Band termination of collective rotation: Dynamical mechanism of occurrence

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The phenomenon of band termination of the nuclear collective rotation has been originally discussed by Bohr and Mottelson. The scenario is the following: In the high-spin rotational nucleus, the effect of the Coriolis term produces a tendency to align the angular momenta of individual single particles in a deformed rotating mean field in the direction of the rotation axis. This rotational alignment of the orbits of individual particles tends to create a density distribution symmetric about the rotation axis. The band termination of collective rotation is thus expected, when the density distribution about the rotation axis becomes symmetric, with the total angular momentum being the sum of the contributions of aligned individual particles. The main purpose of this paper is to formulate this scenario of the band termination from the standpoint of nuclear many-body problems and disclose the *dynamical mechanism of occurrence* of the band termination. It is clarified that the band termination occurs when the intrinsic state in the rotating frame cannot be stable against a variation toward an increase of the collective angular momentum. It is also shown that the value of the collective angular momentum at the band termination is simply an inflection point of the collective rotational energy. The behavior of the single-particle orbitals in the rotating frame is justified and visualized to be in accordance with the scenario of Bohr and Mottelson. [S0556-2813(97)02807-0]

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I. INTRODUCTION

The nucleus is an isolated finite many-body quantum system in which the self-consistent mean field is realized. Its collective modes of motion, which are associated with the time-evolution of the mean field, are inevitably of largeamplitude and are nonlinearly interwoven with the singleparticle modes of motion in a self-consistent way. One of the most typical modes of such a large-amplitude collective motion is the collective rotation. When the system has a deformed stationary mean field which can define an orientation of the system as a whole, one inevitably needs the concept of *spontaneous breakdown* of the rotation symmetry. Thus, the very occurrence of *collective rotational degrees* of freedom originates in restoring the broken rotation symmetry.

The focus in this paper is to disclose the *dynamical mechanism of occurrence* of the band termination phenomena of collective rotation. The band termination of collective rotation is a characteristic quantum property of a *finite* manybody system such as the nucleus. It was originally discussed by Bohr and Mottelson [1,2]: In the high-spin rotational nucleus, the effect of the Coriolis term can be viewed as a

tendency to align the angular momenta of individual singleparticles in a rotating mean field in the direction of the axis of rotation. This rotational alignments of the orbits of individual particles tend to create a density distribution symmetric about the rotation axis. Thus, one may expect the band termination of collective rotation, when the density distribution about the rotation axis becomes symmetric with the total angular momentum being the sum of the contributions of aligned individual particles.

In the heavier nuclei, the ground-state band does not terminate until very high spins, although the termination phenomena have been observed along the yrast line after several band crossings [3]. In the *sd*-shell nuclei at high-spin, however, one can observe the band termination of a single rotational band [3,4].

The scenario of band termination discussed by Bohr and Mottelson were first numerically realized by Bengtsson and Ragnarsson [5] on the basis of the cranked Nilsson-Strutinsky method, and successfully applied to *sd*-shell nuclei [4] and is being applied to medium-heavy nuclei. In this method, the band termination is described as a state having the maximum possible spin for the configuration in which the band begins. In order to analyze the behavior of the configuration and to find the maximum angular momentum, therefore, one *must* numerically calculate each state of the configuration at each point of the deformation (β , γ) and the collective angular momentum *I*.

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In this paper, we try to formulate the scenario of band termination by Bohr and Mottelson from the *standpoint of nuclear many-body problem*. In order to avoid unnecessary confusions, we restrict ourselves to such a *band termination of a single rotational band* (as observed in *sd*-shell nuclei), in which the evolution of the rotational band to its termination does not encounter the band crossing. Our formulation can clearly disclose the dynamical interweaving between the collective rotation and the single-particle motion throughout the evolution of a rotational band to its termination.

Our first task is to precisely formulate the very concept of collective rotation from the standpoint of nuclear many-body problem. Such a formulation has been fully developed [6] by means of the self-consistent collective coordinate (SCC) method [7] on the basis of the time-dependent Hartree-Fock (TDHF) method. For the sake of self-containedness, it is recapitulated in Sec. II in a form suitable for later discussions.

In Sec. III, the formulation of the collective rotation by the SCC method is compared with that of the conventional cranked Hartree-Fock (HF) method. It is shown that the formulation by the SCC method reproduces the intrinsic state in rotating frame as well as the intrinsic Hamiltonian in the rotating frame discussed in the cranked HF method.

Only one essential difference follows: In the SCC formulation of the collective rotation, it is necessary to define a *collective angle operator* which is a local infinitesimal generator for a variation of the intrinsic state toward the increase of the collective angular momentum I, while the cranked HF method does not specify any collective angle operator explicitly. The intrinsic excitation modes in rotating frame are described by the random-phase approximation (RPA) equations for the intrinsic Hamiltonian. With the use of the intrinsic excitation modes, the stability condition of the intrinsic state in rotating frame is discussed.

In Sec. IV, we discuss equations for the generators of collective rotation, i.e., for the collective angle operator and the angular momentum operator. It is shown that the equations are a typical set of RPA equations associated with the Nambu-Goldstone mode, based on the broken rotation symmetry of the intrinsic state. The stability condition of the intrinsic state in rotating frame toward a variation of the collective angular momentum I is given by employing the RPA equation for the collective angle operator. From the stability condition, one can see that the intrinsic state in rotating frame cannot be stable against the variation toward the increase of the collective angular momentum I arrives to an inflection point I_0 of the collective rotational energy.

In Sec. V, it is shown that the collective angle operator vanishes at this inflection point I_0 , demonstrating the *occurrence of the band termination* of collective rotation. We can also justify that the scenario of band termination by Bohr and Mottelson (in terms of the behavior of single-particle orbitals) is actually realized at this inflection point I_0 . Section VI is devoted to visualizing the behavior of single-particle orbitals by numerical investigations for the observed rotational bands in ²⁴Mg and ¹⁶O*. Concluding remarks are given in Sec. VII.

II. DEFINITION OF COLLECTIVE ROTATION

In order to precisely formulate the band termination of collective rotation, one has to start with formulating the very concept of collective rotation. The occurrence of collective rotational degrees of freedom is well understood [1,2] to originate in a *breaking of rotational invariance*, which introduces a "deformation" that makes it possible to specify an orientation of the system. With the use of the SCC method [6,7], let us formulate the collective rotation.

