Extension and parameterization of high-order density dependence in Skyrme forces

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The three-body force is indispensable in nuclear energy density functionals which leads to a density dependent two-body term in the Hartree-Fock approach. Usually a single fractional power of density dependency has been adopted. We consider the possibility of an additional higher-order density dependence in extended Skyrme forces. As a result, new extended Skyrme parameterizations based on the SLy4 force are obtained and the improvements in descriptions of global nuclei have been demonstrated. The higher-order term can also substantially affect nuclear properties in the high density region in general ways.

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I. INTRODUCTION

The nuclear energy density functional theory (EDF) is a principal theoretical tool for descriptions of bulk properties and dynamics of the entire nuclear landscape. The main issues for nuclear EDF theory are concerns about its accuracy and uncertainties. After early Skyrme Hartree-Fock calculations [1], the Skyrme interactions [2] have been widely used and have been demonstrated to be very powerful [3]. In particular, the latest UNEDF Skyrme forces [4-6] based on large scale fitting procedures have remarkably improved the accuracy. On the other hand, the limits of standard Skyrme forces have been reached and new ideas are desirable. The Skyrme force is a very low-momentum (or soft) interaction with a second-order momentum dependence and a three-body interaction that plays an indispensable role in nuclear saturation [7]. In ab initio calculations, it is well known that the three-body force and many-body forces are generated due to suppressed (or renormalization cutoff) degrees of freedom of the two-body potential [8]. Following this picture, the remarkable three-body force contribution in soft Skyrme forces as well as Gogny forces [9] is then understandable. Recently the three-body force has become an attractive issue in ab initio calculations [10, 11] and Brueckner-Hartree-Fock calculations [12, 13]. In Hartree-Fock calculations, the three-body interaction can be considered as a density dependent two body term with \( \rho^3 \), in which the density dependency power \( \gamma \) should be 1. However, the power \( \gamma \) should be smaller than 2/3 to get reasonable nuclear matter incompressibility [14, 15]. In fact, a fractional power of density dependency, ranging from 1/6 to 1, has been adopted in various Skyrme parameterizations [16]. The parameterized density dependence is supposed to simulate complicated many-body correlations in addition to the three-body force and is still an open question.

In the dilute Fermi systems of repulsive cores, the energy density functional can in principle be expanded in powers of \( k_F \) (or \( \rho^{1/3} \)). The EDF expansion coefficients were calculated in a series of papers in 1957, by Huang-Yang [17], Lee-Yang [18], Martin and De Dominicis [19], which takes the form,

\[
\varepsilon = \frac{3\hbar^2}{10m} (3\pi^2)^{2/3} \rho^{5/3} + \frac{\hbar^2 \pi a}{m} \rho^2 \\
+ \frac{2\hbar^2 a \gamma^4 \pi^{2/3}}{35m} (11 - 2 \ln 2) \rho^{7/3} \\
+ 0.78 \frac{\hbar^2 a^{3 \gamma^3 / 3} \rho^{10/3}}{2m} \rho^{8/3}
\]

in which \( a \) denotes a finite radius of particles. These high order terms reflect the increased kinetic energy by considering the finite radius of particles. In the Local Density Approximation for dilute Fermi gases, its EDF form is the same as Skyrme EDF except for different density dependent terms [20]. The EDF of dilute Fermi gases involves terms with \( \rho^{7/3}, \rho^{8/3} \), etc. While the standard Skyrme EDF involves a single density dependent term with \( \rho^{2+\gamma} \). Actually, the \( \rho^{7/3} \) term (corresponding to \( \gamma=1/3 \)) can be mimicked by an effective three-body interaction [21]. In contrast to the dilute Fermi systems, we note that generally the finite radii (volume effects) of nucleons have not been explicitly considered, neither in realistic nor phenomenological nuclear forces.

