Deuteron correlation energy (DCE) of the valence proton-neutron subsystem is evaluated by utilizing a simple three-body model. We focus on the $^6$Li and $^{18}$F nuclei assuming the doubly-closed core and the valence proton and neutron. Two interaction models, schematic density-dependent contact (SDDC) and Minnesota potentials, are utilized to describe the proton-neutron interaction. Evaluating DCE, we conclude that the proton-neutron binding in $^6$Li can be stronger than its counterpart in a deuteron in vacuum. On the other hand, in $^{18}$F, the energetic correlation is remarkably weak, and does not favor the bound, deuteron-like configuration. This significant difference between two systems can be understood from a competition between the proton-neutron kinetic and pairing energies, which are sensitive to the spatial extension of the wave function. This result indicates a remarkable dependence of the deuteron correlation to its environment and the valence orbits.

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I. INTRODUCTION

Deuteron ($J^e = 1^+, S = 1$) is the only possible bound system of two nucleons in vacuum. This common sentence in nuclear physics indicates that, in the spin-triplet (isospin-singlet) channel, nuclear attraction is stronger than that in the spin-singlet (isospin-triplet) channel. In spite of this unique importance, the spin-triplet proton-neutron ($pn$) subsystem in finite nuclei has been less investigated than the spin-singlet pair of the same type of nucleons.

Thanks to the recent developments of radioactive isotope-beam experiments, the access to the spin-triplet ($pn$) pairing correlation in $N = Z$ nuclei is getting possible. In these nuclei, in which the valence proton and neutron occupy the same major shell, $pn$ correlation is expected to be very relevant. Comparing this proton-neutron subsystem with that in vacuum, a natural question arises: “Does a proton-neutron pair at the surface of the nucleus behave like a deuteron?”

The answer to the previous question is, however, not simple to address. In recent theoretical studies, it has been shown that the spin-orbit splitting is a key feature of the deuteron correlation in nuclei. Utilizing the labels, $j_\pm \equiv l \pm 1/2$ to indicate the spin-orbit partners in the same shell, the $pn$ correlation becomes enhanced when the energy gap between $j_+$ and $j_-$ is small. Indeed, a strong spin-triplet $pn$ coupling, possibly with spatial localization that indicates a sort of deuteron condensation at the surface of the nucleus, has been predicted. In Ref. [19], the importance of mixing with continuum states in the $pn$ correlation was also shown. The quasi-deuteron configuration, as well as the isospin-singlet condensate, in heavy nuclei have been discussed with similar intents. It is worthwhile to remind that a similar discussion on the spin-singlet dineutron and diproton correlation has been also carried out.

In spite of all the accumulated knowledge, it is still an open question whether the $pn$ pair can be considered as bound or not in finite nuclei. Especially, its dependence on the selected orbit(s) or on the stability of the whole system has not been clarified as yet. This information should be essential also for the phenomenology of the Gamow-Teller transition, nuclear magnetic mode, and meta-stable states.

In this article, we present a phenomenological evaluation of the so-called deuteron-correlation energy (DCE). We also investigate its sensitivity to the properties of finite nuclei by comparing two systems: $^6$Li and $^{18}$F.

Concerning the first topic, we employ core-orbital three-body model, assuming a doubly-closed core plus the valence proton and neutron. Then, we evaluate the mean energy of the partial $pn$ Hamiltonian, which can be well separated from the total energy. An advantage of our definition of DCE is that it becomes equivalent to the deuteron binding energy, if the $pn$ subsystem is isolated. Thus, it gives us direct information on the changes that appear in finite systems with respect to the counterpart in vacuum.

For the second topic, we discuss the deuteron correlation in valence orbits in light $N = Z$ nuclei, $^6$Li and $^{18}$F. By evaluating DCE in three-body systems, we can investigate the sensitivity of deuteron-like subsystem to its environment. Here we point out a qualitative difference between these two systems: in $^{18}$F, the $A = 17$ core-nucleon subsystem are bound, whereas this is not the case for the $A = 5$ subsystems of $^6$Li. Thus, it is suitable to compare the deuteron correlation in systems where it is strongly or weakly bound. We also discuss the reliability of several interaction models, which play an essential role in the deuteron correlation problem. For simplicity, in this article, we utilize only the two-body interactions.
which should be tuned for each subsystem. 

In Sec. II the formalism of our three-body model is presented. Our results and discussion for $^6$Li are also summarized there. Section III is devoted to $^{18}$F, with a comparison to $^6$Li. Finally, in Sec. IV we summarize the main points of this article, as well as the possible improvements for future studies.

II. $^6$LI NUCLEUS

A. Three-Body Model

Our investigation starts with the $^6$Li nucleus, employing the core-orbital coordinates, $\{r_p, r_n\}$, for the three-body system, $\alpha + p + n$. The detailed formalism of these coordinates is summarized in Appendix. Within this framework, our three-body Hamiltonian is given as,

\[ H_{3b} = h_p + h_n + x_{\text{rec}} + v_{p-n}(r_p, r_n), \]

\[ h_i = \frac{p_i^2}{2\mu_i} + V_{c-i}(r_i), \]

\[ x_{\text{rec}} = \frac{p_p \cdot p_n}{m_c} \quad \text{(recoil term)}, \]

where $i = p$ and $n$ for the valence proton and neutron, respectively. Here, $r_i$ is the relative coordinate between the core and the $i$-th nucleon. Mass parameters are fixed as follows: $\mu_i = m_i m_c/(m_i + m_c)$, $m_p = 938.272$ MeV/$c^2$, $m_n = 939.565$ MeV/$c^2$, and $m_c = 3727.379$ MeV/$c^2$ (a-particle mass). Namely, $h_i$ is the single particle (s.p.) Hamiltonian between the core and the $i$-th nucleon.

