Description of the yrast states in ^{24}Mg by the self-consistent 3D-cranking model

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(Received 2 August 2005; published 30 November 2005)

With the self-consistent 3D-cranking model, the ground-state rotational band in ^{24}Mg is analyzed. The role of triaxial deformation is discussed, in particular in a description of the observed two $I^\pi = 8^+$ states.

DOI: 10.1103/PhysRevC.72.057304 PACS number(s): 21.60.−n, 21.10.Re, 27.30.+t

$^{24}_{12}$Mg has been well studied as a typical case of a well-deformed light-mass nuclear system. After self-consistent microscopic calculations of the nonrelativistic [1] and relativistic methods [2] in the late 1980s, the nucleus is believed to have an axially symmetric and prolate shape in the ground state. Assuming the core of ^{16}O, the ground-state configuration is supposed to have eight valence particles occupying the $d_{5/2}$ orbits (four neutrons and four protons). Because the Fermi level of this nucleus is in the beginning of the *sd* shell (corresponding to the $N = 2$ harmonic-oscillator shell), there are many open valence orbitals above the Fermi level, which may induce deformation and consequently a collective rotation. Such a rotational band has been already identified in experiments (for instance, see Refs. [3,4]). A particular interest is the existence of the two $I^\pi = 8^+$ states observed in experiment. These two states are energetically close to each other (the difference is about 2 MeV). After the study of Sheline *et al*. [5], it is believed that the second 8^+ belongs to the ground-state rotational band (*g* band). Valor *et al*. analyzed the *g* band with the cranked Skyrme HF + BCS approach as well as the configuration mixing approach based on the generator coordinate method (GCM) [6]. However, their calculations assume axial symmetry for descriptions of intrinsic states. Up to $I^\pi = 4^+$, they were able to reproduce the experimental data very well. The cranked mean-field calculation gave a fairly good agreement for $I^\pi = 6^+$, while the configuration mixing approaches returned larger energies for the state. This is simply because these states at high spin were projected out from the noncranked mean-field state. Interestingly, the cranked mean-field calculation for $I^\pi = 8^+$ matches the observed energy of the first 8^+ state, but the authors dismissed the agreement on the basis of the analysis of Sheline *et al*. [5], and they speculated that the disagreement might mainly come from the triaxial effects at high spin induced by the disappearance of the pairing correlation in their calculation.

Inspired by the study by Valor *et al*. [6], I performed the self-consistent cranking calculation, allowing triaxial deformation in a self-consistent manner. As a new aspect in my study, not only 1D-cranking but also 3D-cranking calculations were carried out. An advantage of the 3D-cranking model is that low- and high-K intrinsic structures can be systematically studied [7].

The Hamiltonian used in my study reads

$$\hat{H} = \hat{H}_0 + \hat{V}, \tag{1}$$

where the first term describes the one-body part, which is the spherical Nilsson Hamiltonian in this study, and the second part is the two-body interaction, which is the pairing-plus-quadrupole force (the so-called P+QQ force). The model space (valence space) to diagonalize the two-body part contains two major shells ($N = 2, 3$) in the spherical Nilsson model, in accordance with the Kummar-Baranger criteria for the P+QQ force [8]. The variational state is the HF-Bogoliubov (HFB) ansatz, which is a generalized product state. With quasiparticle annihilation operators β_q, the ansatz is expressed as

$$|\mathrm{HFB}\rangle = \prod_q \beta_q |0\rangle, \tag{2}$$

where $|0\rangle$ is the vacuum for the canonical bases a_m and $a_m^\dagger$. (In my case, the canonical basis corresponds to the spherical Nilsson basis.) The canonical basis and the quasiparticle basis are connected by a unitary transformation called the general Bogoliubov transformation [9]. The variational equation is derived for

$$\delta\langle \mathrm{HFB}|\hat{H} - \sum_{i=1}^{3}(\omega_i \hat{J}_i + \mu_i \hat{B}_i) - \sum_{\tau=p,n} \lambda_\tau \hat{N}_\tau |\mathrm{HFB}\rangle = 0. \tag{3}$$

In the above equation, $\hat{J}_i$ is the ith component of the angular-momentum operator (the index i takes $i = 1, 2, 3$), and $\hat{N}_\tau$ describes the number operator for protons ($\tau = p$) and neutrons ($\tau = n$). $\hat{B}_i$ is an off-diagonal component of the quadrupole operator, defined as

