Microscopic study on the origin of the rotational band of nuclei

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(Dated: March 3, 2022)
Abstract

The origin of the rotational band of nuclei has been investigated by the angular momentum projection (AMP) on the axial Hartree-Fock solutions, by using the semi-realistic effective Hamiltonian M3Y-P6. The rotational energy is decomposed into contributions of the individual terms of the Hamiltonian, and their ratios to the total rotational energy are calculated. Except for light or weakly-deformed nuclei, the ratios of the individual terms of the Hamiltonian are insensitive to nuclides and deformation. The contributions of kinetic energies are large and close to the rigid-rotor values, although those of central forces are sizable. For light or weakly-deformed nuclei, the ratios significantly depend on nuclei and deformation. The contributions of noncentral forces are not negligible. Regardless of nuclides, the attractive forces decrease the moment-of-inertia, and the repulsive forces increase it. A general formula for the rotational energy is derived on the basis of the AMP, which suggests that higher-order terms of the cumulant expansion play roles in the rotational energy and the moment-of-inertia for light or weakly-deformed nuclei.

I. INTRODUCTION

The rotational band is a well-known energy spectrum, $E_x(J) \approx J(J + 1)/2 I \frac{1}{2}$. It is observed experimentally over a wide range of the nuclear chart, including not only stable nuclei but also unstable ones \cite{2}. It indicates that the intrinsic state of nuclei is deformed and rotates with the moment-of-inertia $I$.

From a microscopic standpoint, nuclei have been described self-consistently by the mean-field (MF) theory, such as the Hartree-Fock (HF) and the Hartree-Fock-Bogolyubov (HFB) approximations \cite{3}. Because nuclei are isolated systems, the nuclear Hamiltonian has rotational symmetry, and the angular momentum is a good quantum number in energy eigenstates. However, spontaneous breaking of the rotational symmetry often occurs in the MF approximation. In the case of nuclei, the rotational symmetry breaking of the MF state corresponds with a deformation of the intrinsic state. The deformed intrinsic state is not observed directly. The Nambu-Goldstone (NG) mode is accompanied by the symmetry breaking, and then it restores the corresponding symmetry in energy eigenstates. The restoration of the rotational symmetry corresponds with a whole rotational motion of the deformed nuclei.

Several methods that treat the rotation of nuclei have been developed. As a microscopic theory, the cranking model \cite{3} has been proposed. The Inglis formula \cite{4} and the Belyaev
formula \[5\] have been derived for the moment-of-inertia from the cranking model. The Thouless-Valatin formula \[6\] has been obtained in connection to the random phase approximation (RPA). The angular momentum projection (AMP) has been developed \[3, 7–12\], in which the degenerate intrinsic states along the NG mode are superposed. The AMP enables to calculate rotational energies straightforwardly. The \(J(J+1)\) rule of the excitation energy with the moment-of-inertia is derived from the AMP under a reasonable approximation for well-deformed heavy nuclei \[3, 7, 8, 13–15\]. However, for light or weakly-deformed nuclei, it has not yet become clear whether the same arguments hold.

In the classical mechanics, the rotational energy arises from the kinetic energy. However, the rotational band in nuclei should be formed from the effective Hamiltonian. In principle, the nucleonic interaction originates from the quantum chromodynamics (QCD) \[16\]. However, it is not yet easy to derive the nucleonic interaction from the QCD which is applicable to a variety of nuclei with good accuracy. Because the nucleonic interactions are mediated by mesons which have masses, they are represented by the Yukawa functions \[17\]. The nucleonic interactions also have spin-dependence, both in central and noncentral channels. The spin-dependent forces could contribute to the rotational energy.

The Michigan-three-range-Yukawa (M3Y)-type interactions \[18–20\] are composed of the Yukawa functions except for density-dependent terms. The parameters of the effective interactions have been determined based on the G-matrix with some phenomenological modifications \[19\]. In this respect, the M3Y-type interactions are \textit{semi-realistic} effective interactions. The tensor force is also included, whose parameters are fixed from the G-matrix. The MF calculations using the M3Y-P6 have described well the magic number of nuclei over a wide range of the nuclear chart \[21\]. Because it has a certain connection to the bare nucleonic interaction and is applicable to self-consistent MF calculations including deformation, the M3Y-type interaction is suitable for studying the origin of the rotational band of nuclei.

Under these backgrounds, we shall re-examine and reveal from the microscopic point of view how the rotational band of nuclei is formed. For this purpose, the AMP is applied to the MF wave functions obtained by self-consistent axial-HF calculations using the effective interaction M3Y-P6. The contributions of the individual terms of the semi-realistic Hamiltonian are focused on; in concrete, those of the kinetic energy, the density-independent and dependent central forces, the LS force, the tensor force, and the central part of the one-pion-exchange-potential (OPEP), which is the longest range term and an example of
spin-dependent channels. Additionally, we present a general formulation for the rotational energy. The derived formula is a generalization of the previous ones in Ref. \[3, 7, 8, 13–15\], while the additional terms could be important in the rotational energy and the moment-of-inertia for light or weakly-deformed nuclei.

II. THEORETICAL BACKGROUND

A. Theory of AMP and rotation

The AMP is the method by which an intrinsic state is projected on angular momentum eigenstates \[3\]. In the following, we assume that \(\hat{S}\) is a scalar operator about the three-dimensional rotation, and the intrinsic state is an eigenstate of \(\hat{J}_z\) whose eigenvalue is \(M\).

The intrinsic state \(|\Phi_M\rangle\) is expanded by angular momentum eigenstates \(|JM\rangle\),

\[
|\Phi_M\rangle = \sum_J |JM\rangle \langle JM|\Phi_M\rangle, \tag{1}
\]

where we omit indices other than \(J\) and \(M\) for simplicity. The projection operator on the angular momentum eigenstates \(\hat{P}_{MM}^{(j)}\) is a special case of Eq. (A4), which is hermitian and idempotent,

\[
(\hat{P}_{MM}^{(j)})^\dagger = \hat{P}_{MM}^{(j)}, \tag{2a}
\]
\[
(\hat{P}_{MM}^{(j)})^2 = \hat{P}_{MM}^{(j)}. \tag{2b}
\]

By using the orthogonal property of the Wigner D-function in Eq. (A3), the projection operator is represented by the rotational operator in Eq. (A1) and the Wigner D-function in Eq. (A2) (see also Eq. (A4)). The expectation values of the scalar operator \(\hat{S}\) on the angular momentum eigenstates are represented as follows,

\[
\langle J|\hat{S}|J\rangle = \frac{\langle \Phi_M|\hat{P}_{MM}^{(j)}\hat{S}\hat{P}_{MM}^{(j)}|\Phi_M\rangle}{\langle \Phi_M|\hat{P}_{MM}^{(j)}\hat{P}_{MM}^{(j)}|\Phi_M\rangle} = \frac{\langle \Phi_M|\hat{S}\hat{P}_{MM}^{(j)}|\Phi_M\rangle}{\langle \Phi_M|\hat{P}_{MM}^{(j)}|\Phi_M\rangle} \tag{3}
\]

\[
= \frac{\int_0^\pi d\beta \sin \beta d_{MM}^{(j)}(\beta) \langle \Phi_M|\hat{S} e^{-i\hat{J}_y}\beta|\Phi_M\rangle}{\int_0^\pi d\beta \sin \beta d_{MM}^{(j)}(\beta) \langle \Phi_M|e^{-i\hat{J}_y}\beta|\Phi_M\rangle},
\]
where $\beta$ is the Euler angle around the $y$-axis and $d_{MM}^{(J)}(\beta)$ is the Wigner small d-function in Eq. (A22). Because the intrinsic state is the eigenstate of $\hat{J}_z$, the integrals of $\alpha$ and $\gamma$ in Eq. (A4) are done analytically. Though the LHS of Eq. (3) may look depending on the index $M$, it is omitted with taking into account the rotational symmetry.

By using the property of the Wigner d-function \[ d^{(J)}_{MM}(-\beta) = d^{(J)}_{MM}(\beta), \] the following relation is derived for $\hat{S}$ and $|\Phi_M\rangle$,

\[
\langle \Phi_M | \hat{S} e^{-i\hat{J}_y \beta} | \Phi_M \rangle = \sum_J | \langle J \Phi_M | \hat{S} e^{-i\hat{J}_y \beta} | \Phi_M \rangle |^2 \langle J | \hat{S} | J \rangle d^{(J)}_{MM}(\beta) \\
= \langle \Phi_M | \hat{S} e^{i\hat{J}_y \beta} | \Phi_M \rangle.
\]

(4)

Because of the property of even functions,

\[
d_{2n+1}^{2n+1} | \langle \Phi_M | \hat{S} e^{-i\hat{J}_y \beta} | \Phi_M \rangle |_{\beta=0} = 0, \quad (n = 0, 1, 2, \ldots),
\]

(5)
we have,

\[
\langle \Phi_M | \hat{S} \hat{J}_y^{2n+1} | \Phi_M \rangle = 0,
\]

(6)

whose particular case is $\langle \Phi_M | \hat{J}_y | \Phi_M \rangle = 0$. The fluctuation of an operator $\hat{A}$ is defined as $\sigma[A] := \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$. The relation of the overlap function $\langle \Phi_M | e^{-i\hat{J}_y \beta} | \Phi_M \rangle$ and the fluctuation of $\hat{J}_y$ is,

\[
\frac{d^2}{d\beta^2} \langle \Phi_M | e^{-i\hat{J}_y \beta} | \Phi_M \rangle |_{\beta=0} = -(\sigma[\hat{J}_y])^2.
\]

(7)

In the points or regions of $\langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle \neq 0$, the following function is defined,

\[
S^{01}(\beta) := \frac{\langle \Phi_M | \hat{S} e^{-i\hat{J}_y \beta} | \Phi_M \rangle}{\langle \Phi_M | e^{-i\hat{J}_y \beta} | \Phi_M \rangle},
\]

(8)

which is an even function of $\beta$. The correlation function between operators $\hat{A}$ and $\hat{B}$ is defined as $C[\hat{A}, \hat{B}] := \langle \hat{A} \hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$. The above $S^{01}(\beta)$ is related to the correlation function between $\hat{S}$ and $\hat{J}_y^2$ as follows,

\[
\frac{d^2}{d\beta^2} S^{01}(\beta) |_{\beta=0} = -C[\hat{S}, \hat{J}_y^2].
\]

(9)

The following equations hold,

\[
(\sigma[\hat{J}_x])^2 = (\sigma[\hat{J}_y])^2 = \frac{1}{2} \left( \langle \Phi_M | \hat{J}_y^2 | \Phi_M \rangle - M^2 \right),
\]

(10a)

\[
C[\hat{S}, \hat{J}_x^2] = C[\hat{S}, \hat{J}_y^2] = \frac{1}{2} C[\hat{S}, \hat{J}_y^2].
\]

(10b)
The \( J(J+1) \) rule of rotational energy and the moment-of-inertia of nuclei connected with Eq. (3) were discussed in Refs. [3, 7, 8, 13–15]. If the overlap function \( \langle \Phi_0 | e^{-i\hat{J}_y\beta} | \Phi_0 \rangle \) has a sharp peak at \( \beta \approx 0 \), the energy spectrum is close to the \( J(J+1) \) rule. However, it is not always clear whether \( \langle \Phi_0 | e^{-i\hat{J}_y\beta} | \Phi_0 \rangle \) has a sharp peak at \( \beta \approx 0 \). In the following, we present a more general argument on the rotational energy than those in Refs. [7, 13] by using the cumulant expansion (see Appendix B). This formulation is useful in some cases, as will be discussed in Section III.