Our objective of this work is to consider the possibility of an additional higher order density dependence on top of the standard Skyrme force. In deeded, in the standard Skyrme force, a single density dependent term might be too simplistic. It is also of interdisciplinary interests to study the role of higher order density dependencies and the EDF connection between nuclei and dilute Fermi gases. We speculate that the high-order density dependencies can reflect short-range correlations beyond standard Skyrme forces, and impact in particular the high-density behaviors and isovector properties.

The extensions of Skyrme forces have been developed by many efforts. For example, the Brussels forces by considering the density dependence in the momentum-dependent terms have been very successful [22]. The effective pseudopotential of Skyrme-type EDF has been derived up to the sixth order [23]. On the other hand, the connection between nuclear EDF parameters and ab initio calculations has not yet been clear, although progresses have been achieved in the Density Matrix Expansion [24] and the Effective Field Theory [20].

The higher-order density dependent terms have been considered in Refs. [28, 29] in analogy to those for the dilute...
Fermi gases, but with limited applications. In this work, we are not intended to refit a fully new Skyrme parameter set from scratch but to improve the existed successful Skyrme parameters with an additional higher-order density dependent term. To this end, we concentrate on the momentum-independent terms, and manipulate the $t_0$, $t_3$ parameters and the extended term with $t_{3E}$. Indeed, $t_0$, $t_3$ and $t_{3E}$ are directly entangled in the $s$-wave channel although they are also connected with other parameters. For example, the correlations between parameters have been demonstrated by the Bayesian analysis [23]. We choose to refit the momentum-independent terms based on the SLy4 force [26] and keep other parameters unchanged. The SLy4 force is an ideal start because it has been widely used and has been the references for other parameterizations such as UNEDF forces. Furthermore, SLy4 has a density dependence of $\gamma=1/6$ which is relatively small and may leave room for higher-order density dependencies. Other successful Skyrme forces such as SkM* [27] with $\gamma=1/6$ may also be improved with higher-order density dependencies. Or say we consider an additional higher-order density dependent term for complementary to SLy4 in a perturbative manner. It is turned out that the density dependent terms we employed are different from Refs. [28] [29]. We will then evaluate the performance of the extended new parameterizations compared to the original SLy4.

II. THEORETICAL METHODS

We begin with the standard Skyrme interaction including the two-body and three-body terms [2], which takes the form,

$$ V_{\text{Skyrme}} = \sum_{i<j} v^{(2)}_{ij} + \sum_{i<j<k} v^{(3)}_{ijk} $$

(2)

$$ v^{(2)}_{ij} = t_0 (1 + x_1 P_\sigma) \delta(r_i - r_j) $$

$$ + \frac{1}{2} t_1 (1 + x_1 P_\sigma) \left[ \delta(r_i - r_j) k^2 + k^2 \delta(r_i - r_j) \right] $$

$$ + t_2 (1 + x_2 P_\sigma) \left[ \delta(r_i - r_j) k \cdot (r_i - r_j) \right] $$

$$ + i W_0 (\sigma_i + \sigma_j) \cdot \mathbf{k} \times \delta(r_i - r_j) k $$

(3)

The three-body interaction in the Hartree-Fock calculations can be transformed into a density dependent two-body interaction with $\rho^\gamma$. Correspondingly the power $\gamma$ should be 1 but usually is adjusted to be less than 1 in modern Skyrme forces to get reasonable incompressibilities.

$$ v^{(3)}_{ijk} = t_3 (1 + x_3 P_\sigma) \delta(r_i - r_j) \delta(r_j - r_k) $$

(4)

$$ \Rightarrow v^{(2)'}_{ij} = \frac{1}{6} t_3 (1 + x_3 P_\sigma) \rho(R)^\gamma \delta(r_i - r_j) $$

(5)

In Eq (3) and Eq (4), $t_i$, $x_i$ and $W_0$ are the parameters of the Skyrme interaction, and $R = (r_i + r_j)/2$.

