Optimal pair density functional for description of nuclei with large neutron excess

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I. INTRODUCTION

The energy density functional (EDF) theory provides a comprehensive microscopic framework for description of bulk nuclear properties, low-lying excitations, giant vibrations, and rotational excitations [1]. From the pioneering work by Vautherin and Brink [2], diverse endeavors have been made for finding the best EDF aiming at the description of the nuclear properties across the mass table. For example, the Skyrme functional for the particle-hole (p-h) channel has been improved by taking into account the incompressibility modulus of nuclear matter [3], the spin- and spin-isospin channels [4], the deformation properties [5], the spin-orbit terms [6], and the isospin properties [7]. Efforts to include the new terms such as the tensor terms are also being made (for the recent situation, see Ref. [8]).

The particle-particle (p-p) channel of the EDF (pair density functional, pair-DF) is also an indispensable element for description of nuclear systems [9]. The study of the nuclear matter predicts a very weak $^1S_0$ pairing at the normal density, and the pairing correlation in finite nuclei is considered to be nuclear surface effects [10]. The induced pairing interaction due to phonon exchange also enhances the surface effect [10-12]. These facts suggest the density dependence of the effective pairing force.

The standard parametrization of the pair-DF has the isoscalar density ($\rho = \rho_n + \rho_p$) dependence only [13-14]. The coupling constant should be constrained by the requirement to reproduce the experimental data such as masses, low-lying excited states, and rotational properties. However, the functional form of the density dependence is still under discussion [14-15].

In nuclei near the $\beta$-stability line, the effect of the p-p field characterized by the Fermi energy is much stronger than the p-h field. Therefore the pairing correlations can be treated within the BCS approximation [5-13]. On the other hand, the strengths for the p-p and p-h channels become comparable in magnitude for weakly-bound nuclei [9-13]. Therefore it is desirable to constrain the functional form of the pair-DF by using the experimental data of unstable nuclei.

The isovector density ($\rho_1 = \rho_n - \rho_p$) dependence can have sizable effects in nuclei apart from the $\beta$-stability line. In Ref. [25], the linear $\rho_1$ terms were introduced so as to simulate the neutron pairing gaps in symmetric and neutron matters obtained with either the bare interaction or the interaction screened by the medium polarization effects. It was pointed out that the pairing properties in semi-magic nuclei can be better described by the $\rho_1$-dependent pair-DF than that without $\rho_1$ terms [26].

We also recognized the importance of the linear $\rho_1$ term in the pair-DF [24]. By performing the Hartree-Fock-Bogoliubov (HFB) calculation with various coupling constants of the $\rho$ and $\rho_1$ terms, we emphasized the strong sensitivity to the pairing properties and the influence on rotational excitations in deformed nuclei near the neutron drip line.

In principle, it is desirable to derive the pair-DF from the bare interaction based on the microscopic pairing theory including both the medium polarization effect and the surface phonon coupling effect in finite nuclei. However, it seems very difficult at present in spite of recent progress toward this direction [12-27].

In this paper, we extend the pair-DF by including the linear and quadratic $\rho_1$ terms based on the phenomenological considerations. The pair-DF is designed so as to reproduce the dependence of pairing gaps on both the mass number $A$ and the asymmetry parameter $\alpha = (N - Z)/A$. The parameters in the pair-DF are optimized so as to minimize the root-mean-square (r.m.s.) deviation between the experimental and calculated pairing gaps. The necessity of the $\rho_1$ dependence in pair-DF is emphasized in connection with the effective mass
We extend the analysis with up-to-date measured masses in the wider mass region of \( N, Z \geq 40 \) (except for nuclei with either \( Z = 50, 82 \) or \( N = 50, 82, 126 \)) \cite{37}. The result is shown in Fig. 1. The average \( A \)- and \( \alpha \)-dependence is determined for the neutron and proton pairing gaps separately by \( \chi^2 \)-fitting:

\[
\Delta_n^{(\text{exp})} (\alpha) / \Delta_n^{(A)} \equiv C_n^{(0)} - C_n^{(1)} \alpha^2 \\
\Delta_p^{(\text{exp})} (\alpha) / \Delta_p^{(A)} \equiv C_p^{(0)} - C_p^{(1)} \alpha^2
\]

with \( \Delta_n^{(A)} = 6.75 / A^{1/3} \text{ MeV} \) and \( \Delta_p^{(A)} = 6.36 / A^{1/3} \text{ MeV} \). Here the experimental pairing gaps are extracted by the odd-even mass difference with the three-point staggering parameters \cite{18}.

The Coulomb force is an important building block of nuclear systems. The 20 - 30 \% reduction of \( \Delta_p \) by the self-consistent treatment of the Coulomb force was reported in Ref. \cite{38}. The authors of Ref. \cite{39} also arrived at the same conclusion by performing the HFB calculation with the non-empirical pair-DF. On the other hand, the experimental evidence is unclear in our analysis. The ratio is \( \Delta_p^{(\text{exp})} (\alpha) / \Delta_p^{(\text{exp})} (\alpha) \approx 0.94 (1 - 0.51 \alpha^2) \geq 0.91 \) for \( 0 \leq \alpha \leq 0.25 \). This is smaller than the uncertainty of our analysis about 10 \% shown by error bars in Fig. 1. The elaborate investigation is required to clarify the Coulomb effect. Therefore we neglect this effect in our analysis and leave it as an open problem in the future study.