$$\hat{B}_i = \tfrac{1}{2}(\hat{Q}_{jk} + \hat{Q}_{kj}), \tag{4}$$

where the indices (i, j, k) should be placed in a cyclic manner. Each term with the Lagrange multipliers (ω_i, μ_i, and λ_τ) is necessary to put constraints in intrinsic states: $(\langle \hat{J}_1\rangle, \langle \hat{J}_2\rangle, \langle \hat{J}_3\rangle) = (J\cos\theta, J\sin\theta\sin\phi, J\sin\theta\cos\phi)$; $\langle \hat{N}_\tau\rangle = N_\tau$; $\langle \hat{B}_i\rangle = 0$. The last constraint is necessary so as to keep the orientation of the angular-momentum vector against the intrinsic coordinate axes [9]. The variational equation is solved by means of the method of steepest descent. Details of the method are presented in Ref. [9]. A deformed Nilsson + BCS state is used for an initial trial state at $J = 0$. Deformation parameters and gap energies for the trial state are determined by reference to the calculations of the liquid-drop model by the Möller *et al*. [10]. In the present study, the deformation parameters for the ground state are chosen to be $(\beta, \gamma) = (0.347, 0.0^\circ)$ and the pairing gap

TABLE I. Evolution of the deformation in β as a function of the total spin J, which is obtained from the 1D-cranking calculation.

J	0	2	4	6	8	9
β	0.37	0.38	0.37	0.35	0.31	0.29

energies are $(\Delta_p, \Delta_n) = (1.840\ \text{MeV}, 1.962\ \text{MeV})$. All the physical quantities, such as energy, quadrupole moments (deformation), single-particle spin components, and gap energies, are self-consistently calculated under the above constraints in this framework.

First, the results from the 1D-cranking calculation are reported. Despite the use of a simple separable interaction, the ground-state rotational spectra are reproduced reasonably well (Fig. 1). As Valor *et al*. commented in Ref. [6], the gap energies disappear for both protons and neutrons before $J = 6\hbar$ (Fig.1). Triaxial deformation gradually decreases from $\gamma = 0^\circ$. However, in $J \leqslant 4\hbar$, triaxial deformation can still be regarded as negligible. In other words, axial symmetry is kept fairly well and large (see Table I). On the other hand, at high spin ($J = 8, 10\hbar$), substantial triaxial deformation is formed ($\gamma \gtrsim -10^\circ$), and axial symmetry is clearly broken. It should be noted here that the convention for the quadrupole deformation parameters (β, γ) in this study follows the Hill-Wheeler coordinates, which give the opposite sign in γ to the so-called Lund convention. A fact that the γ deformation becomes negatively larger implies that the nucleus is reaching the noncollective rotational state ($\gamma = -60^\circ$), where the rotational axis corresponds to the shortest principal axis of the deformation.

TABLE II. Single-particle components of the total spin in the 1D-cranking calculation.The first two rows correspond to proton orbitals, and the last two to neutron orbitals. The numbers in parantheses are ratios of single-particle spins against the total spin. The unit of spin is $\hbar$.

Orbital	$J = 2$	$J = 4$	$J = 6$	$J = 8$	$J = 9$
$\pi d_{5/2}$	1.0 (50%)	2.0 (50%)	2.9 (48%)	3.6 (45%)	3.9 (43%)
$\pi d_{3/2}$	0.0 (0%)	0.0 (0%)	0.1 (2%)	0.4 (5%)	0.6 (7%)
$\nu d_{5/2}$	1.0 (50%)	2.0 (50%)	2.9 (48%)	3.6 (45%)	3.9 (43%)
$\nu d_{3/2}$	0.0 (0%)	0.0 (0%)	0.1 (2%)	0.4 (5%)	0.6 (7%)

From this result, it is understandable why the cranking calculation by Valor *et al*. [6] was successful up to $J = 6\hbar$ and why the deviations from the experimental values become larger at higher spins. As mentioned earlier, they solved the HFB equation within the axial symmetry constraint.

In the HFB theory, the total spin is expressed as the sum of single-particle spins, that is,

$$\langle \hat{J}_i \rangle = \sum_m \left\langle j_i^{(m)} \right\rangle = \sum_{mn} (j_i)_{mn} \rho_{nm}, \tag{5}$$