In our extension, by including an additional higher-order density dependent term, the density dependent term is modified as,

$$ v^{(2)'}_{ij} = \frac{1}{6} t_3 (1 + x_3 P_\sigma) \rho(R)^\gamma \delta(r_i - r_j) $$

In this case, there will be 2 more additional parameters $t_{3E}$ and $x_{3E}$. In the SLy4 force [26], the power factor $\gamma$ takes 1/6 and then we consider the next higher order power of 1/2 = 1/6 + 1/3. Actually such an extension is straightforward and can be easily implemented. We noticed that similar extensions exactly according to the density dependent terms for dilute Fermi gases have been discussed in the case of nuclear matter properties [28]. Later it has been investigated in finite nuclei but negative coefficients are obtained for higher-order terms [29]. The density dependent terms we employed are different from [28] [29] since our studies are based on SLy4, although we have similar motivations. It is useful to explore different combinations of density dependencies. Considering recent UNEDF forces with $\gamma$ around 1/3 [28] that is between 1/6 and 1/2, the two density dependent terms we employed should be reasonable.

Next we refit the extended Skyrme parameters for finite nuclei with the Simulated Annealing Method [30]. In this work, we only refit the momentum-independent parameters, $t_0$, $t_3$, $t_{3E}$, $x_0$, $x_3$, $x_{3E}$, and keep others $t_1$, $t_2$, $x_1$, $x_2$, $W_0$ unchanged based on the SLy4 force. In this way the influences of the extended higher-order density dependent term can be clearly illustrated, to avoid the influences due to terms which involve momentum dependencies.

Our fitting procedure is similar to SLy4 as described in Ref. [26]. Briefly, we minimize the quantity,

$$ \chi^2 = \left( \frac{e_\infty + 16}{0.2} \right)^2 + \sum_i \left( \frac{E_{n(i)} - E_{UV14+UVII(i)}}{\Delta E_i} \right)^2 $$

$$ + \sum_i \left( \frac{B_{i(i)} - B_{i(i)}^{\text{exp}}}{2} \right)^2 + \sum_i \left( \frac{R_{c(i)} - R_{c(i)}^{\text{exp}}}{0.02} \right)^2 $$

(6)

where $e_\infty$ is the average energy per nucleon at the saturation point; $E_{n(i)}$ and $E_{UV14+UVII(i)}$ are energies of the neutron matter from Skyrme forces and calculations of Wiringa et al. [33] at different density points; $B_i$ and $R_i$ denote total binding energies and charge radii of selected nuclei respectively. In Eq (6), the fitting uncertainties $\Delta E_i$ are not a constant but increase as densities increase [31]. The nuclear matter properties at the saturation point are important inputs for constraining parameters. In the extended Skyrme functional, we have to slightly modify the equations of the pressure $P$, the incompressibility coefficient $K$, the symmetry energy coefficient $\alpha_s$. The saturation density of 0.1595 fm$^{-3}$, the symmetry energy coefficient $\alpha_s$ of 32 MeV and the effective mass $m^*/m$ of 0.7 have not been adjusted [26]. Therefore, we adjust 6 parameters and have 4 free parameters $e_\infty$, $t_3$, $x_3$ and $x_{3E}$ to fit after taking into account the equations of nuclear matter properties. Then Skyrme parameters $t_0$, $x_0$, $t_{3E}$ can be determined through these expressions.

Our calculations are based on the axially-symmetric Hartree-Fock+BCS approach and the Simulated Annealing
Method (SAM). The Hartree-Fock+BCS equation is solved within axially-symmetric coordinate spaces using the SKYAX solver [32]. In this case deformed nuclei can be included in the fitting procedure compared to the original SLy4 force. The calculations are performed in a 2D box of 30 fm and the uniform lattice space is taken as 0.5 fm. The mixed pairing interaction [33] has been adopted and the pairing strength is taken as \( V_{p,n} = 500 \text{ MeV fm}^{-3} \) for protons and neutrons. SAM [30] is a general purpose algorithm for multi-parameter fittings, based on the Monte Carlo iterative solution method. SAM starts with a high temperature and randomly searches the minimum, which accepts a worse solution than the current one with a certain probability. As the temperature cools down, the searching space becomes smaller and the optimization is then realized. The SAM has already been adopted in the fitting of full Skyrme parameters [34].

