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Neutron-skin uncertainties of Skyrme energy density functionals

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Background: Neutron-skin thickness is an excellent indicator of isovector properties of atomic nuclei. As such, it correlates strongly with observables in finite nuclei that depend on neutron-to-proton imbalance and the nuclear symmetry energy that characterizes the equation of state of neutron-rich matter. A rich worldwide experimental program involving studies with rare isotopes, parity-violating electron scattering, and astronomical observations is devoted to pinning down the isovector sector of nuclear models.
Purpose: We assess the theoretical systematic and statistical uncertainties of neutron-skin thickness and relate them to the equation of state of nuclear matter, and in particular to nuclear symmetry energy parameters.
Methods: We use the nuclear superfluid density functional theory with several Skyrme energy density functionals and density dependent pairing. To evaluate statistical errors and their budget, we employ the statistical covariance technique.
Results: We find that the errors on neutron skin increase with neutron excess. Statistical errors due to uncertain coupling constants of the density functional are found to be larger than systematic errors, the latter not exceeding 0.06 fm in most neutron-rich nuclei across the nuclear landscape. The single major source of uncertainty is the poorly determined slope L of the symmetry energy that parametrizes its density dependence.
Conclusions: To provide essential constraints on the symmetry energy of the nuclear energy density functional, next-generation measurements of neutron skins are required to deliver precision better than 0.06 fm.

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Introduction. The radioactive beam facilities of the next generation will enter the vast, currently unexplored territory of the nuclear landscape towards its limits [1]. This voyage is not going to be easy, especially on the neutron-rich side, but the scientific payoff is expected to be rich and multifaceted [2]. A major quest, at the heart of many fascinating questions, will be to explain the neutron-rich matter in the laboratory and the cosmos across a wide range of nucleonic densities. To this end, an interdisciplinary approach is essential to integrate laboratory experiments with astronomical observations, theory, and computational science.

In heavy neutron-rich nuclei, the excess of neutrons gives rise to a neutron skin, characterized by the neutron distribution extending beyond the proton distribution. The skin can be characterized by its thickness, which is commonly defined in terms of the difference of neutron and proton point root-mean-square (rms) radii: $r_{\rm skin} = \langle r_{\rm n}^2\rangle^{1/2} - \langle r_{\rm p}^2\rangle^{1/2}$. (As discussed in Ref. [3], it is better to define the neutron skin through neutron and proton diffraction radii and surface thickness. However, for well-bound nuclei, which do not exhibit halo features, the above definition of $r_{\rm skin}$ is practically equivalent, see also [4].) The neutron-skin thickness has been found to correlate with a number of observables in finite nuclei related to isovector nuclear fields [5–11]. Furthermore, it has a close connection to the neutron matter equation of state (EOS) and properties of neutron stars [6,7,12–23]. In this context, precise experimental data on $r_{\rm skin}$ are indispensable; they are crucial for constraining the poorly known isovector sector of nuclear structure models.

Various experimental probes have been used to determine $r_{\rm skin}$ [3,9,24]. The Lead Radius Experiment (PREX) recently measured the parity-violating asymmetry coefficient $A_{\rm PV}$ for ^{208}Pb [25], which yielded $r_{\rm skin} = 0.33^{+0.16}_{-0.18}$ [26]. Unfortunately, the experimental error bar of PREX is too large to provide any practical constraint on well-calibrated theoretical models [9]. At present, the most precisely determined [27] isovector indicator in heavy nuclei is the electric dipole polarizability $\alpha_{\rm D}$ in ^{208}Pb [7,28], which has been used to put constraints on $r_{\rm skin}$ of ^{208}Pb [9,27]. However, a number of important measurements are in the works. A follow-up measurement to PREX, PREX-II [29], has been designed to improve experimental precision to 0.06 fm. A Calcium Radius Experiment (CREX) measurement of the neutron skin in ^{48}Ca [30] is promising an unprecedented precision of 0.02 fm. Last but not least, on-going experimental studies of $\alpha_{\rm D}$ in several neutron-rich nuclei [31] will soon provide key data.

The goal of this study is to survey $r_{\rm skin}$ across the nuclear landscape using nuclear density functional theory (DFT) [32]—a global theoretical approach to nuclear properties and a tool of choice in microscopic studies of complex heavy nuclei. By considering several effective interactions, represented by different Skyrme energy density functionals (EDFs) optimized to experimental data, we assess the model (systematic) error on $r_{\rm skin}$. Moreover, by means of the statistical covariance technique, we quantify statistical uncertainties of model predictions and identify those nuclear matter properties (NMPs) of EDFs that are the main sources of statistical error.