Let us consider the case of the even-even nuclei with \( M = 0 \). In the case of \( M \neq 0 \), the following formulation can be extended almost straightforwardly. We further assume the reflection symmetry with respect to the \( x-y \) plane which is called \( \hat{R} \) symmetry,

\[
\hat{R} |\Phi_0 \rangle = |\Phi_0 \rangle, \\
\hat{R} := e^{-i\hat{J}_y\pi}.
\]

Then, by using Eq. (4), the following equation is derived,

\[
\langle \Phi_0 | \hat{S} e^{-i\hat{J}_y(\pi-\beta)} | \Phi_0 \rangle = \langle \Phi_0 | \hat{S} e^{-i\hat{J}_y\beta} | \Phi_0 \rangle.
\]

From Eq. (12) and \( d^{(J)}_{00}(\pi - \beta) = (-)^J d^{(J)}_{00}(\beta) \), \( \langle \Phi_0 | \hat{S} \hat{J}^{(J)}_{00} | \Phi_0 \rangle = 0 \) follows for odd \( J \). Thus, \( \langle J | \hat{S} | J \rangle \) is meaningful only for even \( J \), and the range of \( \beta \) integration can be reduced to \([0, \pi/2]\) [11, 13].

The Wigner d-function can be expanded by the power series of \( \beta \) as follows,

\[
d^{(J)}_{00}(\beta) = \sum_{n=0}^{\infty} c_{2n}\beta^{2n}, \\
c_{2n} = \frac{(-)^n}{(2n)!} \langle J0 | \hat{J}^{2n}_y | J0 \rangle \\
= \frac{\langle J0 | (\hat{J}_+ - \hat{J}_-)^{2n} | J0 \rangle}{(2n)! 2^{2n}},
\]

where \( \hat{J}_+ := \hat{J}_x + i\hat{J}_y \), \( \hat{J}_- := (\hat{J}_+)^\dagger \). Equation (13b) leads to,

\[
c_0 = 1, \\
c_2 = -\frac{1}{2! 2} J(J+1), \\
c_4 = \frac{1}{4! 2^3} J(J+1) [3J(J+1) - 2], \ldots.
\]
The coefficient $c_{2n}$ depends only on $J$. In terms of the cumulant in Eq. (B5), $S^{01}(\beta)$ in Eq. (8) is expanded as follows,

$$S^{01}(\beta) = \sum_{n=0}^{\infty} s_{2n} \beta^{2n},$$  \hspace{1cm} (15a)

$$s_{2n} = \frac{(-\beta)^n}{(2n)!} \langle \Phi_0 | \hat{S}; \hat{J}_y; \cdots; \hat{J}_y | \Phi_0 \rangle_{\text{cum}}. \hspace{1cm} (15b)$$

Equation (15b) leads to,

$$s_0 = \langle \Phi_0 | \hat{S} | \Phi_0 \rangle, \hspace{1cm} (16a)$$

$$s_2 = -\frac{1}{2!} C[\hat{S}, \hat{J}_y^2], \hspace{1cm} (16b)$$

$$s_4 = \frac{1}{4!} \left( C[\hat{S}, \hat{J}_y^4] - 6 C[\hat{S}, \hat{J}_y^2](\sigma[\hat{J}_y]^2) \right), \cdots. \hspace{1cm} (16c)$$

The coefficient $s_{2n}$ is independent of $J$, depending only on $|\Phi_0\rangle$ and $\hat{S}$. By defining the following quantities,

$$N_{2n} := \int_0^{\pi/2} d\beta \sin \beta \beta^{2n} \langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle, \hspace{1cm} (17a)$$

$$A_{2n} := \frac{N_{2n}}{N_0}, \hspace{1cm} (n = 0, 1, 2, \cdots), \hspace{1cm} (17b)$$

which are determined only by $|\Phi_0\rangle$, Eq. (8) is represented as follows,

$$\langle J | \hat{S} | J \rangle = \frac{\int_0^{\pi/2} d\beta \sin \beta \beta^{2n} \langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle S^{01}(\beta)}{\int_0^{\pi/2} d\beta \sin \beta d_{00}^{(J)}(\beta) \langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle} \sum_{m,n=0}^{\infty} c_{2m}s_{2n}N_{2m+2n}$$

$$= \sum_{\ell=0}^{\infty} c_{2\ell} N_{2\ell} \sum_{m,n=0}^{\infty} c_{2m}s_{2n}A_{2m+2n}$$

$$= \sum_{\ell=0}^{\infty} c_{2\ell} A_{2\ell}. \hspace{1cm} (18)$$

In the case of $J = 0$, $c_{2n}$ equals to zero for $n \geq 1$, and the following equation is obtained,

$$\langle 0 | \hat{S} | 0 \rangle = \sum_{n=0}^{\infty} s_{2n} A_{2n}$$

$$= \langle \Phi_0 | \hat{S} | \Phi_0 \rangle + \sum_{n=1}^{\infty} s_{2n} A_{2n}. \hspace{1cm} (19)$$
Let us assume,
\[ \left| \sum_{n=1}^{\infty} c_{2n} A_{2n} \right| < 1. \] (20)

We then expand Eq. (18) as follows,
\[
\langle J | \hat{S} | J \rangle = \left( \sum_{m,n=0}^{\infty} s_{2n} c_{2m} A_{2n+2m} \right) \left( 1 + \sum_{\ell=1}^{\infty} c_{2\ell} A_{2\ell} \right)^{-1} \\
= \left( \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} s_{2n} c_{2m} A_{2n+2m} \right) \\
\times \left[ 1 - \sum_{\ell=1}^{\infty} c_{2\ell} A_{2\ell} + \left( \sum_{\ell=1}^{\infty} c_{2\ell} A_{2\ell} \right)^2 - \cdots \right]. \] (21)

In order to analyze \( J \) dependence of \( \langle J | \hat{S} | J \rangle \), it is appropriate to arrange Eq. (21) by \( c_{2n} \) as follows because \( c_{2n} \sim J^{2n} \),
\[
\langle J | \hat{S} | J \rangle = \left( \sum_{n=0}^{\infty} s_{2n} A_{2n} + c_2 \sum_{n=0}^{\infty} s_{2n} A_{2n+2} + c_4 \sum_{n=0}^{\infty} s_{2n} A_{2n+4} + \cdots \right) \\
\times \left[ 1 - (c_2 A_2 + c_4 A_4 + \cdots) + (c_2 A_2)^2 + \cdots \right] \\
= \sum_{n=0}^{\infty} s_{2n} A_{2n} + c_2 \sum_{n=0}^{\infty} s_{2n} (A_{2n+2} - A_{2n} A_2) \\
+ c_4 \left( \sum_{n=1}^{\infty} s_{2n} (A_{2n+4} - A_{2n} A_4) \right) \\
- (c_2)^2 \left( \sum_{n=1}^{\infty} s_{2n} [A_{2n+2} A_2 - A_{2n} (A_2)^2] \right) + \cdots. \] (22)

Compared with the Kamlah expansion \([3, 15]\), the cumulant expansion of Eq. (15) enables a more organized expansion. We call the \( n \geq 2 \) terms of \( c_{2n} \) higher-\( c_{2n} \)-terms, and those of \( s_{2n} \) higher-\( s_{2n} \)-terms. If the higher-\( c_{2n} \)-terms are neglected, Eq. (22) is approximated as,
\[
\langle J | \hat{S} | J \rangle \approx \langle 0 | \hat{S} | 0 \rangle + \frac{J (J + 1)}{2 \mathcal{I}[\hat{S}]} , \] (23)
where,
\[
\frac{1}{\mathcal{I}[\hat{S}]} := \sum_{n=1}^{\infty} s_{2n} \left[ -\frac{1}{2} (A_{2n+2} - A_{2n} A_2) \right]. \] (24)

For \( \hat{S} = \hat{H} \), where \( \hat{H} \) is the Hamiltonian, the parameter \( \mathcal{I}[\hat{H}] \) is interpreted as the moment-of-inertia. If the higher-\( s_{2n} \)-terms are neglected in Eqs. (19) and (24), \( \langle 0 | \hat{S} | 0 \rangle \) and \( \mathcal{I}[\hat{S}] \) are
approximated as,

\[ \langle 0 | \hat{S} | 0 \rangle \approx \langle \Phi_0 | \hat{S} | \Phi_0 \rangle - \frac{1}{2} C[\hat{S}, \hat{J}_y^2] A_2, \]  
\[ \frac{1}{\mathcal{I}[\hat{S}]} \approx \frac{1}{4} C[\hat{S}, \hat{J}_y^2] [A_4 - (A_2)^2]. \]  

Equation (25b) is the Peierls-Yoccoz moment-of-inertia \[7, 13\]. Further approximation based on the Gaussian approximation \[3, 8, 14, 15\] is discussed in Appendix C. Equation (24) is regarded as a generalization of Eq. (25b). From Eqs. (19), (24) and (25), it is noticed that the higher-s\(_{2n}\)-terms may contribute to \( \langle 0 | \hat{S} | 0 \rangle \) and \( \mathcal{I}[\hat{S}] \). We shall see such a situation in Sec. III B.

B. Semi-realistic effective Hamiltonian

We have implemented AMP calculations in Eq. (3) for the axial-HF solutions using the semi-realistic interaction M3Y-P6 \[19, 20, 24–26\]. It is the first application of the M3Y-type interactions to the AMP calculations.

Because nuclei are finite and isolate systems, their effective Hamiltonian should have rotational, parity, and time-reversal symmetry, with number conservation. We assume that the individual terms of the Hamiltonian also have isospin symmetries except for the Coulomb force. The Hamiltonian is composed of the following terms,

\[ H = K + V_{\text{nucl}} + V_{\text{Coulomb}} - H_{\text{c.m.}}. \]  

The kinetic energy is \( K = \sum_i p_i^2 / 2M \), the nucleonic interaction is \( V_{\text{nucl}} := \sum_{i < j} v_{ij} \), the Coulomb interaction between protons is denoted as \( V_{\text{Coulomb}} \), and the center-of-mass term is \( H_{\text{c.m.}} = P^2 / 2AM \), with the total momentum \( P = \sum_i p_i \) and the mass number \( A = Z + N \).