We suppose for the sake of simplicity that a twodimensional nuclear system consisting of even nucleons is given with a rotational invariant Hamiltonian \hat{H} with an effective (smooth) interparticle force, and the Hartree-Fock (HF) minimization with \hat{H} gives a stationary local-minimum state $|\phi_0\rangle$, satisfying

$$\delta \langle \phi_0 | \hat{H} | \phi_0 \rangle = 0, \tag{1}$$

with an axially symmetric deformation. We further suppose that the HF state $|\phi_0\rangle$ has a property

$$\langle \phi_0 | \hat{J} | \phi_0 \rangle = 0, \tag{2}$$

where \hat{J} is the angular momentum operator along an axis perpendicular to the symmetry axis of the deformation. The deformation of $|\phi_0\rangle$ leads us to a localization of the orientation of the system, which inevitably needs the concept of spontaneous breakdown of the rotation symmetry. In the finite quantum system under consideration, the broken symmetry has to be restored by proper inclusion of the residual interaction which has been neglected under the HF approximation. Thus, the microscopic structure of the collective rotation, which restores the broken rotation symmetry, is essentially related to the problem of how to treat the residual interaction so as to restore the broken symmetry.

In the SCC method the collective rotation, which restores the broken rotation symmetry due to the deformation of $|\phi_0\rangle$, is described by the following class of TDHF equations called the "invariance principle of the Schrödinger equation"¹

$$\delta \langle \phi(I,\theta) | \left\{ \left(i \frac{\partial}{\partial t} - \hat{H} \right) | \phi(I,\theta) \rangle \right\} = 0, \tag{3}$$

where a single Slater-Determinant wave function $|\phi(I, \theta)\rangle$ is related to the HF state $|\phi_0\rangle$ by a time-dependent unitary transformation depending on collective variables $\{I, \theta\}$:

$$|\phi(I,\theta)\rangle = \hat{U}(I,\theta)|\phi_0\rangle.$$
 (4)

The invariance principle means that the time dependence of the collective variables, i.e., the collective angular momentum I(t) and the collective angle $\theta(t)$, has to be determined so as to satisfy Eq. (3).

With the state $|\phi(I,\theta)\rangle$, one can define infinitesimal generators $\{\hat{I}(I,\theta), \hat{\Theta}(I,\theta)\}$ for variations of the collective variables $\{I, \theta\}$, respectively, through the equations

¹Throughout the formulation of this paper, we adopt the convention $\hbar = 1$.

$$\begin{split} i\frac{\partial}{\partial\theta}|\phi(I,\theta)\rangle &= \hat{I}(I,\theta)|\phi(I,\theta)\rangle, \quad \hat{I}(I,\theta)\\ &= \left\{i\frac{\partial}{\partial\theta}\hat{U}(I,\theta)\right\}\hat{U}^{\dagger}(I,\theta), \end{split}$$
(5)

$$\begin{split} \frac{1}{i} \frac{\partial}{\partial I} |\phi(I,\theta)\rangle &= \hat{\Theta}(I,\theta) |\phi(I,\theta)\rangle, \quad \hat{\Theta}(I,\theta) \\ &= \left\{ \frac{1}{i} \frac{\partial}{\partial I} \hat{U}(I,\theta) \right\} \hat{U}^{\dagger}(I,\theta). \end{split}$$

In the SCC method, with the use of the generators $\{\hat{I}(I,\theta), \hat{\Theta}(I,\theta)\}\$, we impose the canonical-variable condition [6]

$$\langle \phi(I,\theta) | \hat{I}(I,\theta) | \phi(I,\theta) \rangle \equiv \left\langle \phi(I,\theta) | i \frac{\partial}{\partial \theta} | \phi(I,\theta) \right\rangle$$
$$= I + \frac{\partial}{\partial \theta} S(I,\theta), \tag{6}$$

$$\langle \phi(I,\theta) | \hat{\Theta}(I,\theta) | \phi(I,\theta) \rangle \equiv \left\langle \phi(I,\theta) \left| \frac{1}{i} \frac{\partial}{\partial I} \right| \phi(I,\theta) \right\rangle$$
$$= -\frac{\partial}{\partial I} S(I,\theta),$$

which guarantees the collective variables $\{I, \theta\}$ to be a pair of *canonical conjugate variables*. In Eq. (6), $S(I, \theta)$ is an arbitrary (single-valued) real function of $\{I, \theta\}$, and expresses the freedom in choosing an appropriate set of the collective variables $\{I, \theta\}$ from among possible canonical transformations of them. From Eq. (6), one can easily derive the "weak" canonical commutation relation²

$$\langle \phi(I,\theta) | [\hat{\Theta}(I,\theta), \hat{I}(I,\theta)] | \phi(I,\theta) \rangle = i.$$
(7)

One of the most appropriate choices of the collective variables $\{I, \theta\}$ for our purpose is to fix

$$S(I,\theta) = 0 \tag{8}$$

so as to obtain, from Eq. (6),

$$\langle \phi(I,\theta) | \hat{I}(I,\theta) | \phi(I,\theta) \rangle = I.$$
 (9)

In this case, one can choose the generator $\hat{I}(I,\theta)$ for the collective rotation under consideration to be identical with the angular momentum operator \hat{J} of the system:

$$\hat{I}(I,\theta) = \hat{J},\tag{10}$$

²From Eq. (6) one has

$$\frac{\partial}{\partial I} \left\langle \phi(I,\theta) \left| i \frac{\partial}{\partial \theta} \right| \phi(I,\theta) \right\rangle + \frac{\partial}{\partial \theta} \left\langle \phi(I,\theta) \left| \frac{1}{i} \frac{\partial}{\partial I} \right| \phi(I,\theta) \right\rangle = 1,$$

which is expressed as Eq. (7) with the use of the definition of generators in Eq. (5).

which demonstrates that the collective rotation under consideration is not an *externally* "cranked" one but selfconsistently originates from the very system itself. This choice is compatible with the condition given in Eq. (2) provided that $|\phi(I=0,\theta=0)\rangle = |\phi_0\rangle$, i.e., $\hat{U}(I=0,\theta=0)=1$, and enables us to reduce the unitary transformation in Eq. (4) to the following simple form:

$$|\phi(I,\theta)\rangle = e^{-i\theta J}|\phi(I)\rangle, \quad |\phi(I)\rangle = e^{iG(I)}|\phi_0\rangle, \quad (11)$$

$$i\hat{G}(I) = \sum_{\mu m} \{g_{\mu m}(I)\hat{c}_{\mu}^{\dagger}\hat{c}_{m} - \text{H.c.}\}, \quad i\hat{G}(0) = 0,$$