III. MODEL

A. Parametrization of pair-DF

We extend the pair-DF by including the linear and quadratic \( \rho_1 \) terms in the following form:

\[
H_{\text{pair}} (r) = \frac{V_0}{4} \sum_{\tau=n,p} \int \left\{ \rho_\tau (r) \right\}^2
\]

with

\[
g_\tau \left[ \rho_\tau \rho_1 \right] = 1 - \eta_0 \rho (r) \rho_0 + \eta_1 \tau_3 \rho_1 (r) \rho_0 - \eta_2 \left( \frac{\rho_1 (r)}{\rho_0} \right)^2
\]

Here \( \tau = n \) (neutron) or \( p \) (proton), and \( \rho_0 = 0.16 \text{ fm}^{-3} \) is the saturation density of symmetric nuclear matter. The \( \tau_3 = 1 \) (n) or \( -1 \) (p) in the linear \( \rho_1 \) term is introduced so as to preserve the charge symmetry of the pair-DF. In nuclei with large \( \alpha \), the \( \rho_1 \) terms produce two effect for pairing correlations. The one is the volume effect inside the nucleus, which is relevant to all nuclei. The other is the skin effect in nuclei apart from the \( \beta \)-stability line.

The pair-DF with \( \eta_0 = 0.5 \) and \( \eta_1 = \eta_2 = 0 \) is one of the current standard parameterizations called the mixed-type pairing force. This pairing force reproduces the average \( A \) dependence of pairing gaps \cite{18}. We also justify
this choice in Sec. [VI]. Therefore, we fix \( \eta_0 = 0.5 \) unless otherwise noted.

### B. Setup

We use the standard Skyrme interaction for the p-h channel in the HFB calculation. The Skyrme SLy4 [7] parametrization is mainly used. In Sec. [VI], we will extend our analysis with 13 Skyrme parameters.

For the determination of \( \eta_1 \) and \( \eta_2 \), we perform the Skyrme-HFB calculation for 156 ground states of even-even, open-shell nuclei in the region of \( Z = 56 - 76 \), and either \( N = 56 - 76 \) or \( 88 - 120 \), which covers the range of \( 0 < \alpha < 0.25 \). We utilize the computer code of the Skyrme-HFB calculation developed by M. Stoitsov et al. [40]. Starting from the spherical, prolate and oblate initial conditions, the lowest energy solution is searched in the space of axially symmetric quadrupole deformation.

We estimate the r.m.s. deviations between the experimental and calculated pairing gaps in order to optimize the \( \eta_1 \) and \( \eta_2 \). The neutron and proton r.m.s. deviations are defined by

\[
\sigma_\tau = \left[ \frac{1}{N_\tau^{\text{exp}}} \sum_{\text{all data}} (\Delta_\tau - \Delta_\tau^{\text{exp}})^2 \right]^{1/2}.
\]

The total r.m.s. deviation is also given by

\[
\sigma_{\text{tot}} = \left[ \frac{N_n^{\text{exp}} \sigma_n^2 + N_p^{\text{exp}} \sigma_p^2}{N_n^{\text{exp}} + N_p^{\text{exp}}} \right]^{1/2}.
\]

Here \( N_\tau^{\text{exp}} \) is the number of existing data of \( \Delta_\tau^{\text{exp}} \) in the region of the present investigation; \( N_n^{\text{exp}} = 93 \) and \( N_p^{\text{exp}} = 84 \). The theoretical pairing gap is defined by \[41\] \[42\] \[43\]

\[
\Delta_\tau = -\int dr \tilde{\rho}_\tau(r) \tilde{h}_\tau(r) / \int dr \tilde{\rho}_\tau(r),
\]

where the local pairing potential is given by

\[
\tilde{h}_\tau(r) = \frac{\partial}{\partial \tilde{\rho}_\tau(r)} \int dr' H_{\text{pair}}(r') .
\]

We extract the coefficients \( C_\tau^{(i)} \) which represent the average \( \alpha \)-dependence of pairing gaps,

\[
\Delta_\tau(\alpha) = \left( C_\tau^{(0)} - C_\tau^{(1)} \alpha^2 \right) \Delta_\tau^{(A)},
\]

by \( \chi^2 \)-fitting analysis for \( \Delta_\tau \) of the 156 nuclei. Here \( \Delta_\tau^{(A)} \) is the same quantity determined for Eqs. [11] and [12].

