Treating Coulomb exchange contributions in relativistic mean field calculations: why and how

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Abstract
The energy density functional (EDF) method is very widely used in nuclear physics, and among the various existing functionals those based on the relativistic Hartree (RH) approximation are very popular because the exchange contributions (Fock terms) are numerically rather onerous to calculate. Although it is possible to somehow ‘mock up’ the effects of meson-induced exchange terms by adjusting the meson–nucleon couplings, the lack of Coulomb exchange contributions hampers the accuracy of predictions. In this work, we show that the Coulomb exchange effects can be easily included with good accuracy in a perturbative approach. Therefore, it would be desirable for future relativistic EDF models to incorporate Coulomb exchange effects, at least to some order of perturbation.

Keywords: Coulomb exchange energy, relativistic mean field, relativistic Slater approximation, nuclear ground states

(Some figures may appear in colour only in the online journal)

1. Introduction

Our current microscopic understanding of the properties of atomic nuclei is based on two main approaches: using the nuclear shell model, on the one hand, and the energy density functional (EDF) method, on the other hand. The real start of application of the EDF method to nuclear systems can be traced back to the early 1970 s when Vautherin and Brink [1] revived the effective Skyrme interaction [2] and proposed a local EDF for nuclear systems. Since then, a vast number of articles dealing with a Skyrme-type EDF have appeared, and this trend will certainly continue for years to come. The main reason for this success is that the Skyrme EDF is a local functional, thus leading to local self-consistent mean fields. Even the Coulomb part of the Skyrme EDF was made local through the Slater approximation for the exchange Coulomb contribution [3]. The validity of the Slater approximation in Skyrme EDF calculations of atomic nuclei has been discussed in the literature [4], and it was found to be accurate at the level of a few per cent throughout the mass table, with better results for medium and heavy nuclei.

In the late 1980 s a new type of EDF became also very popular, namely the so-called relativistic mean field (RMF) approach, which is essentially a relativistic Hartree model with a no-sea assumption. The effective nucleon–nucleon interactions were mediated by meson exchanges with adjusted
coupling strengths. From Walecka’s toy model of the early 1970s [5], it evolved into a sophisticated Hartree-type description of atomic nuclei [6]. Later on, it was extended into a relativistic Hartree–Bogoliubov (RHB) version to take into account the effects of nuclear pairing. For the sake of numerical simplicity all exchange (Fock) terms were dropped, their effects being, one hopes, taken care of by readjusting appropriately the meson–nucleon couplings.

The RMF and RHB approaches are generally quite successful [7] and they are currently as widely applied as the non-relativistic Skyrme-type EDF approach. However, one aspect has so far been overlooked: the Coulomb exchange effects are absent from the RMF description, although it is well known that they are non-negligible, especially in lighter systems (the asymptotic behaviour of the Coulomb mean field in a nucleus having \( Z \) protons is \( (Z - 1)/r \), but it is \( Z/r \) if only the Hartree mean field is considered). In this contribution, we recall that a relativistic version of the Slater approximation is at hand, based on a local density approximation (LDA) for the Coulomb exchange energy [8]. This procedure leads to a set of RMF-type equations where the Coulomb part of the self-consistent mean field is a sum of a direct (local) Coulomb potential, and an exchange Coulomb potential which is also local.

The relativistic Slater approximation for the Coulomb exchange field would be very useful for the newly developed covariant point-coupling models [9, 10] where meson–nucleon vertices are assumed to be of the contact type. Then, all nuclear and Coulomb mean fields would contain exchange contributions and still remain local. In the rest of this short work, we will recall the main expressions which enable one to calculate the Coulomb exchange energy and potential using the relativistic LDA (RLDA), and then we comment on the first applications [8] carried out recently with this method.

2. Approximate forms of the relativistic Coulomb exchange energies and potentials

In the non-relativistic mean field treatment of a finite nucleus having nucleonic densities \( \rho_n(r) \) and \( \rho_p(r) \) the Hartree–Fock (HF) single-particle wavefunctions for protons are solutions of the Schrödinger-type equations containing a Coulomb mean field \( V_C \). This Coulomb potential has a direct (Hartree) component \( V_C^{\text{dir}}(r) \) which is local, and an exchange (Fock) non-local component \( V_C^{\text{ex}}(r, r') \). The LDA consists in approximating the Coulomb exchange energy density at point \( r \) of the inhomogeneous system by that of a homogeneous system having a proton density value equal to \( \rho_p(r) \). Since the single-particle wavefunctions in a homogeneous medium are plane waves, the Coulomb exchange energy per unit volume can be expressed in the simple form [8]

\[
e_{\text{ex}} = -\frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} e^2 p_p^{4/3}.
\]

