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Convergence Behavior of the Nuclear Energy Density Functional for Nuclei

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We investigate the feasibility of a systematic expansion scheme for the study of nuclear structure. We employ a new nuclear energy density functional (EDF) proposed by P. Papakonstantinou *et al.* [Phys. Rev. C **97**, 014312 (2018)], where the EDF is expanded in powers of the Fermi momentum k_F. First, we consider the two lowest-order terms proportional to k_F^3 and k_F^4 in the interaction part and calculate the properties of several spherical magic nuclei. We repeat the calculation by adding higher-order terms proportional to k_F^5 and k_F^6 and investigate the resulting predictions for the nuclear properties. The prediction is significantly improved when three interaction terms, k_F^3, k_F^4 and k_F^5, are considered. The fourth term proportional to k_F^6 corrects the preceding results in a limited range and improves the result marginally. This investigation sheds light on the possibility for accessing a perturbative understanding of nuclear structure.

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I. INTRODUCTION

One of the recent hot issues in the research of nuclear structure is to make an essential improvement in the theory for finite nuclei and infinite nuclear matter. There are many requirements to overcome the limit, ambiguity and shortcomings of the conventional models and traditional approaches. Two important subjects among them may be to establish rules to: i) estimate the uncertainty of calculation, and ii) identify the range of density and asymmetry where extrapolation is reliable. Advent of the issues is closely related to the construction of rare isotope accelerators [1] and launch of projects for accurate observation of neutron stars in space [2]. The two issues can be cast into one category of a problem: Can we have a perturbation theory for the nuclear structure?

Based on several observations in literature and arguments, we realized that k_F/m_ρ could be an expansion parameter of the nuclear energy density functional (EDF) [3], where k_F and m_ρ denote Fermi momentum and rho-meson mass, respectively. EDF thus constructed shows good hierarchical behavior in the result of fitting to homogeneous nuclear matter. A due subsequent question may be whether similar result would be expected when the model is applied to the structure of nuclei. In this work, we will find answer, or hints for answer to the question by calculating properties of several magic nuclei with two-, three- and four-term EDFs and analyzing convergence behavior of the result.

In Sec. II, we illustrate the basic formulae of the model and fitting strategy. In Sec. III, we present the results and discuss the implication of them. We summarize the paper in Sec. IV.

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Table 1. Parameters for SNM at each order and for PNM with four interaction terms. For $N = 1$, k value has the dimension equal to that of c_2, but it is dimensionless for $N = 2$, 3.

	N	c_0 (MeV·fm^3)	c_1 (MeV·fm^4)	c_2 (MeV·fm^5)	c_3 (MeV·fm^6)	k	W_0 (MeV)	χ^2
SNM	1	−676.344222	807.119929	-	-	−172.605530	256.923645	5.45×10^{-3}
	2	−664.516332	763.545612	40.132289	-	0.110636	108.345230	1.76×10^{-5}
	3	−648.720089	676.254826	200.923292	−98.726520	0.095042	109.723679	1.62×10^{-5}
PNM	3	−411.13	1007.78	−1354.64	956.47			

II. MODEL

Energy density functional for homogeneous nuclear matter is assumed to have the form [3]

$$\mathcal{E}(\rho,\delta) = \mathcal{T}(\rho,\delta) + \sum_{i=0}^{N} c_i(\delta)\rho^{1+i/3}, \tag{1}$$

where the total nuclear density ρ is the sum of neutron and proton density $\rho_n + \rho_p$, and δ denotes asymmetry defined as $\delta \equiv (\rho_n - \rho_p)/\rho$.

$\mathcal{T}(\rho,\delta)$ is the free kinetic energy per particle in homogeneous nuclear matter given by the usual expression

$$\begin{aligned}\mathcal{T}(\rho,\delta) \;=\; & \frac{3}{5}\frac{\hbar^2}{2m_p}\left(\frac{1-\delta}{2}\right)^{5/3}(3\pi^2\rho)^{2/3} \\ & + \frac{3}{5}\frac{\hbar^2}{2m_n}\left(\frac{1+\delta}{2}\right)^{5/3}(3\pi^2\rho)^{2/3}. \end{aligned} \tag{2}$$

Summation term represents the interaction energy per particle expanded in powers of $\rho^{1/3}$.