In this way, we provide a benchmark for the precision of future experiments on $r_{\rm skin}$ aiming at informing theory about isovector properties of effective nuclear interactions or functionals. This work builds on the previous global survey [1], which investigated model uncertainties on drip-line positions and several global nuclear properties. In particular, for the positions of the drip lines, systematic and statistical errors were found to be quite similar giving us some confidence in the robustness of our extrapolations into the *terra incognita* [1,33]. Here, we investigate whether the same also holds for $r_{\rm skin}$.

Theoretical background. The theoretical framework applied in this study is the same as in Refs. [1,33]. Namely, we use self-consistent Hartree-Fock-Bogoliubov (HFB) theory with six effective Skyrme interaction parameterizations in the particle-hole channel (SkM* [34], SkP [35], SLy4 [36], SV-min [37], UNEDF0 [38], and UNEDF1 [39]) augmented by the density-dependent, zero range pairing interaction. This set of EDF parameterizations has characteristics that are distinct enough to assess the systematic error within this family of Skyrme models. The rms proton and neutron radii of even-even nuclei across the mass table were obtained in large-scale deformed HFB calculations [40] using the solver HFBTHO [41]. To approximately restore the particle number symmetry broken in HFB, we used the Lipkin-Nogami scheme of Ref. [42]. All remaining details are exactly as in Refs. [1,40].

The Skyrme energy density is parametrized by about a dozen coupling constants that are determined by confronting DFT predictions with experiment. To relate to the nuclear matter EOS, the volume part of the energy density is often parametrized in terms of the NMPs [37,38]. Typically, the phenomenological input used in parameter adjustment consists of nuclear masses and their differences, radii, surface thickness, mean energies of giant resonances, and other data (see Refs. [32,38,43] for a list of observables commonly used in the EDF optimization). The actual fit is done by minimizing the objective function

$$\chi^2(\mathbf{x}) = \sum_p \left(\frac{O_p^{(\rm th)}(\mathbf{x}) - O_p^{(\rm exp)}}{w_p} \right)^2, \qquad (1)$$

with respect to EDF parameters $\mathbf{x} = \{x_i\}$. In Eq. (1), O_p is a selected observable and w_p is the corresponding weight that represents the adopted error.

Once the minimum $\mathbf{x}_{\rm min}$ of (1) is found, a statistical covariance analysis can be carried out to obtain standard deviations and correlations between EDF parameters [37–39,44]. The statistical standard deviation of an observable O is given by

$$\sigma_O^2 = \sum_{i,j} {\rm Cov}(x_i, x_j) \left[\frac{\partial O}{\partial x_i} \frac{\partial O}{\partial x_j} \right], \qquad (2)$$

where ${\rm Cov}(x_i, x_j)$ is the covariance matrix for the model parameters. In the calculation of the covariance matrix, a linearized least-square system in the vicinity of the minimum $\mathbf{x}_{\rm min}$ is usually assumed. Within this approximation [45] the covariance matrix is obtained in terms of the weights w_p and the partial derivatives $\partial_{x_i} O_p^{(\rm th)}|_{\mathbf{x}_0}$, which are usually approximated by finite differences. Thus, the magnitude of the covariance matrix and consequently the magnitude of the standard deviation (2) depend on the chosen weights w_p. The covariance matrix can be linked to the covariance ellipsoid between two parameters [7].

Since the accuracy of Skyrme EDFs, for example, for nuclear binding energies, is usually worse compared to the experimental error bars, the weights w_p should be chosen to reflect the expected accuracy of the model as opposed to the actual experimental error. As argued in Ref. [46], a balanced parameter optimization should lead to uncertainty comparable to the magnitude of the optimization residuals. For example, with UNEDF0, the residuals in binding energies are typically similar in magnitude to the adopted weights [38]. In the optimization of SV-min, the adopted errors were additionally scaled to give a lower weight to nuclei influenced by collective correlations [37]. With a proper choice of weights, calculated statistical errors (2) provide a realistic picture of theoretical uncertainties and predictive capabilities of a model.

In the present work, two different model uncertainties are considered. The systematic error represents the rms spread of predictions of different Skyrme EDFs obtained by means of diverse fitting protocols. In the absence of the exact reference model, such an inter-model deviation represents a rough approximation to the systematic error, and it should be viewed as such. The statistical error represents the theoretical uncertainty associated with model parameters and is obtained using least-squares covariance analysis [7,28,37,46].