The effective nucleonic interaction is formed by the following terms,

\[ V_{\text{nucl}} = V^{(C)} + V^{(LS)} + V^{(TN)} + V^{(C\rho)}, \]  
\[ V^{(X)} := \sum_{i < j} v^{(X)}_{ij}, \quad (X = C, LS, TN, C\rho), \]  

where \( V^{(C)} \), \( V^{(LS)} \), and \( V^{(TN)} \) are the central, the LS, and the tensor forces. The central density-dependent term is distinguished from \( V^{(C)} \) and represented by \( V^{(C\rho)} \). The individual terms of Eq. (27a) have the following forms,
\[
v_{ij}^{(C)} = \sum_n \left( t_n^{(SE)} P_{SE} + t_n^{(TE)} P_{TE} + t_n^{(SO)} P_{SO} + t_n^{(TO)} P_{TO} \right) f_n^{(C)}(r_{ij}),
\]
\[
v_{ij}^{(LS)} = \sum_n \left( t_n^{(LSE)} P_{TE} + t_n^{(LSO)} P_{TO} \right) f_n^{(LS)}(r_{ij}) L_{ij} \cdot (s_i + s_j),
\]
\[
v_{ij}^{(TN)} = \sum_n \left( t_n^{(TNE)} P_{TE} + t_n^{(TNO)} P_{TO} \right) f_n^{(TN)}(r_{ij}) \hat{r}_{ij}^2 S_{ij},
\]
\[
v_{ij}^{(C\rho)} = \left( t_\rho^{(SE)} P_{SE} \cdot \rho(r_i) \right)^{\alpha^{(SE)}} + t_\rho^{(TE)} P_{TE} \cdot \rho(r_i)^{\alpha^{(TE)}} \right) \delta(r_{ij}),
\]
where \( r_{ij} := r_i - r_j, \hat{r}_{ij} := |r_{ij}|, \hat{r}_{ij} := r_{ij}/r_{ij}, p_{ij} := (p_i - p_j)/2, L_{ij} := r_{ij} \times p_{ij}, \)
\[
S_{ij} := 3(\sigma_i \cdot \hat{r}_{ij})(\sigma_j \cdot \hat{r}_{ij}) - \sigma_i \cdot \sigma_j.
\]

The spin-exchange operator and isospin-exchange operator between two nucleons whose indices are \( i \) and \( j \), are defined as,
\[
P_\sigma := \frac{1 + \sigma_i \cdot \sigma_j}{2}, \quad P_\tau := \frac{1 + \tau_i \cdot \tau_j}{2},
\]
then the projection operators on singlet-even (SE), triplet-even (TE), singlet-odd (SO), and triplet-odd (TO) channels are defined as,
\[
P_{SE} := \frac{1 - P_\sigma}{2} \frac{1}{2} + P_\tau \frac{2}{2}, \quad P_{TE} := \frac{1 + P_\sigma}{2} \frac{1}{2} - P_\tau \frac{2}{2},
\]
\[
P_{SO} := \frac{1 - P_\sigma}{2} \frac{2}{2} - P_\tau \frac{2}{2}, \quad P_{TO} := \frac{1 + P_\sigma}{2} \frac{2}{2} + P_\tau \frac{2}{2}.
\]

We use the Yukawa function \( f_n(r) = e^{-\mu_n r}/(\mu_n r) \) for the radial functions, except for the density-dependent term. The density-dependent term contains the Dirac’s delta function. The longest range term in \( v_{ij}^{(C)} \) is fixed to be that of the OPEP. This central OPEP, which is denoted by \( V^{(OPEP)} \), is an example of spin-dependent interactions. The values of the parameters for M3Y-P6 are given in Ref. [19].

\textbf{C. Implementation of AMP}

In this work, we apply the projection after variation (PAV) for the AMP. The numerical method of Eq. \( [3] \) has been discussed in Refs. \([3, 11]\). Some details of Eq. \( [3] \) for non-orthogonal bases are given in Appendices \([D] \) and \([E] \). While the intrinsic state could gradually change for increasing \( J \), such effects are ignored in the present study. Furthermore, the AMP calculations for the HFB solutions are left for future works.
The Gaussian expansion method (GEM) has been applied in which complex range Gaussian bases are used to expand the radial part of the single-particle wave function \[27, 28\]. The angular function is the spinor-spherical-harmonics. The advantages of the GEM in the MF calculations are taken over to the AMP calculations. Additionally, the spherical bases enable precise numerical calculations of the AMP relatively easily.

The parity, the time-reversal, and the reflection operator (see Eq. (11)) are represented as \( \hat{P} \), \( \hat{T} \), and \( \hat{R} \), respectively. For the sake of simplicity, we say “\( \hat{O} \) symmetry” when \( \hat{O} |\Phi_0\rangle = |\Phi_0\rangle \) is satisfied. In the MF calculations, \( \hat{P} \), \( \hat{T} \), \( \hat{R} \), and axial symmetries are assumed. The MF solutions are represented by real numbers (\( U_{ki} \) and \( V_{ki} \) for HFB in Eq. (D5)), owing to the \( \hat{R}\hat{T} \) symmetry. The MF state \( |\Phi_0\rangle \) is a direct product of the parts having specific isospin and parity,

\[
|\Phi_0\rangle = |\Phi_0(p+)\rangle \otimes |\Phi_0(p-)\rangle \otimes |\Phi_0(n+)\rangle \otimes |\Phi_0(n-)\rangle.
\]  

(32)

The overlap function \( \langle \Phi_0 | e^{-i\hat{J}_y\beta} | \Phi_0 \rangle \) has been calculated by the Onishi formula \[9\] (see Eq. (D22)),

\[
\langle \Phi_0 | e^{-i\hat{J}_y\beta} | \Phi_0 \rangle = \sqrt{\text{det} T_{22}^{\beta}},
\]  

(33)

where \( \beta \) in the RHS of Eq. (33) is a shorthand notation of \( \Omega = (\alpha = 0, \beta, \gamma = 0) \). The sign problem of the Onishi formula is well-known, and some solutions have been proposed \[29, 30\]. In the present work, we have confirmed that this sign problem does not seriously influence the results, probably owing to the above symmetries and even-even nuclei. The sign of the square root has been chosen positive in Eq. (33) for any \( \beta \), which is consistent with \( \langle \Phi_0 | \Phi_0 \rangle = 1 \).

There is also an unclear problem in the treatment of the density-dependent coefficients in \( v_{ij}^{(C\rho)} \) in the AMP calculations \[12, 31\]. The density-dependent term in Eq. (28) is not a scalar operator when the density does not have the spherical symmetry. In the present calculations, the standard treatment in Ref. \[11\] has been adopted, replacing the density \( \rho(r) \) in Eq. (28) with “generalized density” \( \bar{\rho}(r; \beta) \) in Eq. (E8). However, a problem has occurred: there is a case in which the generalized density \( \bar{\rho}(r; \beta) \) becomes negative and its fractional power \( \bar{\rho}^\alpha(r; \beta) \) may become multivalued. In the M3Y-P6 interaction, the fractional powers \( \alpha \) are \( \alpha^{(SE)} = 1 \) and \( \alpha^{(TE)} = 1/3 \) \[19\]. The phase of \( \bar{\rho}^\alpha(r; \beta) \) has been chosen negative when
$\tilde{\rho}(r; \beta)$ is negative. For the scalar operator $\hat{S}$, the following equation should hold,

$$
\langle \Phi_0 | \hat{S} | \Phi_0 \rangle = \sum_J \langle \Phi_0 | \hat{S} \hat{d}^{(J)}_{00} | \Phi_0 \rangle = \sum_J (2J + 1) \int_0^{\pi/2} d\beta \sin \beta d^{(J)}_{00} (\beta) \langle \Phi_0 | \hat{S} e^{-iJy\beta} | \Phi_0 \rangle.
$$

(34)

When $\hat{V}^{(C\rho)}[\tilde{\rho}(r)]$ is substituted for $\hat{S}$ in the LHS and $\hat{V}^{(C\rho)}[\bar{\rho}(r; \beta)]$ in the RHS of Eq. (34), there is no mathematical guarantee that Eq. (34) holds. Nonetheless, in the present calculations, Eq. (34) is satisfied for $\hat{V}^{(C\rho)}$ comparably well to those for the other terms of the Hamiltonian in Eqs. (26) and (27).

III. NUMERICAL RESULTS

In the present work, the AMP calculations have been applied to deformed $^{12}{\text{Mg}}$ [20, 24], $^{40}{\text{Zr}}$ [26], $^{60}{\text{Nd}}$ and $^{62}{\text{Sm}}$ isotopes, including stable and unstable nuclei. An important evidence for the deformation is their ratios of excitation energies $E_x(4^+)/E_x(2^+)$ close to 10/3 [2, 32–34]. $^{12}{\text{Mg}}$ is known as a light stable well-deformed nucleus. $^{34}{\text{Mg}}$ is a well-deformed unstable nucleus in the island of inversion [34], $^{40}{\text{Mg}}$ is near the neutron dripline [35], and a deformed halo structure of the intrinsic state has been suggested [25]. $^{80}{\text{Zr}}$ is a deformed unstable nucleus near the proton dripline [36]. $^{100-110}{\text{Zr}}$ are neutron-rich well-deformed nuclei [2, 32, 33]. $^{150-154}{\text{Nd}}$ and $^{152-156}{\text{Sm}}$ are well-known as deformed nuclei [1, 2, 37].

A. Contribution of individual terms of effective Hamiltonian to rotational energy

In this subsection, we present composition of rotational energy. The expectation values of the individual terms of the effective Hamiltonian on angular momentum eigenstates are calculated, respectively. The following quantity is defined,

$$
S_x(J^+) := \langle J^+ | \hat{S} | J^+ \rangle - \langle 0^+ | \hat{S} | 0^+ \rangle,
$$

for an scalar operator $\hat{S}$. For $\hat{S} = \hat{H}$, Eq. (35) corresponds with the excitation energy,

$$
E_x(J^+) = \langle J^+ | \hat{H} | J^+ \rangle - \langle 0^+ | \hat{H} | 0^+ \rangle.
$$

(36)
By taking \( \hat{S} \) to be individual terms of \( \hat{H} \), the values \( S_x(J^+) \) give their contributions to the rotational energy. In the following, \( \hat{S} \) is an element of the following set,

\[
\hat{S} \in \{ \hat{H}, \hat{K}, \hat{V}^{(C)}, \hat{V}^{(LS)}, \hat{V}^{(TN)}, \hat{V}^{(C\rho)}, \hat{V}^{\text{OPEP}} \},
\]

where details of the effective Hamiltonian have been described in Section IIIB.

![Graph](image)

**FIG. 1.** The ratios \( E_x(J^+)/E_x(2^+) \) and \( S_x(J^+)/S_x(2^+) \) for the deformed \(^{80,100,104}\text{Zr}, \(^{154}\text{Nd}, \) and \(^{154}\text{Sm} \) nuclei at their lowest minima. The white circles are the ratios \( E_x(J^+)/E_x(2^+) \) of experiments \(^2\), and the black circles are those obtained by the present work. The ratios \( S_x(J^+)/S_x(2^+) \) are also shown for \( \hat{S} = \hat{K} \) (red circles), \( \hat{S} = \hat{V}^{(C)} \) (blue circles), \( \hat{S} = \hat{V}^{(LS)} \) (yellow circles), \( \hat{S} = \hat{V}^{(TN)} \) (green circles), \( \hat{S} = \hat{V}^{(C\rho)} \) (pink circles), and \( \hat{S} = \hat{V}^{\text{OPEP}} \) (sky-blue circles). The rigid-rotor value of \( J(J+1)/6 \) is presented by the horizontal lines.