 $\{\hat{c}^{\dagger}_{\mu},\hat{c}_{m}\}\$ being the particle and hole creation operators³ satisfying

$$\hat{c}_{\mu} |\phi_0\rangle = \hat{c}_m^{\dagger} |\phi_0\rangle = 0.$$
(12)

With the form given in Eq. (11), the canonical-variable condition in Eq. (6) is written as

$$\begin{bmatrix} I \end{bmatrix} \begin{pmatrix} \phi(I,\theta) & i \frac{\partial}{\partial \theta} & \phi(I,\theta) \end{pmatrix} = \langle \phi(I) & |\hat{J}| & \phi(I) \rangle = I, \\ \phi(I,\theta) & \frac{1}{i} \frac{\partial}{\partial I} & \phi(I,\theta) \end{pmatrix} = \langle \phi(I) & |\hat{\Theta}(I)| & \phi(I) \rangle = 0, \\ (13)$$
$$\hat{\Theta}(I) = \left\{ \frac{1}{i} \frac{d}{dI} e^{i\hat{G}(I)} \right\} e^{-i\hat{G}(I)}, 4$$

$$\langle \phi(I) | [\hat{\Theta}(I), \hat{J}] | \phi(I) \rangle = i.$$
(14)

Here it should be emphasized an important fact which plays a decisive role in later discussions to define the concept of band termination: Although the infinitesimal generator \hat{J} for the collective rotation is a *global* operator, the *angle operator* $\hat{\Theta}(I)$ for the collective rotation is a *local* one which depends on the collective angular momentum variable *I*.

With the use of Eq. (11), the invariance principle given in Eq. (3) is simply written as

$$\delta \langle \phi(I) | \hat{H} - \dot{\theta} \hat{J} + \dot{I} \hat{\Theta}(I) | \phi(I) \rangle = 0.$$
 (15)

³We use the convention of denoting occupied single-particle orbitals by indices m, n, \ldots , and unoccupied single-particle orbitals by indices μ, ν, \ldots . We also use labels α, β, \ldots , to indicate the single-particle orbitals when we need not specify to be occupied or unoccupied.

⁴The generator $\hat{\Theta}(I)$ is a one-body operator, because of the relation

$$\hat{\Theta}(I) = \left\{ \frac{1}{i} \frac{d}{dI} e^{i\hat{G}(I)} \right\} e^{-i\hat{G}(I)} = \frac{d\hat{G}(I)}{dI} + \frac{i}{2!} \left[\frac{d\hat{G}(I)}{dI}, \hat{G}(I) \right] \\ + \frac{i^2}{3!} \left[\left[\frac{d\hat{G}(I)}{dI}, \hat{G}(I) \right], \hat{G}(I) \right] + \cdots.$$



$$:\hat{\Theta}(I):=\hat{\Theta}(I) - \langle \phi(I) | \hat{\Theta}(I) | \phi(I) \rangle,$$
$$:\hat{J}:=\hat{J} - \langle \phi(I) | \hat{J} | \phi(I) \rangle, \tag{16}$$

and by employing the commutation relation (14), one obtains the *equation of collective rotation*

$$\begin{bmatrix} \text{II} \end{bmatrix} \quad \dot{\theta} = \frac{\partial}{\partial I} \mathcal{H}_{\text{rot}}(I), \quad \dot{I} = -\frac{\partial}{\partial \theta} \mathcal{H}_{\text{rot}}(I) = 0, \\ \mathcal{H}_{\text{rot}}(I) \equiv \langle \phi(I) | \hat{H} | \phi(I) \rangle = \langle \phi(I, \theta) | \hat{H} | \phi(I, \theta) \rangle.$$
(17)

By taking a variation $|\delta\phi(I)\rangle = |\delta_{\perp}\phi(I)\rangle$ satisfying

$$\langle \delta_{\perp} \phi(I) | \delta_{\parallel} \phi(I) \rangle = 0,$$
 (18)

one obtains from Eq. (15) the equation of collective submanifold $\Sigma_{rot}(I)$,

$$\delta_{\perp} \langle \phi(I) | \hat{H} | \phi(I) \rangle = \delta_{\perp} \langle \phi(I, \theta) | \hat{H} | \phi(I, \theta) \rangle = 0.$$
 (19)

This means that the optimum collective submanifold $\Sigma_{rot}(I)$ should be extracted in such a way that the expectation value of the Hamiltonian with respect to $|\phi(I)\rangle$ is *stationary* at each point on the collective submanifold for the variations *perpendicular* to it. Without the explicit use of $|\delta_{\perp}\phi(I)\rangle$, Eq. (19) can be expressed as

$$\begin{bmatrix} \text{III} \end{bmatrix} \quad \delta \left\langle \phi(I) \middle| \hat{H} - \left\{ \frac{d\mathcal{H}_{\text{rot}}(I)}{dI} \right\} \hat{J} \middle| \phi(I) \right\rangle = 0, \quad (20)$$

because the variation $|\delta_{\parallel}\phi(I)\rangle$ in Eq. (20) identically leads to zero by the definition in Eq. (16).

Equations [I], [II], and [III] form a set of basic equations of the SCC method for the collective rotation. It has been shown [6] that the set of basic equations enables us to selfconsistently determine the unknown functions $g_{\mu m}(I)$ of $i\hat{G}(I)$ in the state $|\phi(I)\rangle$ defined by Eq. (11) together with the Hamiltonian $\mathcal{H}_{rot}(I)$ of collective rotation. After getting $i\hat{G}(I)$, one obtains a concrete expression of the angle operator $\hat{\Theta}(I)$ through the definition in Eq. (13).

