Relativistic deformed mean-field calculation of binding energy differences of mirror nuclei

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Abstract

Binding energy differences of mirror nuclei for \(A=15, 17, 27, 29, 31, 33, 39\) and 41 are calculated in the framework of relativistic deformed mean-field theory. The spatial components of the vector meson fields and the photon are fully taken into account in a self-consistent manner. The calculated binding energy differences are systematically smaller than the experimental values and lend support to the existency of the Okamoto–Nolen-Schiffer anomaly found decades ago in nonrelativistic calculations. For the majority of the nuclei studied, however, the results are such that the anomaly is significantly smaller than the one obtained within state-of-the-art nonrelativistic calculations.
1. Introduction. Conventional nuclear theory, based on the Schrödinger equation, has difficulties in explaining the binding energy differences of mirror nuclei \([1,2]\). The major contribution to the energy difference comes from the Coulomb force, and a variety of isospin breaking effects provide small contributions. The difficulty in reproducing the experimental values is known in the literature as the Okamoto-Nolen-Schiffer anomaly (ONSA). Several nuclear structure effects such as correlations, core polarization and isospin mixing have been invoked to resolve the anomaly without success \([3]\).

Since Okamoto and Pask \([4]\) and Negele \([5]\) suggested that the discrepancy could be due to a small charge symmetry breaking component in the nuclear force, a variety of calculations have been performed following this suggestion, and a widespread consensus has emerged that the anomaly can eventually be explained by a charge symmetry violation in the nucleon-nucleon interaction \([\mathbf{8}]\). In particular, class III (pp-nn) and class IV (pn) \([\mathbf{6}]\) charge symmetry breaking (CSB) forces can affect the binding energy differences of mirror nuclei \([\mathbf{8}]\), with the effects of the \(\rho^0 - \omega\) mixing being responsible for the bulk of the anomaly \([\mathbf{9,10}]\). However, although the situation regarding the resolution of the ONSA in terms of the \(\rho^0 - \omega\) mixing interaction looks very satisfactory, there have been several recent discussions in the literature \([\mathbf{11}]\) suggesting that the amplitude of the mixing is strongly momentum dependent such that the resulting CSB potential is small at internucleon separations relevant for the anomaly.

In view of such results, it is important to investigate the issue of the binding energy differences of mirror nuclei also in the framework of a relativistic nuclear structure model \([\mathbf{12,13}]\), where the cancellation of very strong scalar and vector potentials is responsible for the binding. Particularly important, in that realm, is the full inclusion of the effects of the polarization of the nuclear core due to an extra particle or hole that are mediated through those strong fields. In the language of relativistic mean-field theory, this requires that the spatial components of the vector fields and the photon are taken into account in a self-consistent manner. The latter are usually neglected in investigations in that realm, and they actually vanish if the system under consideration is invariant under the operation of time-reversal,
which is the case, for instance, for the ground-state of even-even nuclei. However, where
time-reversal invariance is violated, as, for example, in odd mass or rotating nuclei, the
polarization effects generated by the space-like components of the vector fields turned out
to be very important. In the framework of relativistic mean-field theory, this was observed
in studies of the magnetic moments in odd mass nuclei [15] and in an investigation of the
moments of inertia in rotating nuclei [16].

It is well known that the major contribution to the binding energy difference of mirror
nuclei arises from the Coulomb force, and it is therefore essential to take the effects of the
electromagnetic interaction into account as accurately as possible. In this work, we evaluate
the Coulomb field in the nuclei under consideration self-consistently, and we fully include
the effects of the nucleon’s anomalous magnetic moments by means of a tensor-coupling
to the electromagnetic field strength tensor. Furthermore, we include the Fock exchange
contribution to the Coulomb energy in the Slater approximation [17], whereas all other
fields are treated in the Hartree approximation only.

Also, we do not imply the constraint of spherical symmetry, which would greatly simplify
the numerical evaluation, but we allow the self-consistent solutions of the respective field
equations, the Dirac equation for the nucleon spinors and inhomogeneous Klein-Gordon
equations for the mesonic and the Coulomb fields, to be axially deformed.

