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Coulomb Displacement Energies in Relativistic and Non-Relativistic Self-Consistent Models

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Abstract:

Coulomb displacement energies in mirror nuclei are comparatively analyzed in Dirac-Hartree and Skyrme-Hartree-Fock models. Using a non-linear effective Lagrangian fitted on ground state properties of finite nuclei, it is found that the predictions of relativistic models are lower than those of Hartree-Fock calculations with Skyrme force. The main sources of reduction are the kinetic energy and the Coulomb-nuclear interference potential. The discrepancy with the data is larger than in the Skyrme-Hartree-Fock case.

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1. Introduction

The relativistic approach to nuclear structure and reactions has met a considerable success in many nuclear physics problems. Its most characteristic feature is the appearance of a strongly attractive scalar potential U_s and a strongly repulsive vector potential U_v in terms of which the single-particle motion of nucleons in a nucleus can be described via a Dirac equation. In Dirac phenomenology these potentials are directly parametrized so as to correctly reproduce medium-energy nucleon-nucleus scattering[1]. For nuclear structure problems it is usual to start with an effective meson-nucleon Lagrangian which is solved in Dirac-Hartree (i.e., mean field) approximation or Dirac-Hartree-Fock approximation[2]. Then, the scalar and vector potentials result from the interaction of scalar and vector mesons with nucleons. This self-consistent approach has been much used for calculating ground state properties of nuclei. In this work, we examine in this relativistic, self-consistent framework the long-standing problem of Coulomb Displacement Energies (CDE) in nuclei.

The CDE problem got its fame from the observation that reasonable Woods-Saxon models largely underestimate CDE in all nuclei, a fact known as the Nolen-Schiffer anomaly[3]. Of course, numerous correction terms have been listed and evaluated[4,5] but the net result was still a discrepancy of a few percent. However, it was soon realized that a better starting point than Woods-Saxon potentials is to use Hartree-Fock potentials because self-consistency gives rise in a natural way to such effects as Thomas-Ehrman shift or isospin impurity of the N=Z core. Using Hartree-Fock models with Skyrme forces[6] it was found that the discrepancy in mirror nuclei was much reduced[7,8]. Recently, the question was taken up again by Suzuki et al.[9] who started also with Skyrme-Hartree-Fock and did a careful evaluation of all conventional correction terms including effects of charge symmetry breaking (CSB) forces. Their results show that the discrepancy is down to the 1% level in A=17 and 2% in A=41, i.e., 3 to 4 times below the original anomaly.

In the light of these non-relativistic results, it is interesting to look at the predictions of relativistic models. The works of Ref.[10] and Ref.[11] discuss the question of Coulomb energies in the framework of parametrized relativistic potentials U_s and U_v. Their conclusions seem somewhat contradictory. In Ref.[10] it is found that CDE calculated with the (U_s, U_v) model are comparable with those obtained with Skyrme forces. On the other hand, Ref.[11] points out the existence of a negative nuclear-Coulomb interference potential which leads to a small yet significant decrease in Coulomb energy. However, self-consistency effects could be important, as we have learned in the non-relativistic case. Therefore, we use in the present study relativistic models which are treated in the Dirac-Hartree approximation and we compare them to the Skyrme-Hartree-Fock model.

2. Self-consistent models

2.1 Definitions

In the present work, nuclei are described in the framework of microscopic self-consistent models. Starting from an effective Lagrangian or Hamiltonian, the Dirac-Hartree approximation in the relativistic case, or the Hartree-Fock approximation in the non-relativistic case, are made in order to calculate the nuclear ground states. For the purpose of studying CDE in pairs of mirror nuclei, self-consistent models are quite appropriate because one can rely on Koopmans' theorem[12]:

$$E(A+1) - E(A) = \epsilon, \tag{1}$$

where E(A) and E(A+1) are the Hartree or Hartree-Fock total energies of the A- and (A+1)-systems, and ϵ is the single-particle energy of the orbit in which the additional nucleon has been put. Thus, calculating CDE in self-consistent models amounts essentially to compare single-particle energies of proton and neutron orbitals near the Fermi level of the closed-shell A-nucleus. For the relation (1) to hold, one must assume that adding or removing a nucleon does not change the self-consistent field. This is not strictly true, but it has been shown[7] that the effect on CDE of the core polarization due to the last particle is quite small. The reason is that the core is polarized approximately in the same way by a neutron or a proton, and this polarization effect is largely cancelled out in calculating $E(A+p) - E(A+n)$.