The core-nucleon potential is taken as

\[ V_{c-i}(r_i) = V_{WS}(r_i) + V_{\text{Coul}}(r_i)\delta_{i,p}, \]

where the Coulomb potential of an uniformly charged sphere with radius $R_0$ is included for the core-proton subsystem only. For nuclear force, a Woods-Saxon plus spin-orbit potential is employed as

\[ V_{WS}(r) = V_0 f(r) + U_{ls}(l \cdot s)\frac{1}{r} \frac{df(r)}{dr}, \quad (3) \]

\[ f(r) = \frac{1}{1 + e(r-R_0)/a_0}, \quad (4) \]

where $f(r)$ is a standard Fermi profile. In this paper, we adopt the parameters as $R_0 = r_0 \cdot 4^{1/3}$, $r_0 = 1.25$ fm, $a_0 = 0.65$ fm, $V_0 = -47.4$ MeV, and $U_{ls} = -0.4992 V_0 r_0^2$ [36, 44]. From phase-shift analysis, we confirmed that this parameter set fairly reproduces the empirical $\alpha - n$ and $\alpha - p$ scattering data in the $(p_3/2)$-channel [15, 47], as summarized in Table I.

We expand the relevant $pn$-states on an uncorrelated basis, that is the tensor product of proton and neutron states:

\[ |\Phi_{\kappa\lambda}^{m,J,\pi}(\rho,\sigma)\rangle = |\phi_{\kappa}^{m}(\rho)\rangle \otimes |\phi_{\lambda}^{n}(\sigma)\rangle, \quad (5) \]

where $\kappa$ is the shorthand label for all the quantum numbers of the proton states, $\{n_p, l_p, p_p, m_p\}$, and similarly with $\lambda$ for neutron states. Those include the radial quantum number $n$, the orbital angular momentum $l$, the spin-coupled angular momentum $j$ and the magnetic quantum number $m$. Each s.p. state satisfies,

\[ h_p \phi_{\kappa}^{m}(\rho_p) = E_{\kappa} \phi_{\kappa}^{m}(\rho_p), \]

\[ h_n \phi_{\lambda}^{n}(\rho_n) = E_{\lambda} \phi_{\lambda}^{n}(\rho_n), \quad (6) \]

where $E_{\kappa,\lambda}$ is the single-proton (neutron) eigen-energy. Notice that these states describe the $A = 5$ unbound systems, $^5$Li and $^5$He. We employ the s.p. states up to the $(h_{11/2}, g_{9/2})$-channel ($l_{\text{max}} = 5$). We confirmed that this truncation provides a sufficient convergence of the ground state energy of $^6$Li. In order to take into account the Pauli principle, we exclude the first $(s_{1/2})$ state occupied by the core nucleus. The continuum s.p. states are discretized in the radial box of $R_{\text{box}} = 20$ fm. We also fix the energy cut-off, $E_{\text{cut}} = 15$ MeV, in this article. Because we limit our investigation to the low-energy region only, this truncation of core nucleon space indeed provides a sufficient convergence for our results.

### Table I: Resonance energy and width obtained with the alpha-nucleon potential. Those are evaluated from the scattering phase-shift in the $(p_3/2)$-channel.

|           | $E_{\alpha-n}$ (MeV) | $\Gamma_{\alpha-n}$ (MeV) | $E_{\alpha-p}$ (MeV) | $\Gamma_{\alpha-p}$ (MeV) |
|-----------|---------------------|---------------------|---------------------|---------------------|
| This work | $-47.4$             | $0.77, 0.67$        | $1.61, 1.31$        |                     |
|           | $-49.0$             | $0.54, 0.38$        | $1.37, 0.94$        |                     |
| Exp. [45] | $0.89, 0.60$        | $1.97, (\simeq 1.5)$|                     |                     |
| Exp. [46] | $0.798, 0.578$      | $1.69, 1.06$        |                     |                     |
| Exp. [47] | $0.735, 0.60$       | $1.96(5), (\simeq 1.5)$|                     |                     |
B. Proton-Neutron Interactions

1. Schematic Density-Dependent Contact Interaction

For \( pn \) subsystem, we employ two simple interaction models in this article. Our first choice is the so-called schematic density-dependent contact (SDDC) potential \([17, 19]\). That is,

\[
v_{p-n}(r_p, r_n) = w \left( \frac{r_p + r_n}{2} \right) \cdot \delta(r_p - r_n),
\]

\[
w(r) = w_0 \left[ 1 - \eta f(r) \right],
\]

where \( \eta \) is an adjustment parameter. We utilize the same density profile, \( f(r) \), in Eqs. (3) and (7), in order to take the schematic density-dependence into account. Notice that \( w(r \to 0) = w_0 \) for an isolated proton-neutron pair from the core. Thus, its bare strength, \( w_0 \), should be determined consistently to the energy cutoff, \( E_{\text{cut}} \), and the vacuum scattering length, \( a^{(S)}_v \) \([44, 48]\):

\[
a^{(S)}_v = \left[ \frac{2k_{\text{cut}}}{\pi} + 4\pi \frac{h^2}{2\mu_{p-n}w_0^{(S)}} \right]^{-1} \text{(fm)},
\]

or equivalently,

\[
w_0^{(S)} = \frac{h^2}{2\mu_{p-n}} \cdot \frac{4\pi^2a_v^{(S)}}{\pi - 2a_v^{(S)}k_{\text{cut}}} \text{(MeV} \cdot \text{fm}^3),
\]

where \( \mu_{p-n} = m_p m_n / (m_p + m_n) \) and \( k_{\text{cut}} = \sqrt{2\mu_{p-n}E_{\text{cut}}}/\hbar \). The superscripts \( S = 0 \) and 1 indicate the spin-singlet and triplet channels, respectively.