For each set of \( (\eta_0, \eta_1, \eta_2) \), the strength \( V_0 \) is fixed so as to reproduce the \( \Delta_n^{\text{exp}} \) of 156Dy. We use the abbreviation \( V_0[\Delta_n^{156\text{Dy}}] \) for this choice. This nucleus has quadrupole deformation \( \beta \approx 0.28 \) [44]. The experimental

| \( E_{\text{cut}} \) | \( V_0[\Delta_n^{156\text{Dy}}] \) | \( \sigma_{\text{tot}} \) | \( \sigma_n \) | \( \sigma_p \) | \( C_n^{(0)} \) | \( C_n^{(1)} \) | \( C_p^{(0)} \) | \( C_p^{(1)} \) |
|---|---|---|---|---|---|---|---|---|
| 50 | -346.5 | 0.17 | 0.16 | 0.17 | 1.08 | 9.42 | 1.00 | 8.13 |
| 75 | -320.0 | 0.17 | 0.16 | 0.18 | 1.07 | 9.26 | 1.01 | 8.44 |

TABLE I: The cutoff quasiparticle energy \( E_{\text{cut}} \) dependence of the r.m.s. deviations [MeV] and the coefficients \( C_\tau^{(i)} \) are listed. The parameters \( (\eta_0, \eta_1, \eta_2) = (0.5, 0.2, 2.5) \) are fixed. The strength \( V_0 \) [MeV fm\(^{-3}\)] is constrained by the \( \Delta_n^{\text{exp}} \) of \( ^{156}\text{Dy} \).

FIG. 2: (Color online) Neutron and proton pairing gaps obtained with \( \eta_0 = 0.5 \) and \( \eta_1 = \eta_2 = 0 \) are plotted as a function of \( \alpha \). The pairing gaps are divided by \( \Delta_\tau^{(A)} \). The \( ^{40}\text{Nd} \) and \( ^{70}\text{Yb} \) isotopes possessing the large proton shell gaps are indicated by circles with horizontal and vertical bars respectively in the bottom panel.

pairing gaps are \( \Delta_n^{\text{exp}} = 1.17 \) MeV and \( \Delta_p^{\text{exp}} = 0.98 \) MeV, which are close to \( \Delta_n^{\text{exp}}(\alpha) = 1.04 \) MeV and \( \Delta_p^{\text{exp}}(\alpha) = 0.96 \) MeV estimated by Eqs. [11] and [12]. The justification of \( V_0 \) will be discussed in Sec. [VII].

The cutoff quasiparticle energy \( E_{\text{cut}} = 50 \) MeV is fixed in this paper. We checked the dependence of \( \sigma_\tau \) and \( C_\tau^{(i)} \) on the \( E_{\text{cut}} \) in Table II. The results with \( E_{\text{cut}} = 50 \) and 75 MeV agree within a few percent accuracy. Here the parameters of the pair DF are fixed to be \( (\eta_0, \eta_1, \eta_2) = (0.5, 0.2, 2.5) \), which are the optimal choice (See Sec. [V]).
The ∆ and C gap in weak pairing region. Actually, it would be than the particle number projection (PNP). The improvement approximation [45], and can be overcome by performing efficient \( \rho \). We show the drawback of the pair-DF without the terms. The pairing gaps obtained with \( \eta_0 = 0.5, \eta_1 = \eta_2 = 0 \) and \( \eta_1(\eta_0, \eta_2) \) is compared. Here \( \eta_1(\eta_0, \eta_2) \) is the value of \( \eta_1 \) minimizing \( \sigma_{\text{tot}} \) for each \( (\eta_0, \eta_2) \) with \( V_0[\Delta_n(156\text{Dy})] \).

IV. PAIR-DF WITHOUT \( \rho_1 \) TERM

We show the drawback of the pair-DF without the \( \rho_1 \) terms. The pairing gaps obtained with \( \eta_0 = 0.5, \eta_1 = \eta_2 = 0 \), and the strength \( V_0[\Delta_n(156\text{Dy})] = -324.0 \) MeV fm\(^{-3} \) are plotted in Fig. 2. The extracted \( C_r^{(0)} \) and \( C_r^{(1)} \) are shown by the dashed lines in Figs. 3 and 4. The \( \Delta_n \) and \( \Delta_p \) are almost \( \alpha \)-independent. The coefficient \( C_{\phi}^{(1)} \) is 1.11 which is much smaller than the experimental value \( C_{\phi,\exp} = 7.74 \). Although the \( C_{\phi}^{(1)} \) is larger than \( C_{\phi}^{(1)} = 1.11 \), this is due to the collapse of the pairing gap in weak pairing region. Actually, it would be \( C_{\phi}^{(1)} = 1.38 \) if we restrict the data to \( \Delta_p > 0.25 \) MeV. Here the \( \text{isoNd} \) and \( \text{isoYb} \) isotopes possessing the large proton shell gaps are indicated by circles with horizontal and vertical bars respectively in the bottom panel of Fig. 2. The collapse of \( \Delta_p \) is a drawback of the mean-field approximation [43], and can be overcome by performing the particle number projection (PNP). The improvement for the \( C_{\phi}^{(1)} \) values, however, cannot be expected by the PNP procedure [46], because the PNP method does not have any specific isovector effect. Therefore, we neglect the effect of PNP in this study.