Let us denote by $A = (N, Z)$ a closed-shell nucleus with $N = Z$. A pair of mirror nuclei of mass number A+1 consists of a parent nucleus $(N+1, Z)$ and its analog $(N, Z+1)$. For a (A-1) pair, the parent nucleus is $(N, Z-1)$ and its analog is $(N-1, Z)$. The physical CDE, ΔE_c, is defined as the difference between the total energies of the analog nucleus and its parent. Here and in the following, total energies are defined without the nucleon rest masses. In the self-consistent models, we introduce the energy difference:

$$\Delta \equiv \epsilon_p - \epsilon_n, \tag{2}$$

where ϵ_p and ϵ_n are the single-particle energies of the proton and neutron one has to add to, or remove from the A-core. This quantity Δ forms the major part of ΔE_c but it cannot be directly compared to the CDE yet because a number of small but significant contributions must be added. These contributions include the core polarization discussed above, the proton finite size and center of mass effects, the dynamical effect of proton-neutron mass difference, the electromagnetic spin-orbit effects, the vacuum polarization and the effects of CSB forces. They have been extensively discussed and evaluated by many authors [4,5,9]. These corrections are outside the models studied in this work and we shall not calculate them but rather adopt the values of the current literature. On the other hand, our aim is to compare the predictions for Δ given by relativistic and non-relativistic models, and we shall analyze in some detail the various contributions to Δ. In these models, only the direct contribution of the Coulomb interaction has been included and therefore the exchange Coulomb contribution to the CDE is absent from Δ. This exchange contribution must be added to the other correction terms listed above in order to obtain the CDE predicted by our models.

2.2 Relativistic models

Dirac-Hartree descriptions of nuclear ground states have been extensively studied in the past[2]. If one starts from an effective meson-nucleon Lagrangian (e.g., the Walecka's model) and solves it in the mean field approximation, the results are satisfactory as far as nuclear densities and radii are concerned but binding energies tend to be systematically underestimated. Also, the nuclear matter compression modulus K_{nm} turns out to be rather large with such a Lagrangian. The value of K_{nm} can be lowered and brought close to its empirical value[13] if the Lagrangian contains higher power terms in the σ-field[14,15]. This non-linear version of the Walecka's model gives a very good account of ground state properties (binding energies, densities, single-particle spectra) in all magic nuclei[16], the agreement with data being at the same level as that of standard Hartree-Fock calculations[17]. Thus, our relativistic models will use the non-linear σ-model of Ref.[16].

The effective Lagrangian density $\mathcal{L}$ is a sum of a free Lagrangian $\mathcal{L}_0$ and an interaction Lagrangian $\mathcal{L}_i$. The free part is:

$$
\begin{aligned}
\mathcal{L}_0 &= \overline{\psi}(i\gamma_\mu\partial^\mu - M)\psi + \frac{1}{2}\partial_\mu\sigma\partial^\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{3}b\sigma^3 - \frac{1}{4}c\sigma^4 \\
&+ \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}m_\rho^2\underset{\sim}{\rho}_\mu\cdot\underset{\sim}{\rho}^\mu \\
&- \frac{1}{4}\underset{\sim}{\mathbf{G}}_{\mu\nu}\cdot\underset{\sim}{\mathbf{G}}^{\mu\nu} - \frac{1}{4}H_{\mu\nu}H^{\mu\nu},
\end{aligned}
\tag{3}
$$

where

$$
\begin{aligned}
F_{\mu\nu} &\equiv \partial_\nu\omega_\mu - \partial_\mu\omega_\nu, \\
\underset{\sim}{\mathbf{G}}_{\mu\nu} &\equiv \partial_\nu\underset{\sim}{\rho}_\mu - \partial_\mu\underset{\sim}{\rho}_\nu, \\
H_{\mu\nu} &\equiv \partial_\nu A_\mu - \partial_\mu A_\nu.
\end{aligned}
\tag{4}
$$

Here, M, m_σ, m_ω and m_ρ are the rest masses of the nucleon and mesons whereas ψ, σ, ω_μ and $\underset{\sim}{\rho}_\mu$ are the corresponding field operators and A_μ is the electromagnetic field. The non-linearity of the model shows up in the terms σ^3 and σ^4.