III. INTRINSIC STATE IN ROTATING FRAME

With the purpose of comparing the above description of collective rotation by the SCC method with that of the conventional cranking model, let us start with a recapitulation of the basic idea of the cranking model. In this model, we are interested in a HF wave function $|\phi(I)\rangle$, which minimizes the total energy under the constraint so that the angular momentum operator \hat{J} has a fixed expectation value

$$I = \langle \phi(I) | \hat{J} | \phi(I) \rangle \equiv \langle \hat{J} \rangle.$$
(21)

This state is obtained by adding the condition with the Lagrange multiplier ω to the Hamiltonian \hat{H} and by minimizing $\langle \hat{R} \rangle \equiv \langle \hat{H} \rangle - \omega \langle \hat{J} \rangle$. After obtaining the solution of this problem, ω is determined as a function of *I* through the

condition in Eq. (21). The functional form of ω is known to be of the form $\omega = d\langle \hat{H} \rangle / dI$. Thus, the set of basic equations of the cranking model is given by

$$\delta \langle \phi(I) | \hat{H} - \omega \hat{J} | \phi(I) \rangle = 0, \qquad (22a)$$

$$\langle \phi(I)|\hat{J}|\phi(I)\rangle = I,$$
 (22b)

and the Lagrange multiplier ω has to be of the form

$$\omega = \frac{d\mathcal{H}_{\text{rot}}(I)}{dI}, \quad \mathcal{H}_{\text{rot}}(I) \equiv \langle \phi(I) | \hat{H} | \phi(I) \rangle.$$
(23)

Now, let us compare Eqs. (22a), (22b), and (23) with the set of basic equations [I], [II] and [III] in the SCC method. It is self-evident that the basic equation [III] given in Eq. (20) is nothing but Eq. (22a) together with Eq. (23), and the first one of the canonical-variable condition [I] given in Eq. (13) just corresponds to the constraint condition (22b). Only one essential difference rests on the point that to precisely specify the *collective rotation* of the system by the SCC method, it is inevitable to define the collective angle operator $\hat{\Theta}(I)$ in Eq. (13), which satisfies the weak canonical commutation relation with the angular momentum operator \hat{J} , while the cranking model does not specify any collective angle operator explicitly.

With the analogy of the conventional cranking model, hereafter we call $|\phi(I)\rangle$ defined in Eq. (11) the *intrinsic state* in rotating frame, and the operator $\hat{R}(I) \equiv \hat{H} - \omega(I)\hat{J}$ [with $\omega(I) \equiv d\mathcal{H}_{rot}(I)/dI$] the *intrinsic Hamiltonian in rotating* frame. Since the intrinsic state $|\phi(I)\rangle$ is a *stationary state* satisfying Eq. (20), the intrinsic Hamiltonian in rotating frame can be generally expressed as

$$\hat{R}(I) \equiv \hat{H} - \omega(I)\hat{J} = \langle \phi(I) | \hat{R}(I) | \phi(I) \rangle$$

$$+ \sum_{\mu} \epsilon_{\mu}(I)\hat{c}^{\dagger}_{\mu}(I)\hat{c}_{\mu}(I) - \sum_{m} \epsilon_{m}(I)\hat{c}_{m}(I)\hat{c}^{\dagger}_{m}(I)$$

$$+ :\hat{R}_{\text{int}}(I):, \qquad (24)$$

where $\{\hat{c}^{\dagger}_{\mu}(I), \hat{c}_{m}(I)\}$ are particle and hole creation operators in *rotating frame* defined by

$$\hat{c}_{\mu}(I) |\phi(I)\rangle = \hat{c}_{m}^{\dagger}(I) |\phi(I)\rangle = 0.$$
(25)

The operator $:\hat{R}_{int}(I):$ denotes two-body interaction terms consisting of normal-ordered four-particle-hole operators in rotating frame. With the intrinsic Hamiltonian $\hat{R}(I)$ in Eq. (24), one can describe *intrinsic excitation modes in rotating frame* by the RPA eigenvalue equation

$$\hat{X}^{\dagger}_{\lambda}(I) = \sum_{\mu m} \{ \psi_{\lambda}(\mu m: I) \hat{c}^{\dagger}_{\mu}(I) \hat{c}_{m}(I) + \varphi_{\lambda}(\mu m: I) \hat{c}^{\dagger}_{m}(I) \hat{c}_{\mu}(I) \},$$

$$\delta \langle \phi(I) | [\hat{R}(I), \hat{X}^{\dagger}_{\lambda}(I)] - \Omega_{\lambda}(I) \hat{X}^{\dagger}_{\lambda}(I) | \phi(I) \rangle = 0, \quad \Omega_{\lambda}(I) > 0,$$
(26)

 $\langle \phi(I) | [\hat{X}_{\lambda}(I), \hat{X}^{\dagger}_{\lambda'}(I)] | \phi(I) \rangle = \delta_{\lambda, \lambda'},$

$$\langle \phi(I) | [\dot{X}_{\lambda}(I), \dot{X}_{\lambda'}(I)] | \phi(I) \rangle = 0.$$

The intrinsic excitation modes in rotating frame have a direct clear-cut correspondence to the "particle-hole" excitations in the conventional cranking shell model, where the interaction : $\hat{R}_{int}(I)$: is disregarded. When : $\hat{R}_{int}(I)$: is neglected, the intrinsic excitation modes $\hat{X}^{\dagger}_{\lambda}(I)$ with excitation energies $\Omega_{\lambda}(I)$ are reduced to the particle-hole excitations $\hat{c}^{\dagger}_{\mu}(I)\hat{c}_{m}(I)$ with excitation energies $\epsilon_{\mu}(I) - \epsilon_{m}(I)$.