The \( C_{\phi}^{(0)} = 0.84 \) is smaller than \( C_{\phi,\exp} = 1 \). The \( C_{\phi}^{(0)} = 0.67 \) is smaller than \( C_{\phi}^{(0)} \) due to the quenching of \( \Delta_p \) attributed to the neutron skin effect [24]: The neutron skin reduces the overlap between the form factor \( [1 - \eta_0 \rho(r)/\rho_0] \) and \( \tilde{\rho}_p(r) \) in Eq. (3).

The quenching of \( \Delta_p \) due to the neutron skin effect becomes stronger with larger \( \eta_0 \) [24]. The \( \sigma_p \) is shown as a function of \( \eta_0 \) by the dashed line in Fig. 5. Because the \( \sigma_p \) rapidly increases with \( \eta_0 \), the minimum of \( \sigma_{\text{tot}} \) is absent. In addition, the \( C_r^{(0)} \) and \( C_r^{(1)} \) remain small if restricted to \( \eta_1 = \eta_2 = 0 \) (See Figs. 3 and 4).

V. ROLE OF \( \rho_1 \) DEPENDENCE

It is possible to compensate the quenching of \( \Delta_p \) by using a stronger pairing strength for proton (for example, Ref. [48, 55, 56]). However it violates the charge symme-
try of the pair-DF. This is the important symmetry in the theoretical framework, and indispensable for global description of pairing properties from neutron to proton drip line.

This consideration leads to introduction of the linear $\rho_1$ term in Eq. (4). This pair-DF preserves the charge symmetry. The $\rho_1$ term induces the difference of the neutron and proton pairing strengths automatically \[24\]. The $\sigma_p$ has the minimum value at $\eta_1 = 0.15$, while the $\sigma_n$ is almost constant as a function of $\eta_1$. This is shown by the dashed lines in Fig. 8. We obtain the $C_n^{(0)} = 0.93$ and $C_p^{(0)} = 0.83$ with $\eta_1 = 0.15$ and $\eta_2 = 0$, which are better than those with $\eta_1 = \eta_2 = 0$. However, the $C_n^{(1)} = 3.75$ and $C_p^{(1)} = 1.89$ at $\eta_1 = 0.15$ do not improve as a function of $\eta_1$.

The quadratic $\rho_1$ term in the pair-DF improves the r.m.s. deviations. To see this, the r.m.s. deviations are plotted as a function of $\eta_1$ while keeping $\eta_2 = 2.5$ in Fig. 6. Those with $V_{\text{opt}}(\text{def})$, $V_{\text{opt}}(\text{sph})$, $V_0[\Delta_{\text{n}}(\text{156Dy})]$, and $V_0[\Delta_{\text{n}}(\text{120Sn})]$ are compared. The experimental values of $C_r^{(i)}$ are also listed.

| criterion | $V_0$ | $\sigma_{\text{tot}}$ | $\sigma_n$ | $\sigma_p$ | $C_n^{(0)}$ | $C_n^{(1)}$ | $C_p^{(0)}$ | $C_p^{(1)}$ |
|-----------|-------|-----------------------|------------|------------|-------------|-------------|-------------|-------------|
| $V_{\text{opt}}(\text{def})$ | -344.0 | 0.16 0.14 0.18 | 0.93 0.97 0.99 | 0.74 0.76 0.78 | 1.03 0.98 0.99 | 1.00 1.00 1.00 | 0.52 0.52 0.52 | 6.62 6.62 6.62 |
| $V_{\text{opt}}(\text{sph})$ | -308.0 | 0.50 0.47 0.52 | 0.91 0.92 0.93 | 0.97 0.97 0.97 | 0.50 0.50 0.50 | 0.50 0.50 0.50 | 4.62 4.62 4.62 |
| $V_0[\Delta_{\text{n}}(\text{156Dy})]$ | -346.5 | 0.17 0.16 0.17 | 0.92 0.93 0.94 | 0.91 0.91 0.91 | 1.08 1.08 1.08 | 1.00 1.00 1.00 | 0.52 0.52 0.52 | 6.62 6.62 6.62 |
| $V_0[\Delta_{\text{n}}(\text{120Sn})]$ | -322.0 | 0.34 0.30 0.37 | 0.90 0.91 0.92 | 0.89 0.89 0.89 | 0.76 0.76 0.76 | 0.76 0.76 0.76 | 6.11 6.11 6.11 |
| Exp | - | - | - | - | 1.00 1.00 1.00 | 6.25 6.25 6.25 | 8.25 8.25 8.25 |

The pairing gaps obtained with $(\eta_1, \eta_2) = (0.2, 2.5)$ are shown in Fig. 9. The r.m.s. deviations and the coef-
ficients $C^{(i)}_\tau$ are listed in Table III. We see the significant improvement compared to those with $\eta_1 = \eta_2 = 0$.