For the interaction Lagrangian, we consider two cases. In the first case, hereafter referred to as model R-I, we take the same interaction as in Ref.[16], i.e., protons are treated as point-like charged particles coupled directly to the electromagnetic field:

$$
\mathcal{L}_I = -g_\sigma\overline{\psi}\sigma\psi - g_\omega\overline{\psi}\gamma_\mu\omega^\mu\psi - g_\rho\overline{\psi}\gamma_\mu\underset{\sim}{\rho}^\mu\cdot\underset{\sim}{\tau}\psi - e\overline{\psi}\gamma_\mu\frac{1}{2}(1+\tau_3)A^\mu\psi,
\tag{5}
$$

where $\underset{\sim}{\tau}$ is twice the nucleon isospin and the effective coupling constants g_i have been determined, together with the parameters b and c of Eq.(3), by a fit to nuclear matter and finite nuclei properties. In obtaining the results discussed in the next section we have used the parameter values of set II of Ref.[16].

In the relativistic approach it is possible to incorporate in the Lagrangian density the electromagnetic structure of nucleons within the framework of the vector-meson dominance (VMD) model[18] which assumes that nucleons are not directly coupled to the electromagnetic field but only via the ω- and ρ-fields. The Dirac-Hartree equations including the VMD model have been solved for finite nuclei in Ref.[19] where it was shown that this model leads to a satisfactory description of charge densities. It is interesting to examine the possible implications of the VMD model on the CDE problem, and we have therefore considered as an alternative to model R-I the interaction Lagrangian of Ref.[19]:

$$\mathcal{L}_{II} = - g_\sigma \overline{\psi}\sigma\psi - g_\omega \overline{\psi}\gamma_\mu \omega^\mu \psi - \frac{f_\omega}{2M}\overline{\psi}\sigma^{\mu\nu}\partial_\mu \omega_\nu \psi$$
$$- g_\rho \overline{\psi}\gamma_\mu \underset{\sim}{\rho}^\mu . \underset{\sim}{\tau}\psi - \frac{f_\rho}{2M}\overline{\psi}\sigma^{\mu\nu}\partial_\mu \underset{\sim}{\rho}_\nu . \underset{\sim}{\tau}\psi \tag{6}$$
$$+ \frac{e^2}{8}(\frac{m_\rho^2}{g_\rho^2} + \frac{m_\omega^2}{g_\omega^2})A_\mu A^\mu - \frac{\epsilon m_\omega^2}{2g_\omega}A^\mu \omega_\mu - \frac{\epsilon m_\rho^2}{2g_\rho}A^\mu \rho_\mu^{(3)},$$

$\rho_\mu^{(3)}$ being the third isospin component of the ρ-meson field. The Lagrangian (6) will be referred to as model R-II. Again, the coupling constants g_i are to be determined by a fit to nuclear matter and finite nuclei properties whereas the values of the ratios f_ω/g_ω=-0.12 and f_ρ/g_ρ=3.70 are fixed by the anomalous moments of free nucleons. In this work, we want to compare the CDE predictions of models R-I and R-II. To make this comparison meaningful we simply use for R-II the same parameter values (g_i,b,c) (and meson masses) as for R-I and we set $f_\omega = f_\rho$=0. We have checked that the results of R-II are very little changed in the nuclei we have considered (^{16}O and ^{40}Ca) if we use for f_ω and f_ρ their non-zero values.

Let us denote by α the quantum numbers of a single-particle state and by $\psi_\alpha(\underset{\sim}{r})$ the corresponding wave function. In the Dirac-Hartree approximation $\psi_\alpha(\underset{\sim}{r})$ is a solution of the following Dirac equation:

$$[-i\hbar\underset{\sim}{\alpha}.\underset{\sim}{\nabla} + \beta(M + U_s(\underset{\sim}{r})) + U_v(\underset{\sim}{r})]\psi_\alpha(\underset{\sim}{r}) = E_\alpha \psi_\alpha(\underset{\sim}{r}), \tag{7}$$

where U_s and U_v are the self-consistent scalar and vector potentials created respectively by the scalar (σ) and vector (ω, ρ) mesons. These potentials are different for neutrons and protons, and in the latter case the Coulomb field U_c must be added to U_v. Their detailed expressions can be found for instance in Ref.[16]. As for R-II, the potential $U_v(\underset{\sim}{r})$ is composed of the nuclear and Coulomb components of the ω- and ρ-fields(for details, see Ref.[19]). In eq.(7) the energy E_α contains the nucleon rest mass: $E_\alpha = M + \epsilon_\alpha$. It is easy to find a Schrödinger-type equation equivalent to the Dirac equation (7). Denoting by ϕ_α and χ_α the upper and lower components of the four-component spinor ψ_α and introducing the normalized function

$$\tilde{\phi}_\alpha(\underset{\sim}{r}) \equiv B^{-\frac{1}{2}}\phi_\alpha(\underset{\sim}{r})/\langle\phi_\alpha|B^{-1}|\phi_\alpha\rangle^{\frac{1}{2}}, \tag{8}$$