By calculating the ground-state binding energies of various light odd mass nuclei in that
manner, we essentially perform a state-of-the-art evaluation of the Okamoto-Nolen-Schiffer
anomaly in the framework of the modern relativistic mean-field theory. Many contributions
to the anomaly, that in other works in that realm had been accounted for only perturbatively,
are fully included in our description. Amongst them are the core polarization, i.e., the isospin
impurity of the $N = Z$ nuclear core [18], dynamical effects of the proton-neutron mass
difference [19], contributions of the electromagnetic spin-orbit interaction and the Darwin
term [120], the so-called Thomas-Ehrman shift [21] and the Coulomb exchange term [1,19].

In detail, in this paper we calculate the binding energies of mirror nuclei with $A=15,17,27,29,31,33,39$ and 41 using a deformed relativistic mean-field model. The first
published calculation of binding energy differences of mirror nuclei using a relativistic nuclear model is by Nedjadi and Rook [22]. In their calculation, however, the nuclear structure was described in single-particle approximation in terms of a Dirac equation with spherical scalar and vector Woods-Saxon potentials, and no self-consistency between the potentials and the respective solutions of the Dirac equation was enforced. In a recent publication [23], self-consistency between the potentials and the Dirac sources was achieved, but again while assuming spherical symmetry, and also the effects of the $\rho^0 - \omega$ mixing interaction on the binding energies of mirror nuclei in the region of $A=16$ and $A=40$ were calculated within this approach. Here, we evaluate the binding energy differences employing the relativistic state-of-the-art model outlined above.

2. The model. The starting point of any investigation in the realm of relativistic mean-field theory is the local Lagrangian density,

$$
\mathcal{L} = \bar{\psi}_N (i\gamma^\mu - g_\sigma \sigma - g_\omega \phi - g_\rho \phi \tau - e_N A^\mu - \kappa_N \sigma_{\mu\nu} F^{\mu\nu} - M_N) \psi_N
+ \frac{1}{2} \partial_\mu \sigma \partial^\mu \sigma - U(\sigma) - \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu
- \frac{1}{4} R_{\mu\nu} R^{\mu\nu} + \frac{1}{2} m_\rho^2 \rho_\mu \rho^\mu - \frac{1}{4} F_{\mu\nu} F^{\mu\nu},
$$

(1)

consisting of nucleonic, mesonic and electromagnetic fields. The Dirac spinor nucleons ($\psi_N$) couple to the isoscalar-scalar $\sigma$-meson, the isoscalar-vector $\omega$-meson, the isovector-vector $\rho$-meson and the electromagnetic field, and $g_\sigma$, $g_\omega$, $g_\rho$ and $e_N$ are the respective coupling constants. The field tensors for the vector mesons and the photon field are:

$$
\Omega_{\mu\nu} = \partial_\mu \omega_\nu - \partial_\nu \omega_\mu, \quad R_{\mu\nu} = \partial_\mu \rho_\nu - \partial_\nu \rho_\mu, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu.
$$

(2)

The $\sigma$-meson has a nonlinear self-coupling given by the potential $U(\sigma)$

$$
U(\sigma) = \frac{1}{2} m_\sigma^2 \sigma^2 + \frac{1}{3} g_2 \sigma^3 + \frac{1}{4} g_3 \sigma^4,
$$

(3)

which was found to be important, in particular, for an adequate description of nuclear surface and compression properties [24]. Note that in addition to the standard description
In Eq. (1) also the tensor coupling of the nucleon’s anomalous magnetic moments, \(\kappa_p = 1.793\) and \(\kappa_n = -1.913\), with the electromagnetic field has been included.