$c_i(0)$ can be determined from the properties of symmetric nuclear matter (SNM; $\delta = 0$), and $c_i(1)$ from the data of asymmetric nuclear matter. It has been shown in Ref. [3] that the fitting of $c_i(0)$ up to $\rho^{5/3}$ ($N = 2$) reproduces the properties of SNM very well, and addition of ρ^2 term shows small change to the quantitative improvement of fitting. This behavior could be interpreted as a saturation of fitting at the order of $\rho^{5/3}$, and high order terms may give very slight corrections. On the other hand, the chi-square value is significantly reduced when ρ^2 term is added to the EDF up to $\rho^{5/3}$ in the fitting of $c_i(1)$ to the equation of state (EoS) of pure neutron matter (PNM) in Ref. [4] (APR in short). One can guess that contrary to the SNM, fitting could be improved furthermore if we add more terms in the PNM. Saturating behavior of fitting for PNM should be investigated furthermore, but up to ρ^2 order, we could check that the 11 properties of nuclear matter at various densities and asymmetries [5] are satisfied well within the experimental errors.

In the first step for the application of expansion method to the structure of nuclei, we begin with the order $N = 1$ (two terms ρ and $\rho^{4/3}$) for the SNM part of interaction, and increase the order by one up to $N = 3$ (terms to ρ^2). On the other hand, in order to remove the ambiguity from the PNM part, we always keep the four terms (from ρ to ρ^2) in the interaction for PNM.

For the parameters in the PNM part, we adopt the values determined in Ref. [3], and $c_i(0)$ are fitted to saturation density (0.16 fm^{-3}), binding energy per particle (16.0 MeV) for two-term interaction EDF ($N = 1$), compression modulus (240 MeV) for $N = 2$, and the effective mass of the nucleon at saturation (0.7 m_N) for $N = 3$. Parameters thus determined in homogeneous nuclear matter are kept unchanged when the EDF is applied to nuclei.

In Refs. [6,7] we obtained one-to-one mappings from our EDF to Skyrme-type EDF. In order to describe nuclei, derivative and spin-orbit coupling terms should be added to the EDF for homogeneous matter, which introduces two additional parameters k and W_0. Explicit forms of the EDF for nuclei can be found in Ref. [7]. These two new parameters are determined to reproduce the empirical data of the binding energy per nucleon (E_0) and charge radius (R_c) of spherical magic nuclei ^{40}Ca, ^{48}Ca and ^{208}Pb. Parameters at each order are summarized in Table 1. We note that the dimension of k is MeV·fm^5 for $N = 1$ because there is no term proportional to $\rho^{5/3}$ in the EDF for homogeneous matter so k which is the coefficient of $\rho^{5/3}$ term has the dimension equal to that of c_2. However, k is dimensionless for $N = 2$, 3.

Table 2. E_0 and R_c of first three-row nuclei are used in the fitting of k and W_0, and the values for the nuclei in the low five rows are prediction of the model. All the neutron skin thickness Δr_{np} values are predictions. Numbers in the parentheses represents the difference from experiment.

Nuclei	E_0 (MeV)			R_c (fm)			Δr_{np} (fm)		
	$N=1$	$N=2$	$N=3$	$N=1$	$N=2$	$N=3$	$N=1$	$N=2$	$N=3$
^{40}Ca	8.4583 (1.088%)	8.5565 (0.061%)	8.5546 (0.039%)	3.5004 (0.656%)	3.4781 (0.014%)	3.4761 (0.043%)	−0.0377	−0.0444	−0.0444
^{48}Ca	8.9196 (2.918%)	8.6564 (0.119%)	8.6558 (0.126%)	3.3847 (2.657%)	3.4867 (0.276%)	3.4850 (0.227%)	0.33004	0.1764	0.17624
^{208}Pb	7.4491 (5.317%)	7.8809 (0.171%)	7.8801 (0.161%)	5.3357 (3.008%)	5.4887 (0.227%)	5.4872 (0.254%)	0.76681	0.18931	0.18806
^{16}O	7.7620 (2.686%)	7.8684 (1.352%)	7.8685 (1.350%)	2.8037 (3.875%)	2.7618 (2.323%)	2.7591 (2.223%)	−0.0192	−0.0235	−0.0234
^{28}O	4.9098	6.0646	6.0649	2.5784	2.8371	2.8354	1.36041	0.66357	0.66218
^{60}Ca	6.6067	7.6561	7.6553	3.4179	3.6465	3.6448	1.4988	0.49595	0.49485
^{90}Zr	8.9722 (3.011%)	8.7328 (0.262%)	8.7311 (0.242%)	4.1567 (2.640%)	4.2476 (0.511%)	4.2462 (0.557%)	0.20264	0.07116	0.07117
^{132}Sn	7.9967 (5.317%)	8.3563 (0.017%)	8.3565 (0.012%)	4.5235 (3.008%)	4.7089 (0.008%)	4.7075 (0.038%)	0.87652	0.24532	0.24443

