Structure of deuterons in nuclei

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Abstract. Although the isoscalar ($T = 0$) nucleon pair forms a bound state in vacuum, it is not evident whether the isoscalar pair condensation exists in nuclei. We perform calculations of the transition density for two-nucleon removal modes, to study deuteron-like pair states with spin $S = 1$ and isospin $T = 0$ in ^{16}O. The isoscalar proton-neutron (pn) pair states in the nucleus vary, depending on the strength of the isoscalar pn pairing interaction and on the location of the pair inside the nucleus.

1 Introduction

The deuteron is a bound state composed of a proton and a neutron (pn pair). In fact, it is the only bound two-nucleon system, while like-nucleon pairs (pp and nn) do not form bound states in a vacuum. There are two kinds of pn pairs that have different quantum numbers of the total spin S and the total isospin T. The deuteron is labeled by $(S, T) = (1, 0)$. This suggests that the attraction in the $(S, T) = (1, 0)$ channel is stronger than that in the $(S, T) = (0, 1)$ channel. Searches have been conducted for evidence of isoscalar pairing condensation in nuclei. However, so far, no definitive experimental data have been obtained [1].

In nuclei with the same number of neutrons and protons ($N = Z$), the protons and neutrons are expected to occupy the same single-particle orbitals, thus, we expect that the pn correlations are strong in the $N = Z$ nuclei. Since the strength of the isoscalar pair correlation in the nuclear medium is not well known, it is desired to find observables to provide constraints on the pairing strength. In this paper, we study the isoscalar pn pair states in nuclei that has the same quantum number as the deuteron. In reference [2], the proton-induced deuteron knockout reactions, ^{16}O$(p, pd)^{14}$N, has been studied to investigate the isoscalar pn pair states in ^{16}O. The ground state of the ^{16}O nucleus is described by the energy density functional (EDF) method, then, the deuteron states are investigated assuming a product form of the transition density as $\delta\rho(\vec{R}, \vec{r}) = \varphi_{pn}(R)\phi_d(r)$ where $\phi_d(r)$ is the deuteron wave function[1] and $\varphi_{pn}(R)$ is the wave function describing the distribution of the isoscalar pn pairs in the ^{16}O nucleus [2]. The triple differential cross sections for the ^{16}O$(p, pd)^{14}$N reaction is calculated in the distorted wave impulse approximation with $\varphi_{pn}(R)$. The calculation turns out to significantly underestimate the experimental cross sections [3]. However, in reference [2], $\varphi_{pn}(R)$ was estimated using the product form, $\delta\rho(\vec{R}, \vec{0}) = \varphi_{pn}(R)\phi_d(0)$ at $r = 0$. Therefore, the purpose of the present study is to investigate properties of isoscalar pn pairs (deuterons) inside ^{16}O, location and structure of the deuteron states, and to examine the validity of the product form. Here and hereafter, the wave function $\phi_d(r)$ is referred to as "deuteron state" for simplicity.

We perform calculations of the removal transition density for isoscalar pn pairs in the doubly magic nucleus ^{16}O, based on the (time-dependent) density functional theory [4]. Although the method is analogous to the previous study [2], we further investigate the structure without assuming the product form of the transition density. The ground state of ^{16}O is calculated to be spherical. Because of its doubly-closed-shell character, both $T = 0$ and $T = 1$ pair condensations vanish in the mean-field approximation. We employ the pn-pair-removal random-phase approximation (RPA) to incorporate pairing correlations beyond the mean-field approximation, and investigate the properties of pn pairs (deuterons) in ^{16}O with quantum numbers of $T = 0$ (isoscalar) and $S = 1$ (spin triplet). This paper presents numerical results for the transition density in a specific configuration of pn pairs. The structure changes of the deuteron states according to their location in the nucleus and to the isoscalar pairing strength are discussed.

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[1]In general, the isoscalar pn-pair state $\phi_d(r)$ depends on the location, $\phi_d(\vec{r}; \vec{R})$. Precisely speaking, it is not necessarily the deuteron, but the state with the same spin-isospin quantum numbers as the deuteron, $(S, T) = (1, 0)$.

The paper is organized as follows. In section 2, we present the proton-neutron hole-hole RPA method. To study the deuteron states in the ground state of ^{16}O, *pn*-pair-removal transition density is given in section 2.2. In section 3, the numerical results are presented. The transition densities are shown for different locations in the nucleus. The summary and the future perspectives are given in section 4.