where

$$B \equiv E_\alpha + M + U_s(\underset{\sim}{\mathbf{r}}) - U_v(\underset{\sim}{\mathbf{r}}), \tag{9}$$

one can see that $\tilde{\phi}_\alpha$ satisfies:

$$[-\frac{\hbar^2}{2M}\nabla^2 + V_{cent}(\underset{\sim}{\mathbf{r}}) + V_{s.o}(\underset{\sim}{\mathbf{r}})]\tilde{\phi}_\alpha(\underset{\sim}{\mathbf{r}}) = \epsilon_\alpha(1 + \frac{\epsilon_\alpha}{2M})\tilde{\phi}_\alpha(\underset{\sim}{\mathbf{r}}). \tag{10}$$

In this equation, the central and spin-orbit effective potentials depend on the scalar and vector potentials and on ϵ_α. For a neutron they are[10]:

$$\begin{aligned} V_{cent} =& U_s(1 + \frac{U_s}{2M}) + U_v(1 + \frac{\epsilon_\alpha}{M} - \frac{U_v}{2M}) \\ &+ \frac{\hbar^2}{2M}[\frac{1}{4}(\frac{V_0'}{1-V_0})^2 + \frac{1}{r}(\frac{V_0'}{1-V_0}) + \frac{1}{2}(\frac{V_0'}{1-V_0})'], \end{aligned} \tag{11}$$

$$V_{s.o} = \frac{\hbar^2}{2M}\frac{2}{r}(\frac{V_0'}{1-V_0})\underset{\sim}{\mathbf{L}}.\underset{\sim}{\mathbf{s}}, \tag{12}$$

where

$$V_0 \equiv \frac{U_v - U_s}{2M + \epsilon_\alpha}. \tag{13}$$

For a proton, U_v must be replaced by $U_v + U_c$ in eqs.(11-13). If one looks at the Coulomb energy of a proton orbital α one can see that the main contribution U_c is modified by correction terms of first and higher orders in U_c. A rather large first order correction is apparently produced by the interference term $-U_cU_v/M$ but in fact the values of $U_v(r)/M$ which can be 0.3-0.4 in the nuclear center become somewhat smaller at the surface where the valence orbital is located. Furthermore, other correction terms as well as the energy dependence of V_{cent} reduce considerably the decreasing effect of the interference term on the CDE[11].

From eq.(10) we obtain for a neutron state (we omit the subscript α for simplicity):

$$\begin{aligned} \epsilon^{(n)}(1 + \frac{\epsilon^{(n)}}{2M}) &= \langle\tilde{\phi}^{(n)}| - \frac{\hbar^2}{2M}\nabla^2 + V_{cent}^{(n)} + V_{s.o}^{(n)}|\tilde{\phi}^{(n)}\rangle \\ &\equiv \langle T\rangle_n + \langle V_{cent}^{(n)}\rangle_n + \langle V_{s.o}^{(n)}\rangle_n. \end{aligned} \tag{14}$$

In the case of R-II, the potential $U_v(\underline{r})$ for a neutron state, besides the nuclear part contains also the difference of the Coulomb components of the ω- and ρ-fields[19]. However, this difference is negligible and we shall ignore it in what follows. For a proton state, it is convenient to separate out the different components of the effective potential:

$$\begin{aligned} V_{cent}^{(p)} &= U_c + V_{cent}^{(p),N} + \delta V_{cent}^{(p)}, \\ V_{s.o}^{(p)} &= V_{s.o}^{(p),N} + \delta V_{s.o}^{(p)}, \end{aligned} \tag{15}$$

where the potentials $V^{(p),N}$ are calculated from eqs.(11-13) using $U_s^{(p)}$ and $U_v^{(p)}$ without U_c, and the potentials $\delta V^{(p)}$ contain corrections due to U_c at all orders except for the main Coulomb potential U_c which has been written out explicitly. Then, the relation analogous to eq.(14) is:

$$\begin{aligned} \epsilon^{(p)}(1 + \frac{\epsilon^{(p)}}{2M}) &= \langle\tilde{\phi}^{(p)}| - \frac{\hbar^2}{2M}\nabla^2 + U_c + V_{cent}^{(p),N} + \delta V_{cent}^{(p)} + V_{s.o}^{(p),N} + \delta V_{s.o}^{(p)}|\tilde{\phi}^{(p)}\rangle \\ &\equiv \langle T\rangle_p + \langle U_c\rangle_p + \langle V_{cent}^{(p),N}\rangle_p + \langle\delta V_{cent}^{(p)}\rangle_p + \langle V_{s.o}^{(p),N}\rangle_p + \langle\delta V_{s.o}^{(p)}\rangle_p. \end{aligned} \tag{16}$$