It is well known that the RPA eigenvalue equation in Eq. (26) is related to the stability problem of the intrinsic state $|\phi(I)\rangle$. Let $i\hat{F}(I)$ be an infinitesimal generator of a variation of $|\phi(I)\rangle$. Then, the caused variation of the mean intrinsic energy in rotating frame is given by

$$\langle \phi(I) | e^{-iF(I)} \hat{R}(I) e^{iF(I)} | \phi(I) \rangle - \langle \phi(I) | \hat{R}(I) | \phi(I) \rangle$$

= $\langle \phi(I) | [\hat{R}(I), i\hat{F}(I)] | \phi(I) \rangle$
+ $\frac{1}{2!} \langle \phi(I) | [[\hat{R}(I), i\hat{F}(I)], i\hat{F}(I)] | \phi(I) \rangle + \cdots$. (27)

Since the intrinsic state $|\phi(I)\rangle$ is a stationary state for the intrinsic Hamiltonian $\hat{R}(I)$, the first term of the right-hand side in Eq. (27) vanishes. The stability condition of the intrinsic state for the variation is thus given by

$$\delta^{(2)} \langle \phi(I) | \hat{R}(I) | \phi(I) \rangle = \frac{1}{2!} \langle \phi(I) | [[\hat{R}(I), i\hat{F}(I)], i\hat{F}(I)] | \phi(I) \rangle > 0.$$
(28)

Now infinitesimal generators for variations toward the intrinsic excitation modes $\{\hat{X}^{\dagger}_{\lambda}(I), \hat{X}_{\lambda}(I)\}$ may be defined by

$$\hat{q}_{\lambda}(I) \equiv \frac{1}{\sqrt{2}} \{ \hat{X}_{\lambda}^{\dagger}(I) + \hat{X}_{\lambda}(I) \}, \quad \hat{p}_{\lambda}(I) \equiv \frac{i}{\sqrt{2}} \{ \hat{X}_{\lambda}^{\dagger}(I) - \hat{X}_{\lambda}(I) \}.$$
(29)

One then obtains

$$\begin{split} \delta_{\lambda}^{(2)} \langle \phi(I) | \hat{R}(I) | \phi(I) \rangle \\ &\equiv \frac{1}{2!} \langle \phi(I) | [[\hat{R}(I), i\hat{q}(I)], i\hat{q}(I)] | \phi(I) \rangle \\ &= \frac{1}{2!} \langle \phi(I) | [[\hat{R}(I), i\hat{p}(I)], i\hat{p}(I)] | \phi(I) \rangle = \frac{1}{2} \Omega_{\lambda}(I) > 0, \end{split}$$

$$\end{split}$$
(30)

which means that the intrinsic state $|\phi(I)\rangle$ is *stable* against the intrinsic excitation modes. The level-crossing condition $\epsilon_{\mu_0}(I) - \epsilon_{m_0}(I) = 0$ in the rotating shell model, which is closely related to the band-crossing phenomenon, thus simply corresponds to $\Omega_{\lambda_0}(I) = 0$ for the lowest-energy intrinsic excitation mode $\hat{X}^{\dagger}_{\lambda_0}(I)$ at a given *I* value. As mentioned in Sec. I, in this paper we have restricted ourselves to the problem of band termination of a single rotational band in which the evolution of the band to its termination does not encounter the band crossing. Thus, we may suppose that we only have real and nonvanishing eigenvalues $\Omega_{\lambda}(I)$ of the intrinsic excitation modes.

IV. EQUATIONS FOR GENERATORS OF COLLECTIVE ROTATION AND THE OCCURRENCE OF BAND TERMINATION

The generators $\{\hat{J}, \hat{\Theta}(I)\}$ of the collective rotation given in Eq. (13) satisfy the canonical commutation relation in Eq. (14), i.e.,

$$\langle \phi(I) | [\hat{\Theta}(I), \hat{J}] | \phi(I) \rangle = i.$$
 (31)

It is shown that they obey the equations

$$\delta\langle\phi(I)|[\hat{R}(I),\hat{J}]|\phi(I)\rangle = 0, \qquad (32)$$
$$\left\langle\phi(I)\Big|[\hat{R}(I),i\hat{\Theta}(I)] - \frac{d\omega(I)}{dI}\hat{J}\Big|\phi(I)\right\rangle = 0.$$

The first one of Eq. (32) is trivial because of $[\hat{H}, \hat{J}] = 0$. The second one is derived in the following way [8]. From Eq. (20), it follows for a small variation δI of the collective angular momentum I that

$$\delta \langle \phi(I+\delta I) | \hat{R}(I+\delta I) | \phi(I+\delta I) \rangle = 0, \qquad (33)$$

where

 δ

$$|\phi(I+\delta I)\rangle = \{1 + i\,\delta I\hat{\Theta}(I)\}|\phi(I)\rangle,\tag{34}$$

$$\hat{R}(I+\delta I) = \hat{R}(I) - \delta I \frac{d\omega(I)}{dI} \hat{J}.$$

Within the first order of δI , we thus obtain the second one of Eq. (32).

Equation (32) with Eq. (31) is a typical set of RPA equations [8,9] associated with the Nambu-Goldstone mode, based on the broken rotation symmetry of the intrinsic state $|\phi(I)\rangle$. The dynamical moment of inertia $\mathcal{J}_{TV}(I)$ for the collective rotation, called *Thouless-Valatin moment of inertia at a given value I* [8], is defined by

$$\{\mathcal{J}_{\mathrm{TV}}(I)\}^{-1} \equiv \frac{d\omega(I)}{dI} = \frac{d^2 \mathcal{H}_{\mathrm{rot}}(I)}{dI^2},$$
$$\mathcal{H}_{\mathrm{rot}}(I) = \langle \phi(I) | \hat{H} | \phi(I) \rangle. \tag{35}$$

Since the generators $\{\hat{J}, \hat{\Theta}(I)\}$ fulfill the RPA equation given by Eq. (32), they have to be orthogonal to the intrinsic excitation modes $\{\hat{X}^{\dagger}_{\lambda}(I), \hat{X}_{\lambda}(I)\}$ which are also the solutions of the RPA equation in Eq. (26):

$$\langle \phi(I) | [\hat{X}^{\dagger}_{\lambda}(I), \hat{J}] | \phi(I) \rangle = \langle \phi(I) | [\hat{X}^{\dagger}_{\lambda}(I), \hat{\Theta}(I)] | \phi(I) \rangle = 0.$$
(36)

We are now ready to investigate the stability of the intrinsic state $|\phi(I)\rangle$ for the variation δI of the collective angular momentum *I*. By taking $i\hat{F}(I) = i\hat{\Theta}(I)$ in Eq. (28), the stability condition toward the variation δI is given by

$$\begin{split} \delta_{I}^{(2)} \langle \phi(I) | \hat{R}(I) | \phi(I) \rangle \\ &= \frac{1}{2!} \langle \phi(I) | [[\hat{R}(I), i\hat{F}(I)], i\hat{F}(I)] | \phi(I) \rangle \\ &= \frac{1}{2!} \langle \phi(I) | [[\hat{R}(I), i\hat{\Theta}(I)], i\hat{\Theta}(I)] | \phi(I) \rangle \\ &= \frac{1}{2} \frac{d\omega(I)}{dI} = \frac{1}{2} \frac{d^{2} \mathcal{H}_{\text{rot}}(I)}{dI^{2}} = \frac{1}{2} \{ \mathcal{J}_{\text{TV}}(I) \}^{-1} > 0, \end{split}$$
(37)

where we have used Eq. (32).