The optimized set of $(\eta_1, \eta_2)$ gives the justification of the mixed type pairing force $(\eta_0 = 0.5)$. The $\sigma_v$ with $\eta_2 = 2.5$ and $\eta_1(\eta_0, \eta_2)$ is shown as a function of $\eta_0$ by the solid line in Fig. 6. The improvement over the choice $\eta_1 = \eta_2 = 0$, especially the large reduction of $\sigma_v$, is obvious. Therefore, the minimum of $\sigma_{tot}$ can appear at $\eta_0 \approx 0.5$. Here $\eta_1(\eta_0, \eta_2)$ is the value of $\eta_1$ minimizing $\sigma_{tot}$ for each $(\eta_0, \eta_2)$ with $V_0[\Delta_n^{(156}\text{Dy}]$. The $\eta_1(\eta_0, \eta_2)$ at $\eta_2 = 2.5$ is shown as a function of $\eta_0$ in Fig. 6.

The coefficients $C^{(0)}_\tau$ and $C^{(1)}_\tau$ with $\eta_2 = 2.5$ and $\eta_1(\eta_0, \eta_2)$ are shown as a function of $\eta_0$ by the solid lines in Fig. 3 and 4. The $C^{(0)}_\tau$ is insensitive to $\eta_0$, while the $C^{(1)}_\tau$ becomes close to the experimental value at $\eta_0 \approx 0.5$.

VI. EFFECTIVE MASS AND $\rho_1$-DEPENDENCE OF PAIR-DF

A. Isoscalar and isovector effective masses

Pairing correlations are sensitive to the single-particle structure around the Fermi level. For a suggestive example, the pairing gap is a function of $gG$ and given by $\Delta \propto e^{-1/gG}$ for $gG \ll 1$ in the schematic model of the seniority pairing force with the strength $G$ and the uniform single-particle level density $g$. On the other hand, the effective mass has a strong influence on the single-particle energies. The average level density is proportional to the effective mass. Therefore, we expect the close connection between the effective mass and the pair-DF in order to reproduce the global trend of the experimental pairing gaps.

For the investigation, we extend our analysis with 13 Skyrme parametrizations; SKM* [3], SGII [4], LNS [17], SkP [18], BSk17 [49], SkT6 [50], SLy4, SLy5 [51], SkI1, SkI3, SkI4 [5], SkO, and SkO' [54].

$\eta_2 = 2.5$

SLy4

FIG. 10: (Color online) The value of $\eta_1$ minimizing the $\sigma_{tot}$ for each $(\eta_0, \eta_2)$ with $V_0[\Delta_n^{(156}\text{Dy}]$ is plotted as a function of $\eta_0$. The $\eta_2 = 2.5$ is fixed.

FIG. 11: (Color online) The strength $V_0$ reproducing the $\Delta_n^{(exp)}$ of $^{156}\text{Dy}$ for each Skyrme force is plotted in relation to $m^*_s/m$. The results with $\eta_2 = 2.5$ and the optimal $\eta_1$ in Table III are compared to those with $\eta_1 = \eta_2 = 0$. The $\eta_0 = 0.5$ is fixed.

The effective mass of the Skyrme force is given by

$$\frac{\hbar^2}{2m^*_s(r)} = \frac{\hbar^2}{2m} + b_1 \rho - b_1^* \rho_\tau \quad (10)$$

with $I(r) = \rho_1/\rho$ and $\Delta m_1(r) = m/m^*_s - m/m^*_v$. The isoscalar and isovector effective masses are defined by

$$\frac{m}{m^*_s(r)} = 1 + 2m/\hbar^2 \left( b_1 - b_1^* \right) \rho \quad (11)$$

$$\frac{m}{m^*_v(r)} = 1 + 2m/\hbar^2 b_1 \rho = 1 + \kappa. \quad (12)$$

The $m^*_s$ is directly connected to the enhancement factor $\kappa$ of the Thomas-Reiche-Kuhn sum rule [51]. We esti-
TABLE III: The parameter set of the optimal pair-DF for each Skyrme parameterization is listed. The optimal value of \( \eta_1 \) minimizing \( \sigma_{\text{tot}} \) with the strength \( V_0[\Delta m(156\text{Dy})] \) [MeV fm\(^{-3}\)] the r.m.s. deviations [MeV], and the coefficients \( C^{(1)}_0 \) are shown. The parameters \((\eta_0, \eta_2) = (0.5, 2.5)\) are fixed for them. The effective masses \( m^*_p \) and \( m^*_n \) at the saturation density of symmetric nuclear matter, the difference \( \Delta m_1 = m/m^*_n - m/m^*_p \), and the \( W_0/W_0' \) and \( \eta_1 \) of the spin-orbit potential are also listed.

![Graph](image-url)

FIG. 13: (Color online) The same with Fig. [12] but in relation to \( \Delta m_1 \).