III. RESULT AND DISCUSSION

Parameters in Eq. (1) have been adjusted to the properties of nuclear matter, and two parameters k and W_0 to the binding energy per particle and charge radius of ^{40}Ca, ^{48}Ca and ^{208}Pb. Without any further modification or adjustment in the parameters, we calculate E_0, R_c and the neutron skin thickness Δr_{np} of ^{16}O, ^{28}O, ^{60}Ca, ^{90}Zr, ^{132}Sn. Results are shown in Table 2.

First it should be noted that the difference from experiment is greatly reduced if we include $\rho^{5/3}$ ($N=2$) term. On the other hand, change or improvement is very small when ρ^2 term is added. A similar behavior of saturation of precision has already been observed in the fitting of nuclear matter [3]. This result suggests that three may be the minimal number of terms for a precise description of nuclear properties.

Looking at the results of input nuclei ^{40}Ca, ^{48}Ca and ^{208}Pb, lead shows the largest deviation from experiment, 0.16% and 0.25% for E_0 and R_c, respectively. This magnitude is similar to or about 0.1% larger than the those in the GSk model [8]. However our model shows better agreement to data for ^{40}Ca than the GSk model. Since the difference between our model and the GSk model is at the order of 0.1% or less, the two models reproduce the input data fairly precisely. We should stress, however, that the basic assumption of two models is different by principle in the following respects.

1. Our model assumes a rule to construct an EDF systematically, while the conventional models start with a specific form of Skyrme force.

2. There is no rule to determine the parameters in the conventional model, so some parameters assume arbitrary numbers. In addition, there are numerous ways to select input data and fitting method, which has eventually produced hundreds of Skyrme force models. On the other hand we assume to determine the starting EDF only from the properties of homogenous nuclear matter, and introduce minimal numbers of additional parameters when nuclei are considered.

Now let us compare the prediction to experiment. ^{16}O exhibits difference from experiment at the level of 1%. This result is much larger than the GSk model in which E_0 differs from experiment less than 0.2%. In the GSk model, experimental data of ^{16}O is included in the fitting data set, so small difference is an expected result. In our calculation results of ^{16}O are pure predictions. Nevertheless one can see that the difference from experiment for other nuclei are one or two orders of magnitude smaller than ^{16}O. This constrasting behavior of oxygen may be attributed to the limitation of mean-field approximation in the density functional theory. Microscopic method may be more favorable to the description

of light or semi-light nuclei. This could serve as a warning that the use of data on light nuclei might introduce unwanted bias in the fits of phenomenological EDFs.

Contrary to oxygen, predictions of ^{90}Zr and ^{132}Sn differ from experiment at the order of 0.1% or less, so the result is as exact as the nuclei used in the fitting. For the binding energy per nucleon, GSk model gives deviations about $-0.6 \sim -0.1\%$ for ^{90}Zr, and $-0.1 \sim -0\%$ for ^{132}Sn. Our model prediction is no worse than that of the GSk model. We remind again that while the binding energies of ^{90}Zr and ^{132}Sn are used in the fitting of GSk model, our results are genuine predictions.