In Fig. 2, the relationship between the bare contact strength and the vacuum scattering length is presented. Empirical values are \( a^{(S=0)}_v = -23.748 \text{ fm} \) and \( a^{(S=1)}_v = 5.424 \text{ fm} \) for the spin-singlet and triplet channels, respectively \([49, 50]\). Since neutron and proton can become bound in the spin-triplet channel, \( a^{(1)}_v \) is positive finite, and its corresponding bare strength, \( w_0 \simeq -2600 \text{ MeV} \cdot \text{fm}^3 \) for \( E_{\text{cut}} = 15 \text{ MeV} \), provides a strong attraction in vacuum. On the other hand, in the spin-singlet channel, \( a^{(0)}_v \) stays negative and the pairing attraction is incapable to bind the \( pn \) system.

In this article, we only deal with the \( J^\pi = 1^+ \) configuration. Thus, from angular momentum algebra, the spin-singlet component of the \( pn \)-interaction can be neglected \([17]\).

2. Minnesota Interaction

As our second option, we employ the spin-triplet Minnesota potential for the \( pn \) subsystem \([32, 51, 52]\). Using the spin-triplet projection, \( \hat{P}_{S=1} \), that is,

\[
v_{p-n}(r_p, r_n) = V^{(S=1)}_{\text{Min}}(|r_p - r_n|)\hat{P}_{S=1},
\]

\[
V^{(S=1)}_{\text{Min}}(r) = \frac{V_r e^{-K_r r^2}}{r^2} + \frac{V_t e^{-K_t r^2}}{r^2},
\]

where \( V_r = 200 \text{ MeV}, V_t = -178 \text{ MeV}, K_r = 1.487 \text{ fm}^{-2} \) and \( K_t = 0.639 \text{ fm}^{-2} \) \([53]\). This potential correctly reproduces the deuteron binding energy, \( \simeq 2.2 \text{ MeV} \), for the isolated \( pn \) system.

C. Ground State of \( ^6\text{Li} \)

We solve the ground state (g.s.) of \( ^6\text{Li} \) by diagonalizing the three-body Hamiltonian. This leads to the solution,

\[
\Psi_{g.s.}(r_p, r_n) = \sum_M U_M \Phi^{(1,+)}_M(r_p, r_n),
\]

with expansion coefficients, \( \{ U_M \} \). Here \( M = \{ \kappa, \lambda \} \) is the simplified label for the uncorrelated basis. In our computation, \( M_{\text{max}} \simeq 200 \) basis states are employed.

From experimental data \([43, 47]\), the three-body separation energy is,

\[
S_{pn}(^6\text{Li}) = S_d(^6\text{Li}) + S_d(^d) ,
\]

or equivalently,

\[
= S_n(^6\text{Li}) + S_p(^5\text{Li}) \simeq 3.70 \text{ (MeV)}. \]

In order to reproduce this empirical energy, we employ \( \eta = 1.27 \) for the SDDC potential in Eq. (7).

With the Minnesota potential, on the other hand, its original parameters fail to reproduce the empirical energy, with a positive deviation of almost 1 MeV. Namely, for the fitting, we need an enhancement of the \( pn \) attraction. Thus, in addition, we repeat the same calculation but with the enhancement factor, \( f = 1.13 \). That is,

\[
v_{p-n}(r_p, r_n) = f \cdot V^{(S=1)}_{\text{Min}}(|r_p - r_n|)\hat{P}_{S=1}.
\]
TABLE II. Ground state of $^6$Li (1$^+$) obtained with several pn-interaction models. The empirical three-body binding energy is $E_{3b} = -S_{3b}(^6\text{Li}) = -3.70$ MeV. The 4 major configurations are also tabulated: $\pi$ and $\nu$ indicate the $\alpha$-proton and $\alpha$-neutron orbits, respectively. $E_c(d)$ is the two-body binding energy of deuteron in vacuum, obtained with the Minnesota potential. For other quantities, see text for details.