The spin-orbit potential \( W_s(r) \) also has the \( \rho_1 \) dependence. The \( W_s(r) \) of Skyrme DF is defined by

\[
W_s(r) = \frac{1}{2} (W_0 \nabla \rho + W'_0 \nabla \rho_t) + \eta_1 W^{(1)}_s = \left( W_0 + \frac{W'_0}{4} \right) \nabla \rho + \frac{W'_0}{4} \nabla \rho_t + \eta_1 W^{(1)}_s
\]

where \( W^{(1)}_s(r) = C_0 J + \tau_1 C_1 J_1 \) with the parameter \( \eta_1 \) of either 0 or 1. The \( J \) (\( J_1 \)) is the isoscalar (isovector) spin-current density. The \( C_0 \) and \( C_1 \) are given by \( t_1, t_2, x_1 \) and \( x_2 \) of the Skyrme parameter [52]. Most Skyrme functionals have the spin-orbit terms with \( W_0 = W'_0 \). However, the SkI4, SkO, and SkO' have the generalized \( \rho_1 \) dependence by introducing the different strengths \( W_0 \) and \( W'_0 \). The Sk3 has \( W'_0 = 0 \).

We search the optimal value of \( \eta_1 \) which minimizes \( \sigma_{\text{tot}} \) under the conditions; 1) the fixed \((\eta_0, \eta_2) = (0.5, 2.5)\), and 2) the strength \( V_0 \) reproducing the \( \Delta m(156\text{Dy}) \). The numerical uncertainty is \( \delta \eta_1 = 0.025 \). The results are summarized in Table III.

The strengths \( V_0 \) reproducing the \( \Delta m(156\text{Dy}) \) are plotted in relation to \( m^*_s/m \) in Fig. [11]. For \( \eta_1 = \eta_2 = 0 \), the \( V_0 \) increases linearly. This trend is in agree with the general consideration that the pairing strength should be increased if the level density is low. The relation is given by \( V_0 = -505.05 + 264.47 m^*_s/m \text{ MeV fm}^{-3} \) with the correlation coefficient \( r = 0.99 \), except for SkT6 and SkI3 (See Appendix A for the procedure of the correlation analysis). In general, the linear correlation disappears with the \( \rho_1 \) terms due to the \( \eta_1 \) and \( \eta_2 \) dependence of \( V_0 \). However, it is interesting to mention that the linear correlation is recovered with \( \eta_2 = 2.5 \) and the optimal \( \eta_1 \). The extracted correlation is \( V_0 = -531.45 + 266.46 m^*_s/m \text{ MeV fm}^{-3} \) with \( r = 0.99 \).

The optimal values of \( \eta_1 \) are shown in relation to \( m/m^*_v \) in Fig. [12]. The linear correlation between \( \eta_1 \) and \( m/m^*_v \) is obvious, irrespective of the choice of \( W_0 \) and \( \eta_1 \). The extracted relation is given by

\[
\eta_1 = -0.340 + 0.464 m / m^*_v, \tag{16}
\]

or, in terms of the enhancement factor

\[
\eta_1 = 0.124 + 0.464 \kappa, \tag{17}
\]
except for SkI3 and SkT6. The correlation coefficient between $\eta_1$ and $m/m^*_n$ is $r = 0.85$. This indicates that these parameters is almost linearly dependent. The possible reason for the deviation of SkI3 and SkT6 is the special assumption on the Skyrme DF. The SkT6 sets $m^*_n = m^*_p = m$ by definition. The SkI3 neglects the $\rho_1$ term in the spin-orbit potential by setting $W'_\rho = 0$.

During the optimization of the pair-DF, the $\eta_2 = 2.5$ for SLy4 is used for other Skyrme parameters to avoid the huge computational task. However, the improvement obtained by the optimization of the parameter $\eta_2$ should be small. The effect can be estimated as follows: We define the r.m.s. deviation of $C^{(1)}$ by

$$\Delta C^{(1)} = \sqrt{\langle (C^{(1)}_{\tau, \exp} - C^{(1)}_{\tau, \text{opt}})^2 \rangle}.$$  

Here $C^{(1)}_{\tau, \text{exp}}$ is the experimental value of Eqs. (1) and (2). The $\Delta C^{(1)} = 1.5$ is obtained by taking the average $<>$ over $\tau = n, p$ and the 13 Skyrme parameters. If the linearity $\Delta \eta_2 \approx \Delta C^{(1)}/2.3$ of Fig. 8 and the parabolic approximation for $\sigma_{\text{tot}}$ as a function of $\eta_2$ from Fig. 4 are assumed for the other Skyrme parameters, the expected improvement for $\sigma_{\text{tot}}$ is about 0.002 MeV. In addition, we will show that the difference in the pairing gaps for different Skyrme forces is small if the pair-DF with $\eta_2 = 2.5$ and the optimal $\eta_1$ is used in Sec. VII.

From the present analysis, we conclude that the pair-DF should include the $\rho_1$ dependence in order to take into account the effect of the $m^*_n$ and $m^*_p$ for the global description of pairing correlations.

**B. $\Delta m_1$ dependence**

The effective masses $m^*_n$ and $m^*_p$ have strong correlation with the $V_0$ and $\eta_1$ of the pair DF respectively. On the other hand, the splitting of neutron and proton effective masses directly depends on the local asymmetry parameter $I(r)$ through the combination of $m^*_n$ and $m^*_p$: $\Delta m_1 = m^*_n - m^*_p$. If $\Delta m_1$ is negative, the $m^*_p$ ($m^*_n$) is a decreasing (increasing) function of $I$. In order to compensate the effect, the larger $\eta_1$ is necessary so as reproduce the same magnitude of the $\Delta_{\rho}^{(\text{exp})}(\alpha)$ and $\Delta_{\rho}^{(\text{exp})}(\alpha)$ (See Eqs. (1) and (2)). On the other hand, the smaller $\eta_1$ is required for the positive $\Delta m_1$.