### III. RESULTS AND DISCUSSIONS

We refit the extended Skyrme force based on SLy4 with different groups of selected nuclei. In particular, we select 4 groups aiming at different mass regions,

- **Group1:** \(^{40}\text{Ca}, ^{48}\text{Ca}, ^{56}\text{Ni}, ^{132}\text{Sn}, ^{208}\text{Pb} \), for magic nuclei as adopted in the SLy4 fitting;
- **Group2:** \(^{16}\text{O}, ^{36}\text{Mg}, ^{40}\text{Ca}, ^{48}\text{Ca}, ^{50}\text{Cr}, ^{56}\text{Ni}, ^{78}\text{Ni}, ^{100}\text{Zr}, ^{120}\text{Sn}, ^{132}\text{Sn} \), for light nuclei with \( 8 \leq Z \leq 50 \);
- **Group3:** \(^{120}\text{Sn}, ^{132}\text{Sn}, ^{166}\text{Gd}, ^{176}\text{Hf}, ^{198}\text{Pb}, ^{208}\text{Pb}, ^{236}\text{U}, ^{252}\text{Fm}, ^{260}\text{Sg} \), for heavy nuclei with \( Z \geq 50 \);
- **Group4:** \(^{16}\text{O}, ^{36}\text{Mg}, ^{40}\text{Ca}, ^{48}\text{Ca}, ^{50}\text{Cr}, ^{56}\text{Ni}, ^{78}\text{Ni}, ^{100}\text{Zr}, ^{120}\text{Sn}, ^{132}\text{Sn}, ^{166}\text{Gd}, ^{176}\text{Hf}, ^{198}\text{Pb}, ^{208}\text{Pb}, ^{236}\text{U}, ^{252}\text{Fm}, ^{260}\text{Sg} \), for the global mass region.

The experimental binding energies of these nuclei are taken from [35]. The charge radii of 5 magic nuclei are taken from [26].

Figure 1 illustrates the obtained \( \chi^2 \) of different SAM fittings as the temperature cools down. In the fitting procedure, the initial temperature is 2 and decreases by a factor of 0.5 each step. The initial parameters are given as random values in selected sets. The initial ranges of \( T \) and \( x_{3E} \) are from \(-2 \) to 2. The range of \( r_3 \) is from 8000 to 13777. At the beginning, the \( \chi^2 \) is very large and becomes much smaller as the temperature lower than 0.125. One full fitting procedure takes about 200 iterations for the fitting of light nuclei and about 350 iterations for the global fitting, which takes 2~3 days. After that, we polish these parameters by a second fitting with obtained parameters as initial values.

Table I lists the obtained different parameterizations of extended SLy4 forces compared to the original SLy4 force. Generally, the obtained \( \chi^2 \) values of charge radii and binding energies are reduced significantly, compared to the \( \chi^2 \) values of...
TABLE I. Refits of SLy4 parameters with extend density dependent terms, compared to the original SLy4 force. The different parameter sets are obtained by fitting different groups of nuclei, see text for details. We also refit SLy4 without the extended term as labeled by SLy4'. Other parameters in SLy4 not listed here are not adjusted. The corresponding minimized $\chi^2$ of binding energies ($\chi^2_B$) and charge radii ($\chi^2_{R}$) of SLy4 are given in the brackets.