In the mean-field approximation, the meson and photon fields are treated classically, and the variational principle leads to time-independent inhomogeneous Klein-Gordon equations for the mesonic fields with source terms involving the various nucleonic densities and currents:

\[
\begin{align*}
\{-\Delta + m^2_\sigma\} \sigma(r) &= -g_\sigma [\rho^p_s(r) + \rho^n_s(r)] - g_2\sigma^2(r) - g_3\sigma^3(r), \\
\{-\Delta + m^2_{\omega_0}\} \omega_0(r) &= g_\omega [\rho^p_\omega(r) + \rho^n_\omega(r)], \\
\{-\Delta + m^2_\omega\} \omega(r) &= g_\omega [j^p_\omega(r) + j^n_\omega(r)], \\
\{-\Delta + m^2_{\rho_0}\} \rho_0(r) &= g_\rho [\rho^p_\rho(r) - \rho^n_\rho(r)], \\
\{-\Delta + m^2_\rho\} \rho(r) &= g_\rho [j^p_\rho(r) - j^n_\rho(r)],
\end{align*}
\]

\[
\begin{align*}
-\Delta A_0(r) &= e \rho^p_\rho(r) + 2i \nabla \cdot [\kappa_p j^p_\rho(r) + \kappa_n j^n_\rho(r)], \\
-\Delta A(r) &= e j^p_\rho(r) + 2 \nabla \times [\kappa_p j^p_\Sigma(r) + \kappa_n j^n_\Sigma(r)].
\end{align*}
\]

The corresponding source terms are:

\[
\begin{align*}
\rho^N_s &= \sum_{i=1}^{N,Z} \bar{\psi}_i \psi_i, \quad \rho^N_\rho = \sum_{i=1}^{N,Z} \psi_i^+ \bar{\psi}_i, \\
j^N_\omega &= \sum_{i=1}^{N,Z} \bar{\psi}_i \gamma \psi_i, \quad j^N_\rho = \sum_{i=1}^{N,Z} \psi_i^+ \gamma \bar{\psi}_i, \quad j^N_\Sigma = \sum_{i=1}^{N,Z} \bar{\psi}_i \Sigma \psi_i,
\end{align*}
\]

where the sums run over the valence nucleons only. As usual, we neglect the contributions from negative energy states (no-sea approximation).

In this investigation, we limit ourselves to the Hartree approximation. The only exception is the Coulomb interaction for which a Fock exchange contribution is included in the Slater approximation. Then, the Dirac equation for the nucleons can be written as:

\[
\begin{align*}
\left\{ \alpha (-i \nabla - V(r)) + V_0(r) + \beta [M_N + S(r)] \right\} \psi_i &= \epsilon_i \psi_i.
\end{align*}
\]

It contains an attractive scalar potential,

\[
S(r) = g_\sigma \sigma(r) - 2 \kappa_N \Sigma \cdot [\nabla \times A(r)],
\]
a repulsive vector potential,

\[ V_0(r) = g_\omega \omega_0(r) + g_\rho \tau_3 \rho_0(r) + e_N A_0(r), \quad (8) \]

and a magnetic potential,

\[ V(r) = g_\omega \omega(r) + g_\rho \tau_3 \rho(r) + e_N A(r) - 2i \kappa_N \beta \nabla A_0(r), \quad (9) \]

which lifts the degeneracy between nucleonic states related by time-reversal.

Since we are considering nuclei with odd particle numbers, time-reversal invariance is broken in our calculations, and we have to take into account also the nuclear currents of Eq. (5b). The latter are usually neglected in investigations in that realm, although they have proven to be important, for instance, for a successful description of the magnetic moments of odd mass nuclei [15] as well as the moments of inertia in rotating nuclei [16] – where time-reversal is broken by the Coriolis field – in a description in relativistic self-consistent cranking theory, as developed in Ref. [23]. Those currents are the sources for the space-like components of the vector \( \omega(r) \), \( \rho(r) \) and \( A(r) \) fields – see, e.g., Eqs. (4c), (4e) and (4g) – which, in turn, give rise to polarization effects in the Dirac spinors through the magnetic potential \( V(r) \) of Eq. (4). As the latter destroys the degeneracy between nucleonic states related via time-reversal, for instance, for odd mass nuclei as studied here, the odd nucleon polarizes the even-even nuclear core. This effect is commonly referred to as nuclear magnetism.

