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Strong-interaction isospin-symmetry breaking within the density functional theory*

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The conventional Skyrme interaction is generalized by adding zero-range charge-symmetry-breaking and charge-independence-breaking terms, and the corresponding energy density functional is derived. It is shown that the extended model accounts for experimental values of mirror and triplet displacement energies (MDEs and TDEs) in *sd*-shell isospin triplets with, on average, ∼100 keV precision using only two additional adjustable coupling constants. Moreover, the model is able to reproduce, for the first time, the $A = 4n$ versus $A = 4n + 2$ staggering of the TDEs.

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1. Introduction

Mean-field (MF) method based on isospin-invariant Skyrme [1] interaction is proven to be extremely successful in reproducing bulk nuclear properties, see [2] and Refs. cited therein. There is, however, a clear experimental evidence that the strong nucleon-nucleon (NN) interaction violates the isospin symmetry. Based on the differences in phase shifts and scattering lengths, it was shown that the nn interaction is ∼1% stronger than pp interaction and that the np interaction is ∼2.5% stronger than the average of nn and pp interactions [3].

The Coulomb force plays very important role in the formation of nuclear structure. At the same time, acting only between protons, it is the main source of breaking of the isospin symmetry. A systematic study by

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Nolen and Schiffer [4] showed that the experimental differences between the binding energies (BE) of the mirror nuclei, mirror displacement energies (MDEs):

$$\mathrm{MDE} = BE\left(T, T_z = -T\right) - BE\left(T, T_z = +T\right), \tag{1}$$

cannot be reproduced with the Coulomb interaction as the only source of the isospin-symmetry breaking (ISB), see also [5, 6, 7]. Another effect which cannot be reproduced by means of an approach involving only isoscalar strong force is the so called triplet displacement energy (TDE) [8]:

$$\begin{aligned}\mathrm{TDE} = BE\left(T = 1, T_z = -1\right) + BE\left(T = 1, T_z = +1\right) \\ -2BE\left(T = 1, T_z = 0\right),\end{aligned} \tag{2}$$

which measures the curvature of binding energies of isospin triplets. The MDEs and TDEs are related to the charge-symmetry breaking (CSB) and charge-independence breaking (CIB) components of the *NN* interaction, respectively. The aim of this work is to present the preliminary results of the generalized Skyrme approach that includes the CSB and CIB zero-range terms and quantifies their impact on the MDEs and TDEs.

2. Classification of the ISB interactions

On a fundamental level, the isospin symmetry is broken due to (i) different masses and electromagnetic interactions of u and d quarks (which translates at a hadronic level into differences of the masses of hadrons within the same isospin multiplet), (ii) meson mixing, and (iii) irreducible meson-photon exchanges. The CSB mostly originates from the difference in masses of protons and neutrons, leading to the difference in the kinetic energies and influencing the boson exchange. For the CIB, the major cause is the pion mass splitting. For more details see Refs. [3, 9].

Henley and Miller introduced a convenient and commonly used classification of various ISB terms [9, 10]. According to this classification, the isospin-invariant (isoscalar) *NN* interactions are called the class I forces. The class II isotensor forces preserve the charge symmetry, breaking charge independence at the same time. The class III forces break both the charge independence and charge symmetry, staying fully symmetric under interchange of nucleonic indices in the isospace. Finally, forces of class IV break both symmetries and mix isospin already at the two-body level. The classification is commonly used in the framework of models based on boson-exchange formalism, like CD-Bonn [3] or AV18 [11]. So far, apart from Ref. [5], it has not been directly used within the DFT formalism, which is usually based on isospin-invariant strong forces.

3. Extended Skyrme model

To account for the CIB and CSB effects, we have extended the conventional Skyrme interaction by adding zero-range interactions of class II and class III:

$$\hat{V}^{\mathrm{II}}(i,j) = \frac{1}{2}t_0^{\mathrm{II}}\,\delta\left(\boldsymbol{r}_i-\boldsymbol{r}_j\right)\left(1-x_0^{\mathrm{II}}\,\hat{P}_{ij}^{\sigma}\right)\left[3\hat{\tau}_3(i)\hat{\tau}_3(j)-\hat{\vec{\tau}}(i)\circ\hat{\vec{\tau}}(j)\right], \quad (3)$$

$$\hat{V}^{\mathrm{III}}(i,j) = \frac{1}{2}t_0^{\mathrm{III}}\,\delta\left(\boldsymbol{r}_i-\boldsymbol{r}_j\right)\left(1-x_0^{\mathrm{III}}\,\hat{P}_{ij}^{\sigma}\right)\left[\hat{\tau}_3(i)+\hat{\tau}_3(j)\right], \quad (4)$$

where t_0^{II}, t_0^{III}, x_0^{II}, and x_0^{III} are adjustable parameters and $\hat{P}_{ij}^{\sigma}$ is the spin-exchange operator. The corresponding contributions to energy density functional (EDF) read:

$$\mathcal{H}_{\mathrm{II}} = \tfrac{1}{2}t_0^{\mathrm{II}}\left(1-x_0^{\mathrm{II}}\right)(\rho_n^2+\rho_p^2-2\rho_n\rho_p-2\rho_{np}\rho_{pn} -\boldsymbol{s}_n^2-\boldsymbol{s}_p^2+2\boldsymbol{s}_n\cdot\boldsymbol{s}_p+2\boldsymbol{s}_{np}\cdot\boldsymbol{s}_{pn}), \quad (5)$$

$$\mathcal{H}_{\mathrm{III}} = \tfrac{1}{2}t_0^{\mathrm{III}}\left(1-x_0^{\mathrm{III}}\right)\left(\rho_n^2-\rho_p^2-\boldsymbol{s}_n^2+\boldsymbol{s}_p^2\right), \quad (6)$$

where ρ and $\boldsymbol{s}$ are scalar and spin (vector) densities, respectively. Note, that the effect of spin exchange leads to a trivial rescaling of the coupling constants, and can be omitted by setting $x_0^{\mathrm{II}} = x_0^{\mathrm{III}} = 0$. Hence, the extended formalism depends on two new coupling constants.

The contribution to EDF from the class III force depends entirely on the standard *nn* and *pp* densities and, therefore, can be taken into account within the conventional *pn*-separable DFT approach. The contribution from the class II force, on the other hand, depends explicitly on the mixed densities, ρ_{np} and $\boldsymbol{s}_{np}$, and requires the use of *pn*-mixed DFT [12, 13], augmented by the isospin projection to control this degree of freedom.

The proposed extension was implemented within the code HFODD [14] that allows for the *pn*-mixing in the particle-hole channel. The isospin degree of freedom is controlled using the isocranking method – an analogue of the cranking technique, which is widely used in high-spin physics [12]. The method allows us to calculate the entire isospin multiplet, T, by starting from an isospin-aligned state $|T, T_z = T\rangle$ and isocranking it by an angle θ around the x-axis in the isospace. The isocranking can be regarded as an approximate method to perform the isospin projection. The rigorous treatment of the isospin quantum number within the *pn*-mixed DFT formalism requires full, three-dimensional isospin projection, which is currently under development.

4. Numerical results

To investigate the influence of new terms on the ground-state (g.s.) binding energies, we first performed a test calculation without Coulomb for a

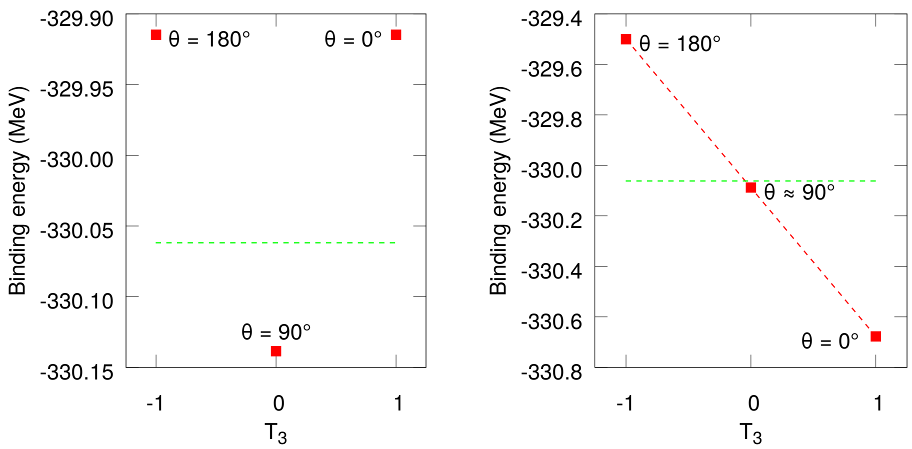

Fig. 1. Calculated g.s. energies of the $A = 30$ isospin-triplet nuclei. Calculations were performed without Coulomb interaction. Full squares in the left and right panels show the results obtained using the class II and III forces, respectively. The dashed lines show the g.s. energies calculated without any ISB terms included. The solid line indicates an almost perfect linear trend of points calculated with the class III force only.

case of the isospin triplet in the $A = 30$ isobars. By adding to the isospin-invariant Skyrme interaction either the class II or class III forces we were able to delineate the influence of hadronic ISB forces on the binding energies and TDE and MDE energy indicators. The results are depicted in Fig. 1. As anticipated, the CIB class II force changes the curvature (TDE) of binding energies within the triplet but almost does not affect the MDE of its $T_z = \pm 1$ members. Conversely, the class III force, which breaks the charge symmetry, strongly affects the values of MDE, introducing only minor corrections to the TDE, which are due to the self-consistency.