Results. The mean value of $r_{\rm skin}$ and the corresponding rms deviation $\Delta r_{\rm skin}^{\rm syst}$ are shown in Fig. 1 for all even-even nuclei with $Z \leqslant 120$ predicted to be particle bound in all our models. (The results for $r_{\rm skin}$ for each individual model can be found in the Supplementary Information of Ref. [1].) As expected, the average value of the neutron-skin thickness $r_{\rm skin}^{\rm av}$ increases steadily with N for each isotopic chain [3,24]. The

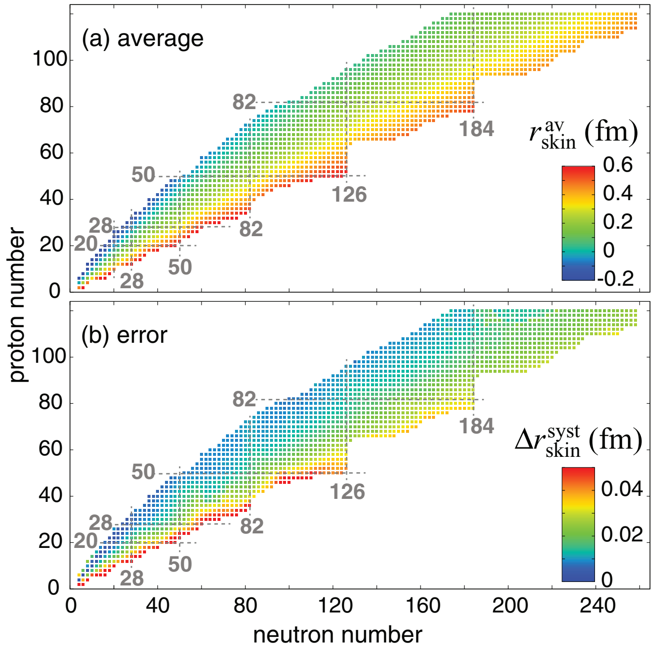

FIG. 1. (Color online) (a) The model-averaged value of $r_{\rm skin}$ and (b) the systematic error $\Delta r_{\rm skin}^{\rm syst}$ for the six EDFs used for the particle-bound even-even nuclei with $Z \leqslant 120$.

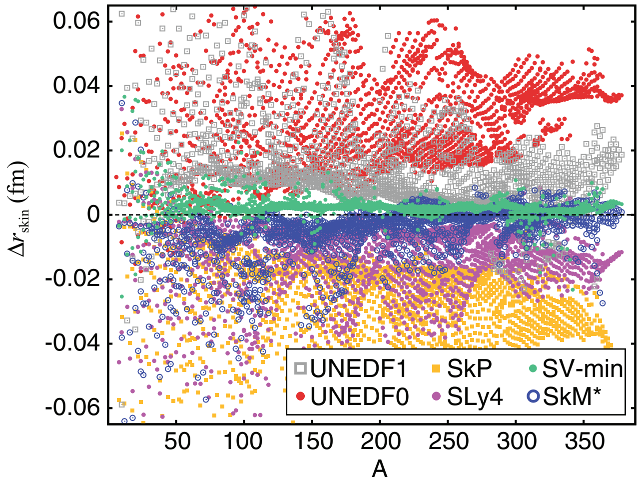

FIG. 2. (Color online) Scatter plot of the deviation of neutron-skin thickness from the mean value $r_{\rm skin}^{\rm av}$ for the six models used as a function of mass number A.

systematic error also increases gradually when approaching the neutron drip line. However, the range of $\Delta r_{\rm skin}^{\rm syst}$ is surprisingly small: the model spread does not exceed 0.05 fm for extremely neutron-rich systems. This suggests that in spite of different optimization strategies, the EDFs considered give a very consistent answer when it comes to $r_{\rm skin}$.

To get a deeper insight into the budget of $\Delta r_{\rm skin}^{\rm syst}$, Fig. 2 shows the individual residuals of $r_{\rm skin}$ with respect to $r_{\rm skin}^{\rm av}$. While SV-min closely follows the average trend, SkP and UNEDF0 show large deviations. By inspecting NMP of the used EDFs [23,38,39,47] one can see that low values of $r_{\rm skin}$ for SkP can be attributed to its particularly low value of the slope of the symmetry energy, $L = 19.7$ MeV (as compared to $L = 44.8$ MeV for SV-min). Still, the parameter L cannot be the whole story, as, for instance, its value for UNEDF0, $L = 45.1$ MeV, is very close to that in SV-min.

