MIRROR AND TRIPLET DISPLACEMENT ENERGIES WITHIN NUCLEAR DFT: NUMERICAL STABILITY*

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Isospin-symmetry-violating class II and III contact terms are introduced into the Skyrme energy density functional to account for charge dependence of the strong nuclear interaction. The two new coupling constants are adjusted to available experimental data on triplet and mirror displacement energies, respectively. We present preliminary results of the fit, focusing on its numerical stability with respect to the basis size.

1. Introduction

An accurate description of atomic nucleus, a system of protons and neutrons interacting with electromagnetic and strong forces, is a difficult task. It can be simplified considerably by introducing the concept of isospin symmetry [1] that relies on charge independence, that is, on equality of nucleon–nucleon (NN) forces $V_{pp} = V_{pn} = V_{nn}$ in the same space-spin channel. The NN scattering experiments indicate, however, that the strong interaction depends slightly on a pair of nucleons involved in the process [2]. On a fundamental level, violation of the isospin symmetry is due to the mass splitting and different charges of the *up* and *down* quarks and the difference in quark composition of proton and neutron.

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In atomic nuclei, the main source of isospin-symmetry breaking (ISB) is the Coulomb force, which shifts binding energies of nuclei forming a multiplet of a given isospin T. This property is used to construct various mass indicators which are sensitive to the ISB effects. The most common among such indicators are the mirror (MDE) and triplet (TDE) displacement energies involving data on isospin doublets ($T = \frac{1}{2}$) and triplets ($T = 1$). It turns out, however, that the Coulomb interaction alone is not sufficient to fully explain neither the MDEs nor the TDEs, and the additional ISB mechanism due to the strong nuclear force might be of importance in the understanding of the experimental data [3, 4].

Contemporary *ab initio* models are able to account for ISB effects in both NN scattering data and light nuclei [5–7]. However, they are still not suitable for describing heavier systems which is a domain of mean-field (MF) or density functional theory (DFT). These approaches are excellent tools to study bulk properties (masses, radii or quadrupole moments) in atomic nuclei regardless of their mass and parity of proton and neutron numbers, see [8] and references therein. Among different variants of MF or DFT approaches, the models based on the Skyrme interaction [9] are the most efficient computationally and fairly well describe nuclear binding energies. However, the isospin invariant Skyrme energy density functionals (S-EDF) [10, 11], which are typically used in practical applications, systematically fail to reproduce the experimental data on MDEs and TDEs. In our recent work [12], we introduced two new ISB terms into the S-EDF. They read[1]:

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

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

The first calculations performed with these modifications proved the ability of the extended model to correctly grasp the missing ISB effects in both the MDEs and TDEs, however, a systematic fitting of the new coupling constants t_0^{II} and t_0^{III} is necessary (x_0^{II} and x_0^{III} turned out to be redundant).

In this paper, we present a discussion on the numerical stability of MDEs and TDEs with respect to the choice of the basis size. The study allows us to estimate a theoretical uncertainty associated with a given basis cut-off. The discussion is followed by a presentation of preliminary results of the fitting procedure performed with a certain basis cut-off.

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[1] Formulas given in Eqs. (3) and (4) in Ref. [12] contain, by mistake, a redundant factor $\frac{1}{2}$. It does not affect numerical calculations.

2. Numerical stability

Nuclear calculations often depend on a choice of the basis size. Their reliability and, in particular, predictive power requires an estimate of theoretical uncertainties related to the basis size. The HFODD code [13, 14] used in this work solves the HF equation in the Cartesian harmonic oscillator (HO) basis. Its size can be controlled by providing a number of spherical HO shells N. In practical applications, the choice of N is always a matter of trade-off between computation time and expected precision of the calculations.

To evaluate theoretical uncertainty of the calculated MDEs and TDEs due to the basis size, we have performed test calculations for $T = \frac{1}{2}$ doublets with $A = 25$, 33, 57, and 75 and for $T = 1$ triplets with $A = 22$, 34, and 58. Calculations have been performed using the spherical HO bases consisting of $N = 10$, 12, 14, and 16 shells. For the heaviest doublets with $A = 57$ and 75, we have extended the test by including the bases consisting of $N = 18$ and 20 shells. In each case, we have computed the MDEs and TDEs using three different S-EDF parametrizations, including the density-independent SV_T S-EDF of Refs. [15, 16], and two popular density-dependent S-EDFs SkM* [17] and SLy4 [18]. Additionally, it has been checked that the new ISB terms affect rather weakly the stability of the MDEs and the TDEs and, in effect, the calculations were performed with t_0^{II} and t_0^{III} as in Table I. Results are collected in Figs. 1 and 2.

TABLE I

Values of the t_0^{II} and t_0^{III} parameters with uncertainty and standard deviations for MDE and TDE, σ_{fit}, resulting from the fit to all available data on isospin doublets and triplets. The calculations has been done for three different S-EDFs considered in this work.