This correlation can be seen in Fig. 13. The extracted correlation is

$$\eta_1 = 0.261 - 0.193\Delta m_1$$  

with $r = -0.63$, except for SkT6 and SkI3. Although this correlation is weaker than that between $\eta_1$ and $m/m^*_n$ due to the scattering of the $m^*_n/m$ value, it is meaningful to conclude the linear dependence between $\eta_1$ and $\Delta m_1$. The $\eta_1 \approx 0.26$ at $\Delta m_1 \approx 0$ can be the rough estimation of the $\eta_1$ compensating the artificial $\Delta_{\rho}$ suppression due to the neutron skin effect.

**VII. CHOICE OF $V_0$**

It is desirable to optimize the strength $V_0$ for experimental data in wide region of nuclear chart. However, the procedure demands heavy computational efforts. Therefore the $V_0$ is usually fixed so as to reproduce a pairing gap of specific nucleus. Several authors adopted the $\Delta_n^{(\text{exp})}$ of $^{120}$Sn [46, 53, 54]. The strength $V_0[\Delta_n^{(120\text{Sn})}] = -322.0$ MeV fm$^{-3}$ with SLy4 force and $(\eta_1, \eta_2) = (0.2, 2.5)$ gives $\epsilon_{\text{tot}} = 0.34$ MeV (see Table III). On the other hand, if the $V_0$ is fixed in deformed region, for example, $V_0[\Delta_n^{(156\text{Dy})}] = -346.5$ MeV fm$^{-3}$...
FIG. 16: (Color online) The same with Fig. 15 but for the proton pairing gaps of \( N = 50 \) and 82 isotones.

FIG. 17: (Color online) The difference in the pairing gaps for the different Skyrme parameters. See text for details.

the r.m.s. deviation reduces to \( \sigma_{\text{tot}} = 0.17 \text{ MeV} \). The \( V_0 \) dependence of the \( \sigma_{\text{tot}} \) is shown in Fig. 14. The optimal value \( V_{\text{opt}} \text{(def)} = -344.0 \text{ MeV fm}^{-3} \) for the deformed nuclei is close to the \( V_0[\Delta_n^{(156\text{Dy})}] \).

In Figs. 15 and 16, the \( \Delta_n \) of Sn and Pb isotopes and the \( \Delta_p \) of \( N = 50 \) and 82 isotones obtained with SLy4 force and \( (\eta_1, \eta_2) = (0.2, 2.5) \) are shown. The results with \( V_{\text{opt}} \text{(def)} \), \( V_0[\Delta_n^{(156\text{Dy})}], V_0[\Delta_n^{(120\text{Sn})}] \) are compared. The difference of the results with \( V_{\text{opt}} \text{(def)} \) and \( V_0[\Delta_n^{(156\text{Dy})}] \) is negligible along the isotopic and isotonic chains. However, the choice of \( V_0[\Delta_n^{(156\text{Dy})}] \) overestimates the experimental pairing gaps \( \Delta_p^{(\exp)}(A) \) in these spherical nuclei. The strength optimized only for the spherical nuclei \( V_{\text{opt}} \text{(sph)} = -308.0 \text{ MeV fm}^{-3} \) is 10.4 % weaker than \( V_{\text{opt}} \text{(def)} \).

It is an open problem to construct the pair-DF which allows us to describe the pairing properties along the chains of semi-magic nuclei at the same quality achieved for deformed region. The authors of Ref. 52 considered that the overestimation in spherical nuclei may be partly attributed to the effect of the particle number fluctuation. They showed that the HFB calculation with the approximate particle number projection using the Lipkin-Nogami method improves the agreement with experiment for spherical nuclei. We do not discuss this point further in detail, and the choice of \( V_0[\Delta_n^{(156\text{Dy})}] \) is employed in this work.

The strengths \( V_0 \) for other Skyrme parameters are also determined by the same procedure. The \( \sigma_{\text{tot}} \) with the choice of \( V_0[\Delta_n^{(156\text{Dy})}] \) is almost the same quality compared to SLy4 (see Table III). In Fig. 17, the \( \Delta_n/\Delta_n^{(A)} \) of Sn and Pb isotopes and the \( \Delta_p/\Delta_p^{(A)} \) of \( N = 50 \) and 82 isotones obtained with Skyrme BSk17, LNS and SkM* are shown. The \( \eta_1 \) and \( V_0[\Delta_n^{(156\text{Dy})}] \) in Table III are used for the Skyrme forces. For comparison, the value obtained with the SLy4 force is subtracted:

\[
\delta(\Delta_p/\Delta_p^{(A)})(X) = \Delta_p/\Delta_p^{(A)}(X) - \Delta_p/\Delta_p^{(A)}(\text{SLy4})
\]

for \( X = \text{BSk17}, \text{LNS} \) and \( \text{SkM}^* \). Their \( \Delta m_1, m^*_e/m \) are \((0.190, 0.800), (0.028, 0.780), (0.164, 0.727), \) and \((-0.262, 0.653) \) for SLy4, BSk17, LNS, and \( \text{SkM}^* \) respectively. The \( \sigma_{\text{tot}} \) of the BSk17 is smallest, and the \( \kappa \) of \( \text{SkM}^* \) is largest in this work. The LNS parametrization was built to match the \( \ell \) dependence of the effective masses and the neutron matter EOS predicted by Brückner-Hartree-Fock calculation.