2 Pair-removal RPA

2.1 Calculation of states in ^{14}N

First, the ground state of the target nucleus, ^{16}O, is obtained by self-consistently solving the Hartree-Fock (HF) equations.

$$h_{\rm HF}[\rho]\,|\varphi_i\rangle = \epsilon_i\,|\varphi_i\rangle\,. \tag{1}$$

The HF single-particle Hamiltonian $h_{\rm HF}[\rho]$ is given by the derivative of the energy density functional $E[\rho]$ with respect to the one-body density, $h_{\rm HF} = \delta E[\rho]/\delta\rho$. The ground-state density is constructed as $\rho = \sum_{i<F}|\varphi_i\rangle\langle\varphi_i|$, where the summation is restricted to the single-particle orbits whose energies are below the Fermi energy (hole orbits), $\epsilon_i < \epsilon_F$.

Next, the states in ^{14}N, produced by the *pn*-pair knockout reaction, are described by the proton-neutron hole-hole RPA (*pn*-hhRPA) theory. Although the ground state of ^{16}O is described by the HF state in which the pair gaps vanish ($\Delta_n = \Delta_p = 0$), the RPA theory is able to include the residual pairing correlation beyond the mean field. The transition density $\delta\rho(\vec{r}_1,\vec{r}_2)$ for the annihilation of a *pn* pair of given spin and isospin quantum numbers, where $\vec{r}_1$ and $\vec{r}_2$ indicate the coordinates of two nucleons (proton and neutron), provides information on where the *pn* pairs are located and their structure inside the nucleus.

In *pn*-hhRPA, the ground state of ^{16}O is taken as the RPA ground state ($|A_0\rangle$), and the excited states are defined as $|B_\lambda\rangle = \Gamma^\dagger_\lambda|A_0\rangle$. Here, the operator $\Gamma^\dagger_\lambda$ is the *pn*-hhRPA normal-mode creation operator that removes a *pn* pair from the ground state of ^{16}O and induces a transition to the λ-th excited state of ^{14}N, which is expressed as

$$\Gamma^\dagger_\lambda = \sum_{\pi,\nu<F} X^\lambda_{\pi\nu} c_\pi c_\nu - \sum_{\pi',\nu'>F} Y^\lambda_{\pi'\nu'} c_{\nu'} c_{\pi'}\,. \tag{2}$$

Here, c_π (c_ν) are the operators that annihilate a proton (a neutron) in single-particle states π (ν) below the Fermi level, while $c_{\pi'}$ ($c_{\nu'}$) are those that annihilate a proton (a neutron) in single-particle states π' (ν') above the Fermi level. These single-particle states are obtained in equation (1) using the Skyrme SGII EDF [5]. The pairing part of the EDF is obtained with the density-dependent contact interaction in the isoscalar channel

$$V = V_0 \frac{1+P_\sigma}{2}\frac{1-P_\tau}{2}\left(1-\frac{\rho(\vec{r})}{\rho_0}\right), \tag{3}$$

where $\rho_0 = 0.16$ fm^{-3} and $\rho(\vec{r})$ is the nucleon density. P_σ (P_τ) is the spin (isospin) exchange operator [6].

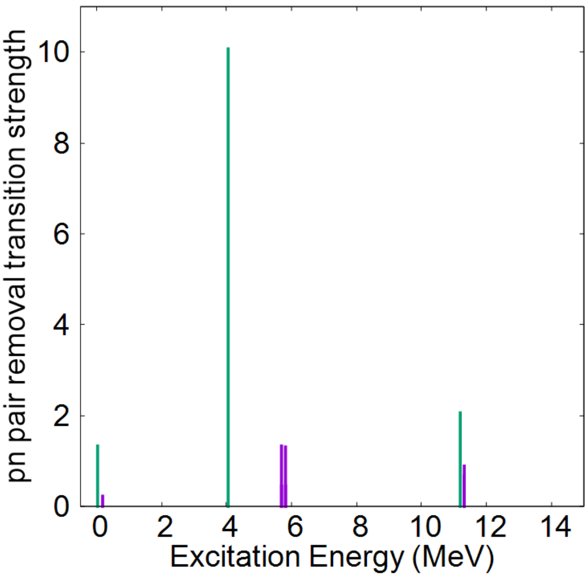

Figure 1. Calculated *pn* pair removal transition strength $S^{\lambda_J}_\mu$ with $M = \mu = 1$, as a function of the excitation energy in ^{14}N. The magenta lines represent the transition strengths for the isoscalar *pn* pairing strength $V_0 = 0$, while the green lines correspond to those for $V_0 = -490$ MeV fm^3. To make the bar at $E = 0$ visible, the magenta lines are shifted by 0.1 MeV to the right.

