Large-amplitude collective dynamics of shape phase transition in the low-lying states of $^{30-38}$Mg is investigated by solving the five-dimensional (5D) quadrupole collective Schrödinger equation. The collective masses and potentials of the 5D collective Hamiltonian are microscopically derived with use of the constrained Hartree-Fock-Bogoliubov plus local quasiparticle random phase approximation method. Good agreement with the recent experimental data is obtained for the excited $0^+$ states as well as the ground bands. For $^{30}$Mg, the shape coexistence picture that the deformed excited $0^+$ state coexists with the spherical ground state approximately holds. On the other hand, large-amplitude quadrupole-shaped fluctuations dominate in both the ground and the excited $0^+$ states in $^{32}$Mg, providing a picture that is different from the interpretation of the “coexisting spherical excited $0^+$ state” based on the naive inversion picture of the spherical and deformed configurations.

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Nuclei exhibit a variety of shapes in their ground and excited states. A feature of the quantum phase transition of a finite system is that the order parameters (shape deformation parameters) always fluctuate and vary with the particle number. Especially, the large-amplitude shape fluctuations play a crucial role in transitional (critical) regions. Spectroscopic studies of low-lying excited states in transitional nuclei are of great interest to observe such unique features of the finite quantum systems.

Low-lying states of neutron-rich nuclei at approximately $N = 20$ attract great interest, as the spherical configurations associated with the magic number disappear in the ground states. In neutron-rich Mg isotopes, the increase of the excitation energy ratio $E(4_{1}^+)/E(2_{1}^+)$ [1–3] and the enhancement of $B(E2; 2_1^+ \rightarrow 0_1^+)$ from $^{30}$Mg to $^{34}$Mg [4–6] indicate a kind of quantum phase transition from spherical to deformed shapes taking place around $^{32}$Mg. These experiments stimulate microscopic investigations on quadrupole collective dynamics unique to this region of the nuclear chart with various theoretical approaches: the shell model [7–10], the Hartree-Fock-Bogoliubov (HFB) method [11,12], the parity-projected Hartree-Fock (HF) [13], the quasiparticle random phase approximation (QRPA) [14,15], the angular-momentum projected generator coordinate method (GCM) with [16] and without [17,18] restriction to the axial symmetry, and the antisymmetrized molecular dynamics [19].

Quite recently, excited $0^+$ states were found in $^{30}$Mg and $^{32}$Mg at 1.789 MeV and 1.058 MeV, respectively, and their characters are presently under hot discussion [20–23]. For $^{30}$Mg, the excited $0^+$ state is interpreted as a prolately deformed state which coexists with the spherical ground state. For $^{32}$Mg, from the observed population of the excited $0^+$ state in the $t,p$ reaction on $^{30}$Mg, it is suggested [22] that the $0^+$ state is a spherical state coexisting with the deformed ground state and that their relative energies are inverted at $N = 20$. However, available shell-model and GCM calculations considerably overestimate its excitation energy (1.4–3.1 MeV) [9,10,16,21]. It is therefore a challenge for modern microscopic theories of nuclear structure to clarify the nature of the excited $0^+$ states. For understanding shape dynamics in low-lying collective excited states of Mg isotopes near $N = 20$, it is certainly desirable to develop a theory capable of describing various situations in a unified manner, including, at least, (1) an ideal shape coexistence limit where the wave function of an individual quantum state is well localized in the deformation space and (2) a transitional situation where the large-amplitude shape fluctuations dominate.

In this Rapid Communication, we microscopically derive the five-dimensional (5D) quadrupole collective Hamiltonian using the constrained Hartree-Fock-Bogoliubov (CHFB) plus local QRPA (LQRPA) method [24]. The 5D collective Hamiltonian takes into account all the five quadrupole degrees of freedom: the axial and triaxial quadrupole deformations $(\beta, \gamma)$ and the three Euler angles. This approach is suitable for our purpose of describing a variety of quadrupole collective phenomena in a unified way. Another advantage is that the time-odd mean-field contributions are taken into account in evaluating the vibrational and rotational inertial functions. In spite of their importance for correctly describing collective excited states, the time-odd contributions are ignored in the widely used Inglis-Belyaev cranking formula for inertial functions. The CHFB + LQRPA method has been successfully applied to various large-amplitude collective dynamics, including the oblate-prolate shaped coexistence phenomena in Se and Kr isotopes [24,25], the $\gamma$-soft dynamics in $sd$-shell nuclei [26], and the shape phase transition in neutron-rich Cr isotopes [27]. A preliminary version of this work was reported in Ref. [28].