| Type of $v_{p-n}$ | Label | Li-S | Li-S2 | Li-SCC with $f(r)$ of $\alpha$ | Li-MO | Li-MF | Li-MO2 |
|-------------------|-------|------|-------|--------------------------------|-------|-------|-------|
| Adjustment of $v_{p-n}$ | $\eta = 1.27$ | $\eta = 1.44$ | $f = 1$ | $f = 1.13$ | $f = 1$ |
| $E_c(d)$ (MeV) | $E_c(d)$ | $a_v^{(S=1)}(5.424$ fm) | $-2.22$ | $-4.07$ | $-2.22$ |
| $V_0$ of WS Pot. (MeV) | -47.4 | -49.0 | -47.4 | -47.4 | -49.0 |
| $E_{3b} = \langle H_{3b} \rangle$ (MeV) | -3.70 | -3.70 | -2.69 | -3.70 | -3.64 |
| $\langle v_{p-n} \rangle$ (MeV) | -8.96 | -8.22 | -7.65 | -8.91 | -8.17 |
| $\langle x_{sec} \rangle$ (MeV) | -0.44 | -0.44 | -0.38 | -0.37 | -0.34 |
| $\langle \theta_{pn} \rangle$ (deg) | 83.9 | 83.8 | 84.6 | 85.2 | 85.9 |
| $\pi(p_{3/2}) \cdot \nu(p_{3/2})$ (%) | 54.7 | 56.4 | 60.4 | 58.7 | 62.5 |
| $\pi(p_{3/2}) \cdot \nu(p_{1/2})$ (%) | 18.8 | 18.1 | 16.9 | 17.8 | 16.5 |
| $\pi(p_{1/2}) \cdot \nu(p_{3/2})$ (%) | 18.3 | 17.7 | 16.3 | 17.3 | 15.9 |
| $\pi(s_{1/2}) \cdot \nu(s_{1/2})$ (%) | 2.9 | 1.3 | 2.3 | 2.2 | 1.3 |
| DCE $\equiv \langle h_{p-n} \rangle$ (MeV) | -4.34 | -3.54 | -3.21 | -4.35 | -3.46 |
| $\langle h_{c-pn} \rangle$ (MeV) | +0.64 | -0.16 | +0.52 | +0.65 | +0.18 |
| $\langle \pi_{p-n}^2/2 \mu_{p-n} \rangle$ (MeV) | 4.62 | 4.68 | 4.44 | 4.56 | 4.71 |
| $\langle \pi_{c-pn}^2/2 \mu_{c-pn} \rangle$ (MeV) | 4.29 | 4.84 | 4.43 | 4.63 | 5.07 |
| $\sqrt{\langle \xi_{p-n}^2 \rangle}$ (fm) | 5.72 | 5.55 | 5.61 | 5.64 | 5.46 |
| $\sqrt{\langle \xi_{c-pn}^2 \rangle}$ (fm) | 3.46 | 3.42 | 3.38 | 3.28 | 3.11 |

This modification, of course, leads to an inconsistency with the deuteron energy in vacuum.

In Table II our results with the SDDC and Minnesota interactions (original and fitted) are summarized as “Li-S”, “Li-MO”, and “Li-MF” sets. Generally, they will coincide with each other. One can find that both $pn$ interactions play a major role: the mean $pn$ interaction energy, $\langle v_{p-n} \rangle$, show deeply negative values within the g.s. solutions.

The mean opening angle of $pn$, $\langle \theta_{pn} \rangle$, is less than 90 degrees in the three cases. This indicates a spatial correlation between two nucleons [24]. Indeed, as shown in Ref. [30], this is a product of the mixture of different parities with respect of the core-nucleon subsystems: if one employs only the odd or even-$l$ states in the uncorrelated basis, the resultant mean opening angle should be exactly 90 degrees, lacking the spatial correlation. In our present result, however, this angular correlation is weak compared with the isospin-triplet dineutron or diproton correlation [28, 30, 35, 55]. This is consistent with the fact that the contamination from channels other than $(p_{3/2})$ and $(p_{1/2})$ is minor in this system.

Comparing the original and enhanced Minnesota cases, indicated by Li-MO and Li-MF in Table II, the $pn$ interaction potential is more attractive in the latter case. This is simply due to our fitting manipulation to the empirical binding energy. However, the above structural information is qualitatively similar, and we conclude its weak sensitivity to the binding energy.

### D. Deuteron Correlation Energy

In order to evaluate the deuteron correlation energy (DCE), it is more convenient to work with the T-Jacobi coordinates. Namely, we can transform our core-orbital coordinates, $\{r_p, r_n\}$, to the T-Jacobi ones, $\{\xi_{p-n}, \xi_{c-pn}\}$, as seen in Eq. (12). Exact formulas can be found in Appendix. In these T-Jacobi coordinates, our three-body Hamiltonian is decomposed as,

$$H_{3b} = h_{p-n} + h_{c-pn},$$

(13)
II. There, we also tabulate the mean kinetic energies there, the SDDC interaction needs to be refitted ($\eta = 1.44$), whereas the Minnesota can be unchanged from its original value. Eventually, the core-$pn$ channel is stable with negative mean energies. Furthermore, also in these cases, our previous statement can be kept: the $pn$ subsystem is more strongly bound (about 50%) than in vacuum. Consequently, in all the calculations we have performed, an enhancement of DCE has been observed.

E. Geometric Structure

In order to evaluate the spatial extent of the wave function, we compute the mean relative distances, $\langle \xi_{p-n}^2 \rangle$ and $\langle \xi_{c-pn}^2 \rangle$. From Appendix, the corresponding operators are given by

$$\xi_{p-n}^2 = |\xi_{p-n}|^2 = |r_p - r_n|^2,$$
$$\xi_{c-pn}^2 = |\xi_{c-pn}|^2 = |(r_p + r_n)/2|^2. \quad (15)$$

Thus, the mean distances depend on $\langle \xi_{p-n}^2 \rangle$ and $\langle r_p \cdot r_n \rangle$. Especially for $\langle \xi_{c-pn}^2 \rangle$, if the total three-body system is loosely bound with an extended wave function, this value is also large, but with a notable exception: when the resultant $pn$-opening angle is sufficiently narrow, then $\langle \xi_{c-pn}^2 \rangle \simeq 0$.