Equation (37) denotes the important fact that when the collective angular momentum *I* arrives to an inflection point I_0 of the collective rotational energy $\mathcal{H}_{rot}(I) \equiv \langle \phi(I) | \hat{H} | \phi(I) \rangle$, satisfying

$$\{\mathcal{J}_{\rm TV}(I_0)\}^{-1} \equiv \lim_{I \to I_0 = 0} \left[\frac{d^2 \mathcal{H}_{\rm rot}(I)}{dI^2} \right] = 0,$$
(38)

the intrinsic state $|\phi(I)\rangle$ constructed upon the band-head state $|\phi_0\rangle$ in Eq. (1) *cannot be stable* against the variation toward increase of the collective angular momentum *I*. This is a precise *physical definition of the band termination of collective rotation*. Namely, at the inflection point $I=I_0$, the collective rotation to restore the broken rotation symmetry terminates. This definition is not *directly* connected with whether all the valence nucleons under consideration are coupled to a maximum angular momentum or not.

V. STRUCTURE OF SINGLE-PARTICLE ORBITALS AT BAND TERMINATION

With the explicit use of the expression of the two-body interaction terms : $\hat{R}_{int}(I)$: in the intrinsic Hamiltonian

$$:\hat{R}_{\text{int}}(I):=\frac{1}{4}\sum_{\alpha\beta\gamma\delta}v_{\alpha\beta,\gamma\delta}(I):\hat{c}^{\dagger}_{\alpha}(I)\hat{c}^{\dagger}_{\beta}(I)\hat{c}_{\delta}(I)\hat{c}_{\gamma}(I):,$$
(39)

$$v_{\alpha\beta,\gamma\delta}(I) = -v_{\beta\alpha,\gamma\delta}(I) = -v_{\alpha\beta,\delta\gamma}(I) = v_{\beta\alpha,\delta\gamma}(I),$$

the equations for generators of the collective rotation given in Eq. (32) are now explicitly written down as

$$\{\epsilon_{\mu}(I) - \epsilon_{m}(I)\}J_{\mu m}(I) + \sum_{\nu n} \{v_{\mu n, m\nu}(I)J_{\nu n}(I) - v_{\mu\nu, mn}(I)J_{\nu n}^{*}(I)\} \equiv 0,$$
(40a)

$$\{\epsilon_{\mu}(I) - \epsilon_{m}(I)\}\Theta_{\mu m}(I) + \sum_{\nu n} \{v_{\mu n, m\nu}(I)\Theta_{\nu n}(I) - v_{\mu\nu, mn}(I)\Theta_{\nu n}^{*}(I)\} = -i\{\mathcal{J}_{\mathrm{TV}}(I)\}^{-1}J_{\mu m}(I),$$
(40b)

where $J_{\mu m}(I)$ and $\Theta_{\mu m}(I)$ are the coefficients of particlehole components of $\{\hat{J}, \hat{\Theta}(I)\}$, respectively:

$$\hat{J}_{ph}(I) \equiv \sum_{\mu m} \{ J_{\mu m}(I) \hat{c}^{\dagger}_{\mu}(I) \hat{c}_{m}(I) + J^{*}_{\mu m}(I) \hat{c}^{\dagger}_{m}(I) \hat{c}_{\mu}(I) \}, \\ \hat{\Theta}_{ph}(I) \equiv \sum_{\mu m} \{ \Theta_{\mu m}(I) \hat{c}^{\dagger}_{\mu}(I) \hat{c}_{m}(I) + \Theta^{*}_{\mu m}(I) \hat{c}^{\dagger}_{m}(I) \hat{c}_{\mu}(I) \}.$$
(41)

When $I < I_0$, one always has Eq. (31) by which one obtains

$$\sum_{\mu m} \{ J_{\mu m}(I) \Theta_{\mu m}^{*}(I) - J_{\mu m}^{*}(I) \Theta_{\mu m}(I) \} = i.$$
 (42)

Equations (40b) and (42) are sufficient to determine $\Theta_{ph}(I)$ and the moment of inertia $\mathcal{J}_{TV}(I)$. By neglecting the twobody interaction terms in Eq. (40b), one obtains the Inglis formula in the cranking shell model, with the aid of Eq. (42), as

$$\Theta_{\mu m}(I) = -i \frac{\{\mathcal{J}_{\mathrm{TV}}(I)\}^{-1} J_{\mu m}(I)}{\epsilon_{\mu}(I) - \epsilon_{m}(I)}, \qquad (43)$$
$$\mathcal{J}_{\mathrm{TV}}(I) = 2 \sum_{\mu m} \frac{|J_{\mu m}(I)|^{2}}{\epsilon_{\mu}(I) - \epsilon_{m}(I)}.$$

At the band termination point $I = I_0$ defined by Eq. (38), one *cannot enforce* the weak canonical commutation relation in Eq. (31) so that Eq. (43) *cannot be adopted*. In this case, we therefore have to start with extending the condition in Eq. (13) to the following form. In the neighborhood of $I = I_0$, the condition may be written as

$$\langle \phi(I) | \hat{J} | \phi(I) \rangle = I - (I - I_0) \vartheta (I - I_0) = \begin{cases} I & \text{for } I < I_0, \\ I_0 & \text{for } dI \ge I_0, \end{cases}$$
(44)

$$\langle \phi(I) | \hat{\Theta}(I) | \phi(I) \rangle = 0,$$

where $\vartheta(I-I_0)$ is the function defined by

$$\vartheta(I-I_0) = \begin{cases} 0 & \text{for } I < I_0, \\ 1 & \text{for } I > I_0. \end{cases}$$
(45)