Figure 3 shows the statistical error of $r_{\rm skin}$ for the isotopic chains of Ca, Zr, Er, and $Z = 120$ obtained with UNEDF0 and SV-min. Even though the magnitude of statistical error, $\Delta r_{\rm skin}^{\rm stat}$, is somewhat different for the two models, especially in the heavier isotopes, the model predictions for $r_{\rm skin}$ are consistent. Apparent discontinuities, e.g., for the $Z = 120$ isotopic chain, are due to sudden changes in quadrupole deformation (see Ref. [1], Supplementary Information). Also, similar to the systematic error of Fig. 1, $\Delta r_{\rm skin}^{\rm stat}$ propagates with N. The gradual growth of statistical error with the neutron excess is primarily caused by the isovector coupling constants of the functional that are poorly constrained by the current data.

The statistical error of UNEDF0 and SV-min on $r_{\rm skin}$ is significantly larger than the systematic error of Fig. 1. As discussed earlier, the statistical error of a computed observable depends on the adopted errors used in (1). Since the weights w_p reflect the expected accuracy of the model, the error bars given in Fig. 3 do provide a good measure of the model uncertainty. The reason for the difference in the magnitude of $\Delta r_{\rm skin}^{\rm stat}$ between UNEDF0 and SV-min can be traced back to the different optimization protocols in both cases. Namely, in the optimization of SV-min, lower weights were assumed for certain nuclei to account for collective correlations, and this explicitly impacts the standard deviation (2). At the same time, the experimental data pool for SV-min includes, in addition to charge radii, diffraction radii and surface thickness [37], thus reducing the statistical uncertainty compared to UNEDF0.

For UNEDF0 and SV-min, the dominant contributions to $\Delta r_{\rm skin}^{\rm stat}$ come from L and $a_{\rm sym}$. This is illustrated in Fig. 4, where the contributions to the sum of Eq. (2) are plotted for Pb isotopes (the second index j is summed over all the parameters). The contribution from L is by far the largest one in all isotopes, and it yields over 50% of the total error. We checked that this also holds for other semi-magic isotopic chains. The strong impact of L on the statistical error of neutron rms radii was also found in Ref. [46]. For SV-min, some of the isoscalar coupling constants also provide contributions comparable in the magnitude to the $a_{\rm sym}$ parameter. However, when these contributions are summed up, they cancel out rather precisely and the net value is small. This is expected, since correlations between isoscalar and isovector parameters in SV-min are low [7].

While $a_{\rm sym}$ is determined fairly precisely for both UNEDF0 (30.5 ± 3.1 MeV) and SV-min (30.7 ± 1.9 MeV), the uncertainty in L is much greater: $L = 45 \pm 40$ and 45 ± 26 MeV for UNEDF0 and SV-min, respectively. The fact that the symmetry

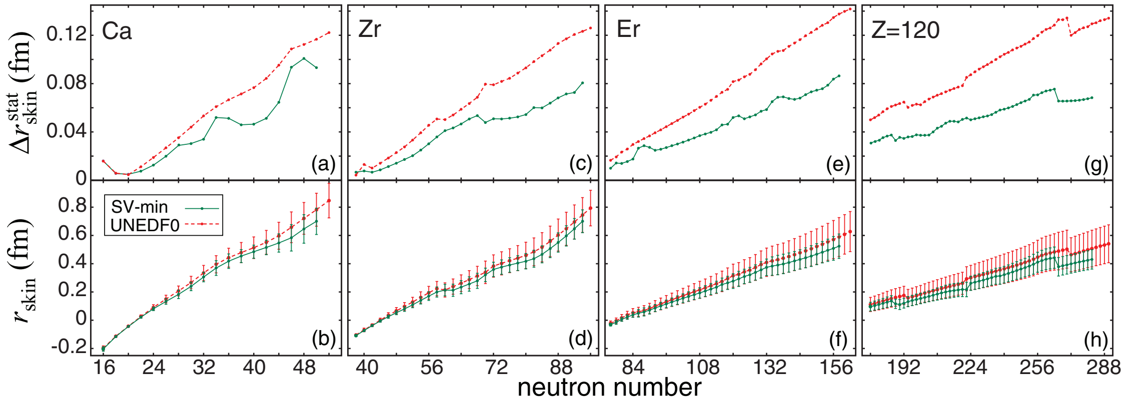

FIG. 3. (Color online) Top: calculated statistical error on $r_{\rm skin}$ in Ca, Zr, Er, and $Z = 120$ isotopic chains for UNEDF0 (dashed line) and SV-min (solid line). Bottom: corresponding neutron skins with statistical uncertainties (error bars).