At the bottom of Table II our results are tabulated. Comparing those with the kinetic energies, one can find a common feature: when the relative distance gets narrow, its corresponding kinetic energy increases. This can be naturally understood from the uncertainty principle between the relative coordinates and the conjugate momenta.

For the comparison with another system, $^{18}$F, in the next section, we point out a general feature of DCE. When the total three-body system is loosely bound, the $pn$-relative distance, $\langle \xi_{p-n}^2 \rangle$, is large if $\cos (\theta_{pn}) \simeq 0$, and consistently, the kinetic energy, $\langle \xi_{p-n}^2 / 2 \mu_{p-n} \rangle$, becomes small. Consequently, the $pn$ subsystem can get energetically “stable”, in spite of the loose stability of the whole partial two-body system is affected by the presence of the third cluster.

Besides these interesting results, however, we should face one shortcoming, namely the instability problem in the core-$pn$ channel: the expectation value, $\langle h_{c-pn} \rangle$, is positive both in the SDDC and Minnesota cases. Thus, the core-$pn$ subsystem should be unbound with our parameters. To remedy this problem, we employ a slightly deeper Woods-Saxon potential for the core-nucleon channels: $V_0 = -49.0$ MeV in Eq. (3), whereas the other parameters are not changed. With this potential, the core-nucleon levels are slightly deviated from the experimental data, but the whole picture still keeps a qualitative consistency: both core-proton and core-neutron states are broad resonances, as seen in Table II ($V_0 = -49.0$ MeV).

In “Li-S2” and “Li-MO2” sets in Table II our results with the deeper core-nucleon potential are summarized. In order to reproduce the three-body binding energy there, the SDDC interaction needs to be refitted ($\eta = 1.44$), whereas the Minnesota can be unchanged from its original value. Eventually, the core-$pn$ channel is stable with negative mean energies. Furthermore, also in these cases, our previous statement can be kept: the $pn$ subsystem is more strongly bound (about 50%) than in vacuum. Consequently, in all the calculations we have performed, an enhancement of DCE has been observed.
system. In $^{6}$Li, indeed, this kinetic energy is not sufficient to overcome the pairing energy, and thus, the $pn$ subsystem is quite deeply bound.

Finally, concerning the more realistic computations, of course, we admit that further optimization may be considered. Those include the exact treatment of the continuum levels in the core-nucleon channels $^{15}$[54,56–60], as well as the tensor and spin-orbit components in the $pn$ interaction $^{11}$[61]. Those are, however, technically demanding and beyond the scope of our present model.

III. $^{18}$F NUCLEUS

Next we focus on another system, $^{18}$F, which may also support the deuteron correlation around the core nucleus, $^{16}$O. A major difference from $^{6}$Li is that, in the $^{16}$O—$p$ or $^{16}$O—$n$ subsystem, there are some bound s.p. orbits. Also, the major shell includes $(s_{1/2})$, $(d_{5/2})$ and $(d_{3/2})$. Thus, it can be suitable to investigate the sensitivity of the deuteron correlation to the valence orbit(s).

| TABLE III. Core-nucleon energy levels of $^{17}$O and $^{17}$F with respect to the one-nucleon threshold, obtained with the core-nucleon potentials in this work. The unit is MeV. Subscript $r$ indicates the s.p. resonances, and $\Gamma$ is the resonance width obtained from the scattering phase-shift. |
|-----------------------------------------------|
|                    | This work                    | Exp.$^{[17]}$             |
|-----------------------------------------------|
|                    | default                      | $pf$-mix.                 |
| $^{16}$O—$n$       | $\epsilon(2s_{1/2})$         | $-3.25$                   |
|                    |                              | $-3.272$                  |
|                    | $\epsilon(1d_{5/2})$         | $-4.11$                   |
|                    |                              | $-4.143$                  |
|                    | $\epsilon_{r}(d_{3/2})$      | $+0.90$                   |
|                    | ($\Gamma = 0.10$)            | ($\Gamma = 0.096$)        |
|                    | $\epsilon_{r}(f_{7/2})$      | $+7.01$                   |
|                    | ($\Gamma = 2.74$)            | ($\Gamma = 0.58$)         |
|                    |                              | $+4.13$                   |
|                    | $\epsilon_{r}(f_{5/2})$      | $+11.6$                   |
|                    | ($\Gamma = 12.1$)            | ($\Gamma = 6.04$)         |
|                    |                              | $+9.48$                   |
|                    | $\epsilon_{r}(p_{3/2})$      | $+2.72$                   |
|                    | ($\Gamma = 8.60$)            | ($\Gamma = 1.15$)         |
|                    |                              | $+0.61$                   |
| $^{16}$O—$p$       | $\epsilon(2s_{1/2})$         | $-0.13$                   |
|                    |                              | $-0.105$                  |
|                    | $\epsilon(1d_{5/2})$         | $-0.55$                   |
|                    |                              | $-0.600$                  |
|                    | $\epsilon_{r}(d_{3/2})$      | $+4.01$                   |
|                    | ($\Gamma = 0.89$)            | ($\Gamma = 1.53$)         |
|                    | $\epsilon_{r}(f_{7/2})$      | $+10.0$                   |
|                    | ($\Gamma = 4.02$)            | ($\Gamma = 1.29$)         |
|                    |                              | $+7.22$                   |
|                    | $\epsilon_{r}(f_{5/2})$      | $+14.8$                   |
|                    | ($\Gamma = 14.4$)            | ($\Gamma = 7.83$)         |
|                    |                              | $+12.6$                   |
|                    | $\epsilon_{r}(p_{3/2})$      | no resonance              |
|                    | ($\Gamma = 3.58$)            | $+2.94$                   |