2.2 Calculation of *pn*-pair structure in nuclei

To investigate the *pn* structure in the ^{16}O nucleus, we calculate the following transition density.

$$\delta\rho^{\lambda(JM)}_\mu(\vec{r}_2,\vec{r}_1) = \langle B^{(JM)}_\lambda|[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)]^{T=0}_{S=1,S_z=\mu}|A_0\rangle\,, \tag{4}$$

where (J, M) represent the magnitude and the magnetic quantum number of the angular momentum of the state $|B_\lambda\rangle$. Here, $[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2)]^{T=0}_{S=1,S_z=\mu}$ is the operator that simultaneously removes two nucleons at coordinates $\vec{r}_1$ and $\vec{r}_2$ coupled to $T = 0$ and $(S, S_z) = (1,\mu)$. The origin of the coordinate is set at the center of the ^{16}O nucleus. We neglect the fluctuation of the center of mass in the present study.

To find states in the residual ^{14}N nucleus that are produced by the isoscalar *pn*-pair removal, let us define the pair removal transition strength as

$$S^{\lambda_J}_\mu \equiv \left|\int \delta\rho^{\lambda(J\mu)}_\mu(\vec{r},\vec{r})d\vec{r}\right|^2. \tag{5}$$

Here, when the state $|B_\lambda\rangle$ has the angular momentum J, we adopt its z component (magnetic quantum number) as $M = \mu$. Setting $\vec{r}_1 = \vec{r}_2 = \vec{r}$, the relative orbital angular momentum $l_{\rm rel}$ of the pair is restricted to be zero, $l_{\rm rel} = 0$. Therefore, in equation (5), we are looking at the s-wave *pn* pair with $(S, S_z) = (1,\mu)$ where the total isospin of the pair is automatically determined as $T = 0$ due to the Pauli principle. The value of $S^{\lambda_J}_\mu$ of equation (5) provides information on the character of the state λ in the residual nucleus B.

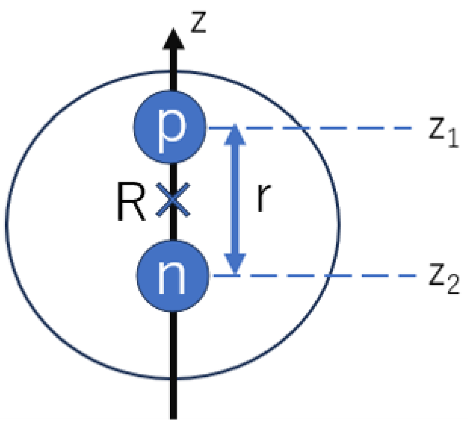

Figure 2. Schematic illustration of the *pn* pair on the *z* axis. The center of mass coordinate *R* and the relative coordinate *r* of the removed proton and neutron along the *z* axis.

3 Results and Discussion

We use a computer program developed in reference [7] to perform the numerical calculation of *pn*-hhRPA. The program assumes axial symmetry, thus, the RPA equation is solved in each sector of the *K* quantum number. Since the ground state of ^{16}O is spherical, *K* is regarded as the magnetic quantum number, $K = M$. For the states $J^\pi = 1^+$ in ^{14}N, we set $M = \mu = 1$ and calculate the *pn* removal transition strength (5). In figure 1, the transition strengths $S_1^{\lambda_1}$ to the states in ^{14}N are shown as a function of the excitation energy. For the vanishing pairing strength $V_0 = 0$, in addition to the transition to the ground state in ^{14}N, finite transition strengths appear at excitation energies around 6 MeV and 11 MeV. The transition strength to the ground state is nonzero but turns out to be very weak. For the finite value of the isoscalar pairing strength $V_0 = -490$ MeV fm^3, the state appears at 4 MeV and 11 MeV, in addition to the ground state. The isoscalar pairing significantly increases the transition strength to the ground state by a factor of about four. The first excited state with $J^\pi = 1^+$ has the largest transition strength, more than five times larger than that to the ground state. The excitation energy of the first excited 1^+ state is also shifted down by the isoscalar pairing correlation. The experimental excitation energy is 3.948 MeV [8], which is close to the value obtained with $V_0 = -490$ MeV fm^3.