The ratios of the individual terms in the effective Hamiltonian \( S_x(J^+)/S_x(2^+) \) have been calculated as well as the ratio of the total excitation energy \( E_x(J^+)/E_x(2^+) \). The results for the deformed \(^{40}\text{Zr}, \(^{154}\text{Nd}, \) and \(^{154}\text{Sm} \) nuclei at their lowest minima are shown in Fig. 1. The ratios \( E_x(4^+)/E_x(2^+) \) obtained by the present work are close to those of the experiments and 10/3. The values of \( S_x(J^+) \) are negative for \( \hat{V}^{(TN)} \) and \( \hat{V}^{(C\rho)} \) as will be shown in Fig. 3. As well as \( E_x(J^+)/E_x(2^+), S_x(J^+)/S_x(2^+) \) well obeys the \( J(J+1) \) rule, up to high angular momentum \( J \approx 12 \). As \( J \) increases, the ratios slightly deviate from the \( J(J+1) \) line. The experimental values gradually get smaller than the \( J(J+1) \) line in many nuclei at high \( J \). Additional quantum correlations such as the shape mixing, a part of which can be handled via the variation after projection (VAP) \(^3,11\), should be considered in order to reproduce experimental values more accurately.
FIG. 2. The ratios $E_x(J^+)/E_x(2^+)$ and $S_x(J^+)/S_x(2^+)$ for the deformed $^{12}$Mg isotopes at their lowest minima. The white circles are the experimental values of $E_x(J^+)/E_x(2^+)$ for $^{24}$Mg [2], $^{34-38}$Mg [34], and $^{40}$Mg [38]. For $^{40}$Mg, the spin and parity of the excited states have not been confirmed yet. See Fig. 1 for conventions.

In Fig. 2, the ratios $E_x(J^+)/E_x(2^+)$ and $S_x(J^+)/S_x(2^+)$ for the deformed $^{12}$Mg isotopes at their lowest minima are shown. Note that for $^{40}$Mg, the spin and parity of the excited states have not yet been confirmed experimentally. The ratios $E_x(4^+)/E_x(2^+)$ obtained by the present work are close to those of the experiments and 10/3 except for $^{40}$Mg. The ratios $S_x(4^+)/S_x(2^+)$ are also close to 10/3, as well. As $J$ increases, the ratios deviate from the $J(J+1)$ lines.

FIG. 3. The ratios $S_x(2^+)/E_x(2^+)$ for the deformed nuclei at their lowest minima.
Because the ratios $S_x(4^+)/S_x(2^+)$ are close to 10/3 irrespective of $\hat{S}$ and nuclides in Figs. 1 and 2, we focus on compositions of the first excitation energies $E_x(2^+)$. Figure 3 shows the ratios $S_x(2^+)/E_x(2^+)$ at their lowest minima, all of which have prolate shapes. Except for the $^{12}$Mg region, these ratios are insensitive to nuclides. The contributions of $\hat{K}$, $\hat{V}^{(C)}$, and $\hat{V}^{(C\rho)}$ are about 75%, 75%, and -50%, respectively. The large positive contribution of $\hat{K}$ is harmonious with the rotational energy in classical mechanics. Both $\hat{V}^{(C)}$ and $\hat{V}^{(C\rho)}$ give sizable contributions, although they tend to cancel each other to certain extent. The contributions of $\hat{V}^{(LS)}$ and $\hat{V}^{(TN)}$ are small. These noncentral forces mainly contribute near the surface of nuclei. Therefore, these forces become relatively small compared to the central forces when the mass number increases. In the $^{12}$Mg region, the ratios significantly depend on nuclei. The LS force widens the rotational band, and the tensor force narrows it, whose ratios are large compared to those of $^{80,104}$Zr, $^{154}$Nd, and $^{154}$Sm nuclei. Regardless of nuclides, $\hat{V}^{(C)}$ and $\hat{V}^{(LS)}$ act attractively, and $\hat{V}^{(TN)}$ and $\hat{V}^{(C\rho)}$ do repulsively on the binding energies. The contributions of the formers are positive, and those of the latters are negative for the rotational energies. In other words, the attractive forces decrease the moment-of-inertia of nuclei, and the repulsive forces increase it. The contributions of $\hat{V}^{(OPEP)}$ are about 10 % at most. The contributions of $\hat{V}_{\text{Coulomb}}$ and $\hat{H}_{\text{c.m.}}$ to the excitation energies are no more than a few percent. The latter results indicate that the center-of-mass motion and the rotational motion, both of which are NG modes in the MF approximation, hardly couple each other.
FIG. 4. The $a_{20}$ (quadrupole deformation parameter) dependence of $E_x(J^+)/E_x(2^+)$ for the $^{34}_{12}$Mg, $^{40}_{12}$Mg, $^{80}_{40}$Zr, and $^{154}_{60}$Nd nuclei. Their lowest minima are represented by the filled circles. The $J(J+1)/6$ values are presented by the horizontal lines.

We define the quadrupole deformation parameter $a_{20}$ as follows:

$$q_0 =: 1.09A^{5/3}a_{20},$$

(38)

where $q_0$ is the mass quadrupole moment of the MF state. Figure 4 shows the $a_{20}$ dependence of $E_x(J^+)/E_x(2^+)$ for energy minima of the $^{34}_{12}$Mg, $^{40}_{12}$Mg, $^{80}_{40}$Zr, and $^{154}_{60}$Nd nuclei, including their local minima. The values of $a_{20}$ for the lowest minima of $^{34}_{12}$Mg, $^{40}_{12}$Mg, $^{80}_{40}$Zr, and $^{154}_{60}$Nd are 0.56, 0.47, 0.52, and 0.31, respectively. The ratios $E_x(4^+)/E_x(2^+)$ are close to 10/3 irrespective of nuclides. For low $J$, the ratios are close to the $J(J+1)$ line, which indicates that the approximation in Eq. (23) is good. For the $^{80}_{40}$Zr and $^{154}_{60}$Nd nuclei, the ratios become closer to the $J(J+1)$ line up to high $J$ as $|a_{20}|$ increases. For the $^{34,40}_{12}$Mg nuclei or the minima having small $|a_{20}|$ values, the $J(J+1)$ rule gets deviating as $J$ increases, though the intrinsic states are fixed. This deviation indicates that the higher-$c_{2n}$-terms are not negligible in Eq. (22).
FIG. 5. The $a_{20}$ dependence of $S_x(4^+)/S_x(2^+)$ for $K$ (red circle), $V^{(C)}$ (blue squares), $V^{(LS)}$ (yellow stars), $V^{(TN)}$ (green triangles), $V^{(C\rho)}$ (pink diamonds), and $V^{(OPEP)}$ (sky-blue pluses).

In Fig. 5 the $a_{20}$ dependence of $S_x(4^+)/S_x(2^+)$ is shown. For $^{80}_{40}$Zr and $^{154}_{60}$Nd, the ratios are close to $10/3$, which is almost independent of $a_{20}$ and $\hat{S}$ with only a few exceptions. For $a_{20} = 0.56$ of $^{34}_{12}$Mg and $a_{20} = 0.47$ of $^{40}_{12}$Mg, the ratios are also close to $10/3$, which is independent of $\hat{S}$. However, at the other minima of $^{34,40}_{12}$Mg, the results strongly depend on $a_{20}$ and $\hat{S}$. 
In Fig. 6 the $a_{20}$ dependence of the ratio $S_x(2^+)/E_x(2^+)$ is shown. For $^{80}_{40}$Zr and $^{154}_{60}$Nd, the ratios become almost constant for $a_{20}$. The contributions of $\hat{V}^{(C)}$ and $\hat{V}^{(LS)}$ become positive, and those of $\hat{V}^{(C_p)}$ and $\hat{V}^{(TN)}$ does negative as $|a_{20}|$ increases. The ratios of these interactions fluctuate in the regions where $|a_{20}|$ is not large, although the ratios of $\hat{K}$ are almost independent of the deformation parameter and nuclides. For $^{34,40}_{12}$Mg nuclei, the ratios strongly depend on the individual MF states. For $^{40}_{12}$Mg, we find an extraordinary result that the ratio of $\hat{K}$ is negative at $a_{20} = -0.34$. At this MF state, $J = 2$ gives the lowest value of $S(J^+)$ for $\hat{S} = \hat{K}$. 

**FIG. 6.** The $a_{20}$ dependence of $S_x(2^+)/E_x(2^+)$.
FIG. 7. The ground state correlations $\Delta E_{\text{g.s.c.}}$ obtained by the AMP calculations for the deformed $^{12}\text{Mg}$ (red crosses), $^{40}\text{Zr}$ (blue triangles), and $^{62}\text{Sm}$ (green squares) isotopes at their lowest minima. The horizontal axes are the mass number $A$ and the quadrupole deformation parameter $a_{20}$.

We define the ground state correlation as follows (see also Eq. (19)),

$$\Delta E_{\text{g.s.c.}} := \langle \Phi_0 | \hat{H} | \Phi_0 \rangle - \langle 0^+ | \hat{H} | 0^+ \rangle,$$

which may be compared with the 2nd term of the RHS of Eq. (25a). The values of $\Delta E_{\text{g.s.c.}}$ obtained by the AMP calculations for the deformed $^{12}\text{Mg}$, $^{40}\text{Zr}$, and $^{62}\text{Sm}$ isotopes at their lowest minima are shown in Fig. 7. While $\Delta E_{\text{g.s.c.}}$ is not sensitive to the mass number, it depends on $a_{20}$, which is a reasonable result. The correlation coefficient between $\Delta E_{\text{g.s.c.}}$ and $a_{20}$ is about 0.89, confirming a positive correlation between them. Thus, $\Delta E_{\text{g.s.c.}}$ increases as deformation of nuclei does.

B. Influence of higher-$c_{2n}$-terms and higher-$s_{2n}$-terms in Eq. (22)

In this subsection, we investigate influence of higher-$c_{2n}$-terms and higher-$s_{2n}$-terms in Eq. (22) in Sec. II A for the $^{34}_{12}\text{Mg}$, $^{40}_{12}\text{Mg}$, $^{80}_{40}\text{Zr}$, and $^{154}_{60}\text{Nd}$ nuclei, including their local minima.
FIG. 8. The $a_{20}$ dependence of $|\langle J_0|\Phi_0\rangle|^2/[(2J+1)N_0]$ in Eq. (40) for the $^{34}$Mg, $^{40}$Mg, $^{80}$Zr, and $^{154}_{60}$Nd nuclei. The colored symbols represent the various values of $a_{20}$ as presented in the insets.

We examine the condition of Eq. (20) numerically. According to Eqs. (13), (17), and (A4), we get the following relation between $\sum_{n=0}^{\infty} c_{2n} A_{2n}$ and the norm $|\langle J_0|\Phi_0\rangle|$ in Eq. (1),

$$1 + \sum_{n=1}^{\infty} c_{2n} A_{2n} = \sum_{n=0}^{\infty} c_{2n} A_{2n} = \frac{\langle \Phi_0| \tilde{P}^{(j)}|\Phi_0\rangle}{(2J+1)N_0} = \frac{|\langle J_0|\Phi_0\rangle|^2}{(2J+1)N_0} \quad (40)$$

The $a_{20}$ dependence of this quantity is shown in Fig. 8. As the angular momentum $J$ increases, the values of Eq. (40) diminish. For the well-deformed minima of $^{80}$Zr and $^{154}_{60}$Nd, they decrease more slowly than the $^{34,40}$Mg nuclei or the weakly-deformed minima. Equation (20) is satisfied for all cases investigated here unless $\langle J_0|\Phi_0\rangle = 0$. 
It is important for the $J(J + 1)$ rule in Eq. (23) that the higher-$c_{2n}$-terms are small compared to the $c_2$ term in Eq. (22). To examine influence of the higher-$c_{2n}$-terms and the higher-$s_{2n}$-terms in Eq. (22), the $a_{20}$ dependence of $A_{2n}$ and $A_{2n+2}/A_{2n}$ is shown in Fig. 9. For the well-deformed minima of $^{80}_{40}$Zr and $^{154}_{60}$Nd, the values of $A_{2n}$ are small compared to the $^{34}_{12}$Mg nuclei or the weakly-deformed minima. As $|a_{20}|$ and the mass number increases, $A_{2n+2}/A_{2n}$ decreases for fixed $n$. Small $A_{2n+2}/A_{2n}$ values help both the $J(J + 1)$ rule and the approximation of Eq. (25), although $c_{2n}$ and $s_{2n}$ also play a role.
FIG. 10. The $a_{20}$ dependence on the relative errors in Eq. (41).