Combining eqs.(14) and (16) we get:

$$\begin{aligned} (1 + \frac{\epsilon^{(p)} + \epsilon^{(n)}}{2M})\Delta = \langle U_c\rangle_p &+ [\langle T\rangle_p - \langle T\rangle_n] + [\langle V_{cent}^{(p),N}\rangle_p - \langle V_{cent}^{(n)}\rangle_n] \\ &+ [\langle V_{s.o}^{(p),N}\rangle_p - \langle V_{s.o}^{(n)}\rangle_n] + \langle\delta V_{cent}^{(p)}\rangle_p + \langle\delta V_{s.o}^{(p)}\rangle_p, \end{aligned} \tag{17}$$

where Δ is the energy difference defined in eq.(2). This decomposition of Δ is the basis of our discussion in section 3.

2.3 Non-relativistic models

Non-relativistic Hartree-Fock models have often been used in CDE studies[7-9]. They provide a well-established framework for evaluating the main contribution Δ to Coulomb energy differences. Indeed, Hartree-Fock calculations with conventional effective interactions predict values of Δ larger than those obtained with simple Woods-Saxon potentials. The recent work of Ref.[9] shows that, in the Hartree-Fock framework a careful calculation of the various correction terms listed in subsection 2.1 leads to a deviation from experiment of the order of 1- 2% in the mirror pairs A=17 and 41, i.e., considerably less than the so-called Nolen-Schiffer anomaly[3]. Thus, we shall consider the Hartree-Fock model with Skyrme interaction as a reference model to which we can compare the predictions of relativistic models.

In the Skyrme-Hartree-Fock approximation the single-particle wave functions ϕ_α are solutions of the following Schrödinger equation:

$$[-\underset{\sim}{\nabla}\cdot\frac{\hbar^2}{2M^*(\underset{\sim}{\mathbf{r}})}\underset{\sim}{\nabla}+\frac{1}{2}(1-\tau_3)U_c(\underset{\sim}{\mathbf{r}})+U_{cent}(\underset{\sim}{\mathbf{r}})+U_{s.o}(\underset{\sim}{\mathbf{r}})]\phi_\alpha(\underset{\sim}{\mathbf{r}})=\epsilon_\alpha\phi_\alpha(\underset{\sim}{\mathbf{r}}), \qquad (18)$$

where M^*, U_c, U_{cent} and $U_{s.o}$ are respectively the non-locality effective mass, direct Coulomb potential, central and spin-orbit potentials. These functions are calculated self-consistently and they may differ for protons and neutrons. Their detailed expressions can be found in Ref.[6]. For a proton state, the single-particle energy is:

$$\begin{aligned}\epsilon^{(p)} &= \langle\phi^{(p)}|-\frac{\hbar^2}{2M}\nabla^2+U_c+[U^{(p)}_{cent}-\frac{\hbar^2}{2}\underset{\sim}{\nabla}\cdot(\frac{1}{M^{*(p)}}-\frac{1}{M})\underset{\sim}{\nabla}]+U^{(p)}_{s.o}|\phi^{(p)}\rangle\\ &\equiv \langle T\rangle_p+\langle U_c\rangle_p+\langle V^{(p)}_{cent}\rangle_p+\langle V^{(p)}_{s.o}\rangle_p,\end{aligned} \qquad (19)$$

where the quantity $\langle V^{(p)}_{cent}\rangle_p$ contains the contribution from the central potential and corrections due to the effective mass. Similarily, the single-particle energy for a neutron state is:

$$\begin{aligned}\epsilon^{(n)} &= \langle\phi^{(n)}|-\frac{\hbar^2}{2M}\nabla^2+[U^{(n)}_{cent}-\frac{\hbar^2}{2}\underset{\sim}{\nabla}\cdot(\frac{1}{M^{*(n)}}-\frac{1}{M})\underset{\sim}{\nabla}]+U^{(n)}_{s.o}|\phi^{(n)}\rangle\\ &\equiv \langle T\rangle_n+\langle V^{(n)}_{cent}\rangle_n+\langle V^{(n)}_{s.o}\rangle_n.\end{aligned} \qquad (20)$$

The energy difference Δ is thus decomposed into its different contributions:

$$\Delta=\langle U_c\rangle_p+[\langle T\rangle_p-\langle T\rangle_n]+[\langle V^{(p)}_{cent}\rangle_p-\langle V^{(n)}_{cent}\rangle_n]+[\langle V^{(p)}_{s.o}\rangle_p-\langle V^{(n)}_{s.o}\rangle_n]. \qquad (21)$$

We have chosen to cast Δ into this form in order to compare to the relativistic result (17). Usually, another decomposition is adopted[7,9] which exhibits explicitly the Thomas-Ehrman shift and the correction due to isospin impurity of the core, but it is of course the same quantity Δ which is discussed.