Next, let us show the transition density $\rho(\vec{r}_1, \vec{r}_2)$ in the ^{16}O nucleus. In the present study, we focus our discussion on the transition to the ground state ($\lambda = 0$) in the ^{14}N nucleus, which has $J = 1$ with positive parity. To investigate the deuteron states, it is useful to visualize the transition density for the removal of the isoscalar ($T = 0$) *pn*-pair states. In this study, we restrict the configuration of the *pn* pair by adopting the positions of two nucleons, $\vec{r}_1$ and $\vec{r}_2$, both on the *z*-axis (see figure 2). In this case, the coordinates of the two nucleons are specified by z_1 and z_2 ($x_1 = x_2 = y_1 = y_2 = 0$). Then, we plot the transition density $\delta\rho_\mu^{\lambda(JM)}(z_1, z_2)$. For later purposes, we also define the center of mass of the *pn* pair as $R = (z_1 + z_2)/2$, and the relative coordinate as $r = z_1 - z_2$. Because of the sphericity of ^{16}O and the symmetric property of $\delta\rho_\mu^{\lambda(JM)}(z_1, z_2)$ with respect to the exchange of z_1 and z_2, we can assume $R > 0$ and $r > 0$ without losing generality.

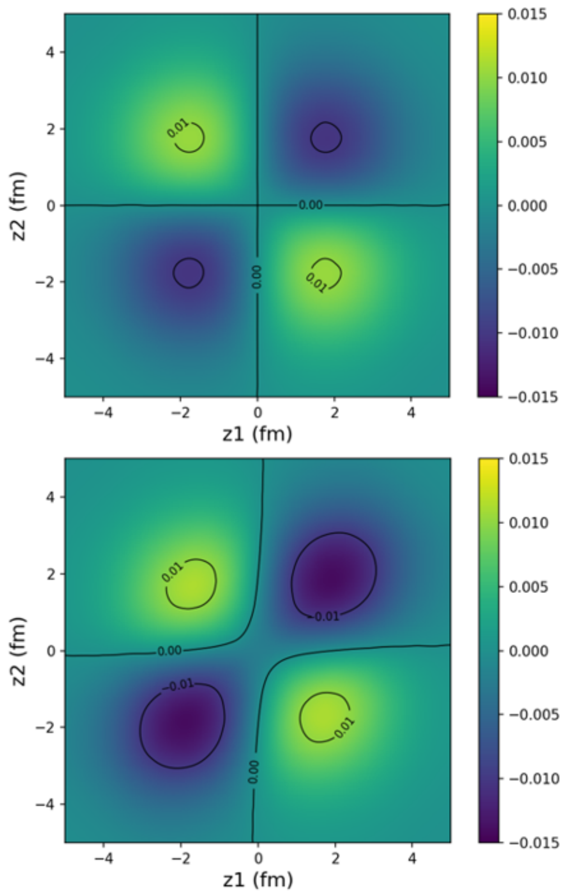

Figure 3. Calculated *pn*-removal transition density $\delta\rho_1^{0(11)}(z_1, z_2)$ from ^{16}O to the ground state in ^{14}N, with z_1 as the horizontal axis and z_2 as the vertical axis. The top panel corresponds to the *pn* pairing strength $V_0 = 0$, and the bottom panel corresponds to that obtained with $V_0 = -490$ MeV fm^3.