We next investigate the validity of the approximation in Eq. (25). The values of $s_2$ and $s_4$ are calculated by using Eq. (15a) via numerical differentiation for $\hat{S} = \hat{H}$. In Fig. 10, the $a_{20}$ dependence of the following relative errors is shown (see also Eqs. (19), (23), (24), (36), and (39)),

$$\varepsilon_{g,s,c.}^{(k)} := \frac{-\sum_{n=1}^{k} s_{2n} a_{2n} - \Delta E_{g,s,c.}}{\Delta E_{g,s,c.}},$$  \hspace{1cm} (41a)$$

$$\varepsilon_{x}^{(k)} := \frac{3 \sum_{n=1}^{k} s_{2n} \left[-\frac{1}{2} (A_{2n+2} - A_{2n} a_{2n})\right] - E_{x}(2^+)}{E_{x}(2^+)},$$  \hspace{1cm} (41b)$$

for $k = 1, 2$. For well-deformed $^{80}$Zr and $^{154}$Nd nuclei, both $\varepsilon_{g,s,c.}^{(1)}$ and $\varepsilon_{x}^{(1)}$ are less than a few percents except for the minima having small $|a_{20}|$ values. However, the errors are not necessarily small for $^{34,40}$Mg nuclei or weakly-deformed minima. Regardless of nuclides, $|\varepsilon_{g,s,c.}^{(2)}|$ is smaller than $|\varepsilon_{g,s,c.}^{(1)}|$. Except for $a_{20} = -0.42$ of $^{34}$Mg, $|\varepsilon_{x}^{(2)}|$ is also smaller than $|\varepsilon_{x}^{(1)}|$. The contributions of the $s_4$ terms in Eq. (41) turn out to be significant for $^{34,40}$Mg nuclei or weakly-deformed minima.
### C. Angle dependence of overlap function

In this subsection, the dependence of the overlap functions \( \langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle \) and \( S^{01}(\beta) \) in Eq. (8) on the angle \( \beta \) are discussed for further understanding of the numerical results in Sections IIIA and IIIB such as the \( J(J+1) \) rule and the ratio \( S_x(2^+) / E_x(2^+) \).

![Graph showing the dependence of the overlap functions on \( \beta \) for deformed nuclei at their lowest minima. Gray lines are obtained by the Gaussian approximation in Eq. (C1).](image)

**FIG. 11.** The dependence of the overlap functions \( \langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle \) on the angle \( \beta \) for the deformed nuclei at their lowest minima. Gray lines are obtained by the Gaussian approximation in Eq. (C1).

In Fig. the dependence of the overlap functions \( \langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle \) on the angle \( \beta \) is shown for the deformed nuclei at their lowest minima. The overlap functions for the \( ^{80}_{40}\text{Zr} \) and \( ^{154}_{62}\text{Sm} \) nuclei have sharper peaks than those for the \( ^{34}_{12}\text{Mg} \) nuclei. From Eq. (7), the fluctuation \( \sigma[\hat{J}_y] \) is connected to the coefficient of the second derivative of \( \langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle \) at \( \beta = 0 \). We have calculated \( \langle \Phi_0 | \hat{J}_y^2 | \Phi_0 \rangle \), from which the values of \( \sigma[\hat{J}_y] \) are obtained (see Eq. (10a)). The values of \( \langle \sigma[\hat{J}_y] \rangle^2 \) for \( ^{24}_{12}\text{Mg} \), \( ^{34}_{12}\text{Mg} \), \( ^{80}_{40}\text{Zr} \), \( ^{104}_{40}\text{Zr} \), and \( ^{154}_{62}\text{Sm} \) are 10.1, 17.2, 51.9, 64.2, and 86.6, respectively. The Gaussian approximation in Eq. (C1) holds well except for \( \beta \approx \pi/2 \) although the overlap functions for \( ^{12}\text{Mg} \) nuclei have broad peak. In this approximation, \( (\sigma[\hat{J}_y])^{-1} \) is the width of the Gaussian.
FIG. 12. The angle dependence of \( \langle \Phi_0(\tau \pi) | e^{-iJ_y\beta} | \Phi_0(\tau \pi) \rangle \) (\( \tau = p, n, \pi = +, - \)) for the deformed \( ^{34}_{12}\text{Mg}, ^{40}_{12}\text{Mg}, ^{80}_{40}\text{Zr}, \) and \( ^{154}_{62}\text{Sm} \) nuclei at their lowest minima.

In the present AMP calculations, because the rotational operator \( e^{-iJ_y\beta} \) does not mix isospin and parity, the overlap function \( \langle \Phi_0 | e^{-iJ_y\beta} | \Phi_0 \rangle \) can be separated via isospin and parity as Eq. (32). Figure 12 shows the angle dependence of the overlap functions \( \langle \Phi_0(\tau \pi) | e^{-iJ_y\beta} | \Phi_0(\tau \pi) \rangle \) (\( \tau = p, n \) and \( \pi = +, - \)), for the deformed \( ^{34}_{12}\text{Mg}, ^{40}_{12}\text{Mg}, ^{80}_{40}\text{Zr}, \) and \( ^{154}_{62}\text{Sm} \) nuclei at their lowest minima. For the \( ^{12}\text{Mg} \) nuclei, some components hardly depend on the \( \beta \) angle and have almost spherical structure. For the \( ^{40}_{12}\text{Mg} \) nucleus, the \( n- \) component is well-deformed, which may be related to the deformed halo structure with peanut shape [28]. For the \( ^{80}_{40}\text{Zr} \) nucleus, all isospin and parity components are similarly deformed, and the Gaussian approximation in Eq. (C1) holds well. For the \( ^{154}_{62}\text{Sm} \) nucleus, the \( n- \) component is strongly deformed, though the others are not so strongly deformed and the Gaussian approximation is not very good.
FIG. 13. The angle dependence of $\langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle$ for the $^{34}_{12}\text{Mg}$, $^{40}_{12}\text{Mg}$, $^{80}_{40}\text{Zr}$, and $^{154}_{60}\text{Nd}$ nuclei, including their local minima. The colors represent the various values of the quadrupole deformation parameter $a_{20}$ shown in the insets.

Figure 13 shows the angle dependence of $\langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle$ for minima of the $^{34}_{12}\text{Mg}$, $^{40}_{12}\text{Mg}$, $^{80}_{40}\text{Zr}$, and $^{154}_{60}\text{Nd}$ nuclei, including their local minima with various values of the quadrupole deformation parameter $a_{20}$. The overlap functions have sharper peaks near $\beta = 0$ irrespective of nuclides as $|a_{20}|$ increases. A similar result is obtained in Ref. [12]. The Gaussian approximation sometimes fails for the $^{12}\text{Mg}$ nuclei or the weakly-deformed minima. The overlap function depends on the mass number as well as $a_{20}$. The sharpness of the peak near $\beta = 0$ of $\langle \Phi_0 | e^{-i\hat{J}_y \beta} | \Phi_0 \rangle$ corresponds with the fluctuation $\sigma[\hat{J}_y]$. The large fluctuation takes place when $|a_{20}|$ is large for the heavy nuclei [3], which leads to a sharp peak near $\beta = 0$. As $\Lambda_{2n}$ in Eq. (17) is determined by the angle dependence of the overlap function.
\[ \langle \Phi_0 | e^{-i \hat{J}_y \beta} | \Phi_0 \rangle, \]

it is fair to say that the results in Figs. 8 and 9 originate from those in Fig. 13.

![Graph](image)

**FIG. 14.** The angle dependence of \(-\Delta S^{01}(\beta)\) for the individual terms of the Hamiltonian for the deformed \(^{24}_{12}\)Mg, \(^{34}_{12}\)Mg, \(^{80}_{40}\)Zr, and \(^{154}_{62}\)Sm nuclei at their lowest minima.

In order to represent angle dependence of \(S^{01}(\beta)\) in Eq. (8), the following quantity is defined,

\[ \Delta S^{01}(\beta) := S^{01}(\beta) - S^{01}(\beta = 0), \]

then, as in Eq. (9),

\[ -\frac{d^2}{d\beta^2} \Delta S^{01}(\beta) \bigg|_{\beta=0} = C[\hat{S}, \hat{J}_y^2]. \] (43)

The angle dependence of \(-\Delta S^{01}(\beta)\) for the deformed \(^{24}_{12}\)Mg, \(^{34}_{12}\)Mg, \(^{80}_{40}\)Zr, and \(^{154}_{62}\)Sm nuclei at their lowest minima are shown in Fig. 14. The value of \(C[\hat{S}, \hat{J}_y^2]\) for \(\hat{K}\) is positive. For \(\hat{V}^{(\text{TN})}\) and \(\hat{V}^{(C\rho)}\), the values of \(C[\hat{S}, \hat{J}_y^2]\) are negative. Considering Eq. (25b), the values of \(C[\hat{S}, \hat{J}_y^2]\) are almost consistent with the results in Fig. 3 as the coefficient \(\Lambda_4 - (\Lambda_2)^2\) is canceled out in \(S_x(2^+)/E_x(2^+)\). As the mass number increases, the value of \(|C[\hat{S}, \hat{J}_y^2]|\) significantly increase except for \(\hat{S} = \hat{V}^{(LS)}\), \(\hat{V}^{(\text{TN})}\), and \(\hat{V}^{(\text{OPEP})}\). This observation seems to account for the results in Fig. 3. Although they are not shown, the angle dependence of \(-\Delta S^{01}(\beta)\) are almost constant and \(C[\hat{S}, \hat{J}_y^2] \approx 0\) for \(\hat{V}_{\text{Coulomb}}\) and \(\hat{H}_{\text{c.m.}}\), independent of
nuclides. The values of $-\Delta S^{01}(\beta)$ far from $\beta \approx 0$ strongly depend on nuclides, which is influenced by the higher-order terms of the cumulant expansion in Eq. (15).

In the present work, the values of $C[\hat{S}, \hat{J}_y^2]$ for $\hat{S} = \hat{K}$ is almost always positive. However, there exists an exception; the local oblate minimum of $^{40}\text{Mg}$. In order to separate $-\Delta S^{01}(\beta)$ for $\hat{K}$ into contributions of the isospin $\tau$ and the parity $\pi$, the following quantity is defined,

$$S^{01}(\beta; \tau \pi) := \frac{\langle \Phi_0(\tau\pi) | \hat{S} e^{-iJ_y^2} | \Phi_0(\tau\pi) \rangle}{\langle \Phi_0 | e^{-iJ_y^2} | \Phi_0 \rangle}, \quad (44a)$$

$$\Delta S^{01}(\beta; \tau \pi) := S^{01}(\beta; \tau \pi) - S^{01}(\beta = 0; \tau \pi), \quad (44b)$$

for $\tau = p,n$ and $\pi = +,−$. The angle dependence of $-\Delta S^{01}(\beta; \tau \pi)$ in Eq. (44) is shown in Fig. 15 for the local oblate minimum of $^{40}\text{Mg}$. The value of $-\Delta S^{01}(\beta; n-)$ at $\beta \approx 0$ is negative and significant although those for the others are positive. This anomalous result is related to the negative contribution of $\hat{K}$ exhibited in Fig. 6.