3. Results and discussion

We have performed Dirac-Hartree calculations with models R-I and R-II, and Skyrme-Hartree-Fock calculations with interaction SGII[20]. The calculations were done for the core nuclei ^{16}O and ^{40}Ca, and the CDE of mirror pairs around these cores will be discussed in this section. In the work of Ref.[9] it was found that CDE in mirror nuclei calculated with the two widely used forces SGII and SIII are very close and therefore we can take the SGII results as representative of Skyrme force predictions. As already mentioned in subsection 2.1 only the direct Coulomb contribution is included in the present self-consistent calculations.

The three models give a good account of total binding energies in ^{16}O and ^{40}Ca. They also reproduce quite well the experimental charge distributions[9,16], an important feature for a quantitative study of CDE. Models R-I and SGII assume point-like protons, therefore the finite-proton distributions are obtained by folding the point-proton distributions with a gaussian form factor adjusted to the value of 0.8 fm for the r.m.s. radius of the proton. On the other hand, the finite proton size is already included in model R-II because of the VMD mechanism and therefore this folding correction must not be done. All three models must be corrected for the center-of-mass effect on the charge distribution, and this can be done only approximately by assuming a harmonic oscillator model, i.e., one has to fold the above finite-proton distributions with a function $\exp(r^2/B^2)/(B\sqrt{\pi})^3$ where $B = \sqrt{\hbar/M\omega A}$ with $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ MeV[21]. In Table 1 the r.m.s. radii of charge distributions thus obtained are compared with experimental values in ^{16}O and ^{40}Ca. All three models give a good account of the experimental charge radii (the present results of model R-I correct those of Ref.[16] which contain a small numerical error).

Let us now examine the various contributions to the r.h.s. of eqs.(17) and (21). They are shown in Table 2 for the A=15 and A=17 pairs, and in Table 3 for the A=39 and A=41 pairs. The direct Coulomb term $\langle U_c \rangle_p$ is the main contribution but there are a number of sizable correction terms which partly cancel one another. The net result is that Δ is always smaller than $\langle U_c \rangle_p$ in the relativistic case whereas in the non-relativistic case Δ is larger than $\langle U_c \rangle_p$ for the A=17 and A=41 pairs. Models R-I and SGII give direct Coulomb contributions which are rather close except in the A=17 case, while predictions of model R-II are 60-100 keV below R-I. The latter result can be understood by recalling that $\langle U_c \rangle_p$

is calculated in models R-I and SGII using the point-proton distribution whereas in model R-II it is the finite-proton distribution which is involved, i.e., the small negative finite size correction is already included in model R-II. The first correction term to $\langle U_c \rangle_p$ is the kinetic energy difference $\langle T \rangle_p - \langle T \rangle_n$ (second row of Tables 2 and 3) which is always negative. It is due to the difference in the proton and neutron wave functions. One can see that this effect is larger for $j = l + 1/2$ orbitals (A=17 and 41) than for $j = l - 1/2$ orbitals (A=15 and 39), and that it is enhanced in relativistic models. The second correction $\langle V^{(p),N}_{cent} \rangle_p - \langle V^{(n)}_{cent} \rangle_n$ originates from the difference between the nuclear part of the proton central potential and the neutron central potential, and to a lesser extent from the wave function difference. This correction is positive and in the non-relativistic case it largely cancels the kinetic energy difference whereas in the relativistic case it is considerably larger. The third correction term $\langle V^{(p),N}_{s.o} \rangle_p - \langle V^{(n)}_{s.o} \rangle_n$ is similar to the previous one but it concerns the spin-orbit potentials. Its magnitude does not change much from relativistic to non-relativistic models. It is negative for $j = l - 1/2$ orbitals and positive for $j = l + 1/2$ ones, i.e., comparable in magnitude but opposite in sign as compared to the usual electromagnetic spin-orbit term which is part of the corrections to the present models. In the non-relativistic case, the sum of the three above corrections to $\langle U_c \rangle_p$ corresponds to the Thomas-Ehrman and the core isospin impurity effects already discussed in the literature[7,9]. The magnitude of this sum does not exceed 200 keV in the nuclei studied here with a negative (positive) sign in $j = l - 1/2$ ($j = l + 1/2$) nuclei. On the other hand, the corresponding sum is positive in the relativistic models and can be larger than 1 MeV for the A=39 and 41 pairs due to the large values of $\langle V^{(p),N}_{cent} \rangle_p - \langle V^{(n)}_{cent} \rangle_n$. This would lead to an overprediction of CDE by relativistic models if not for the presence of the fourth correction term $\langle \delta V^{(p)}_{cent} \rangle_p$ which does not exist in the non-relativistic case. The main contribution to this term is the negative nuclear-Coulomb interference potential $-U_c U_v / M$ which was already discussed in Ref.[11] in the framework of Dirac phenomenology. In our self-consistent relativistic models the term $\langle \delta V^{(p)}_{cent} \rangle_p$ represents about 75% of $\langle V^{(p),N}_{cent} \rangle_p - \langle V^{(n)}_{cent} \rangle_n$ in A=15 and A=39 systems but only 30 to 60% in A=17 or A=41 systems. Finally, the last correction $\langle \delta V^{(p)}_{s.o} \rangle_p$ related to the spin-orbit potential is relatively small and its sign depends on whether $j = l + 1/2$ or $j = l - 1/2$.