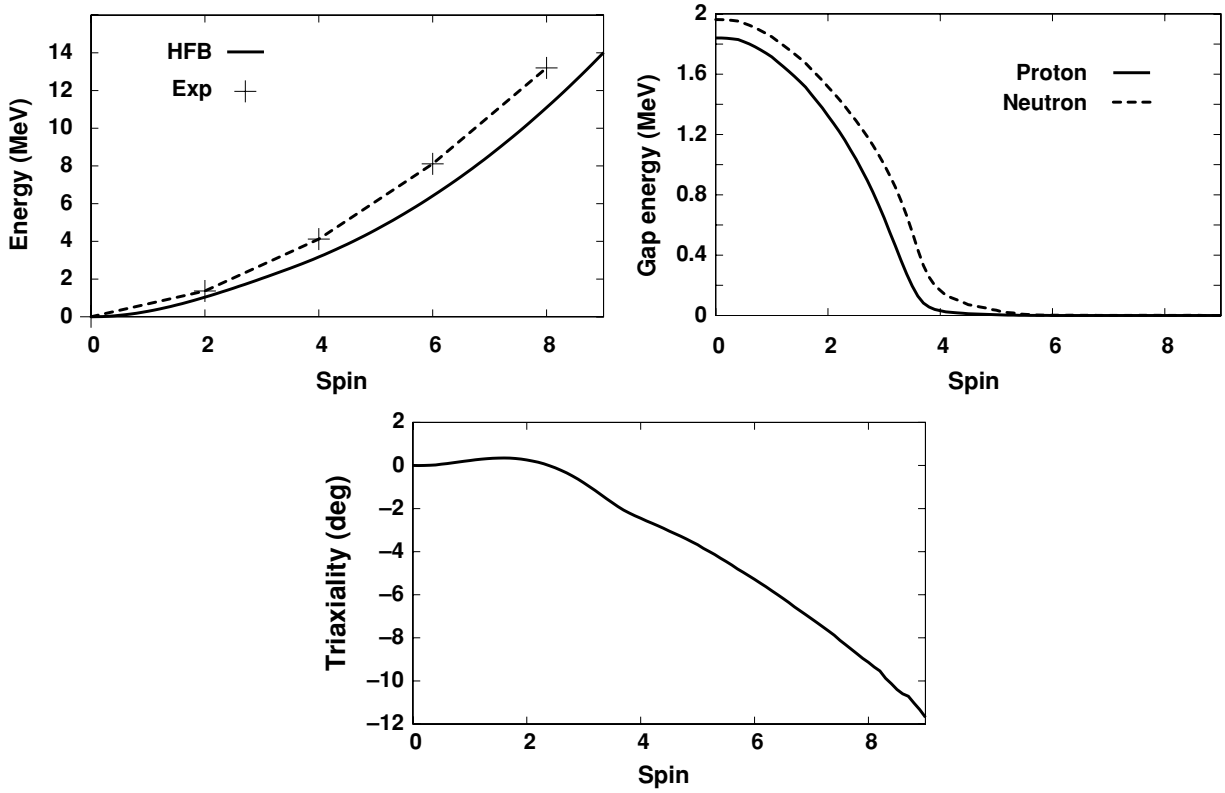

FIG. 1. (Top left) Rotational energy obtained in the 1D-cranking calculation (solid curve), and the experimental data (crosses). (Top right) Gap energies for protons and neutrons, obtained in the 1D-cranking calculation. (Bottom) γ deformation obtained in the 1D-cranking calculation.

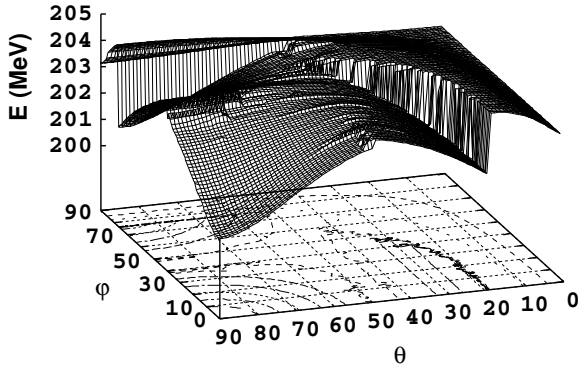

FIG. 2. Energy surface of the $J = 8\hbar$ state, calculated by means of the 3D-cranked HFB method. There are two minima as intrinsic states, which are seen at $(\theta, \phi) = (0^\circ, 0^\circ)$ and $= (90^\circ, 0^\circ)$.

where ρ is the density matrix and j_i is the single-particle angular-momentum operator. The indices m and n are for the canonical bases, and the index i is for the coordinate axes, that is, $i = 1, 2, 3$. Using this information of angular momentum, we can discuss a nuclear structure with single-particle spins. Table II gives the calculated main components of single-particle spins for different total spins J. The result reflects a fact that ^{24}Mg is a $N = Z$ nucleus, that is, the ways of single-particle excitations are the same for both protons and neutrons. For low-spin members in the rotational band, the total spin consists mainly of $d_{5/2}$. The higher the total spin, the more the $d_{3/2}$ orbit is occupied. Therefore the "collectivity" in this nucleus is attributed to gradual excitations into the $d_{3/2}$ orbit.

Next, the results of the 3D-cranking calculations are presented. In this paper, we focus on the analysis of the $J^\pi = 8^+$ state, in which its triaxial deformation becomes substantial ($\gamma \simeq -10^\circ$) in the 1D-cranking calculation.