A. Model Parameters

For $^{18}$F, we perform similar calculations but with an appropriate change of parameters. First, the core-mass parameter, $m_{c}$, is changed as appropriate. In order to take Pauli principle into account, we exclude the $(1s_{1/2}), (1p_{3/2})$, and $(1p_{1/2})$ states, which are occupied by the core nucleus.

For the core-nucleon interaction, we again adopt the Woods-Saxon potential, where Coulomb term is added only for the s.p. proton states. In Eq. (2), some parameters are changed: in our default set, $r_{0} = r_{0} \cdot 161^{1/3}$, $V_{0}^{(l=0)} = -53.1$ MeV, $V_{0}^{(l\neq 0)} = 0.99$, $U_{ls} = 24.9$ MeV·fm$^{2}$, while $r_{0}$ and $a_{0}$ are unchanged. In correspondence, the density profile, $f(r)$, in the SDDC $pn$ interaction is also changed.

Additionally to the default set, in Sec. III C, we also employ $pf$-mixture Woods-Saxon potential. There, its depth parameter is modified only for the odd-$l$ channels: $V_{0}^{(l=odd)} = 1.188 \cdot V_{0}^{(l=0)}$.

In Table III the core-nucleon levels are summarized. Our parameters fairly reproduce the experimental s.p. levels both in the proton and neutron channels. For resonant channels, we also checked the width as obtained from the phase-shift analysis. These results approximately coincide with other theoretical models $^{[17]}$[21].

Because of the well-determined s.p. levels, in contrast to the case of $^{6}$Li, we cannot modify the core-nucleon potentials for the major $sd$-shell. Thus, in order to reproduce the three-body binding energy, the only adoptable way is to modify the $pn$ interaction parameters. For $^{18}$F, this binding energy is measured as 9.75 MeV $^{[17]}$. Thus, the SDDC $pn$-pairing interaction is re-adjusted with $\eta = 1.32$. For the Minnesota interaction, on the other hand, we need a reduction factor, $f = 0.67$, to reproduce this empirical energy similarly to Ref. $^{[21]}$.

B. Ground State of $^{18}$F

In “F-S”, “F-MO”, and “F-MF” sets in Table IV our results are summarized in the same manner as for $^{6}$Li. Generally, $pn$ pairing makes a major contribution also in $^{18}$F. The mean $pn$ interaction energy, $(v_{p-n})$, exhausts 85 % of the three-body binding energy in the F-MO case, whereas it amounts to 70 % in the other two cases.

Checking other results in the three cases, the structural properties are similar, and not too sensitive to the specific $pn$ interaction models. There is a small amount of $pn$-angular correlation, but not very significant. This corresponds to a small mixing of the $sd$-shell with other orbits. Because of the heavy core, the recoil-term energy is almost negligible in this system. The mean relative distances also show similar values, independently of the $pn$ interactions. These values are well consistent with the results in Ref. $^{[17]}$. 
TABLE IV. Same to Table [1] but for the g.s. of $^{18}$F ($1^+$). The empirical binding energy is $E_{3b} = -9.75$ MeV [47].