These equations are solved self-consistently following the method based on an expansion in terms of eigenfunctions of an axially symmetric deformed harmonic oscillator, as developed by the Munich group [23,26], and the basis is truncated such that reliable convergence is achieved. This expansion technique introduces additional basis parameters which are optimally chosen so as to get fast convergence (for details see Ref. [26]). In detail, we fix the oscillator length, \( b_0 = \sqrt{\hbar/M_N \omega_0} \), corresponding to \( \hbar \omega_0 = 41A^{-1/3} \) (for bosons \( b_B = b_0/\sqrt{2} \)), where \( M_N \) is the nucleon mass.

Pairing is not included in our investigation because there is little known about this
correlation in these light nuclei under consideration. Also, as we are only interested in
binding energy differences between mirror nuclei, pairing effects cancel out almost entirely.

We use the recently proposed non-linear Lagrangian parameter set NL-SH [27] which has
been shown to yield excellent results for ground-state binding energies, charge and neutron
radii of spherical as well as deformed nuclei on both sides of the stability line [28]. The exact
values for the various parameters in the Lagrangian of Eq. (1) are given in Table 1.

Table 1. Mass parameters and coupling constants for the non-linear parameter set NL-SH.

| Masses       | Coupling constants |
|--------------|--------------------|
| $m_\sigma = 526.059$ MeV | $g_\sigma = 10.444$ |
|               | $g_2 = -6.910$ fm$^{-1}$ |
|               | $g_3 = -15.834$ |
| $m_\omega = 783.000$ MeV | $g_\omega = 12.945$ |
| $m_\rho = 763.000$ MeV  | $g_\rho = 4.383$ |

Note that in our numerical calculations, the total angular momentum, $j$, is not a good
quantum number – due to the, in general, nonvanishing axial deformation of the nucleon
source terms and mesonic fields – but only its projection onto the symmetry axis, $m_j$, and we
are thus evaluating the respective binding energies in the nucleus’s intrinsic reference frame.
We could improve on that approximation by projecting the corresponding solutions onto
good angular momentum. However, as we are only interested in binding energy differences,
the uncertainties that are associated with the aforementioned approximation are expected
to be small.

3. Numerical results. Table 2 summarizes the results for the binding energy differences
for various nuclei between $A=15$ and $A=41$. The experimental values are presented in
column EXP. In this table we also list the nonrelativistic results obtained by Sato [29] in
the framework of the density matrix expansion (DME) method and Skyrme II Hartree-Fock
calculations (SkII), respectively. The results of the present calculation are presented in
column REL. Columns $\Delta_{\text{DME}}$, $\Delta_{\text{SkII}}$, and $\Delta_{\text{REL}}$ are the differences between the experimental values and the respective results of the nonrelativistic (DME, SkII) and relativistic (REL) theoretical calculations.

Table 2. Binding energy differences in keV. Columns EXP are the experimental values, DME and SkII are the results of the nonrelativistic calculations by Sato [29], and REL refers to the present relativistic calculation. Columns $\Delta_{\text{...}}$ are the respective differences between theory and experiment.