Obviously from Fig. 2, two configurations compete with each other. This competition can be considered as a kind of "level crossing" between two different states (or configurations), but in the 3D-cranking calculation each "level" is represented by a curved surface. There are mainly two minima in the energy surface for the $J = 8\hbar$ state (Fig.2): $(\theta, \phi) = (0^\circ, 0^\circ)$ and $= (90^\circ, 0^\circ)$, and they characterize the two configurations. The former minimum corresponds to the 1D-cranking solution in which triaxiality is calculated to be $\gamma \simeq -10^\circ$. The rotation axis is found to be along the shortest axis, and the corresponding state is expected be of low-K character. The latter minimum is the energetically lowest state (yrast state) at this spin, which is about 2.5 MeV lower than the 1D-cranking solution. This yrast state at $J^\pi = 8^+$ is found to be axially symmetric because the triaxiality is calculated to be $\gamma \simeq 0^\circ$ ($\beta \simeq 0.24$). In this case, the rotational axis points

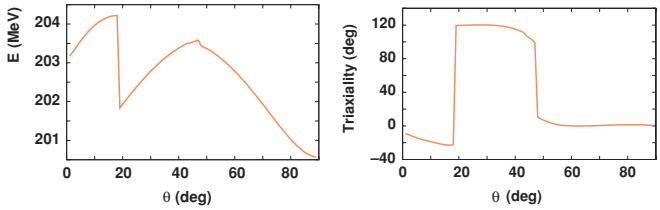

FIG. 3. (Color online)(Left) A cross section of the energy surface at $\phi = 0^\circ$. (Right) Triaxial deformation at $\phi = 0^\circ$.

along the longest axis of the axially symmetric shape, so that the rotation is of single-particle character. As a result, the major components of the state should be of high-K characters. Studying in detail the microscopic structure, we find the total spin to be constructed almost purely by the $d_{5/2}$ orbits (in both protons and neutrons): $3.97\hbar$ each by the $d_{5/2}$ orbits of protons and neutrons. In addition to the difference in the deformation, a lack of the $d_{3/2}$ component in the first 8^+ state implies that the yrast state is surely different from rotational members of the g band from a microscopic point of view. The shell-model calculation by Wiedenhover *et al.* [4] says that such a configuration, that is, $(d_{5/2})^8$, corresponds to the first 8^+ state (which does not belong to the g band) observed in experiment. Therefore my result is consistent with that of the shell-model calculation too.

From this result, we can conclude that the yrast state found in our calculation at $J = 8\hbar$ is a high-K state with $K^\pi = 8^+$. It was experimentally observed to be energetically lower than the second 8^+ state by about 2 MeV.

In the right-hand panel of Fig. 3, the triaxial deformation is seen to have $\gamma \simeq 120^\circ$ at $20^\circ \lesssim \theta \lesssim 45^\circ$. Because the level crossing happens at $\theta \simeq 20^\circ$, we cannot exactly see how the graph continues toward $\theta \to 0$. However, from the trend of the graph, it is possible to guess that the graph forms a symmetric shape with respect to $\theta = 45^\circ$ in the left-hand panel of Fig. 3, and that $\gamma \to 120^\circ$ for $\theta \to 0^\circ$ in the right-hand panel of Fig. 3. This reflection symmetry around $\theta = 45^\circ$ indicates that the state in $0^\circ \leqslant \theta \leqslant 45^\circ$ and the state in $45^\circ \leqslant \theta \leqslant 90^\circ$ have the same intrinsic structure. (The calculated β values are shown in Table III.)

The ground-state rotational band was studied with the self-consistent 1D-cranking calculation. It was confirmed in this study that an effect of triaxiality on the nature of the rotational band is important at high spin, as previously anticipated by Valor *et al.* In addition, two high-spin states at $J = 8^+$ observed in experiment were analyzed by means of the self-consistent 3D-cranking calculation. It concludes (in a qualitative manner) that the yrast 8^+ state is an axially symmetric high-K state created by the deformation-aligned protons and neutrons in the $d_{5/2}$ orbitals whereas the second

TABLE III. Change of β as a function of the tilt angle θ, obtained in the 3D-cranking calculation for $J = 8\hbar$ and $\phi = 0^\circ$.

θ	0	10	20	30	40	50	60	70	80	90
β	0.31	0.25	0.21	0.18	0.14	0.11	0.17	0.21	0.23	0.24

8^+ is a rotational member of the ground-state rotational band with substantial triaxial deformation.

For the first time, with in the framework of the self-consistent and microscopic method, the two $I^\pi = 8^+$ states in ^{24}Mg, which correspond to low- and high-K states, respectively, are explained on the same footing, that is, through the self-consistent 3D-cranking model.

The author thanks P. Ring and P.-H. Heenen for their suggestions to calculate this ^{24}Mg nucleus by using the self-consistent 3D-cranking method. Useful discussions with W. Catford, P. W. Walker, and P. Regan are also acknowledged. This work is supported by EPSRC with an advanced research fellowship GR/R75557/01 as well as a first grant EP/C520521/1.

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