| Parameters          | SLy4     | SLy4'(global) | Group1(magic) | Group2(light) | Group3(heavy) | Group4(global) |
|---------------------|----------|---------------|---------------|---------------|---------------|---------------|
| $t_0$ (MeV · fm$^3$) | -2488.91 | -2493.536     | -2132.57      | -2106.69      | -2310.79      | -2319.15      |
| $t_3$ (MeV · fm$^3(1+\frac{1}{2})$) | 13777.0  | 13809.324     | 9366.12       | 9036.30       | 11549.45      | 11660.70      |
| $t_3-E$ (MeV · fm$^3(1+\frac{1}{2})$) | 0        | 0             | 2756.97       | 2970.72       | 1410.64       | 1334.88       |
| $x_0$                | 0.834    | 0.931         | 0.968         | 0.988         | 0.972         | 0.863         |
| $x_3$                | 1.354    | 1.496         | 1.922         | 1.975         | 1.715         | 1.509         |
| $x_{3E}$             | 0        | 0             | 0.375         | 0.530         | 0.324         | 0.622         |
| $\epsilon_{\infty}$ (MeV) | -15.972  | -15.963       | -16.063       | -16.085       | -16.055       | -16.039       |
| $K_{\infty}$ (MeV)   | 229.9    | 230.31        | 247.33        | 248.84        | 239.19        | 238.58        |
| $\chi^2_R$           | 10.35    | 2.18(4.04)    | 5.00(10.04)   | 0.39(0.62)    | 7.4(10.66)    |
| $\chi^2_B$           | 31.67    | 0.83(2.46)    | 3.83(6.82)    | 19.26(78.28)  | 25.92(84.87)  |
| $\chi^2_{\text{sum}}$ | 42.84    | 3.67(6.91)    | 9.79(17.306)  | 20.52(79.21)  | 33.82(95.94)  |

SLy4 shown in brackets. The incompressibility values $K_{\infty}$ and energies $\epsilon_{\infty}$ at the saturation density are also listed. We can see that the existed parameters $t_0$, $t_3$ are reduced. The obtained $t_{3E}$ parameter of the higher-order term ranges from 1334.88 to 2970.72. We noticed that in Refs. [36, 37], with decreasing momentum cutoffs in second-order Hartree-Fock calculations, the adjusted parameters $t_0$, $t_3$ decrease and the density dependency power increases. Our results with higher order terms are similar to that trend. In the fittings of heavy and global nuclei, the parameters of the higher-order term are relatively small. While in the fitting of light nuclei, the parameter of the higher-order term is the largest, which is mainly responsible for improving the descriptions of charge radii. This indicates that complex density dependencies are required for describing light nuclei. In our tests, by reducing the fitting weights on charge radii, the obtained higher-order term decreases. In the heavy mass region, the obtained new extended parameterizations still produce large deviations in binding energies. We also refit the SLy4 with the global group, as labeled by SLy4'. The resulted $\chi^2$ is significantly reduced except for the descriptions of charge radii. This demonstrated that the extended higher-order density dependent term is important for descriptions of nuclear charge radii.

![FIG. 4. (Color online) Symmetry energies as a function of nuclear matter density, corresponding to different Skyrme parameter sets in Table II.](image-url)
three-body (N2LO) forces [38]. Generally, the SLy4 force underestimates the energies compared to the Chiral force. While the extended SLy4 force can bring more binding energies. This is consistent with the situation of neutron matter energies as shown in Fig. 2.

To study the behaviors of extended SLy4 forces for nuclear matter properties, the incompressibility and the symmetry energy are displayed in Fig. 3 and Fig. 4, respectively. In Fig. 3 the extended forces all generate larger incompressibility values at high densities compared to the SLy4 force. The parameters for light nuclei with the largest higher order term produce the highest incompressibility. This causes very little influences in the low density region. It is understandable that the increased incompressibility is due to the repulsive higher-order density dependence. In Fig. 4 the symmetry energies as a function of densities are displayed. It can be seen that the symmetry energies decrease in the high density region by considering the higher order density dependent term. Again the parameters for light nuclei produce the softest symmetry energy. There has been some favorable arguments about the soft symmetry energy in dense nuclear matter [39]. In fact, by studying the expressions of nuclear matter properties, we note that the behaviors of the extended higher-order density dependence shown in Figs. 3-4 are general. We conclude that the inclusion of a higher-order density dependent term would impact the equation of state and isovector properties in the high density region (supra-saturation density), which are important for studying neutron star structures.

