\eta e$. 

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As referred to the RLDA, another effective way to include the exchange contributions of Coulomb field into the RH approach \cite{27}, a phenomenological formula is firstly developed for the effective charge factor $\eta$. In the RLDA, the $E_{\text{Cex}}$ can be expanded with respect to the $\beta = (3\pi^2 \rho_p)^{1/3}/M$, where $M$ is the proton mass. Up to the second order of $\beta$, the Coulomb exchange energy in the RLDA reads as

$$E_{\text{Cex}}^{\text{RLDA}} = -\frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} e^2 \int d^3r \rho_p^{4/3} \left( 1 - \frac{2}{3} \beta^2 \right).$$  \hspace{1cm} (5)

Empirically the proton density can be approximated as

$$\rho_p(r) = \begin{cases} 
0, & r > R \\
Z/(4\pi R^3/3), & r \leq R
\end{cases},$$  \hspace{1cm} (6)

with nuclear radius $R = r_0 A^{1/3}$ and then

$$\frac{E_{\text{Cex}}^{\text{RLDA}}}{E_{\text{Cdir}}} = -\frac{5}{4} \left( \frac{3}{2\pi} \right)^{2/3} Z^{-2/3} + \frac{15}{8M^2r_0^2} A^{-2/3}.$$  \hspace{1cm} (7)

From the calculations of the RHFB approach with the effective interaction PKA1 \cite{14}, it is found that the exact $E_{\text{Cex}}$ is much smaller than $E_{\text{Cdir}}$. Taking the $^{132}\text{Sn}$ as an example, the absolute ratio between $E_{\text{Cex}}$ and $E_{\text{Cdir}}$ is about 0.05. Therefore, one can expand the effective charge factor $\eta$ as the powers of $E_{\text{Cex}}/E_{\text{Cdir}}$, i.e.,

$$\eta = \sqrt{1 + \frac{E_{\text{Cex}}}{E_{\text{Cdir}}}} = 1 + \frac{E_{\text{Cex}}}{2E_{\text{Cdir}}} - \frac{1}{8} \left( \frac{E_{\text{Cex}}}{E_{\text{Cdir}}} \right)^2 + \cdots.$$  \hspace{1cm} (8)

Up to the linear order of $(E_{\text{Cex}}/E_{\text{Cdir}})$, the effective charge factor determined by the RLDA can be written as

$$\eta = 1 - \frac{5}{8} \left( \frac{3}{2\pi} \right)^{2/3} Z^{-2/3} + \frac{15}{16M^2r_0^2} A^{-2/3}.$$  \hspace{1cm} (9)

Inspired by the above formalism, we employ the expression

$$\eta(Z, A) = 1 - aZ^b + cA^d$$  \hspace{1cm} (10)

to parameterize the effective charge factor, as referred to the exact calculations of RHFB.

In this work, the effective interactions PKA1 \cite{14} and D1S \cite{31} are utilized in the particle-hole and particle-particle channels for the RHFB calculations, respectively. With the calculated $E_{\text{Cex}}$ and $E_{\text{Cdir}}$ in the RHFB approach, the exact effective charge factors can be obtained for each nucleus using Eq. \cite{3}. The exact effective charge factors for traditional
FIG. 1: (Color online) The effective charge factors for the semi-magic Ca, Ni, Sn, and Pb isotopes calculated by the RHFB approach with PKA1. The fitted values with Eq. (10) are shown by solid lines.

semi-magic Ca, Ni, Sn, and Pb isotopes are shown in Fig. 1 by the open circles. By fitting to these exact effective charge factors with Eq. (10), the parameters are determined as $a = 0.366958$, $b = -0.645775$, $c = 0.030379$, $d = -0.398341$ and the corresponding effective charge factors are shown in Fig. 1 by the solid lines. It is clear that the effective charge factor is sensitive to the proton number and increases as the proton number increases. In addition, there also exists a weak isospin dependence along an isotopic chain, which slightly decreases as the neutron number increases in general. With the phenomenological formula in Eq. (11), the fitted effective factors are in excellent agreement with the exact values. Comparing Eq. (10) with Eq. (9), it is found that the value of the parameter $b$ is close to $-2/3$, while the parameter $d$ shows a remarkable deviation from $-2/3$. In fact, the deviation mainly originates from the higher-order dependence on the proton density, i.e., the $\beta^2$ term in Eq. (5), introduced by the relativistic correction to $E_{\text{Cex}}$ in the LDA. For the proton density, we adopt a phenomenological formula in Eq. (6), which is too simple to well describe the real nuclear system. Therefore, by taking the coefficients in Eq. (9) as free parameters, the deviations from real nuclear systems can be taken into account effectively.