The 5D quadrupole collective Hamiltonian is written as

$$\mathcal{H}_{\text{coll}} = T_{\text{ vib}} + T_{\text{ rot}} + V(\beta, \gamma),$$

$$T_{\text{ vib}} = \frac{1}{2} D_{\beta\beta}(\beta, \gamma) \dot{\beta}^2 + D_{\beta\gamma}(\beta, \gamma) \dot{\beta} \dot{\gamma} + \frac{1}{2} D_{\gamma\gamma}(\beta, \gamma) \dot{\gamma}^2,$$

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where $T_{\text{vib}}$ and $T_{\text{rot}}$ are the vibrational and rotational kinetic energies, respectively, and $V$ is the collective potential. The vibrational collective masses $D_{\beta\beta}$, $D_{\beta\gamma}$, and $D_{\gamma\gamma}$ are the inertial functions for the $(\beta, \gamma)$ coordinates. The rotational moments of inertia $J_k$ associated with the three components of the rotational angular velocities $\omega_k$ are defined with respect to the principal axes. In the CHFB + LQRPA method, the collective potential is calculated with the CHFB equation with four constraints on the two quadrupole operators and the proton and neutron numbers. The inertial functions in the collective Hamiltonian are determined from the LQRPA normal modes locally defined for each CHFB state in the $(\beta, \gamma)$ plane. The equations to find the local normal modes are similar to the well-known QRPA equations, but the equations are solved on top of the nonequilibrium CHFB states. Two LQRPA solutions representing quadrupole shaped motion are selected for the calculation of the vibrational inertial functions. After quantizing the collective Hamiltonian, we solve the 5D collective Schrödinger equation and obtain collective wave functions

$$\Psi_{aIM}(\beta, \gamma, \Omega) = \sum_{K=\text{even}} \Phi_{aIK}(\beta, \gamma, \Omega) |I|MK\rangle,$$  

where $\Phi_{aIK}(\beta, \gamma, \Omega)$ are the vibrational wave functions and $|I|MK\rangle$ are the rotational wave functions defined in terms of $D$ functions $D^{|I|MK}_{\beta\gamma}(\Omega)$. We then evaluate $E2$ matrix elements. More details of this approach are given in Ref. [24].

We solve the CHFB + LQRPA equations employing, as a microscopic Hamiltonian, the pairing-plus-quadrupole (P + Q) model including the quadrupole-pairing interaction. As an active model space, the two major harmonic oscillator shells ($sd$ and $pf$ shells) are taken into account for both neutrons and protons. To determine the parameters in the P + Q Hamiltonian, we first perform Skyrme-HFB calculations at the spherical shape. The resulting single-particle energies (in the canonical basis) are then scaled with the effective mass of the SkM* functional $m^*/m = 0.79$, since the P + Q model is designed to be used for single-particle states whose effective mass is equal to the bare nucleon mass. In $^{32}\text{Mg}$, the $N = 20$ shell gap between $d_{3/2}$ and $f_{7/2}$ is 3.7 MeV for the SkM* functional, and it becomes 2.9 MeV after the effective mass scaling. This value is appreciably smaller than the standard modified oscillator value 4.5 MeV [30]. This spacing almost stays constant for $^{30-36}\text{Mg}$. The strengths of the monopole-pairing interaction are determined to reproduce the pairing gaps obtained in the Skyrme-HFB calculations at the spherical shape. The strength of the quadrupole particle-hole interaction is determined to reproduce the magnitude of the axial quadrupole deformation $\beta$ of the Skyrme-HFB minimum. The strengths of the quadrupole-pairing interaction are determined so as to fulfill the self-consistency condition [31]. We use the quadrupole polarization charge $\delta e_{\text{pol}} = 0.5$ for both neutrons and protons when evaluating $E2$ matrix elements. We solve the CHFB + LQRPA equations at 3600 $\beta$-$\gamma$ mesh points in the region $0 < \beta < \beta_{\text{max}}$ and $0^\circ < \gamma < 60^\circ$, with $\beta_{\text{max}} = 0.5$ for $^{30}\text{Mg}$ and 0.6 for $^{32,34,36}\text{Mg}$.