At the band termination point $I=I_0$, Eq. (44) simply becomes

$$\langle \phi(I_0) | \hat{J} | \phi(I_0) \rangle = I_0, \qquad (46a)$$

$$\langle \phi(I_0) | \hat{\Theta}(I_0) | \phi(I_0) \rangle = 0,$$
 (46b)

and Eqs. (40a) and (40b) are reduced to

$$\{\epsilon_{\mu}(I_{0}) - \epsilon_{m}(I_{0})\}J_{\mu m}(I_{0}) + \sum_{\nu n} \{v_{\mu n, m\nu}(I_{0})J_{\nu n}(I_{0}) - v_{\mu\nu, mn}(I_{0})J_{\nu n}^{*}(I_{0})\} = 0, \qquad (47a)$$

$$\{\epsilon_{\mu}(I_{0}) - \epsilon_{m}(I_{0})\}\Theta_{\mu m}(I_{0}) + \sum_{\nu n} \{v_{\mu n, m\nu}(I_{0})\Theta_{\nu n}(I_{0}) - v_{\mu\nu,mn}(I_{0})\Theta_{\nu n}^{*}(I_{0})\} = 0.$$
(47b)

Equation (47b) means that the single-particle orbitals at $I = I_0$ have a special property that all the matrix elements of $\Theta_{\mu m}(I_0)$ vanish, since we have supposed that the stability matrix of the intrinsic Hamiltonian is to be positive definite. This fact together with the condition in Eq. (46b) demonstrates that the collective angle operator $\hat{\Theta}(I)$, which is essential to properly define the collective rotation, vanishes at $I = I_0$. Equation (40a) is the identity for the conserved angular momentum operator. However, at $I = I_0$, it is expressed as Eq. (47a) having the same structure as Eq. (47b). This implies that the single-particle orbitals at $I = I_0$ have a special property that all the particle-hole components of the angular momentum, which are responsible for the collective rotation, vanish and only the diagonal components remain. Physically this means that all valence particles in the occupied orbitals at $I = I_0$ are *in alignment* to be coupled to the angular momentum I_0 as is specified by Eq. (46a), realizing the scenario of band termination by Bohr and Mottelson. Conceptually, the band termination is a dynamical restoration of the broken symmetry, where the one-body density operator and the angular momentum operator are diagonalized simultaneously.

When the particle-hole components of the total angular momentum operator vanishes, its canonical conjugate operator $\Theta(I)$ suddenly vanishes, satisfying the condition (47b). Namely, the collective rotational state and the state with fully aligned single-particles are disconnected with each other, and the band termination occurs at the singular point $I = I_0$. After the band termination of the collective rotation, one may thus has the situation of the so-called rotation about symmetry axis [2] which is also referred to as noncollective rotation [3]. In the numerical calculations of the cranked HF state with the Lagrangian multiplier ω , it should be noticed that the discontinuous change between the collective rotation and the noncollective rotation is often overlooked when one uses the constraint condition in Eq. (21), i.e., $\langle \hat{J} \rangle \equiv \langle \phi(I) | \hat{J} | \phi(I) \rangle = I$. In this case, therefore, one has to properly employ the constraint condition given in Eq. (44), i.e., $\langle \hat{J} \rangle = I - (I - I_0) \vartheta (I - I_0)$. Then, upon the variation of ω , one has

$$d\langle \hat{H} \rangle = \omega d\langle \hat{J} \rangle = \omega dI \{ 1 - \vartheta (I - I_0) \}, \qquad (48)$$

and so $\langle \hat{H} \rangle$, viewed as a function of *I*, satisfies

$$\frac{d}{dI}\langle \hat{H} \rangle = \omega \{1 - \vartheta (I - I_0)\} = \begin{cases} \omega & \text{for} \quad I < I_0, \\ 0 & \text{for} \quad I > I_0. \end{cases}$$
(49)

From Eq. (49), one obtains

$$\frac{d^2}{dI^2}\langle \hat{H}\rangle = \frac{d\omega}{dI} \{1 - \vartheta(I - I_0)\} - \omega \,\delta(I - I_0), \qquad (50)$$

which leads to the *normal* relation when $I \neq I_0$,

$$\frac{d^2}{dI^2} \langle \hat{H} \rangle = \begin{cases} \frac{d\omega}{dI} & \text{for } I < I_0, \\ 0 & \text{for } I > I_0. \end{cases}$$
(51)

At $I = I_0$ where the all valence particles in the occupied orbitals are in full alignment, one has from Eq. (50)

$$\left[\frac{d^2\langle\hat{H}\rangle}{dI^2}\right]_{I=I_0} = \left\{\lim_{I\to I_0=0} \left(\frac{d\omega}{dI}\right)\right\} \{1-\vartheta(0)\} - \omega(I_0)\,\delta(0).$$
(52)

Thus, a physical *finite value* of $[d^2 \langle \hat{H} \rangle / dI^2]_{I=I_0}$ is obtained only when $\lim_{I \to I_0 = 0} (d\omega/dI)$ satisfies⁵

$$\left\{\lim_{I \to I_0 - 0} \left(\frac{d\omega}{dI}\right)\right\} = 2\,\omega(I_0)\,\delta(0),\tag{53}$$

so that one has the value given by $[d^2 \langle \hat{H} \rangle / dI^2]_{I=I_0} = 0$. This means that the value I_0 , where all the valence particles in the occupied orbitals become in full alignment, just corresponds to the inflection point of the collective rotational energy $\langle \hat{H} \rangle$. Equation (53) shows that $d\omega/dI$ cannot be convergent at the inflection point I_0 .

VI. NUMERICAL INVESTIGATION OF SINGLE-PARTICLE ORBITALS NEAR BAND TERMINATIONS IN $$^{24}\mathrm{Mg}$$ AND ${}^{16}\mathrm{O}\,*$

In order to visualize the special character of singleparticle orbitals in the intrinsic state at $I=I_0$, discussed in Sec. V, we have made numerical investigation of the singleparticle orbitals in the intrinsic state near the band terminations in ${}^{24}Mg$ and ${}^{16}O^*$. The band termination in *sd*-shell nuclei at high spin is not a phenomenon specific to the mean field method, but appears in spherical sd-shell model calculations with particle-hole configuration mixing [10], and in the Elliott SU(3) model [11]: It is a basic quantummechanical property of a finite many-body system [3]. In this sense, it is quite intersting to investigate behavior of the single-particle orbitals near the band terminations in ²⁴Mg and ${}^{16}O^*$, whose intrinsic states are expected to be stable for the intrinsic excitation modes. The experimental evidence for the ground-state rotational band structure of ²⁴Mg (both energy spacing and transition probabilities) with I < 8 is definitely convincing [12,13], and it has been suggested [14,15] that its band termination is at $I_0 = 12$ [Fig. 1(a)]. The excited 6.05 MeV 0_2^+ state in ¹⁶O has experimentally suggested as a 4p-4h excitation with a large intrinsic deformation, and to be a band-head state forming a rotational band I=0,2,4,6,8with the band termination at $I_0 = 8$ [Fig. 1(b)].