In order to exclude the effects due to the self-consistency, one-step calculations have been performed to investigate the effects of the LDA on Coulomb exchange energies in Ref. 27, i.e., $E_{\text{Cex}}^{\text{NRLDA}}$ and $E_{\text{Cex}}^{\text{RLDA}}$, are respectively obtained from the nonrelativistic local density approximation (NRLDA) and RLDA with the proton density $\rho_p(r)$ given by the self-consistent RHFB calculations. In terms of the phenomenological effective charge factor,
the Coulomb exchange contributions can be approximated as

\[ E_{\text{Cex}}^{\eta(Z,A)} = \left( 1 - \frac{1}{\eta^2} \right) E_C. \]  

(11)

The relative deviations of the approximate Coulomb exchange energies \( E_{\text{Cex}}^{\text{approx}} \) from the exact RHFB results are defined as

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

(12)

By taking the even-even Pb isotopes from proton drip line to neutron drip line as examples, the calculated Coulomb exchange energies \( E_{\text{Cex}}^{\text{exact}}, E_{\text{Cex}}^{\text{NRLDA}}, E_{\text{Cex}}^{\text{RLDA}}, \) and \( E_{\text{Cex}}^{\eta(Z,A)} \) are shown as a function of mass number in the panel (a) of Fig. 2. The corresponding relative deviations \( \Delta E_{\text{Cex}} \) defined in Eq. (12) are shown in the panel (b) of Fig. 2.

![Figure 2: Coulomb exchange energies and the corresponding relative deviations from the exact results in Pb isotopes obtained from phenomenological effective charge factor (open circles). For comparison, the exact results from the RHFB approach with PKA1 and other results obtained with the NRLDA and RLDA are shown by the filled squares, open triangles, and open squares, respectively.](image)

FIG. 2: (Color online) Coulomb exchange energies and the corresponding relative deviations from the exact results in Pb isotopes obtained from phenomenological effective charge factor (open circles). For comparison, the exact results from the RHFB approach with PKA1 and other results obtained with the NRLDA and RLDA are shown by the filled squares, open triangles, and open squares, respectively.

It is found that the magnitudes of the Coulomb exchange energies \( E_{\text{Cex}} \) generally decrease with increasing mass number. For each nucleus, the magnitude of \( E_{\text{Cex}} \) is overestimated by the NRLDA, and substantially improved when the relativistic corrections are taken into account \[27\]. However, the calculations with the RLDA still overestimated the exact \( E_{\text{Cex}} \) by about 1 MeV, especially for the neutron-deficient nuclei. Further improvement on the description of the exact \( E_{\text{Cex}} \) is achieved for the calculations with the phenomenological
effective charge factors in Eq. (10). From the panel (b) of Fig. 2 it is found that the relative deviations for the calculations with the NRLDA and the RLDA are respectively $5.2\% \sim 8.1\%$ and $1.7\% \sim 3.6\%$, while the relative deviation for the calculations with the phenomenological effective charge factor is smaller than $0.5\%$. Moreover, the systematic deviations from the exact values are eliminated. This shows that the contributions beyond the RLDA can be effectively included by using the phenomenological effective charge factors in Eq. (10).

In order to investigate the effects due to the self-consistency, the self-consistent calculations with phenomenological effective charge factors have been performed as well. The systematics of calculated results for the semi-magic Ca, Ni, Sn, and Pb isotopes from proton drip line to neutron drip line are shown in Fig. 3, where the traditional doubly magic nuclei are marked by the open symbols. Comparing with the exact Coulomb exchange energies from the RHFB calculations, it is found that the relative deviations $\Delta E_{\text{Cex}}$ for the calculations with the phenomenological effective charge factor are less than $1\%$ for the selected semi-magic isotopes, while the results with the NRLDA show remarkable systematic deviations and the maximum deviation even exceeds $8\%$. For the Ca and Ni isotopes, the self-consistent calculations with the phenomenological effective charge factor and the RLDA show a similar accuracy. As the proton number increases, the RLDA calculation systematically overestimates the magnitude of Coulomb exchange energies for the Sn and Pb isotopes, leading to a large relative deviation, while the relative deviation for the calculation with phenomeno-
logical effective charge factor is still within 1%. Therefore, the phenomenological effective charge factor shown in Eq. (10) for the Coulomb exchange term in nuclear CDFT is more robust than the NRLDA and RLDA. In particular, the systematic deviations from the exact Coulomb exchange energies for the NRLDA and RLDA are eliminated not only for the light nuclei, but also for the heavy nuclei.

Since the binding energy differences (BED) of mirror nuclei are sensitive to the nuclear Coulomb field, the exchange term of Coulomb field inevitably plays an important role in understanding the BED of mirror nuclei. In Fig. 4 we display the discrepancy between the BED of mirror nuclei calculated by RHB approach with the parameter sets, i.e., NL3 (triangles), PKDD (squares), or DD-ME2 (circles), and those calculated by RHFB approach with PKA1. The filled and open symbols denote the results with and without the phenomenological effective charge factors, respectively.