| A  | State | EXP | DME | $\Delta_{\text{DME}}$ | SkII | $\Delta_{\text{SkII}}$ | REL | $\Delta_{\text{REL}}$ |
|----|-------|-----|-----|----------------------|------|----------------------|-----|----------------------|
| 15 | $1p_{1/2}^{-1}$ | 3560 | 3180 | 380                  | 3270 | 290                  | 3465 | 95                   |
|    | $1p_{3/2}^{-1}$ | 3460 | 3215 | 245                  | 3270 | 190                  | 3239 | 221                  |
| 17 | $1d_{5/2}^{-1}$ | 3500 | 3200 | 300                  | 3305 | 195                  | 3421 | 79                   |
| 27 | $1d_{5/2}^{-1}$ | 5610 | 5130 | 480                  | 5115 | 495                  | 5059 | 551                  |
| 29 | $2s_{1/2}$     | 5700 | 5415 | 285                  | 5465 | 235                  | 5666 | 34                   |
| 31 | $2s_{1/2}^{-1}$| 6250 | 5710 | 540                  | 5685 | 565                  | 6211 | 39                   |
| 33 | $1d_{3/2}$     | 6350 | 5990 | 360                  | 6070 | 280                  | 6137 | 213                  |
| 39 | $1d_{3/2}^{-1}$| 7430 | 6895 | 535                  | 7000 | 430                  | 7026 | 404                  |
| 41 | $1f_{7/2}$     | 7230 | 6790 | 440                  | 6875 | 355                  | 6826 | 404                  |

The first and most concrete conclusion, one can draw from Table 2, is that – similarly to the DME and SkII calculations – the relativistic results for the binding energy differences are systematically smaller than the experimental values. Second, for the nuclei with $A = 15(1p_{1/2}^{-1}), 17, 29, 31, 33$ and $39$, the relativistic results are significantly closer to experiment than the nonrelativistic ones, and for $A = 15(1p_{3/2}^{-1})$ and $41$, the deviation of the relativistic calculation from experiment is between the SkII and the DME results. Third, it is interesting to observe that for $A=15$ the experiment-theory difference, $\Delta_{\text{REL}}$, is larger for the $1p_{3/2}^{-1}$ than for the $1p_{1/2}^{-1}$ state, contrary to the corresponding nonrelativistic DME and SkII results. Note, also, that the relativistic results go in the same direction as the experimental
values, i.e. REL(3/2) > REL(1/2) and EXP(3/2) > EXP(1/2). This feature was already observed in the previous relativistic calculation of Ref. [23], and it hints the superiority of the relativistic framework in the description of the nuclear spin-orbit interaction, as discussed, for instance, in Ref. [30]. Fourth, only for nuclei with A=27, the differences between theory and experiment are larger in the relativistic calculation than in the nonrelativistic ones. The corresponding numerical calculations converge actually very slowly, indicating that other degrees of freedom, e.g., triaxial deformation or multi-nucleon correlations, play an important role for those nuclei.

3. Conclusions and future perspectives. Although our calculation still leaves room for improvement, such as the inclusion of exchange effects or projection onto good angular momentum, it is, however, fair to conclude that the results support, within the context of a relativistic mean-field description, the existence of the ONSA. However, the relativistic results have a tendency to be closer to experiment than the corresponding state-of-the-art nonrelativistic ones, i.e., the respective ONS anomaly is smaller in the relativistic description.

Nonrelativistic and relativistic calculations have shown that inclusion of $\rho^0 - \omega$ mixing in the NN interaction can resolve the ONSA in a satisfactory way. However, in view of several recent discussions suggesting that the contribution of the $\rho^0 - \omega$ mixing to the ONSA is strongly suppressed, it is extremely important to investigate alternative explanations of the anomaly. Various current unconventional ideas on the origin of the anomaly will be checked to high precision in the framework presented here [31]. Amongst them are a isovector component in the coupling of the otherwise isoscalar $\sigma$-meson, as suggested by Saito and Thomas [32], i.e. a small difference in the couplings of the proton and the neutron to the scalar $\sigma$-field. A similar effect, which will be incorporated into the present model, is the modification of the in-medium up-down quark condensates, which, in turn, implies a change of the neutron-proton mass difference in the nucleus, as proposed by Henley and Krein [33]. Another hypothesis, which can be evaluated very precisely in the model presented here, is a possible isospin violation in various meson-nucleon coupling constants, as suggested
independently by Dmitrašinović and Pollock [34] as well as Gardner et al. [35]. All these
effects can, in principle, arise through the small mass difference of the up- and down-quarks
in the nucleon.

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