FIG. 15. The angle dependence of $-\Delta S^{01}(\beta; \tau \pi)$ in Eq. (44) for $\hat{S} = \hat{K}$ for the oblate minimum of $^{40}\text{Mg}$. Red is proton even parity, blue is proton negative parity, yellow is neutron positive parity, and green is neutron negative parity.

for $\tau = p,n$ and $\pi = +,−$. The angle dependence of $-\Delta S^{01}(\beta; \tau \pi)$ in Eq. (44) is shown in Fig. 15 for the local oblate minimum of $^{40}\text{Mg}$. The value of $-\Delta S^{01}(\beta; n-)$ at $\beta \approx 0$ is negative and significant although those for the others are positive. This anomalous result is related to the negative contribution of $\hat{K}$ exhibited in Fig. 6.
D. Comparison of $E_x(2^+)$ with rigid-rotor model and experiment

\[ E_x(J_+) = \frac{J(J+1)}{2\mathcal{I}^{(RR)}}, \]

\[ \mathcal{I}^{(RR)} \approx 0.0138A^{5/3}. \]
In the classical mechanics, the rotational energy of the rigid-body comes from kinetic energy. Interestingly, the values of $\mathcal{S}_x(2^+)$ for $\mathcal{S} = \hat{K}$ are close to the rigid-rotor value in the $^{40}\text{Zr}$ and $^{62}\text{Sm}$ regions.

Figure 17 shows the excitation energies for the deformed nuclei at their lowest minima, all of which have prolate shapes. The rigid-rotor value is small compared to the experimental values, e.g., for the $^{40}\text{Zr}$, $^{60}\text{Nd}$, and $^{62}\text{Sm}$ regions. The excitation energies obtained by the present calculations are close to the experimental values of $E_x(2^+)$ for all nuclides. However, we should be careful in comparing the values obtained by the AMP calculations with those of the experiment. The pair correlations will reduce the moment-of-inertia and raise the excitation energies. It should also be kept in mind that there is uncertainty in treating the density-dependent terms in the AMP calculations.
IV. CONCLUSION

The origin of the rotational band of nuclei has been investigated by the AMP calculation for the self-consistent axial-HF solutions, using the semi-realistic effective Hamiltonian M3Y-P6. The contributions of the individual terms of the Hamiltonian to the excitation energies have been analyzed. Except for the light nuclei or the weakly-deformed solutions, their ratios are insensitive to nuclides and states. The contributions of the kinetic energies are large and close to the rigid-rotor values. A large cancellation occurs between the density-dependent channel and the density-independent one in the central force, although their sum is still sizable. The contributions of the noncentral forces are small.

In contrast, the results significantly depend on nuclei and deformation for the light nuclei or the weakly-deformed solutions. The contributions of the noncentral forces are not negligible. Regardless of nuclides, the attractive forces decrease the moment-of-inertia, and the repulsive forces increase it. The pair correlations and the shape mixing may influence the results for actual nuclei, and we leave them for future works.

By using the cumulant expansion, a general formula for the rotational energy is derived on the basis of the AMP. This formula is a generalization of those in Refs. [3, 7, 8, 13–15]. The deviation from the $J(J + 1)$ rule could be caused by the higher-order terms of the expansion of the Wigner d-function. It is suggested that the newly found higher-order terms of the cumulant expansion play roles in the light nuclei or the weakly-deformed solutions, contributing to the rotational energy and the moment-of-inertia.

ACKNOWLEDGMENTS

The authors are grateful to H. Kurasawa and S. Iwasaki for discussions. In this research, the numerical calculations were carried out on Yukawa-21 at YITP in Kyoto University. This research also used computational resources of Oakforest PACS provided by the Multidisciplinary Cooperative Research Program in Center for Computational Sciences, University of Tsukuba, and HITACHI SR24000 at the Institute of Management and Information Technologies, Chiba University. This research had been supported by the research assistant program at Chiba University.
Appendix A: Wigner D-function and projection operator

In this appendix, the Wigner D-function and its property are summarized. An arbitrary three-dimensional rotation can be characterized by the Euler angles \( \Omega = (\alpha, \beta, \gamma) \). The corresponding rotational operator \( \hat{R}(\Omega) \) [39] can be represented as follows,

\[
\hat{R}(\Omega) = e^{-iJ_z\alpha} e^{-iJ_y\beta} e^{-iJ_z\gamma}.
\]  

(A1)

The matrix elements of the rotational operator \( \hat{R}(\Omega) \) on the angular momentum eigenstates are well-known as the Wigner D-function [22, 39, 40], which is defined,

\[
D^{(j)}_{mk}(\Omega) := \langle jm | \hat{R}(\Omega) | jk \rangle = e^{-i(m\alpha+k\gamma)}d^{(j)}_{mk}(\beta),
\]  

(A2a)

\[
d^{(j)}_{mk}(\beta) := \langle jm | e^{-iJ_y\beta} | jk \rangle,
\]  

(A2b)

where \( d^{(j)}_{mk}(\beta) \) is often called the Wigner (small) d-function. On the standard phase convention of the angular momentum, \( d^{(j)}_{mk}(\beta) \) takes a real number. The orthogonal property of the Wigner D-function is as follows,

\[
\int d\Omega D^{(j)}_{mk}(\Omega) D^{(j')*}_{m'k'}(\Omega) = \frac{16\pi^2}{2j+1} \delta_{jj'} \delta_{mm'} \delta_{kk'},
\]  

(A3)

By using Eqs. (A2) and (A3), the generalized projection operator on the angular momentum eigenstates is represented as follows,

\[
\hat{P}^{(j)}_{mk} := |jm\rangle \langle jk| = \frac{2j+1}{16\pi^2} \int d\Omega D^{(j)*}_{mk}(\Omega) \hat{R}(\Omega),
\]  

(A4)

which satisfies the following equations,

\[
(\hat{P}^{(j)}_{mk})^\dagger = \hat{P}^{(j)}_{km},
\]  

(A5a)

\[
(\hat{P}^{(j)}_{mk})^2 = \delta_{mk} \hat{P}^{(j)}_{mk}.
\]  

(A5b)

Appendix B: Cumulant expansion

In this appendix, the cumulant expansion [23] is summarized. In the following, the bracket \( \langle \rangle \) represents a general expectation value. The cumulant of operators \( \hat{X}_1, \hat{X}_2, \cdots, \hat{X}_n \) is defined as,

\[
\langle \hat{X}_1; \cdots; \hat{X}_n \rangle_{\text{cum}} := \frac{\partial}{\partial t_1} \cdots \frac{\partial}{\partial t_n} \ln \left\langle \exp \left( \sum_{i=1}^{n} t_i \hat{X}_i \right) \right\rangle_{t_1=\cdots=t_n=0},
\]  

(B1)
where $[\hat{X}_i, \hat{X}_j] = 0$ for all $i$ and $j$. For instance,

$$\langle \hat{X}_1 \rangle_{\text{cum}} = \langle \hat{X}_1 \rangle,$$

$$\langle \hat{X}_1; \hat{X}_2 \rangle_{\text{cum}} = \langle \hat{X}_1 \hat{X}_2 \rangle - \langle \hat{X}_1 \rangle \langle \hat{X}_2 \rangle = C[\hat{X}_1, \hat{X}_2].$$

In particular, $\langle \hat{X}_1; \hat{X}_1 \rangle_{\text{cum}} = (\sigma[\hat{X}_1])^2$. In the case of $\hat{Y} = \hat{X}_i$ for all $i$, and $t = \sum_{i=1}^{n} t_i$, we get the following equation,

$$\langle \hat{Y}; \cdots; \hat{Y} \rangle_{\text{cum}} = \frac{\partial^n}{\partial t^n} \ln \langle e^{t \hat{Y}} \rangle \bigg|_{t=0},$$

then,

$$\ln \langle e^{t \hat{Y}} \rangle = \sum_{n=1}^{\infty} \frac{t^n}{n!} \langle \hat{Y}; \cdots; \hat{Y} \rangle_{\text{cum}}.$$  

We also get the following equation,

$$\frac{\langle \hat{X} e^{t \hat{Y}} \rangle}{\langle e^{t \hat{Y}} \rangle} = \frac{\partial}{\partial s} \ln \langle e^{s \hat{X} + t \hat{Y}} \rangle \bigg|_{s=0}$$

$$= \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{\partial}{\partial s} \frac{\partial^n}{\partial t^n} \ln \langle e^{s \hat{X} + t \hat{Y}} \rangle \bigg|_{s=t=0}$$

$$= \sum_{n=0}^{\infty} \frac{t^n}{n!} \langle \hat{X}; \hat{Y}; \cdots; \hat{Y} \rangle_{\text{cum}}.$$  

**Appendix C: Gaussian approximation connected to AMP**

In this appendix, the Gaussian approximation [3] for the rotational energy in Section II A is discussed. In the case that the overlap function $\langle \Phi_0 | e^{-i \hat{J}_y \beta} | \Phi_0 \rangle$ has a sharp peak near $\beta \approx 0$, then the integrand of $N_{2n}$ in Eq. (17a) is finite only near $\beta \approx 0$ [3]. However, we do not assume the sharpness of the overlap function $\langle \Phi_0 | e^{-i \hat{J}_y \beta} | \Phi_0 \rangle$ here, but just assume that it is approximated by the Gaussian function (see also B4),

$$\langle \Phi_0 | e^{-i \hat{J}_y \beta} | \Phi_0 \rangle = 1 - \frac{1}{2} \langle \Phi_0 | \hat{J}_y^2 | \Phi_0 \rangle \beta^2 + \cdots \approx e^{-\frac{1}{2} (\sigma[\hat{J}_y])^2 \beta^2}.$$  

Similar approximation is also known as the cumulant expansion in statistical mechanics [44]. For $x > 0$, the following functions are defined,

$$N_{2n}^{(G)}(x) := \int_{0}^{\pi/2} d\beta \sin \beta \beta^{2n} e^{-\frac{1}{2} x \beta^2},$$  

$$A_{2n}^{(G)}(x) := \frac{N_{2n}^{(G)}(x)}{N_0^{(G)}(x)}.$$  

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analogously to Eq. (17). The function \( \Lambda^{(G)}_2(x) \) is called universal function \( [45] \). The recurrence relations of \( N^{(G)}_{2n}(x) \) and \( \Lambda^{(G)}_{2n}(x) \) are as follows,

\[
\frac{d}{dx} N^{(G)}_{2n}(x) = -\frac{1}{2} N^{(G)}_{2n+2}(x), \quad \text{(C3a)}
\]

\[
\frac{d}{dx} \Lambda^{(G)}_{2n}(x) = -\frac{1}{2} \left[ \Lambda^{(G)}_{2n+2}(x) - \Lambda^{(G)}_{2n}(x) \Lambda^{(G)}_{2n}(x) \right]. \quad \text{(C3b)}
\]

![Graph of \( \Lambda^{(G)}_{2n}(x) \) for different \( n \) values on a logarithmic scale.](image)

**FIG. 18.** The \( x \) dependence of \( \Lambda^{(G)}_{2n}(x) \) defined by Eq. \( (C2) \) for \( n = 0, ..., 5 \) on a logarithmic scale.