Our theoretical framework is quite general and it can be used in conjunction with various Skyrme forces or modern density functionals going beyond the P + Q model. Then the effects of weakly bound neutrons and coupling to the continuum on the properties of the low-lying collective excitations, discussed in Refs. [14, 15], can be taken into account, for example, by solving the CHFB + LQRPA equations in the three-dimensional (3D) coordinate mesh representation. However, it requires a large-scale calculation with modern parallel processors and it remains a challenging future subject. A step toward this goal has recently been carried out for axially symmetric cases [27].

Figure 1 shows the collective potentials $V(\beta, \gamma)$ for $^{30-36}\text{Mg}$. It is clearly seen that prolate deformation grows with an increase in the neutron number. The collective potential for $^{30}\text{Mg}$ is very soft with respect to $\beta$. It has a minimum at $\beta = 0.11$ and a local minimum at $\beta = 0.33$. The barrier height between the two minima is only 0.24 MeV (measured from the lower minimum). In $^{32}\text{Mg}$, in addition to the prolate minimum at $\beta = 0.33$, a spherical local minimum (associated with the $N = 20$ spherical shell gap) appears. The barrier height between the two minima is 1.0 MeV (measured from the lower minimum). The spherical local minimum disappears in $^{34}\text{Mg}$ and $^{36}\text{Mg}$, and the prolate minima become soft in

\[ T_{\text{rot}} = \frac{1}{2} \sum_{k=1}^{3} J_k(\beta, \gamma) \omega_k^2, \]

\[ \langle \Phi_1 \alpha I K \rangle \]

\[ \langle \Omega_1 \rangle \]

\[ V_{\text{pol}} = -\frac{e^2}{2\epsilon}. \]
the very low excitation energy of the $0^2_2$ states and the increase of $E(2_1^+ + 2_2^+) / E(2_1^+)$ decreases as 2.03, 1.76, 1.43, and 1.47, in going from $^{30}\text{Mg}$ to $^{36}\text{Mg}$. Thus, the properties of the $2_1^+$ and $4_1^+$ states gradually change from vibrational to rotational with increasing neutron number.