| Label | Type of $v_{p-n}$ | F-S | F-S2 | F-MO | F-MF | F-MF2 |
|-------|------------------|-----|------|------|------|-------|
| Adjustment of $v_{p-n}$ | | $\eta = 1.32$ | $\eta = 1.437$ | $\eta = 1.437$ | $\eta = 1.437$ | $\eta = 1.437$ |
| $E_{c}(d)$ (MeV) | (default) | $f = 1$ | $f = 0.67$ | $f = 0.67$ | $f = 0.67$ | $f = 0.67$ |
| WS Pot. | $|a_{\nu}(S=1) = 5.424$ fm | $|a_{\nu}(S=1) = 5.424$ fm | | $|a_{\nu}(S=1) = 5.424$ fm | | $|a_{\nu}(S=1) = 5.424$ fm |
| $E_{3b} = \langle H_{3b} \rangle$ (MeV) | default | pf-mix. | default | default | default | pf-mix. |
| $\langle v_{p-n} \rangle$ (MeV) | $-9.78$ | $-9.74$ | $-13.33$ | $-9.75$ | $-9.72$ | $-9.72$ |
| $\langle x_{pp} \rangle$ (MeV) | $-1.10$ | $-0.63$ | $-0.09$ | $-0.07$ | $-0.45$ | $-0.45$ |
| $\langle \theta_{pn} \rangle$ (deg) | $87.4$ | $72.3$ | $88.7$ | $88.7$ | $80.0$ | $80.0$ |
| $\pi \langle d_{5/2} \rangle \cdot \nu \langle d_{3/2} \rangle$ (%) | $57.9$ | $52.2$ | $48.4$ | $60.7$ | $61.2$ | $61.2$ |
| $\pi \langle d_{3/2} \rangle \cdot \nu \langle d_{3/2} \rangle$ (%) | $13.9$ | $10.9$ | $15.0$ | $10.4$ | $9.1$ | $9.1$ |
| $\pi \langle s_{1/2} \rangle \cdot \nu \langle s_{1/2} \rangle$ (%) | $10.7$ | $10.8$ | $17.6$ | $16.0$ | $14.6$ | $14.6$ |
| $\pi \langle f_{7/2} \rangle \cdot \nu \langle f_{7/2} \rangle$ (%) | $0.4$ | $6.9$ | $0.2$ | $0.1$ | $2.8$ | $2.8$ |
| $\pi \langle p_{3/2} \rangle \cdot \nu \langle p_{3/2} \rangle$ (%) | $0.5$ | $1.9$ | $0.3$ | $0.2$ | $0.7$ | $0.7$ |
| DCE $\equiv \langle h_{p-n} \rangle$ (MeV) | $+0.33$ | $+3.17$ | $-2.05$ | $+1.78$ | $+4.66$ | $+4.66$ |
| $\langle h_{c-pn} \rangle$ (MeV) | $-10.11$ | $-12.91$ | $-11.28$ | $-11.53$ | $-14.38$ | $-14.38$ |
| $\langle \pi_{p-n}^2 / 2 \mu_{p-n} \rangle$ (MeV) | $7.50$ | $11.28$ | $9.27$ | $8.67$ | $11.56$ | $11.56$ |
| $\langle \pi_{c-pn}^2 / 2 \mu_{c-pn} \rangle$ (MeV) | $6.59$ | $1.34$ | $8.89$ | $8.49$ | $4.82$ | $4.82$ |
| $\sqrt{\langle \xi_{p-n}^2 \rangle}$ (fm) | $5.09$ | $4.73$ | $4.96$ | $4.95$ | $4.60$ | $4.60$ |
| $\sqrt{\langle \xi_{c-pn}^2 \rangle}$ (fm) | $2.79$ | $3.37$ | $2.58$ | $2.59$ | $2.83$ | $2.83$ |

C. Energy and Spatial Correlations

When evaluating the DCE, however, the situation becomes contrary to the initial guess of the strong deuteron correlation. First, in the original Minnesota case (F-MO), DCE is smaller than the value in vacuum. Namely, the bound $sd$-shell hardly supports the $pn$-energy correlation. Furthermore, comparing this DCE with other two cases (F-S and F-MF), where the pairing parameters have to be adjusted, a drastic change occurs. In the F-S and F-MF cases, the $pn$-subsystem is unstable around the core, because DCE is positive. This coincides with the reduction of the pairing attraction strength to achieve the empirical binding energy. Indeed, the reduced Minnesota force does not support the spin-triplet $pn$-bound state in vacuum: $E_{c}(d) > 0$. Note also that, even with the positive DCE value, the whole system can still be stable, as long as $|h_{c-pn}|$ is sufficiently negative.

Until this point, within our simple two-body interaction models, there has been no indication of an enhancement of DCE in $^{18}$F, showing a remarkable difference from $^{6}$Li. Also, the opening-angle or equivalently the spatial correlation is not significant. The latter result is in contrast to Ref. [21]. In order to reproduce the spatial $pn$ correlation, and to investigate its effect on DCE, we replace the Woods-Saxon potential with the $pf$-mixture version. With this potential, as shown in Table III, the odd-$l$ states become closer to the Fermi surface, and thus, a certain degree of mixing with the g.s. solutions is more easily realized.

In sets “F-S2” and “F-MF2” of Table IV our results with the $pf$-mixture potential are given. Indeed, we can find an increase of the odd-$l$ contamination. Consistently, the opening angle can get closer with this potential, as we expected. Note also that, for the three-body binding energy, $pn$-pairing interactions are re-adjusted. In these cases with a significant spatial correlation, however, the $pn$ subsystem is not bound in $^{18}$F. Furthermore, its instability becomes enhanced compared with the default Woods-Saxon cases (F-S, F-MO and F-MF), as indicated by the increase of DCE.

The instability of the $pn$ subsystem in the presence of spatial localization can be understood from the uncertainty principle. When the $pn$ subsystem becomes concentrated with the narrow distance, $\xi_{p-n}$, the density distribution with respect of its conjugate momentum, $\pi_{p-n}$, should be dispersed. This leads to the enhancement of the relative kinetic energy, $\langle \pi_{p-n}^2 / 2 \mu_{p-n} \rangle$, which can be
the spatial distribution is more localized. This result reflects the effect of the different spatial distributions: for the short-range attraction like the \( ^6\text{Li} \) nuclei, regarding the \( pn \) correlation in weakly and strongly bound nuclei. This can be mainly understood from the uncertainty principle between the spatial and momentum distributions: because \( ^6\text{Li} \) is a loosely-bound three-body system, its \( pn \)-spatial (momentum) distribution can be dispersed (concentrated), and thus, the mean \( pn \)-kinetic energy, \( \left\langle \frac{\pi_{p-n}^2}{2\mu_{p-n}} \right\rangle \), gets reduced. The comparably small contribution of the \( pn \)-pairing energy, \( \left\langle v_{p-n} \right\rangle \), of the SDDC or Minnesota interaction model is not sufficient to support a strong \( pn \) binding in \(^{18}\text{F} \). Our conclusion provides a phenomenological benchmark to discuss the \( pn \) correlation in various situations or/and systems.