In Fig. 18 the numerical results of the \( x \) dependence of \( \Lambda^{(G)}_{2n}(x) \) in Eq. \( (C2b) \) are shown. For small \( n \) and large \( x \), the following relation is confirmed,

\[
\Lambda^{(G)}_{2n}(x) > \Lambda^{(G)}_{2n+2}(x). \quad \text{(C4)}
\]

With \( \Lambda^{(G)}_{2n}(x) \) and Eq. \( (C3b) \), Eqs. \( (19) \) and \( (24) \) are approximated as follows,

\[
\langle 0|\hat{S}|0 \rangle \approx \sum_{n=0}^{\infty} s_{2n} \Lambda^{(G)}_{2n}(x) \bigg|_{x=(\sigma[\hat{j}_y])^2}, \quad \text{(C5a)}
\]

\[
\frac{1}{\mathcal{T}[\hat{S}]} \approx \sum_{n=1}^{\infty} s_{2n} \frac{d}{dx} \Lambda^{(G)}_{2n}(x) \bigg|_{x=(\sigma[\hat{j}_y])^2}. \quad \text{(C5b)}
\]

If the width of the Gaussian \( (\sigma[\hat{j}_y])^{-1} \) is narrow enough, the integral of \( N^{(G)}_{2n}(x) \) in Eq. \( (C2a) \) is approximated by taking \( \sin \beta \approx \beta \),

\[
N^{(G)}_{2n}(x) \approx \int_0^{\pi/2} d\beta \beta^{2n+1} e^{-\frac{1}{2}x\beta^2} = 2^n \int_0^\lambda du u^n e^{-xu}, \quad \text{(C6a)}
\]

\[
= 2^n \int_0^\lambda du u^n e^{-xu}, \quad \text{(C6b)}
\]
where $\lambda := \pi^2/8$. The integral of Eq. (C6b) is a generalization of the gamma function $\Gamma(n+1)$, which corresponds with $\Gamma(n+1)$ in the case of $x = 1$ and $\lambda \to \infty$. The recurrence relation in Eq. (C3a) is satisfied for $N^{(G)}_{2n}(x)$ in Eq. (C6a). In the case of $n = 0$, the integral of $N^{(G)}_{2n}(x)$ in Eq. (C6a) can be done analytically,

$$N_0^{(G)}(x) \approx \frac{1}{x}(1 - e^{-\lambda x}). \quad \text{(C7)}$$

By using Eqs. (C3a) and (C7), an analytical expression of $N^{(G)}_{2n}(x)$ is obtained,

$$N^{(G)}_{2n}(x) \approx \frac{2^n n!}{x^{n+1}} \left(1 - e^{-\lambda x} \sum_{m=0}^{n} \frac{(\lambda x)^m}{m!}\right), \quad \text{(C8)}$$

and then,

$$A^{(G)}_{2n}(x) \approx \frac{2^n n!}{x^n} \frac{1 - e^{-\lambda x} \sum_{m=0}^{n} \frac{(\lambda x)^m}{m!}}{1 - e^{-\lambda x}}. \quad \text{(C9)}$$

By widening the range of integral $\pi/2 \to \infty$ in Eq. (C6a), i.e., $\lambda \to \infty$ in Eq. (C6b), the following equation is obtained,

$$N^{(G)}_{2n}(x) \approx \frac{2^n n!}{x^{n+1}}, \quad \text{(C10)}$$

and,

$$A^{(G)}_{2n}(x) \approx \frac{2^n n!}{x^n}. \quad \text{(C11)}$$

Equation (C11) satisfies Eq. (C4) for small $n$ and large $x$. Although Eq. (C4) breaks down at extremely large $n$ for any $x$, it does not immediately cause a problem of convergence in Eq. (18) because $c_{2n}$ in Eq. (13b) eases the convergence problem via,

$$\langle J0| (\hat{J}_+ - \hat{J}_-)^{2n}|J0 \rangle \sim \binom{2n}{n} (-)^n J^{2n}, \quad \text{(C12)}$$

and,

$$c_{2n} A^{(G)}_{2n} \sim \frac{1}{n!} \left(\frac{J^2}{2x}\right)^n. \quad \text{(C13)}$$

If we neglect higher-$s_{2n}$-terms in Eq. (C5), $\langle 0|\hat{S}|0 \rangle$ and $\mathcal{I}[\hat{S}]$ are approximated by using Eq. (C11),

$$\langle 0|\hat{S}|0 \rangle \approx \langle \Phi_0|\hat{S}|\Phi_0 \rangle - \frac{C[\hat{S}, \hat{J}_y^2]}{(\sigma[J_y])^2}, \quad \text{(C14a)}$$

$$\frac{1}{\mathcal{I}[\hat{S}]} \approx \frac{C[\hat{S}, \hat{J}_y^2]}{(\sigma[J_y])^4}. \quad \text{(C14b)}$$

Equation (C14b) is the Yoccoz moment-of-inertia [3, 8, 14]. Equation (C14) is the result of the Kamlah expansion [3, 15].
Appendix D: AMP for non-orthogonal bases

A summary of the MF theory for non-orthogonal bases, particularly the HFB theory, is given in the appendix of Ref. [41]. In this appendix, we present the method of AMP on top of that. The single-particle (s.p.) base ket is represented by $|k\rangle$, and $N_{kk'} := \langle k|k' \rangle$ is the norm matrix. The matrix $N$ is hermitian. We assume that $N$ is positive definite. Then, the completeness holds,

$$\sum_{kk'} |k\rangle (N^{-1})_{kk'} \langle k'| = \hat{1},$$  \hspace{1cm} (D1)

where the $\hat{1}$ on the right-hand side is the identity operator in the s.p. space.

The Fock space is represented by the creation and annihilation operators and the particle vacuum [42]. We denote the creation (annihilation) operator for the s.p. basis $k$ by $c_k^\dagger$ ($c_k$).

They obey the fermionic anti-commutation relations,

$$\{c_k, c_{k'}^\dagger\} = N_{kk'}, \quad \{c_k, c_{k'}\} = 0, \quad \{c_{k'}^\dagger, c_{k'}^\dagger\} = 0.$$  \hspace{1cm} (D2)

The particle vacuum $|0\rangle_c$ is defined,

$$c_k |0\rangle_c = 0 \quad \text{for all } k,$$  \hspace{1cm} (D3)

which satisfies $c_c (0|0\rangle_c = 1$. In the following, we consider the Fock space, like $|k\rangle = c_k^\dagger |0\rangle_c$, $|kk'\rangle = c_k^\dagger c_{k'}^\dagger |0\rangle_c$, and so on. Let us consider the case that the Hamiltonian $\hat{H}$ consists of the 1-body term $\hat{K}$ and the 2-body term $\hat{V}$. The Hamiltonian is represented by the non-orthogonal s.p. bases as follows,

$$\hat{H} = \sum_{k_1 \cdots k_4} (N^{-1})_{k_1k_2} \langle k_2|\hat{K}|k_4 \rangle (N^{-1})_{k_4k_3} c_{k_1}^\dagger c_k c_k c_k c_k$$

$$+ \frac{1}{4} \sum_{k_1 \cdots k_8} (N^{-1})_{k_1k_2} (N^{-1})_{k_3k_4} \langle k_2k_4|\hat{V}|k_1k_8 \rangle a (N^{-1})_{k_6k_5} (N^{-1})_{k_8k_7} c_{k_1}^\dagger c_{k_3}^\dagger c_{k_7}^\dagger c_{k_5}^\dagger,$$  \hspace{1cm} (D4)

where the matrix elements of $\hat{V}$ are anti-symmetrized.

The generalized Bogolyubov transformation is defined,

$$\alpha_i^\dagger := \sum_{k=1}^M \left( c_k^\dagger U_{ki} + c_k V_{k_i} \right),$$

$$\alpha_i := \sum_{k=1}^M \left( c_k U^*_{k_i} + c_k^\dagger V^*_{k_i} \right),$$  \hspace{1cm} (D5)
where $M$ is the number of the bases, the matrices $U$ and $V$ are $M \times M$ square matrices. In the vector and matrix representation, Eq. (D5) can be expressed as follows,

$$ (\alpha^\dagger \alpha) = (c^\dagger c)W, \quad W := \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}, $$

(D6)

where $(c^\dagger c)$ represents $(c_1^\dagger \cdots c_M^\dagger c_1 \cdots c_M)$. Note that the transformation in Eq. (D6) is non-unitary transformation, so the matrix $W$ is not an unitary matrix. In contrast, $\alpha_i^\dagger$ and $\alpha_i$ obey the usual fermionic canonical anti-commutation relations,

$$ \{\alpha_i, \alpha_{i'}^\dagger\} = \delta_{ii'}, \quad \{\alpha_i, \alpha_{i'}\} = 0, \quad \{\alpha_i^\dagger, \alpha_{i'}^\dagger\} = 0, \quad (D7) $$
as they are obtained the HFB equation. From Eqs. (D2), (D6), and (D7), the matrix $W$ satisfies the following equation,

$$ W^\dagger N' W = 1, \quad N' := \begin{pmatrix} N & 0 \\ 0 & N^* \end{pmatrix}. $$

(D8)

The HFB vacuum is defined,

$$ \alpha_i |\Phi\rangle = 0 \quad \text{for all} \quad i, \quad (D9) $$

and satisfies $\langle \Phi |\Phi\rangle = 1$.

In the GEM of Ref. [27], we assume the spherically symmetric s.p. bases $k = (\nu \ell j m t_z)$. Therefore, $c_k^\dagger$ is a spherical tensor operator of rank $j$, i.e.,

$$ \hat{R}(\Omega)c_{\nu\ell j m t_z}^\dagger \hat{R}^\dagger(\Omega) = \sum_{m'} c_{\nu\ell j m' t_z}^\dagger D_{m'm}^{(j)}(\Omega), $$

(D10)

where $D_{m'm}^{(j)}(\Omega)$ is the Wigner D-function in Eq. (A2). The hermitian conjugate of Eq. (D10) is as follows,

$$ \hat{R}(\Omega)c_{\nu\ell j m t_z} \hat{R}^\dagger(\Omega) = \sum_{m'} c_{\nu\ell j m' t_z} D_{m'm}^{(j)*}(\Omega). $$

(D11)

Thus, $c_k$ itself is not a spherical tensor. Equations (D10) and (D11) can be expressed as follows,

$$ \hat{R}(c^\dagger c)\hat{R}^\dagger = (c^\dagger c)D', \quad D' := \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix}, $$

(D12)

where $D_{kk'} = \delta_{\nu\nu'}\delta_{\ell\ell'}\delta_{jj'}\delta_{tt}, D_{m'm'}^{(j)}(\Omega)$. 