Let us next discuss the properties of the $0^+_2$ states and the $2^+_2$ and $4^+_2$ states connected to the $0^+_2$ states with strong $E2$ transitions. The result of calculation is presented in Fig. 3, together with the recent experimental data. The calculated excitation energies of the $0^+_2$ states are 1.353 and 0.986 MeV for $^{30}\text{Mg}$ and $^{32}\text{Mg}$, respectively, in fair agreement with the experimental data [21,22]. In particular, the very low excitation energy of the $0^+_2$ state in $^{32}\text{Mg}$ is well reproduced. In our calculation, more than 90% (80%) of the collective wave functions for the yrast (excited) band members are composed of the $K = 0$ component. Therefore, we denote the ground band by “the $K = 0$ band,” and the excited band by “the $K = 2$ band.” The $2^+_2$ and $4^+_2$ states belonging to the $K = 0$ band appear as the second $2^+_2$ and $4^+_2$ states in $^{30,32}\text{Mg}$, while they appear as the third $2^+_2$ and $4^+_2$ states in $^{34,36}\text{Mg}$. Accordingly, we use $2_{2,3}^+$ and $4_{2,3}^+$ to collectively indicate the second or the third $2^+_2$ and $4^+_2$ states. The calculated ratios of the excitation energies relative to the excited $0^+_2$ state $[E(4_{2,3}^+) - E(0^+_2)] / [E(2_{2,3}^+) - E(0^+_2)]$ are 3.18, 2.87, 3.25, and 3.00, for $^{30}\text{Mg}$, $^{32}\text{Mg}$, $^{34}\text{Mg}$, and $^{36}\text{Mg}$, respectively. In the upper panel of Fig. 3 we also plot the rotor-model prediction for the excitation energies of the $4^+_2$ states estimated from the $0^+_2 - 2^+_2$ spacings in the $K = 0_2$ bands. The deviation from the rotor-model prediction is largest in $^{32}\text{Mg}$, indicating importance of shape-fluctuation effects. Although the calculated excitation spectrum of the $K = 0_2$ band in $^{30}\text{Mg}$ looks rotational, we find a significant deviation from the rotor-model prediction in the $E2$ transition properties. The calculated ratios of the $E2$ transition strengths $B(E2; 2_{2,3}^+ \rightarrow 2_{2,3}^+) / B(E2; 2_1^+ \rightarrow 2_{2,3}^+)$ of the interband transition strengths between the $K = 0_2$ and $K = 0_2$ bands (lower panel). Experimental data are taken from Refs. [21,22]. See text for details.
Contour lines are drawn at every eighth part of the maximum value. From the behavior of the interband discussed in our forthcoming full-length paper. As suggested collective kinetic energy (collective masses). This point will be \[ \sum \] shape. From the behavior of the vibrational wave functions, deformed region. In $^{34}\text{Mg}$, it is distributed around the prolate region. In $^{34}\text{Mg}$, it is distributed around the prolate shape. From the behavior of the vibrational wave functions, one can conclude that shape fluctuation in the ground $0_1^+$ state is largest in $^{32}\text{Mg}$. To understand the microscopic mechanism of this change from $^{30}\text{Mg}$ to $^{34}\text{Mg}$, it is necessary to take into account not only the properties of the collective potential in the $\beta$ direction but also its curvature in the $\gamma$ direction and the collective kinetic energy (collective masses). This point will be discussed in our forthcoming full-length paper. As suggested from the behavior of the interband $B(E2)$ ratio, the vibrational wave functions of the $2_1^+$ state are noticeably different from those of the $0_1^+$ state in $^{30}\text{Mg}$ and $^{32}\text{Mg}$, while they are similar in the case of $^{34}\text{Mg}$. Next, let us examine the vibrational wave functions of the $0_2^+$ and $2_1^+$ states in $^{30}$–$^{34}\text{Mg}$. It is immediately seen that they exhibit one node in the $\beta$ direction. This is their common feature. In $^{30}\text{Mg}$ and $^{32}\text{Mg}$, one bump is seen in the spherical to weakly deformed region, while the other bump is located in the prolate deformed region around $\beta = 0.3$–$0.4$. The bump at the deformed region of the $0_2^+$ and $2_1^+$ states and the extended structure of the $2_1^+$ states to the deformed region, which lead to an appreciable overlap of their vibrational wave functions, are responsible for the large interband $B(E2;0_2^+ \rightarrow 2_1^+)$ values. In $^{34}\text{Mg}$, the node is located near the peak of the vibrational wave function of the $0_1^+$ state, suggesting that they have $\beta$-vibrational properties.

To further reveal the nature of the ground and excited $0^+$ states, it is important to examine not only their vibrational wave functions but also their probability density distributions. Since the 5D collective space is a curved space, the normalization condition for the vibrational wave functions is given by

\[
\int \sum_k |\Phi_{\alpha l K}(\beta, \gamma)|^2 |G(\beta, \gamma)|^{1/2} d\beta d\gamma = 1,
\]

with the volume element

\[
|G(\beta, \gamma)|^{1/2} d\beta d\gamma = 2\beta^4 \sqrt{W(\beta, \gamma)} R(\beta, \gamma) \sin 3\gamma \ d\beta d\gamma,
\]

\[
W(\beta, \gamma) = (D_{\beta\beta}(\beta, \gamma)D_{\gamma\gamma}(\beta, \gamma)) - (D_{\beta\gamma}(\beta, \gamma))^2 \beta^{-2},
\]

\[
R(\beta, \gamma) = D_1(\beta, \gamma)D_2(\beta, \gamma)D_3(\beta, \gamma),
\]

where $D_{\alpha l 1,2,3}$ are the rotational masses defined through $J_\alpha = 4\beta^2 D_\alpha \sin^2(\gamma - 2\pi k/3)$. Thus, the probability density of taking a shape with specific values of $(\beta, \gamma)$ is given by $\sum_k |\Phi_{\alpha l K}(\beta, \gamma)|^2 |G(\beta, \gamma)|^{1/2}$. Due to the $\beta^4$ factor in the volume element, the spherical peak of the vibrational wave function disappears in the probability density distribution. Accordingly, it will give us a picture that is quite different from that of the wave function. Needless to say, it is important to examine both aspects to understand the nature of individual quantum states.