There remains several tasks for future studies, toward the phenomenological improvement of our model analysis. The first possible expansion is to implement the spin-orbit or/and tensor forces in the \( pn \) interaction \([11, 54, 61]\). The sophisticated treatment of continuum states may be also profitable for further realistic models \([15, 54, 57, 60, 62, 65]\). In order to precisely discuss the spatial \( pn \) correlation \([20, 21]\), taking the exchange effect of valence particles into account might be required \([60]\). With these possible improvements, a further evaluation of DCE, covering other systems with different spa-
tial extensions, could be reported in future. The model-
dependence of the pn-pairing energy also needs to be re-
garded carefully.

Another direction of progress is, as suggested in Ref. [22], the deuteron emission within a time-dependent
framework [34, 55, 67–70]. From this process, including
[22], the deuteron emission within a time-dependent
generation, could be reported in future. The model-
be defined in matrix form:

\[
[\mathbf{U}]_{\text{P.R.A.T. 2015 project In:Theory of the University of Padova (Project Code: CPDA154713). T. Oishi sincerely thanks Yusuke Tanimura, Kouichi Hagino and Hiroyuki Sagawa for fruitful discussions. The computing facilities offered by CloudVeneto (CSIA Padova and INFN) are acknowledged.}

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**Appendix: Transformation of Coordinates**

In the main text, we employ the core-orbital as well as
T-Jacobi coordinates for the three-body system. In this
section, we give a formalism for these transformations.

First, we need the original coordinates and the conjugate
momenta:

\[
\vec{X} = \begin{bmatrix} x_p \\ x_n \\ x_c \end{bmatrix}, \quad \vec{P} = \begin{bmatrix} p_p \\ q_n \\ q_c \end{bmatrix}. \tag{A.1}
\]

In these coordinates, the three-body Hamiltonian is,

\[
H_{3b} = \sum \frac{\vec{q}_i^2}{m_i} + V_{c-p} + V_{c-n} + v_{p-n}, \tag{A.2}
\]

where \(i = p, n\) and \(c\) for proton, neutron and core, re-
spectively.

With 3 \times 3 matrix, \(U\), the core-orbital coordinates can be
defined in matrix form:

\[
\begin{bmatrix} r_p \\ r_n \\ r_G \end{bmatrix} = U \vec{X}, \quad \bar{\vec{P}} = \begin{bmatrix} p_p \\ p_n \\ p_G \end{bmatrix} = (U^T)^{-1} \vec{P}, \tag{A.3}
\]

where

\[
U = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ \frac{m_p}{M} & \frac{m_n}{M} & \frac{m_c}{M} \end{pmatrix}, \tag{A.4}
\]

with \(M \equiv \sum m_i\) (total mass). A schematic view is displayed in Fig. 3. In these coordinates, the Hamiltonian reads

\[
H_{3b} = \frac{p_G^2}{2M} + \frac{p_p^2}{2\mu_p} + \frac{p_n^2}{2\mu_n} + p_p \cdot p_n + \text{(potentials)}, \quad (A.5)
\]

where the first term represents the center-of-mass kinetic
energy, that can be neglected. This leads to Eq. (1).

On the other side, T-Jacobi coordinates are given as,

\[
\xi = \begin{bmatrix} \xi_{p-n} \\ \xi_{c-pn} \\ r_G \end{bmatrix} = V \vec{X}, \quad \bar{\vec{Q}} = \begin{bmatrix} \pi_{p-n} \\ \pi_{c-pn} \\ p_G \end{bmatrix} = (V)^{-1} \vec{P}, \tag{A.6}
\]

where

\[
V = \begin{pmatrix} \frac{1}{m_p} & 0 & \frac{-1}{m_c} \\ \frac{m_p + m_n}{m_p m_n} & \frac{1}{m_p} & \frac{1}{m_n} \end{pmatrix}. \quad (A.7)
\]

They are also displayed in Fig. 3. In these T-Jacobi coor-
dinates, the Hamiltonian reads

\[
H_{3b} = \frac{p_G^2}{2M} + \frac{\pi_{p-n}^2}{2\mu_{p-n}} + \pi_{c-pn}^2 + \text{(potentials)}, \quad (A.8)
\]

with the relative masses,

\[
\frac{1}{\mu_{p-n}} = \frac{m_p + m_n}{m_p m_n}, \quad \frac{1}{\mu_{c-pn}} = \frac{1}{m_p + m_n} + \frac{1}{m_c}. \quad (A.9)
\]

Thus, one can separate the \(p_n\)-subsystem Hamiltonian,
\(h_{p-n} = \pi_{p-n}^2/2\mu_{p-n} + v_{p-n}\), in these coordinates. Notice also that, both in the core-orbital and T-Jacobi coordinate
systems, the center-of-mass motion is separated.

In order to evaluate the DCE, it is convenient to notice that,

\[
\pi_{c-pn} = p_p + p_n, \quad \pi_{p-n} = m_n p_p - m_p p_n, \quad (A.10)
\]

as well as,

\[
\frac{\pi_{c-pn}^2}{2\mu_{c-pn}} = \frac{M}{2m_c(m_p + m_n)}(p_p^2 + p_n^2 + 2p_p \cdot p_n), \quad (A.11)
\]

for the core-orbital and T-Jacobi kinetic operators.
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