

# Toward *ab initio* charge symmetry breaking in nuclear energy density functionals<sup>†</sup>

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The parameter sets of energy density functionals (EDFs) of the nuclear density functional theory (DFT) are commonly determined phenomenologically to reproduce experimental masses and charge radii as well as nuclear matter properties. To establish a link between microscopic approaches and EDFs, an *ab initio* determination of the parameters of EDFs, as well as their functional forms, is highly desired. To date, however, a direct correspondence between *ab initio* and DFT remains elusive. A sophisticated yet practical approach to pin down the EDF parameters is to combine the *ab initio* and phenomenological EDF calculations.

Even though the isospin symmetry breaking (ISB) terms are small parts of the nuclear interaction, effects of the ISB terms on nuclear properties have received attention, while the ISB terms have often been neglected in EDFs. The ISB interaction can be divided into two parts: the charge symmetry breaking (CSB) and the charge independence breaking (CIB) interactions.

Our aim in this study is to propose a comprehensive methodology to determine the CSB terms in nuclear EDFs adopting the *ab initio* results. We implement the ISB terms in a Skyrme EDF to demonstrate our methodology. We will show that the mass difference of mirror nuclei  $\Delta E_{\text{tot}}$  and the neutron-skin thickness  $\Delta R_{\text{np}}$  of doubly-magic nuclei calculated by *ab initio* methods without and with the CSB terms, once they are available, enable us to determine the CSB strength in the EDF with an uncertainty of less than 6%, independently from other ISB forces such as CIB and Coulomb forces.

The Skyrme-like CSB and CIB interactions read<sup>1)</sup>

$$v_{\text{CSB}}(\mathbf{r}_1, \mathbf{r}_2) = \frac{\tau_{1z} + \tau_{2z}}{4} s_0 (1 + y_0 P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (1a)$$

$$v_{\text{CIB}}(\mathbf{r}_1, \mathbf{r}_2) = \frac{\tau_{1z}\tau_{2z}}{2} u_0 (1 + z_0 P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (1b)$$

respectively, where  $\tau_{iz}$  is the  $z$ -direction of the isospin operator of nucleon  $i$  ( $i = 1, 2$ ) and  $P_\sigma$  is the spin-exchange operator. For simplicity, in the SAMi-ISB EDF,<sup>2)</sup>  $y_0 = z_0 = -1$  are chosen to select the spin-singlet channel. The CIB strength  $u_0 = 25.8 \text{ MeV fm}^3$  has been previously determined using the Brueckner Hartree-Fock calculation of symmetric nuclear matter.<sup>2,3)</sup> The CSB strength  $s_0 = -26.3 \text{ MeV fm}^3$  has

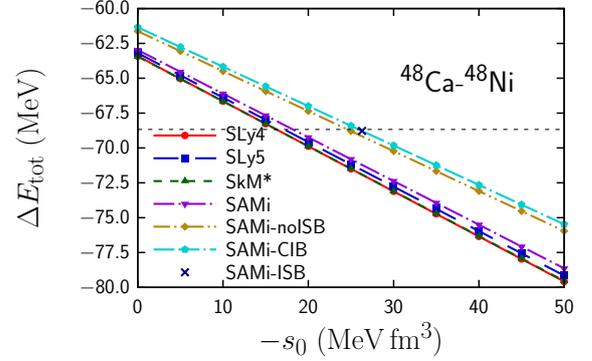


Fig. 1. Dependence of mass difference of mirror nuclei  $^{48}\text{Ca}$  and  $^{48}\text{Ni}$ ,  $\Delta E_{\text{tot}} = E_{\text{tot}}^{\text{Ca}48} - E_{\text{tot}}^{\text{Ni}48}$ , on CSB strength  $s_0$ .

been determined to reproduce the isobaric analog energy of  $^{208}\text{Pb}$ .<sup>2)</sup> In this study, as  $u_0$  has been already determined microscopically, we propose a way to determine  $s_0$  microscopically. Because the isobaric analog energy is not available using *ab initio* methods at this moment, we focus on alternative well-established observables: the nuclear radius and mass, which are more easily accessible than any *ab initio* method.

The dependence of the mass difference of mirror nuclei  $^{48}\text{Ca}$  and  $^{48}\text{Ni}$ ,  $\Delta E_{\text{tot}} = E_{\text{tot}}^{\text{Ca}48} - E_{\text{tot}}^{\text{Ni}48}$ , on the CSB strength  $s_0$  is shown in Fig. 1. For comparison, results calculated with the original SAMi-ISB and experimental data (AME2020) are also shown using crosses and horizontal lines, respectively. Remarkably, one can note that  $\Delta E_{\text{tot}}$  has a strong linear correlation to the CSB strength  $s_0$ , and the correlation is universal among the functionals. Thus, the calculated results are fitted to  $\Delta E_{\text{tot}} = a - bs_0$ . As seen in the figure,  $s_0$  and  $\Delta E_{\text{tot}}$  are highly correlated ( $r = 1.000$ ), and the slope  $b$  is almost universal among Skyrme EDFs. Note that the parameters  $a$  and  $b$  are determined with a 0.5% error. Accordingly, among these functionals, the slope  $b$  deviates within  $\lesssim 6\%$  around the average value of  $b$ . Thus, once the *ab initio* results for  $\Delta E_{\text{tot}}$  calculated without and with the bare CSB interaction,  $\Delta E_{\text{tot}}^{\text{w/o CSB}}$  and  $\Delta E_{\text{tot}}^{\text{w/CSB}}$ , are obtained, using  $\bar{b}$ , we can determine  $s_0$  as  $-s_0 = \left( \Delta E_{\text{tot}}^{\text{w/CSB}} - \Delta E_{\text{tot}}^{\text{w/o CSB}} \right) / \bar{b}$ . As the uncertainty of  $\bar{b}$  is  $\lesssim 6\%$ , the expected uncertainty of  $s_0$  is also  $\lesssim 6\%$ , assuming that the uncertainty associated with the *ab initio* calculations is negligible.

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