Interaction	SV	SkM*	SLy4
t_0^{II} [MeV fm^3]	17 ± 5	24 ± 8	22 ± 7
σ_{fit} [keV]	100	110	100
t_0^{III} [MeV fm^3]	-7.3 ± 1.9	-5.5 ± 1.3	-5.5 ± 1.1
σ_{fit} [keV]	190	150	120

The basis-size-dependence tests suggest that the optimal strategy regarding both efficiency and accuracy of the calculations is to compute light ($10 \le A \le 30$), medium-mass nuclei ($31 \le A \le 56$), and heavy ($A \ge 57$) nuclei using bases consisting of $N = 10$, 12, and 14 spherical HO shells, respectively. For both the MDEs and TDEs, this strategy would result in the basis-size related uncertainty not exceeding $\Delta_{basis} \approx \pm 15$ keV. As we

show in Sec. 3, the basis-size uncertainty is relatively small as compared to the uncertainty resulting from the fitting procedure, which may justify using even smaller bases.
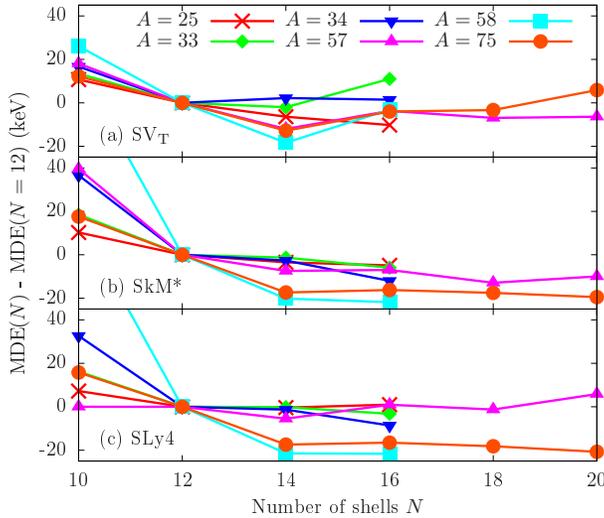

Fig. 1. (Colour on-line) Values of MDEs in function of the number of spherical HO shells used in the basis, plotted with respect to that obtained for $N = 12$. Results for multiplets with different values of A are labelled with different symbols, as shown in the legend. Panels (a), (b), and (c) show values obtained using SV_T, SkM*, and SLy4 S-EDFs, respectively.
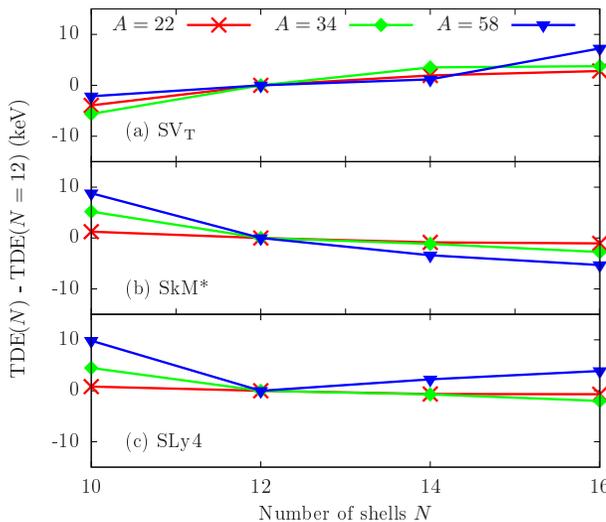

Fig. 2. (Colour on-line) The same as in Fig. 1, but for the TDEs.

3. Results of fitting

As stated in Sec. 2, the optimum choice of the number of spherical HO shells implies dividing the mass region of interest into the three subsets. In the present preliminary study, we use $N = 10$ shells for all nuclei having masses $10 \leq A \leq 56$ and 58, and we use $N = 14$ shells only for the heaviest systems. This choice almost doubles the basis-size related uncertainty of the calculated MDEs to $\Delta_{\mathrm{basis}} \approx \pm 30 \, \mathrm{keV}$ without much affecting the uncertainty of the calculated TDEs. A smaller computational time allows us to explore the richness of experimental data available for ISB effects in the $10 \leq A \leq 58$ nuclei. In future, it may allow us to perform calculations of mirror and triplet energy differences in rotational bands or the ISB effects in electromagnetic and β decays using the recently developed no-core configuration–interaction (NCCI) formalism [19], which involves CPU time demanding isospin and angular momentum projections and configuration mixing.

With the less strict choice of the basis size, the two new coupling constants (see Ref. [12]) were adjusted to all available data [20, 21] on MDEs ($10 \leq A \leq 75$) and TDEs ($10 \leq A \leq 58$). The fitting procedure has been realized independently for t_0^{II} and t_0^{III} parameters using linear regression method and following the guidelines from Ref. [22] and will be described in details in our forthcoming publication. The fitting results as well as the standard deviations from the experimental data points are presented in Table I.

As it turns out, the uncertainty resulting from the choice of the basis cut-off, Δ_{basis}, is small with respect to the values of standard deviations, σ_{fit}, given in Table I. Hence, in the total uncertainty, $\Delta_{\mathrm{T}} = \sqrt{\sigma_{\mathrm{fit}}^2 + \Delta_{\mathrm{basis}}^2}$, the basis-size related uncertainty constitutes only a small correction.

4. Summary

In the paper, we performed preliminary calculations of MDEs and TDEs paying special attention to the numerical stability of the results with respect to the basis size. It turned out that the optimum choice of the number of spherical HO shells, N, which defines the basis size, is $N = 10$ for light nuclei ($10 \leq A \leq 30$), $N = 12$ for medium-mass nuclei ($31 \leq A \leq 56$) and $N = 14$ for heavy nuclei ($A \geq 57$). It is shown that the corresponding uncertainty, $\Delta_{\mathrm{basis}} = \pm 15$ keV, is small as compared to the uncertainty coming from the fitting procedure. This allows us to compute light and medium-mass nuclei using the basis consisting only of $N = 10$ HO shells without loosing much of the precision. Smaller basis, in turn, will be beneficial regarding efficiency of the planned NCCI calculations. Finally, the two new coupling constants were adjusted to all available experimental data. The details of the fitting procedure will be presented in the forthcoming publications.

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