The test shows that the ISB forces of class II and III contribute almost exclusively to TDEs and MDEs, respectively. It justifies our strategy of fitting the $t_0^{\rm II}$ and $t_0^{\rm III}$ coupling constants to the TDE and MDE residuals – the differences between experimental and theoretical results obtained using the conventional MF model that involves only the isospin-invariant Skyrme and Coulomb forces. Moreover, since the residuals are relatively small, the fit can be done in a perturbative way what leads to: $t_0^{\rm II} = 20\,{\rm MeV}$ and $t_0^{\rm III} = -8\,{\rm MeV}$. These values were subsequently used to calculate MDEs and TDEs for isospin triplets in the sd-shell nuclei. The results are presented in Fig. 2. Without the hadronic ISB forces, the discrepancies between the

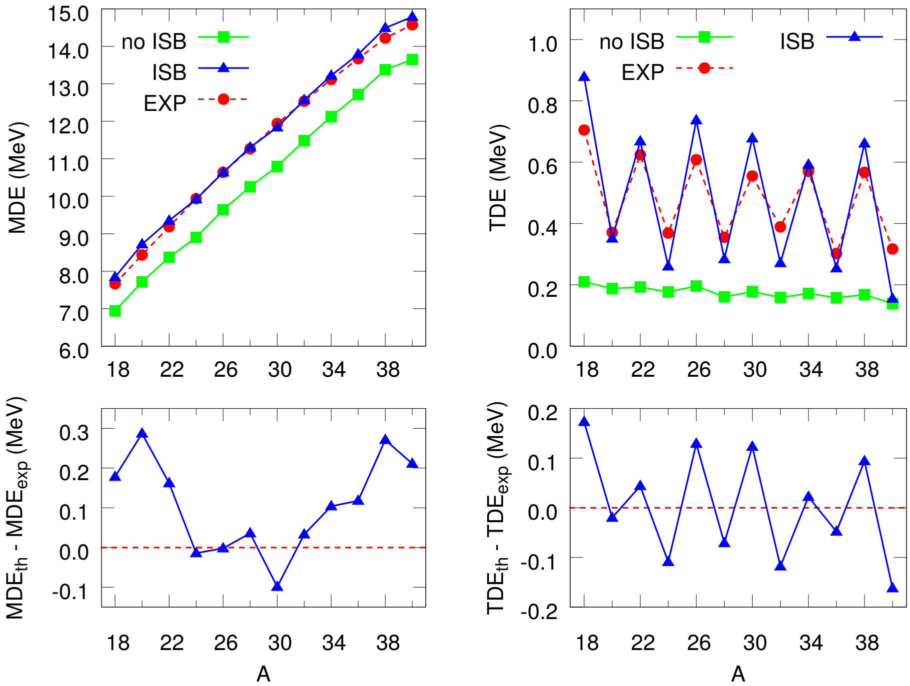

Fig. 2. The upper panels display the values of MDEs (left) and TDEs (right) calculated for the isospin triplets in the *sd*-shell nuclei. Circles show experimental points, squares represent results of calculations involving isospin-invariant Skyrme force SV [15] only, and triangles show results obtained using the extended model with the hadronic ISB terms (3) and (4) included. Coulomb interaction was included. The lower panels show differences between the theoretical calculations with the ISB terms included and experimental values.

experimental and the theoretical values of MDEs (dubbed the Nolen-Schiffer anomaly [4]) are of order of 1 MeV. For TDEs, they are on average 0.3 MeV. Moreover, the conventional model cannot reproduce a very characteristic staggering of TDEs between the $A = 4n$ and $A = 4n + 2$ triplets.

The inclusion of the hadronic ISB terms of class II and class III allows us to reduce the average disagreement between experiment and theory to a level of about 100 keV for TDEs and 130 keV for MDEs. Moreover, as shown in the figure, the extended model allows to account, for the first time, for the $A = 4n$ and $A = 4n+2$ staggering of TDEs. It is worth underlying that the results obtained for the $4n + 2$ triplets were obtained by isocranking the isospin-aligned $|T = 1, T_z = 1\rangle$ MF solutions in even-even nuclei, which are uniquely defined and represent the $J = 0^+$ ground states. The isospin-aligned $|T = 1, T_z = 1\rangle$ MF solutions in the $4n$ triplets, on the other hand, refer to odd-odd nuclei. These solutions are, in general, aligned in space and represents the $J \neq 0$ states. Due to the shape-alignment ambiguity, see Ref. [16], the MF solutions in odd-odd nuclei are not uniquely defined. The results shown in Fig. 2 represent arithmetic averages over the MF solutions that correspond to spin alignments along the short, middle, and long axes of the nuclear shape, respectively.

5. Summary

The conventional MF model involving the isospin-invariant Skyrme force with Coulomb interaction included has been extended by adding two zero-range terms that break charge symmetry and charge independence. The two free parameters were adjusted to reproduce the experimental values of the MDEs and TDEs. This allowed us reduce the discrepancy between experimental and theoretical values to, on average, ∼100 keV, and to reproduce, for the first time, the $A = 4n$ and $A = 4n + 2$ staggering of the TDEs. We plan to apply the extended model to study phenomena sensitive to the isospin symmetry.

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