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We define a matrix $T$, 

$$\hat{R}(\alpha^\dagger \alpha)\hat{R}^\dagger =: (\alpha^\dagger \alpha)T, \quad T := \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix},$$

and we obtain the following relation,

$$T = W^{-1}D'W = W^\dagger N'\hat{D}W.$$  \hfill (D14)

We also define a matrix $\Sigma_x$ as follows \[43\],

$$\Sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$  \hfill (D15)

and get the following relations,

$$\Sigma_x N' \Sigma_x = N''^\ast,$$

$$\Sigma_x W \Sigma_x = W^\ast,$$

$$\Sigma_x D' \Sigma_x = D''^\ast.$$  \hfill (D16)

By using Eqs. (D14), (D16), and $(\Sigma_x)^2 = 1$, the following relation is derived,

$$\Sigma_x T \Sigma_x = T^\ast,$$  \hfill (D17)

i.e., $T_{22} = T_{11}^\ast$ and $T_{21} = T_{12}^\ast$. For simplicity, we express,

$$|0\rangle := |\Phi\rangle,$$  \hfill (D18a)

$$|1\rangle := \hat{R}(\Omega) |\Phi\rangle,$$  \hfill (D18b)

and assume that $\langle 0|1 \rangle$ does not vanish. According to the generalized Wick’s theorem \[10\],

$$\frac{\langle 0|c_{k_1}^\dagger c_{k_2}^\dagger c_{k_3} c_{k_4}|1 \rangle}{\langle 0|1 \rangle} = \frac{\langle 0|c_{k_2}^\dagger c_{k_3}|1 \rangle}{\langle 0|1 \rangle} \frac{\langle 0|c_{k_1}^\dagger c_{k_4}|1 \rangle}{\langle 0|1 \rangle} - \frac{\langle 0|c_{k_1}^\dagger c_{k_3}|1 \rangle}{\langle 0|1 \rangle} \frac{\langle 0|c_{k_2}^\dagger c_{k_4}|1 \rangle}{\langle 0|1 \rangle} + \frac{\langle 0|c_{k_1}^\dagger c_{k_2}^\dagger |1 \rangle}{\langle 0|1 \rangle} \frac{\langle 0|c_{k_3} c_{k_4}|1 \rangle}{\langle 0|1 \rangle},$$

and Eq. (D4), we get the equation,

$$\frac{\langle 0|\hat{H}|1 \rangle}{\langle 0|1 \rangle} = \sum_{k_1 k_2} \langle k_2|\hat{K}|k_1 \rangle \rho_{k_1 k_2}^{k_1} + \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} \langle k_3 k_4|\tilde{V}|k_1 k_2 \rangle \left( 2\rho_{k_1 k_3}^{k_1} \rho_{k_2 k_4}^{k_1} + \kappa_{k_1 k_2}^{k_1} \kappa_{k_3 k_4}^{k_1} \right).$$

\hfill (D20)
where we have defined "generalized density matrix" \( \rho^{01} \), and "generalized pairing tensors" \( \kappa^{01} \) and \( \kappa^{10} \),

\[
(N \rho^{01} N)_{kk'} := \frac{\langle 0| c_k^\dagger c_k |1 \rangle}{\langle 0|1 \rangle},
\]

\[
(N \kappa^{01} N^*)_{kk'} := \frac{\langle 0| c_k c_k^\dagger |1 \rangle}{\langle 0|1 \rangle},
\]

\[
(N \kappa^{10} N^*)_{kk'} := \frac{\langle 1| c_k c_k^\dagger |0 \rangle}{\langle 1|0 \rangle}.
\]

The overlap function \( \langle 0|1 \rangle \) can be calculated by the Onishi formula [9, 10],

\[
\langle 0|1 \rangle = \langle \Phi| \hat{R}(\Omega) |\Phi \rangle = \sqrt{\text{det} T_{22}(\Omega)}. \tag{D22}
\]

By using "generalized contractions" [10], i.e.,

\[
\frac{\langle 0| \alpha_i \alpha_i^\dagger |1 \rangle}{\langle 0|1 \rangle} = \delta_{ii'}, \quad \frac{\langle 0| \alpha_i \alpha_i^\dagger |1 \rangle}{\langle 0|1 \rangle} = X_{ii'};
\]

\[
\frac{\langle 0| \alpha_i^\dagger \alpha_i |1 \rangle}{\langle 0|1 \rangle} = 0, \quad \frac{\langle 0| \alpha_i^\dagger \alpha_i^\dagger |1 \rangle}{\langle 0|1 \rangle} = 0,
\]

\[
X := T_{12} T_{22}^{-1} = -X^T,
\]

and defining the following matrices,

\[
\tilde{V} := V + U^* X^*,
\]

\[
\tilde{U} := U + V^* X^*,
\]

the matrices \( \rho^{01} \), \( \kappa^{01} \), and \( \kappa^{10} \) in Eq. (D21) can be expressed as follows,

\[
\rho^{01} = \tilde{V}^* V^T,
\]

\[
\kappa^{01} = \tilde{V}^* U^T,
\]

\[
\kappa^{10} = V^* \tilde{U}^T. \tag{D25}
\]

Appendix E: Time-reversal symmetry in AMP

In this appendix, we summarize the properties of the generalized density matrix \( \rho^{01} \), and the generalized pairing tensors \( \kappa^{01} \) and \( \kappa^{10} \), which are derived from time-reversal symmetry in the AMP calculations connected to the GEM. For a liner operator \( \hat{A} \), and arbitrary kets \( |a \rangle \) and \( |b \rangle \), we get the following equation [39],

\[
\langle b|\hat{A}|a \rangle = \langle a| \cdot \left( \hat{T} \hat{A}^\dagger \hat{T}^{-1} |b \rangle \right), \tag{E1}
\]

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where $\hat{T}$ represents a time-reversal operator, and $\tilde{a}$ is a shorthand notation of the time-reversed state of $a$. We assume the MF state $|\Phi\rangle$ has the time-reversal symmetry. By applying Eq. (E1) to Eq. (D21) and using $[\hat{R}(\Omega), \hat{T}] = 0$ for any $\Omega$, we get the following equations,

\begin{align*}
(N\rho^{01}N)_{kk'} &= + (N\rho^{01}N)^*_{kk'}, \\
(N\rho^{01}N)_{k\bar{k}'} &= - (N\rho^{01}N)^*_{k\bar{k}'}, \\
(N\kappa^{01}N^*)_{kk'} &= + (N\kappa^{01}N^*)^*_{kk'}, \\
(N\kappa^{01}N^*)_{k\bar{k}'} &= - (N\kappa^{01}N^*)^*_{k\bar{k}'}, \\
(N^*\kappa^{10}N)_{kk'} &= + (N^*\kappa^{10}N)^*_{kk'}, \\
(N^*\kappa^{10}N)_{k\bar{k}'} &= - (N^*\kappa^{10}N)^*_{k\bar{k}'}.
\end{align*}

(E2)

In the case of the spherical bases, the norm matrix $N$ has the following form [27, 41],

$$N_{kk'} = \delta_{\ell\ell'}\delta_{jj'}\delta_{mm'}\delta_{tt'}N((\ell j \nu \nu'))^{(\ell j \nu \nu')}.$$  

(E3)

Therefore, the norm matrix $N$ does not mix the states of $k$ and $\bar{k}$ each other, and we can get the following equations from Eq. (E2),

\begin{align*}
\rho^{01}_{kk'} &= + \rho^{01*}_{kk'}, \\
\rho^{01}_{k\bar{k}'} &= - \rho^{01*}_{kk'}, \\
\kappa^{01}_{kk'} &= + \kappa^{01*}_{kk'}, \\
\kappa^{01}_{k\bar{k}'} &= - \kappa^{01*}_{kk'}, \\
\kappa^{10}_{kk'} &= + \kappa^{10*}_{kk'}, \\
\kappa^{10}_{k\bar{k}'} &= - \kappa^{10*}_{kk'}.
\end{align*}

(E4)

For the AMP calculations in the coordinate space, which is convenient for the density-dependent interaction (see Eq. (28)), the coordinate representation of $\rho^{01}$, $\kappa^{01}$, and $\kappa^{10}$ are needed. The local parts for $\rho^{01}$, $\kappa^{01}$, and $\kappa^{10}$ are as follows,

\begin{align*}
\rho^{01}(r\sigma_1\tau_1; \Omega) &= \sum_{k_1k_2} \rho^{01}_{k_1k_2}(\Omega) \varphi_{k_1}(r\sigma_1\tau_1) \varphi^*_{k_2}(r\sigma_2\tau_1), \\
\kappa^{01}(r\sigma_1\tau_1; \Omega) &= \sum_{k_1k_2} \kappa^{01}_{k_1k_2}(\Omega) \varphi_{k_1}(r\sigma_1\tau_1) \varphi_{k_2}(r\sigma_2\tau_1), \\
\kappa^{10}(r\sigma_1\tau_1; \Omega) &= \sum_{k_1k_2} \kappa^{10}_{k_1k_2}(\Omega) \varphi_{k_1}(r\sigma_1\tau_1) \varphi_{k_2}(r\sigma_2\tau_1).
\end{align*}

(E5)
where \( \varphi_k(\mathbf{r}\sigma\tau) := \langle \mathbf{r}\sigma\tau|k \rangle \), \( \sigma \) is the spin’s index and \( \tau \) is the isospin’s one. The antisymmetric property of the generalized pairing tensors,

\[
\kappa_{kk'}^{01} = -\kappa_{k'k}^{01}, \\
\kappa_{kk'}^{10} = -\kappa_{k'k}^{10},
\]

(E6)

leads ones of the coordinate representation version,

\[
\kappa_{01}^{01}(\mathbf{r}\bar{\sigma}\sigma;\Omega) = -\kappa_{01}^{10}(\bar{\mathbf{r}}\bar{\sigma}\sigma;\Omega), \\
\kappa_{10}^{01}(\mathbf{r}\bar{\sigma}\sigma;\Omega) = -\kappa_{10}^{10}(\bar{\mathbf{r}}\bar{\sigma}\sigma;\Omega),
\]

(E7)

where \( \bar{\sigma} \) denotes the counterpart of \( \sigma \). We define “generalized density” as follows,

\[
\bar{\rho}_{01}(\mathbf{r};\Omega) := \sum_{\tau} \sum_{\sigma} \rho_{01}(\mathbf{r}\sigma\bar{\sigma};\Omega).
\]

(E8)

By using Eq. (E4) and the following relations,

\[
\varphi_{k}(\mathbf{r}\sigma\tau) = +\varphi_{k}^{*}(\bar{\mathbf{r}}\bar{\sigma}\tau), \\
\varphi_{k}(\mathbf{r}\sigma\tau) = -\varphi_{k}^{*}(\bar{\mathbf{r}}\bar{\sigma}\tau),
\]

(E9)

we get the following equations,

\[
\rho_{01}^{01}(\mathbf{r}\sigma\bar{\sigma};\Omega) = +\rho_{01}^{1*}(\mathbf{r}\bar{\sigma}\sigma;\Omega), \\
\rho_{01}^{10}(\mathbf{r}\bar{\sigma}\sigma;\Omega) = -\rho_{01}^{1*}(\mathbf{r}\bar{\sigma}\sigma;\Omega), \\
\kappa_{01}^{01}(\mathbf{r}\sigma\bar{\sigma};\Omega) = +\kappa_{01}^{1*}(\mathbf{r}\bar{\sigma}\sigma;\Omega), \\
\kappa_{10}^{10}(\mathbf{r}\bar{\sigma}\sigma;\Omega) = +\kappa_{10}^{1*}(\mathbf{r}\bar{\sigma}\sigma;\Omega).
\]

(E10)

By using Eq. (E10), the generalized density in Eq. (E8) becomes real number,

\[
\bar{\rho}_{01}(\mathbf{r};\Omega) = \bar{\rho}_{01}^{*}(\mathbf{r};\Omega).
\]

(E11)

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