In spite of the variety of \( \Delta m_1 \) and \( m^*_e/m \), the \( \delta(\Delta_p/\Delta_p^{(A)}) \) is small along the isotopic and isotonic chains, except for around the subshell closure: \( N = 90 \) for \( \Delta_n \), and \( Z = 38 \) and 40 for \( \Delta_p \). This is because the pairing correlations are sensitive to the single-particle structure around the subshell closure.

The small \( \delta(\Delta_n/\Delta_n^{(A)}) \) can be expected due to the weak sensitivity of \( \sigma_{\eta_1} \) to \( \eta_1 \) if the strength \( V_0 \) is constrained by \( \Delta_n^{(\exp)} \) of a specific nucleus. This is seen in Fig. 6. Authors of Ref. 58 also pointed out that the \( \Delta_n \) of Sn and Pb isotope chains are insensitive to \( \Delta m_1 \) by performing the HFB calculation with the mixed type pairing force and various Skyrme forces. On the other hand, the fine tuning of \( \eta_1 \) is indispensable for the small \( \delta(\Delta_p/\Delta_p^{(A)}) \) due to the sensitivity of \( \sigma_{\eta_1} \) to \( \eta_1 \). This is shown in Fig. 6 and discussed in Ref. 24.

The \( \eta_2 = 2.5 \) for SLy4 is commonly used for other Skyrme parameters (see Sec. VII). This is an approximation in our analysis. However, the small \( \delta(\Delta_p/\Delta_p^{(A)}) \) as a function \( \alpha \) means that the difference in the \( \alpha \) dependence of the pairing gaps due to the different Skyrme forces can be small with the fixed \( \eta_2 = 2.5 \).

We refer the pair-DF with the parameters in Table III as the optimal one for each Skyrme parameterization. The optimal pair-DF with \( \rho_1 \) dependence is constructed aiming at unique description of pairing properties toward
the neutron drip line. Our prescription is based on the phenomenological considerations. In this sense, our conclusion is tentative. However, the optimal pair-DF can preserves the good descriptive power of the neutron excess dependence of pairing correlations, and provide the certain foundation for the further improvement with experimental data of nuclei with larger neutron excess.

VIII. CONCLUSION

We proposed a new pair-DF by introducing the \( \rho_1 \) dependence. We emphasized the necessity of both the linear and quadratic \( \rho_1 \) terms in the pair-DF for the global description of pairing correlations; namely the dependence on both the mass number \( A \) and the neutron excess \( \alpha = (N - Z)/A \).

To optimize the parameters in the pair-DF, we performed the HFB calculation for 156 nuclei of \( A = 118 \) – 196 and \( \alpha < 0.25 \). By the extensive investigation with 13 Skyrme parameterizations, we clarify that the pair-DF should include the \( \rho_1 \) dependence in order to take into account the effect of the \( m_1^* \) and \( m_2^* \) in the p-h channel: The \( \eta_1 \) and \( m/m_1^* \) is linearly dependent, and the pairing strength \( V_0 \) linearly increases as a function of \( m_2^*/m \) with the optimal set of \((\eta_0, \eta_1, \eta_2)\). The relationship between the optimal \( \eta_1 \) and the splitting of the neutron and proton effective masses is also discussed. The \( V_0 \) is fixed so as reproduce the \( \Delta (\exp) \) of \( ^{156}\text{Dy} \). With this choice, we can obtain the almost minimum value of the total r.m.s. deviation between the experimental and calculated pairing gaps. The different Skyrme forces with the optimal pair-DF can give the small difference in the pairing gaps toward the neutron drip line.

In this paper, we concentrated on the analysis of pairing gaps in finite nuclei based on the phenomenological consideration. To obtain the deeper insight to the \( \rho_1 \) terms in the pair-DF, it is interesting to investigate pairing correlations in asymmetric nuclear matter by comparing the up-to-date calculations with 3-body force and correlations beyond the mean-field approximation. This analysis is a future subject.

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APPENDIX A: CORRELATION ANALYSIS

We introduce the correlation coefficient \( r \) for a data set 
\[ \{(x_i, y_i)\} \quad (i = 1, 2, \cdots, n) \]
It is defined by
\[
r = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2} \sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}}.
\]

The coefficient \( r \) can take a real value of \(-1 \leq r \leq 1\). In the limit of \( r = 1 \) or \(-1\), the data set is linearly dependent. On the other hand, the correlation between \( x \) and \( y \) is weak if \( r \) is close to zero.

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