Last three columns in Table 2 show the neutron skin thickness Δr_{np}. Since Δr_{np} is not used in the fitting, all the results are prediction of the model. The results of $N = 1$ drastically differ from those of $N = 2$ and 3. One can find a reason from the expansion parameter J and L of the symmetry energy,

$$E_{\rm sym}(\rho) = J + \frac{1}{3}L\left(\frac{\rho-\rho_0}{\rho_0}\right) + \cdots . \qquad (3)$$

We obtain J and L in MeV as (96.6, 368.5) for $N = 1$, and (32.8, 49.1) for $N = 2$ and 3 (to the digit we present, J and L are equal for $N = 2$ and 3). Experiments provide the range of each parameter as $J = 30 \sim 35$ MeV and $L = 40 \sim 76$ MeV. The set of $N = 1$ gives J and L completely out of the experiment range. On the other hand, $N = 2$ and 3 satisfy the experiment, and moreover the change from $N = 2$ to $N = 3$ is small as we observed in E_0 and R_c. From the result of Δr_{np}, we can again draw the conclusion that three leading order terms are essential, and fourth or higher order terms are marginal.

The correlation between Δr_{np} and L has been studied extensively, and it is shown that Δr_{np} can be approximated linear to L for ^{68}Ni, ^{132}Sn and ^{208}Pb [9]. Plugging our prediction $\Delta r_{np} \simeq 0.19$ fm for Pb into a linear fitting relation in Ref. [10],

$$L = (-78.5 \pm 3.2) + (740.4 \pm 20.9) \times \Delta r_{np}, \qquad (4)$$

we obtain $L \simeq 55$ MeV, which is slightly larger than our result $L = 49.1$ MeV.

IV. SUMMARY AND OUTLOOK

In search for an organized framework which allows for systematic extension of energy density functional model of nuclear structure, we propose an ansatz by assuming expansion of nuclear EDF in powers of Fermi momentum. The EDF is fitted to well-known properties of nuclear matter at first. Keeping the parameters thus obtained unchanged, we transform the EDF to Skyrme-type EDF and fit the two additional parameters which account for the derivative interactions and a spin-orbit coupling to binding energy per nucleon and charge radius of ^{40}Ca, ^{48}Ca and ^{208}Pb. In order to investigate the perturbative behavior of the ansatz, we calculate properties of several spherical magic nuclei with two-, three- and four-term interaction EDFs for the symmetric nuclear matter part, while retaining four terms for the PNM part at all orders of SNM calculation.

We observe that model prediction improves significantly when three interaction terms are accounted in the EDF, and fourth term gives tiny corrections. This result could be a signal for a model of nuclear structure in which estimation of uncertainty could be under control. On the other hand, it has been shown that $\rho^{1/3}$ expansion in the PNM is much more non-trivial than the SNM [3,7]. Similar analysis with extended terms in PNM is in progress.

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REFERENCES

[1] S. Jeong, New Phys.: Sae Mulli **66**, 1458 (2016).
[2] K. C. Gendreau *et al.*, in *Proc. SPIE9905, SpaceTelescopes and Instrumentation 2016 Ultraviolet to Gamma Ray* (22 July, 2016), 99051H.
[3] P. Papakonstantinou, T.-S. Park, Y. Lim and C. H. Hyun, Phys. Rev. C **97**, 014312 (2018).

[4] A. Akmal, V. R. Pandharipande and D. G. Ravenhall, Phys. Rev. C **58**, 1804 (1998).
[5] M. Dutra, O. Lourenco, J. S. Sá Martins and A. Delfino, Phys. Rev. C **85**, 035201 (2012).
[6] H. Gil, P. Papakonstantinou, C. H. Hyun, T.-S. Park and Y. Oh, Acta Phys. Polon. B **48**, 305 (2017).
[7] H. Gil, P. Papakonstantinou, C. H. Hyun and Y. Oh, New Phys.: Sae Mulli **67**, 456 (2017).
[8] B. K. Agrawal, S. K. Dhiman and R. Kumar, Phys. Rev. C **73**, 034319 (2006).
[9] A. Carbone, G. Coló, A. Bracco, L.-G. Cao and P. F. Bortignon *et al.*, Phys. Rev. C **81**, 041301 (2010).
[10] L.-W. Chen, C. M. Ko and B.-A. Li, Phys. Rev. C **73**, 064309 (2005).