In Fig. 5, we display the probability density integrated over $\gamma$, $P(\beta) \equiv \int d\gamma |\Phi_{\alpha l 0,0 K=0}(\beta, \gamma)|^2 |G(\beta, \gamma)|^{1/2}$, of finding a shape with a specific value of $\beta$, together with the vibrational wave functions squared $|\Phi_{\alpha l 1,0 K=0}(\beta, \gamma)|^2$ for the ground and excited $0^+$ states ($\alpha = 1$ and 2). Let us first look at the upper panels for the ground states. We note that, as expected, the spherical peak of the vibrational wave function for $^{30}\text{Mg}$ in Fig. 5(a) corresponds to the peak at $\beta \simeq 0.15$ of the probability density in Fig. 5(b). In Fig. 5(b), the peak position moves toward a larger value of $\beta$ in going from $^{30}\text{Mg}$ to $^{34}\text{Mg}$. The distribution for $^{32}\text{Mg}$ is much broader than those for $^{30}\text{Mg}$ and $^{34}\text{Mg}$.

Next, let us look at the lower panels in Fig. 5 for the excited states. In Fig. 5(c), the vibrational wave functions for

\[
\begin{aligned}
0^+_1 & (a) \\
0^+_1 & (e) \\
0^+_2 & (i) \\
2^+_1 & (b) \\
2^+_1 & (f) \\
2^+_1 & (j) \\
0^+_2 & (c) \\
0^+_2 & (g) \\
0^+_2 & (k) \\
2^+_2 & (d) \\
2^+_2 & (h) \\
2^+_2 & (l)
\end{aligned}
\]
SHAPE FLUCTUATIONS IN THE GROUND AND EXCITED . . .

$^{30}$Mg and $^{32}$Mg exhibit the maximum peak at the spherical shape. However, these peaks become small and are shifted to the region with $\beta \simeq 0.1$ and $\beta \simeq 0.2$ in $^{30}$Mg and $^{32}$Mg, respectively, in Fig. (5(d)). On the other hand, the second peaks at $\beta \simeq 0.3$ and $\beta \simeq 0.4$ in $^{30}$Mg and $^{32}$Mg, respectively, seen in Fig. (5(c)), become the prominent peaks in Fig. (5(d)). In $^{30}$Mg, the bump at $\beta \simeq 0.1$ is much smaller than the major bump at $\beta \simeq 0.3$. In this sense, we can regard the $0_{-}^{+}$ state of $^{30}$Mg as a prolate deformed state. In the case of $^{32}$Mg, the probability density exhibits a very broad distribution extending from the spherical to deformed regions up to $\beta \simeq 0.5$ with a prominent peak at $\beta \simeq 0.4$ and a node at $\beta \simeq 0.3$. The position of the node coincides with the peak of the probability density distribution of the $0_{1}^{+}$ state, as expected from the orthogonality condition.

In summary, we have investigated the large-amplitude collective dynamics in the low-lying states of $^{30-36}$Mg by solving the 5D quadrupole collective Schrödinger equation. The collective masses and potentials of the 5D collective Hamiltonian are microscopically derived with use of the CHFB + LQRPA method. Good agreement with the recent experimental data is obtained for the excited $0^{+}$ states as well as the ground bands. For $^{30}$Mg, the shape coexistence picture that the deformed excited $0^{+}$ state coexists with the spherical ground state approximately holds. On the other hand, large-amplitude quadrupole-shaped fluctuations dominate in both the ground and the excited $0^{+}$ states in $^{32}$Mg, in contrast to the interpretation of “deformed ground and spherical excited $0^{+}$ states” based on the simple inversion picture of the spherical and deformed configurations. To test these theoretical predictions, an experimental search for the distorted rotational bands built on the excited $0_{1}^{+}$ states in $^{30}$Mg and $^{32}$Mg is strongly desired.

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