It can be seen from Tables 2 and 3 that the predictions of models R-I and R-II are rather close for all the various contributions to Δ. In the next-to-last row of these Tables are reported the sums of correction terms to $\langle U_c \rangle_p$. Our results for the SGII model are consistent with the values of the δ_{NN} correction of Ref.[9]. The relativistic models lead to summed corrections which are always below those of model SGII. This difference increases from 100 keV in the A=15 system to about 350 keV in the A=41 system. Thus, one can expect that the values of Δ will be generally larger for the non-relativistic model than for the relativistic ones. This is shown in the bottom row of Tables 2 and 3 where the quantity Δ calculated using eq.(17) or (21) is reported.

We can now address the question of comparing with experimental CDE. In the case of models R-I and SGII, the following corrections must be added to Δ: exchange Coulomb contribution, finite size and center of mass corrections, dynamical contribution of proton-neutron mass difference, electromagnetic spin-orbit contribution, core polarization and vacuum polarization corrections[4,5]. In addition there are contributions from CSB nuclear forces. In Ref.[9] the CSB corrections have been carefully evaluated together with the above corrections using model SGII. It was found that the CSB contributions are effective in increasing the calculated CDE. Here, we shall assume that both relativistic and non-relativistic models are subject to the same corrections whose values we take from Ref.[9]. For model R-II the finite size correction should not be included, as we have discussed above. Actually, if we use the values of Ref.[9] for this correction we find that the Δ values of model R-I corrected for finite size effects are very close to those of R-II. Notice that if we had used the VMD model (see eq.(6)) with the coupling constants f_ω/g_ω =-0.12 and f_ρ/g_ρ =3.70 the electromagnetic spin-orbit effect which is due to the neutron and proton anomalous magnetic moments would also be naturally included in the relativistic model. Since we have set $f_\omega = f_\rho = 0$ in model R-II this effect must be explicitly added as in model R-I.

With all corrections included, it is found[9] that the differences between experimental and calculated CDE using the SGII model are 108 keV, 9 keV, 157 keV and 163 keV in the A=15, 17, 39 and 41, respectively. Applying the same corrections to the relativistic models gives 172 keV, 332 keV, 263 keV and 505 keV for the corresponding energies calculated with R-I and 179 keV, 331 keV, 276 keV and 518 keV if one uses R-II. While the non-relativistic model is doing satisfactorily well in reducing the discrepancy with experiment to the level of 1-3%, the relativistic models are underestimating somewhat the CDE especially in the A=41 case. Although the corrections we have applied to them were simply taken from a non-relativistic calculation it is unlikely that a more consistent evaluation of these corrections would change appreciably the present results.

4. Conclusion

In this work we have made a comparative study of the CDE problem in relativistic and non-relativistic self-consistent models. Knowing that non-relativistic Skyrme-Hartree-Fock models can approach the experimental data in mirror nuclei by about 1-3% if conventional corrective effects are included our aim was to examine the situation of relativistic models which are generally doing well in describing bulk properties (binding energies, charge distributions) of nuclear ground states. To make a quantitative comparison meaningful we have performed calculations with models which give similar binding energies and charge radii. To this end, it was necessary to use relativistic models non-linear in the σ-field since bulk properties of finite nuclei predicted by linear models are not very close to Skyrme-Hartree-Fock predictions.