Figure 3 shows the transition density for the isoscalar *pn*-pair removal in which both nucleons are located on the *z*-axis (z_1 and z_2). The calculated transition density can be regarded as a kind of wave function for two nucleons coupled to $T = 0$. In the top panel of figure 3 of the zero pairing strength $V_0 = 0$, the transition density completely vanishes on the lines of $z_1 = 0$ and $z_2 = 0$ on which one of the nucleons of the *pn* pair is at the center of the ^{16}O nucleus. These lines correspond to nodal lines in the two-dimensional plane of (z_1, z_2), at which the transition density $\delta\rho_{01}^{(11)}(z_1, z_2)$ changes its sign. In the case of $V_0 = -490$ MeV fm^3, the obtained values on the lines of $z_1 = 0$ and $z_2 = 0$ are small but finite. Especially, we see a non-zero value at the origin $z_1 = z_2 = 0$, when both the proton and the neutron are at the center of the nucleus. This indicates that, in the absence of pairing correlation, the transition originates purely from a proton and a neutron in the *p* orbits, because the transition to the ground state in ^{14}N is achieved by the removal of two nucleons in

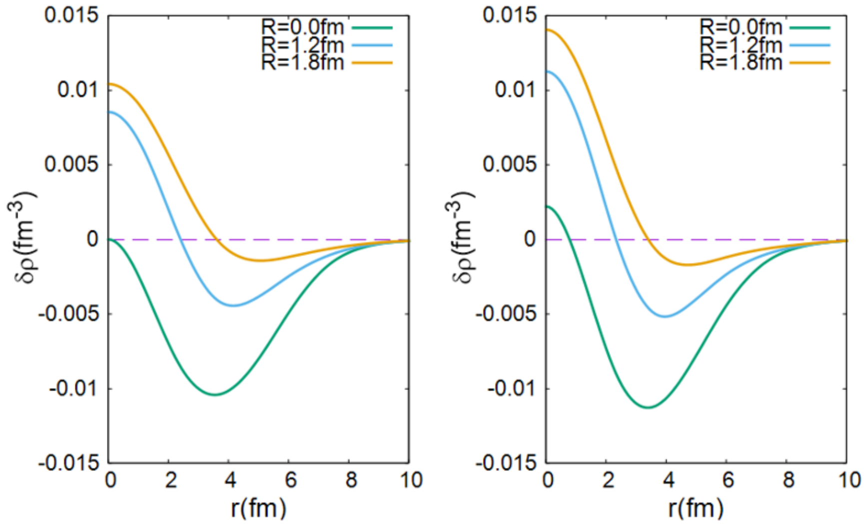

Figure 4. Calculated *pn*-removal transition density $\delta\rho_1^{0(11)}(R, r)$ as functions of r. The left panel shows the case with *pn* pairing strength $V_0 = 0$, and the right panel shows the case with *pn* pairing strength $V_0 = -490$ MeV fm^3. The green lines correspond to $R = 0$, the blue lines to $R = 1.2$ fm, and the orange lines to $R = 1.8$ fm.

the $p_{1/2}$ orbit. In contrast, dynamical correlations of the *pn* pairing make contributions of those in the s orbits possible. Absolute values of the transition density $\delta\rho_1^{0(11)}(z_1, z_2)$ are enhanced by the dynamical *pn* pairing correlations. The largest absolute values are observed at four different configurations, $z_1 = z_2 \approx \pm 2$ fm and $z_1 = -z_2 \approx \pm 2$ fm. This may indicate that the deuteron states are prominent both at the short range (contact configuration, $r = 0$) and at the long range ($r \approx 4$ fm). In reference [2], only the short-range correlation with $r = 0$ is taken into account. It is of significant interest to study the effect of the long-range correlation for the deuteron knockout reaction.

To further provide an intuitive picture of the deuteron states in ^{16}O, we plot the $\delta\rho_1^{0(11)}(r)$ with fixed values of R. See figure 2 for the explanation of the coordinates, R and r. Figure 4 shows the transition density as a function of r for different values of R. For the case of no pairing correlation ($V_0 = 0$), $\delta\rho(r)$ vanishes at $r = 0$ at the center of the nucleus $R = 0$. This is consistent with the analysis for figure 3. The nodal structure is clearly seen in both cases of $V_0 = 0$ and $V_0 = -490$ MeV fm^3. The structure of the deuteron states inside the nucleus depends on the shell structure of the ground state, and exhibit a complicated feature. Among the three lines corresponding to $R = 0$, 1.2 and 1.8 fm, the peak height at $r = 0$ is the highest at $R = 1.8$ fm. In addition, the structure of the deuteron states becomes simple near the surface, showing a single peak at $r = 0$ and the nodal and the oscillatory structures are disappearing. Near the surface with the dilute density, it may suggest a transition to the deuteron in vacuum.