In summary, guiding by the RLDA, we explore a phenomenological formula for the coupling strength of Coulomb field to take into account the Coulomb exchange term effectively.
in the RH approximation. Comparing with the NRLDA and RLDA, the description of exact Coulomb exchange energies in the RHFB calculations is remarkably improved with the phenomenological effective charge factors. In particular, the systematic deviations of the NRLDA and RLDA calculations from the exact Coulomb exchange energies are eliminated not only for the light nuclei, but also for the heavy nuclei. The relative deviations of the Coulomb exchange energies in the calculations with phenomenological effective charge factors are less than 1% for traditional semi-magic Ca, Ni, Sn, and Pb isotopes from proton drip line to neutron drip line. Furthermore, one found that the BED of mirror nuclei are sensitive to the Coulomb exchange term, and the discrepancy between the BED of mirror nuclei calculated by the RHB approach with the RH parameter sets and those calculated by the RHFB approach with PKA1 can be remarkably reduced by using the phenomenological effective charge factors.

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[1] N. Auerbach, Phys. Rep. 98, 273 (1983).
[2] J. Meng, H. Toki, S. Zhou, S. Zhang, W. Long, and L. Geng, Prog. Part. Nucl. Phys. 57, 470 (2006).
[3] D. Vretenar, A. V. Afanasjev, G. A. Lalazissis, and P. Ring, Phys. Rep. 409, 101 (2005).
[4] B. Sun, F. Montes, L. S. Geng, H. Geissel, Yu. A. Litvinov, and J. Meng, Phys. Rev. C 78, 025806 (2008).
[5] Z. M. Niu, B. Sun, and J. Meng, Phys. Rev. C 80, 065806 (2009).
[6] Y. F. Niu, N. Paar, D. Vretenar, and J. Meng, Phys. Rev. C 83, 045807 (2011).
[7] Z. M. Niu, Y. F. Niu, H. Z. Liang, W. H. Long, T. Nikšić, D. Vretenar, J. Meng, arXiv:1210.0680 (2012).
[8] Z. M. Niu and C. Y. Gao, Int. J. Mod. Phys. E 19, 2247 (2010).
[9] J. Meng, Z. M. Niu, H. Z. Liang, and B. Sun, Sci. Chin. Ser. G 54, 119 (2011).
[10] W. H. Zhang, Z. M. Niu, F. Wang, X. B. Gong, and B. H. Sun, Acta Phys. Sin. 61, 112601 (2012).
[11] J. Walecka, Ann. Phys. (N.Y.) 83, 491 (1974).
[12] A. Bouyssy, S. Marcos, J. F. Mathiot, and N. Van Giai, Phys. Rev. Lett. 55, 1731 (1985).
[13] W. H. Long, N. Van Giai, and J. Meng, Phys. Lett. B640, 150 (2006).
[14] W. H. Long, H. Sagawa, N. V. Giai, and J. Meng, Phys. Rev. C 76, 034314 (2007).
[15] W. H. Long, H. Sagawa, J. Meng, and N. Van Giai, Europhys. Lett. 82, 12001 (2008).
[16] W. H. Long, T. Nakatsukasa, H. Sagawa, J. Meng, H. Nakada, and Y. Zhang, Phys. Lett. B680, 428 (2009).
[17] W. H. Long, P. Ring, N. Van Giai, and J. Meng, Phys. Rev. C 81, 024308 (2010).
[18] J.-P. Ebran, E. Khan, D. Peña Arteaga, and D. Vretenar, Phys. Rev. C 83, 064323 (2011).
[19] H. Z. Liang, N. Van Giai, and J. Meng, Phys. Rev. Lett. 101, 122502 (2008).
[20] H. Z. Liang, P. W. Zhao, and J. Meng, Phys. Rev. C 85, 064302 (2012).
[21] H. Z. Liang, N. Van Giai, and J. Meng, Phys. Rev. C 79, 064316 (2009).
[22] J. C. Slater, Phys. Rev. 81, 385 (1951).
[23] C. Titin-Schnaider and P. Quentin, Phys. Lett. B49, 397 (1974).
[24] J. Skalski, Phys. Rev. C 63, 024312 (2001).
[25] J. Le Bloas, M.-H. Koh, P. Quentin, L. Bonneau, and J. I. A. Ithnin, Phys. Rev. C 84, 014310 (2011).
[26] M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A683, 227 (2001).
[27] H. Q. Gu, H. Z. Liang, W. H. Long, N. Van Giai, and J. Meng, arXiv:1210.3162v1 [nucl-th] (2012).
[28] G. A. Lalazissis, J. König, and P. Ring, Phys. Rev. C 55, 540 (1997).
[29] W. H. Long, J. Meng, N. Van Giai, and S. G. Zhou, Phys. Rev. C 69, 034319 (2004).
[30] G. A. Lalazissis, T. Nikšić, D. Vretenar, and P. Ring, Phys. Rev. C 71, 024312 (2005).
[31] J. F. Berger, M. Girod, and D. Gogny, Comput. Phys. Commun. 63, 365 (1991).