Under the LDA assumption, the Coulomb exchange energy of the finite system would then be

\[
E_{\text{ex}}^{\text{LDA}} = -\frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} e^2 \int d^3 p_p^{4/3} (r).
\]

This is the so-called Slater approximation [3] routinely employed in many self-consistent, non-relativistic mean field studies [11]. It leads to a local potential representing the exchange (Fock) Coulomb potential:

\[
V_{\text{LDA}}^{\text{ex}}(r) = \frac{\delta E_{\text{ex}}^{\text{LDA}}}{\delta \rho_p(r)} = -\left(\frac{3}{\pi}\right)^{1/3} e^2 p_p^{4/3} (r).
\]

In the relativistic case, the Coulomb energy is expressed again in terms of the proton density:

\[
\rho_p(r) = \sum_i \nu_i^2 \bar{\psi}_i(r) \gamma^0 \psi_i(r)
\]

and proton current:

\[
\mathbf{j}_p(r) = \sum_i \nu_i^2 \bar{\psi}_i(r) \gamma^\mu \mathbf{p} \psi_i(r),
\]

where \( (\gamma^0, \gamma^\mu) \) are the Dirac matrices, the \( \nu_i \) are four-component spinors and the \( \nu_i^2 \) are occupation probabilities. The relativistic expressions for the direct and exchange Coulomb energies are

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

\[
E_{\text{ex}}^{\text{R}} = -\frac{e^2}{2} \sum_i \nu_i^2 \int d^3 r d^3 r' \cos (|\mathbf{e}_i - \mathbf{e}_s| |\mathbf{r} - \mathbf{r}'|)
\]

The relativistic homogenous nuclear matter, the \( \psi_i \) are plane wave solutions of the Dirac equation, and the time-like and space-like components of \( E_{\text{ex}}^{\text{R}} \) per unit volume, \( \tilde{e}_{\text{ex}}^{\text{R}} \) and \( \tilde{e}_{\text{ex}}^{\text{R}} \), can be related to the non-relativistic energies \( e_{\text{ex}} \) of equation (1) through [12]

\[
\tilde{e}_{\text{ex}}^{\text{R}} = \Phi(\beta),
\]

\[
\tilde{e}_{\text{ex}}^{\text{R}} = \Phi(\beta),
\]

where

\[
\beta = (3 \pi^2 n_p)^{1/3} M.
\]

M being the proton mass, whereas \( \Phi(\beta) \) and \( \Phi'(\beta) \) are analytical functions of \( \beta \) [8]. The relativistic corrections to the Coulomb exchange energy increase with the density, and they are substantial in atomic nuclei. On the other hand, it is sufficient to evaluate them by expanding \( \Phi(\beta) \) and \( \Phi'(\beta) \) up to
Coulomb exchange energies in the relativistic Hartree–Bogoliubov framework, and they can be generalized to the RHFB form. The point-coupling assumption leads to local, self-consistent nuclear potentials and makes the Dirac equations easier to solve numerically. For the Coulomb interaction, it is of course unreasonable to assume the point-coupling case and a good strategy would be to handle fully the direct Coulomb interaction while the exchange Coulomb effects would be described by the \( V^{\text{RLDA}}_{\text{Cex}}(\mathbf{r}) \) potential, similarly to what is done with Skyrme effective interactions.

Another observation that one can deduce from the comparison of the relativistic results of [8] with the study of the non-relativistic Slater approximation carried out by Titin-Schnaider and Quentin [4] using a Skyrme-type EDF is that the RLDA method seems to give more accurate Coulomb exchange energies. In [4] the \( A \approx 16–56 \) region was explored, and it turned out that the non-relativistic Slater approximation overestimates the Coulomb exchange energies by 5–7%. On the other hand, the relative error due to the RLDA is always less than 4% (and could be of either sign) over a wide range of nuclides from \( A = 40 \) to \( A = 266 \).

Thus, one has now a simple and efficient way to incorporate into RMF-type calculations, or more generally into RHFB models with point-coupling vertices, most of the effects due to Coulomb exchange interactions among protons inside a nucleus.

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