4 Summary

Based on the Skyrme EDF of the SGII parameters, the structures of the deuteron states (*pn* pair with isospin $T = 0$ and spin $S = 1$) are investigated with the *pn*-hhRPA method. We study the deuteron states in the ground state of ^{16}O, in which the pairing gaps vanish due to its doubly-closed-shell character. Although the pairing correlation is absent in the ground state, the hhRPA is able to take into account the effects of the dynamical pairing correlation beyond the mean field. The transition density with respect to the deuteron-annihilation operator ($T = 0$ and $S = 1$) is investigated for the case of the transition to the ground state in ^{14}N. Previously, the deuteron knockout reaction was studied with the transition density $\delta\rho(R, r)$ obtained with the *pn*-hhRPA calculation [2], assuming a product form of $\delta\rho(R, r) \approx \varphi_{pn}(R)\phi_d(r)$, where R (r) indicates the center of mass of the deuteron (the relative distance between proton and neutron). Our calculations show that the product form is strongly violated inside the nucleus. The deuteron state $\phi_d(r)$ significantly changes according to its position R. $\phi_d(r)$ is strongly peaked at $r = 0$ at large R (deuteron located near the surface), showing that the proton and the neutron in the deuteron tend to be close to each other. On the other hand, $\phi_d(r)$ has a node for small R (the deuteron deep inside the nucleus). Especially, we find $\phi_d(0) \approx 0$ at the center ($R = 0$). This can be understood by the shell structure of ^{16}O. To have a finite value at $R = r = 0$, nucleons in the $s_{1/2}$ orbits must contribute to the transition density, which is practically forbidden by the deep binding of the $s_{1/2}$ nucleons. The structure of $\phi_d(r)$ at $R = 0$ suggests a long-range correlation between proton and neutron forming a cigar-like configuration. This type of long-range correlation is also enhanced by the isoscalar pairing correlations.

As we have shown in figure 1, the transition strength to the first excited 1^+ state in ^{14}N is significantly stronger than that to the ground state. For the deuteron knockout reaction, it may be important to investigate the deuteron states in ^{16}O associated with the transition to the excited 1^+ state. The calculation and the analysis are in progress. For future studies, the deuteron states in open-shell heavy nuclei are also of significant interest, since the isovector pairing plays an important role in the ground state. The interplay between isoscalar and isovector pairing may produce a new feature in the deuteron states in the heavy systems. To elucidate the structure of *pn* pair inside the nucleus, not only the deuteron-knockout but also *pn*-knockout reaction in general is useful. In particular, the measurement of the relative momentum of the *pn* pairs may provide valuable information on the spatial structure of the pairs.

Acknowledgements

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References

[1] S. Frauendorf, A.O. Macchiavelli, Overview of neutron–proton pairing, Prog. Part. Nucl. Phys. **78**, 24 (2014). 10.1016/j.ppnp.2014.07.001

[2] Y. Chazono, K. Yoshida, K. Yoshida, K. Ogata, Proton-induced deuteron knockout reaction as a probe of an isoscalar proton-neutron pair in nuclei, Phys. Rev. C **103**, 024609 (2021). 10.1103/PhysRevC.103.024609

[3] C. Samanta, N.S. Chant, P.G. Roos, A. Nadasen, A.A. Cowley, Discrepancy between proton- and alpha-induced cluster knockout reactions on ^{16}O, Phys. Rev. C **26**, 1379 (1982). 10.1103/PhysRevC.26.1379

[4] T. Nakatsukasa, K. Matsuyanagi, M. Matsuo, K. Yabana, Time-dependent density-functional description of nuclear dynamics, Rev. Mod. Phys. **88**, 045004 (2016). 10.1103/RevModPhys.88.045004

[5] N.V. Giai, H. Sagawa, Monopole and dipole compression modes in nuclei, Nucl. Phys. A **371**, 1 (1981). https://doi.org/10.1016/0375-9474(81)90741-7

[6] P. Ring, P. Schuck, The Nuclear Many-Body Problem (Springer-Verlag, Berlin, 1980), ISBN 978-3-540-21206-5

[7] K. Yoshida, Spin–isospin response of deformed neutron-rich nuclei in a self-consistent Skyrme energy-density-functional approach, Prog. Theor. Exp. Phys. **2013**, 113D02 (2013). 10.1093/ptep/ptt091

[8] National nuclear data center, `https://www.nndc.bnl.gov/ensdf/index.jsp`