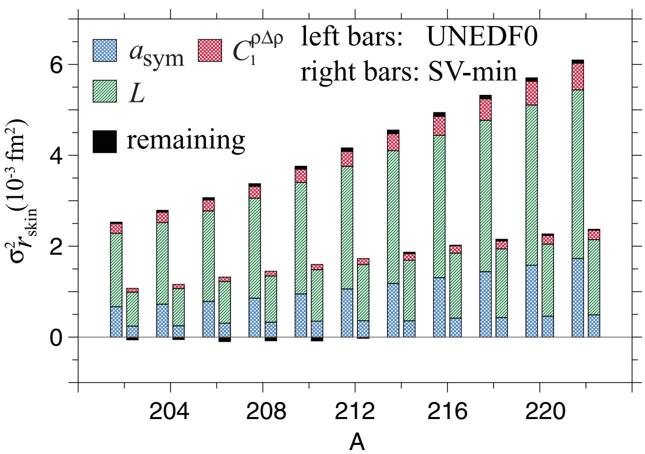

FIG. 4. (Color online) Error budget of $\sigma^2_{r_{skin}}$ (2) for UNEDF0 (left bars) and SV-min (right bars) for even-even isotopes of Pb. The dominant sources of uncertainty are the symmetry energy parameter a_{sym}, the slope of the symmetry energy L, and to a lesser degree, the isovector coupling constant $C_1^{\rho\Delta\rho}$ that governs the surface properties of EDFs.

energy and its slope are less precisely determined in UNEDF0 is reflected in the larger error Δr_{skin}^{stat} seen in Fig. 4.

Finally, to address the required experimental accuracy to constrain Skyrme EDF models by future measurements of r_{skin}, we present in Table I Δr_{skin}^{stat} of UNEDF0 and SV-min, the systematic error Δr_{skin}, and the model-averaged deviation of Ref. [9] constrained by the measured value of α_D in ^{208}Pb [27]. The results are presented for ^{208}Pb and ^{48}Ca. The error bar of PREX [25] is unfortunately too large ($\sim$0.18 fm) to provide a useful constraint on isovector properties of current models. On the other hand, the superb anticipated accuracy of the planned CREX experiment (0.02 fm) [30] will have an impact on reducing the statistical error on r_{skin}.

Conclusions. This survey addresses systematic and statistic errors on the neutron-skin thickness predicted by various Skyrme EDF models. Because r_{skin} has been found to strongly correlate with various isovector indicators, it provides an essential constraint on nuclear EDFs that aim at making extrapolations into the *terra incognita* at the neutron-rich side of the nuclear landscape. We have found that systematic error Δr_{skin}^{syst} obtained in this work and in Ref. [9] is smaller than the statistical error Δr_{skin}^{stat}. As expected, both errors grow with

TABLE I. Theoretical uncertainties on r_{skin} in ^{208}Pb and ^{48}Ca (in fm). Shown are statistical errors of UNEDF0 and SV-min, systematic error Δr_{skin}^{syst}, the model-averaged deviation of Ref. [9], and errors of PREX [25] and planned PREX-II [29] and CREX [30] experiments.

Nucleus	Δr_{skin}^{stat}		Δr_{skin}^{syst}	Ref. [9]	Experiment
	UNEDF0	SV-min			
^{208}Pb	0.058	0.037	0.013	0.022	0.18 [25], 0.06 [29]
^{48}Ca	0.035	0.026	0.019	0.018	0.02 [30]

neutron number due to propagation of uncertainties of poorly determined EDF isovector coupling constants. As far as the systematic error is concerned, one has to bear in mind that it does depend on the particular choice of models used. For instance, there is a systematic shift in r_{skin} predicted by the Skyrme models studied in this work and the relativistic EDFs [9,10], which exceeds Δr_{skin}^{syst} obtained here.

The slope of the symmetry energy L is the single main contributor to Δr_{skin}^{stat}. As already pointed out in many previous studies, this parameter is strongly correlated with many isovector indicators. Therefore, planned precise measurements of r_{skin} will help in pinning down this crucial NMP. Conversely, if L could be constrained by some other experimental data [22], this would also reduce model uncertainty on r_{skin}. The methodology presented in this paper aiming at assessing statistical and systematic uncertainties on calculated quantities can be generally used to determine the uniqueness and usefulness of an observable with respect to current theoretical models and can be used to help in planning future experiments and experimental programs [48].

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