The main result is that relativistic models lead to binding energy differences Δ in mirror pairs which are systematically smaller than those of Skyrme-Hartree-Fock model. This underestimate can exceed 300 keV in the ^{17}F-^{17}O and ^{41}Sc-^{41}Ca pairs, a very large value on the scale of CDE. For a detailed comparison we have cast Δ into its various components. It appears that the two main sources of reduction of Δ are the kinetic energy term and the nuclear-Coulomb correction to the proton central potential. The proton-neutron kinetic energy difference is negative in the non-relativistic case but it is even more negative in the relativistic model. The nuclear-Coulomb proton potential is very specific to the relativistic approach and it has no counterpart in the non-relativistic one. Its dominant term is the nuclear-Coulomb interference potential which gives a large negative contribution to Δ. On the other hand, these negative effects are partly counteracted by the fact that in relativistic models the purely nuclear potential of a proton is much less attractive than that of the corresponding neutron. The net result is nevertheless in favour of the non-relativistic model.

We have estimated the CDE in the relativistic case by assuming that Δ must be affected by the same conventional corrections as in the non-relativistic case. We find that the calculated CDE considerably underestimate the data in mirror nuclei, the discrepancy being up to 500 keV in ^{41}Sc-^{41}Ca. This seems to be a serious shortcoming if one compares with non-relativistic self-consistent predictions where the corresponding discrepancy is at the level of 1%. Perhaps other effects not considered here, such as medium effects on the structure of the nucleon[23,24] have to be invoked, but one would need very reliable estimates of these effects in order to have a really quantitative discussion.

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Table captions

Table 1: Calculated and experimental charge radii (in fm). The data are from Ref.[22].

Table 2: The various contributions to the energy difference Δ, calculated in the mirror pairs ^{15}O-^{15}N and ^{17}F-^{17}O. The different quantities are defined in eqs. (17) and (21). All values are in MeV.

Table 3: Same as Table 2, for the pairs ^{39}Ca-^{39}K and ^{41}Sc-^{41}Ca.

	^{16}O	^{40}Ca
R-I	2.80	3.49
R-II	2.75	3.44
SGII	2.75	3.47
Exp.	2.74	3.45

Table 1

	$^{15}O - ^{15}N$			$^{17}F - ^{17}O$		
	$R-I$	$R-II$	$SGII$	$R-I$	$R-II$	$SGII$
$<U_c>_p$	3.975	3.884	3.979	3.438	3.382	3.580
$(a)\ <T>_p - <T>_n$	−0.528	−0.494	−0.404	−1.243	−1.186	−0.824
$(b)\ <V^{(p),N}_{cent}>_p - <V^{(n)}_{cent}>_n$	1.123	1.081	0.326	1.470	1.413	0.775
$(c)\ <V^{(p),N}_{s.o}>_p - <V^{(n)}_{s.o}>_n$	−0.072	−0.068	−0.093	0.130	0.124	0.134
$(d)\ <\delta V^{(p)}_{cent}>_p$	−0.820	−0.800	− − −	−0.448	−0.439	− − −
$(e)\ <\delta V^{(p)}_{s.o}>_p$	0.019	0.018	− − −	−0.013	−0.012	− − −
$(a)+(b)+(c)+(d)+(e)$	−0.278	−0.263	−0.171	−0.104	−0.100	0.085
Δ	3.744	3.667	3.808	3.342	3.290	3.665

Table 2

	$^{39}Ca - ^{39}K$			$^{41}Sc - ^{41}Ca$		
	$R-I$	$R-II$	$SGII$	$R-I$	$R-II$	$SGII$
$<U_c>_p$	7.665	7.557	7.644	7.121	7.038	7.112
$(a)\ <T>_p - <T>_n$	−0.838	−0.802	−0.676	−1.282	−1.231	−1.008
$(b)\ <V^{(p),N}_{cent}>_p - <V^{(n)}_{cent}>_n$	2.237	2.187	0.596	2.214	2.159	1.033
$(c)\ <V^{(p),N}_{s.o}>_p - <V^{(n)}_{s.o}>_n$	−0.100	−0.096	−0.114	0.136	0.130	0.152
$(d)\ <\delta V^{(p)}_{cent}>_p$	−1.741	−1.717	− − −	−1.242	−1.229	− − −
$(e)\ <\delta V^{(p)}_{s.o}>_p$	0.036	0.035	− − −	−0.029	−0.028	− − −
$(a)+(b)+(c)+(d)+(e)$	−0.406	−0.393	−0.194	−0.203	−0.199	0.177
Δ	7.344	7.249	7.450	6.947	6.868	7.289

Table 3