The intrinsic states for these rotational bands are given by

$$\vartheta(x) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\alpha \frac{e^{i\alpha x}}{\alpha - i\varepsilon} = \begin{cases} 0 & \text{for } x < 0, \\ 1 & \text{for } x > 0, \end{cases}$$

we have $\vartheta(0) = 1/2$.

⁵When we employ the functional form of $\vartheta(x)$,



solving the cranked HF state with the Lagrange multiplier ω , i.e.,

$$\delta \langle \phi(I) | \hat{H} - \omega \hat{J}_x | \phi(I) \rangle = 0, \tag{54}$$

$$\langle \phi(I) | \hat{J}_x | \phi(I) \rangle = I,$$

where we have adopted the three-dimensional harmonic oscillator basis with the Gogny-D1' force [16–18] for the effective interaction, and the rotational axis is chosen as the *x* axis. In numerically solving this cranked HF equation, we have employed a new algorithm [19] developed by Iwasawa *et al.* This algorithm, called the *reference state method*, enables us to solve the constrained HF(CHF) equation without relying on the conventional *adiabatic assumption.*⁶ By this method, one can obtain many CHF lines, which are formed by continuously connected solutions of the CHF equation with a maximum overlap criteria. By applying this algorithm to the cranked HF equation given in Eq. (54), one may thus

FIG. 1. Rotational energy $\mathcal{H}_{rot}(I) - \mathcal{H}_{rot}(0)$ vs angular momentum I of ²⁴Mg and ¹⁶O*. (a) The ground rotational band of ²⁴Mg. We denote the yrast rotational band from the ground state obtained with our method by a solid line, the band obtained by Ragnarsson et al. [14] by a broken line with diamonds, that obtained by Bonche et al. [20] by a dotted line, definite experimental values [12] by crosses. Tentative states [21] are shown in the parentheses. (b) The excited rotational band of ¹⁶O. We denote the excited rotational band from 0^+_2 state obtained with our method by a solid line, the band obtained by Åberg et al. [22] by a broken line with diamonds, definite experimental values [23] by crosses. The tentative state [24] is shown in the parentheses.

obtain many rotational bands in place of many CHF lines. Thus, the structure of single-particle orbitals in the rotational band in ¹⁶O upon the excited 4p-4h 0⁺ state is easily evaluated.

In our program the major shells have been included up to N=4 and the parity and the signature symmetry have been imposed. It has been observed that the Gogny-D1' force well reproduces the binding energies of the ground states of ²⁴Mg and ¹⁶O (see Table I), but does not lead to a good agreement in absolute values between the experimental rotational energies and the calculated ones (see Fig. 1). In this sense, the obtained numerical results for the behavior of single-particle orbitals should be evaluated in a qualitative point of view.

Figures 2 and 3 visualize the behavior of single-particle orbitals at I=0,6,10,12 in the ground-state band of ²⁴Mg and

TABLE I. Binding Energies of Ground States.

Nuclei	²⁴ Mg	¹⁶ O
Our calc. [MeV]	- 196.77	- 129.99
Exp. [25] [MeV]	- 198.26	- 127.62

⁶The terminology *adiabatic assumption* used here means that it is characterized by finding out *only* the most energetically favorable CHF state satisfying a given constraint condition.









 $J_{(n,b)=6}$

I = 10

FIG. 2. Density distribution and matrix elements of \hat{J}_x of ²⁴Mg (see text).





I = 12



at I=0,4,6,8 in the excited-state band of ¹⁶O, respectively. The right-hand side of these figures shows the magnitude of the matrix elements of \hat{J}_x , i.e., $|\langle \alpha(I) | \hat{J}_x | \beta(I) \rangle|$, between the single-particle states $|\alpha(I)\rangle$ and $|\beta(I)\rangle$ at an angular momentum *I*: The vertical axis represents the magnitude $J(\mathbf{a},\mathbf{b};I) \equiv |\langle \alpha(I) | \hat{J}_x | \beta(I) \rangle|$ and the horizontal axes **a** and **b** denote the ID numbers of the eigenstates $\{|\alpha(I)\rangle\}$ in a sub-

space with parity π_{α} = + and signature s_{α} = + of the proton system. (We have the same picture for the neutron system.) The left-hand side shows density distributions projected on the the *yz* plain perpendicular to the rotational axis, i.e., *x* axis. It can be seen from Figs. 2 and 3 that the rotational alignments of the single-particle orbit of individual particles are associated with a trend toward symmetry about the *x*











I = 6









axis. At $I = I_0$, all individual particles are thus in alignment so as to produce an oblate symmetry with respected to the *x* axis in accordance with the scenario of Bohr and Mottelson [1,2]. With the employment of the reference state method in solving the cranked HF equation, we have also been able to justify the singularity shown in Eq. (53).

VII. CONCLUDING REMARKS

By fully employing the concept of the broken rotation symmetry as the origin of the collective rotation, we have shown the dynamical mechanism of occurrence of the band termination of collective rotation from the standpoint of the nuclear many-body problem. It has been disclosed that the collective rotation to restore the broken symmetry vanishes when the intrinsic state in rotating frame cannot be stable against the variation toward increase of the collective angular momentum I. It has also been demonstrated that the value of the collective angular momentum at the band termination is simply an inflection point of the collective rotational energy. The behavior of the single-particle orbitals in rotating frame is justified and visualized to be in accordance with the scenario of the band termination, which was originally discussed by Bohr and Mottelson.

In this paper, we have discussed the band termination of a single collective rotational band, provided that the intrinsic state in rotating frame is stable, throughout the evolution of the rotational band to its termination. It is, therefore, outside of the scope of this paper to discuss the termination phenomenon along the yrast line in the heavier nuclei, where the rotational alignments of particles individually occur accompanied by the level crossings of single-particle orbitals. This problem will be discussed in a separate paper.

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