Finally, the global calculations of binding energies of 603 even-even nuclei are shown in Fig. 5. The calculations are done with the axially-symmetric Hartee-Fock+BCS solver SKYAX, and with the original SLy4, the refitted SLy4′ and the extended SLy4 (global) parameter sets. As we can see that the results of the extended parameterization are similar to the SLy4′ results. The original SLy4 remarkably underestimates the binding energies of heavy and superheavy nuclei. The extended SLy4 and SLy4′ have improved the global descriptions by including some heavy nuclei in the fitting procedure. For all the nuclei, the resulted root-mean-square (rms) deviations of the extended SLy4, SLy4′ and SLy4 are 2.30 MeV, 2.94 MeV and 4.37 MeV, respectively. In the region of \( Z \leq 82 \), the rms deviations of the extended SLy4, SLy4′ and SLy4 are 2.00 MeV, 2.71 MeV, 3.18 MeV, respectively. In the region of \( Z \leq 50 \), the rms deviations of the extended SLy4, SLy4′ and SLy4 are 2.15 MeV, 2.88 MeV, 1.97 MeV, respectively. Therefore we can say that the extended SLy4 force has globally improved the descriptions of binding energies, compared to the refitted SLy4′ and the original SLy4. Note that the extended global parameterization set has a relatively small higher-order density dependent term, as displayed in Table I. We see that SLy4, SLy4′ and the extended SLy4 are not able to describe the binding energies of magic nuclei and deformed nuclei simultaneously. Or say the shell effects are overestimated as they are based on a small effective mass of 0.7 [26]. Presently the effective mass and the related \( t_1 \), \( t_2 \) parameters have not been adjusted in the extended SLy4 forces. Indeed, UNEDF Skyrme forces with large effective masses around 1 are very successful in describing binding energies of the whole nuclear landscape [4]. On the other hand, the Brussels Skyrme force with an effective mass of 0.8 and additional collective corrections for deformations also works very successful [40]. In addition, SLy4 is unable to describe the surface tension compared to calculations with microscopic center-of-mass corrections [41]. Actually, our main goal in this work is to study the influences of the extended higher-order density dependence, by refitting only the momentum-independent parameters. The global performance of the extended SLy4 is very encouraging. To further improve the overall performance, the adjustments of all the Skyrme parameters including the extended term by choosing properly physics inputs will be our next step.

**IV. SUMMARY**

In summary, we studied the extension of Skyrme forces by including a higher-order density dependent term, according to our speculation that a single density dependent term might be too simplistic. This is in analogy to high order density dependent terms in the EDF for dilute Fermi gases. We studied the influences by adjusting only the momentum-independent parameters based on the SLy4 force, with two density depen-
dent terms of $\rho^{1/6}$ and $\rho^{1/2}$. The obtained new extended parameterizations indicate that the strengths of the higher order term $\rho^{1/2}$ are dependent on different fitting regions. We have seen that the higher-order term can improve descriptions of binding energies of global nuclei and neutron droplets as expected. We also noticed that the higher-order term is important for descriptions of charge radii. The extended parameterization set obtained by fitting light nuclei has the largest higher order term, indicating complex density dependencies are required for light nuclei. Furthermore, we demonstrated that the extended density dependence can impact nuclear matter properties particularly in the supra-saturation density region with general behaviors, although the extrapolations of Skyrme forces to the high density region still have large uncertainties. In conclusion, our studies have provided some insights and opportunities for future developments of Skyrme energy density functionals.

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