A region of high-spin toroidal isomers

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Abstract

The combined considerations of both the bulk liquid-drop-type behavior and the quantized angular momentum reveal that high-spin toroidal isomeric states may have general occurrences for light nuclei with $28 \leq A \leq 48$. High-spin $N=Z$ toroidal isomers in this mass region have been located theoretically using cranked self-consistent constraint Skyrme-Hartree-Fock model calculations.

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Nuclei as we now know them have sphere-like geometry. Wheeler suggested that under appropriate conditions the nuclear fluid may assume a toroidal shape \[1, 2, 3\]. Toroidal nuclei are however plagued with various instabilities \[3\], and the search remains elusive \[4, 5, 6\]. It was found previously from the liquid-drop model that a “rotation” about the symmetry axis with an angular momentum $I=I_z$ above a threshold can stabilize the toroidal nucleus and can lead to a high-spin isomer \[7\].

The toroidal high-spin isomer, whose large angular momentum $I=I_z$ must be generated by the alignment of individual nucleon angular momenta along the symmetry axis \[8\], provides an elegant example in quantum mechanics as how an axially-symmetric system can acquire a quantized angular momentum. Furthermore, the nuclear fluid in the toroidal isomeric state may be so severely distorted by the change from sphere-like geometry to the toroidal shape that it may acquire bulk properties of its own, to make it a distinct type of quantum fluid. Finally, the toroidal high-spin isomer may be a source of energy, as its decay to the ground state can release a large amount of excitation energy and the possibility of toroidal high-spin isomers may stimulate also future reaction studies to explore their production and detection by fusion of two ions at high angular momenta \[9,10\]. For all these reasons, the investigation on toroidal high-spin isomers is of general interest.

In the liquid-drop model of a toroidal nucleus, we can select the major radius $R$, the minor radius $d$, the angular momentum $I=I_z$ about the symmetry axis, and the corresponding rigid-body moment of inertia $\mathcal{I}_{\text{rigid}}$ as macroscopic variables. (For a sketch of $R$ and $d$, see Fig. 1 of \[3\].) The energy $I(I+1)/2\mathcal{I}_{\text{rigid}}$ associated with the angular momentum $I$ can be called the “rotational” energy. The variation of the rotational energy and the Coulomb energy tend to counter-balance the variation of the surface energy \[7\]. As a consequence, there is an $I$-threshold above which the rotating toroidal nucleus can be stable against a variation of $R/d$. The toroidal nucleus is stable also against axially-asymmetric sausage distortions within an $I$-window, when the same mass flow is maintained across the toroidal meridian. Beyond the $I$-window, sausage instabilities of higher orders dominate to break the toroid into many beads \[7\].

To study toroidal high-spin states theoretically, we need a systematic way to determine the quantized $I$ value, which is a non-trivial function of $N$ and $Z$. The quantized $I$ can be obtained from the single-particle state diagrams under the constraint of a fixed aligned angular momentum. For simplicity, we limit our present studies to even-even $N=Z$ nuclei. Previously, an investigation of $^{40}$Ca as the evolution of a chain of 10 alpha particles revealed that $^{40}$Ca with $I=60\ h$ may represents a toroidal high K-isomeric state $^{[1]}$, in qualitative agreement with the $I$-threshold and $I$-window concepts in $^{[7]}$.

Accordingly, we need the energy diagram of the single-particle states in a toroidal nucleus for different
aligned angular momenta $I$. For $I=0$, the single-particle potential for a nucleon in a toroidal nucleus with azimuthal symmetry in cylindrical coordinates $(r, z)$ can be represented by \[ V_0(r, z) = \frac{1}{2} m \omega_0^2 (r - R)^2 + \frac{1}{2} m \omega_0^2 z^2, \] where $\hbar \omega_0 = [(3\pi R/2d)^{1/3} 41/A^{1/3}] (\rho_{\text{torus}})/(\rho_0)$. We have included the ratio $\langle \rho_{\text{torus}} \rangle / \langle \rho_0 \rangle$ where $\langle \rho_{\text{torus}} \rangle$ and $\langle \rho_0 \rangle$ are the average nuclear densities in the toroidal and the spherical configurations respectively, because the mean-field potential is proportional approximately to the nuclear density. In microscopic calculations, $\langle \rho_{\text{torus}} \rangle / \langle \rho_0 \rangle$ is found to be approximately 1/2 to 2/3. For $R \gg d$ and low-lying states with the radial nodal quantum number $n_r=0$ and the azimuthal nodal quantum number $n_z=0$, the expectation value of the spin-orbit interaction is approximately zero [3], and we can neglect the spin-orbit interaction.

We label a state by $(n \Lambda \Omega \Omega_z)$, where $n=(n_z + n_r)$, $\pm \Lambda$ is the $z$-component of the orbital angular momentum, and $\Omega = |A \pm 1/2|$ is the single-particle total angular momentum with $z$-components $\Omega_z = \pm \Omega$. For $R \gg d$, the single-particle energy of the $(n \Lambda \Omega \Omega_z)$ state with $I=0 \hbar$ is therefore

\[ E(n \Lambda \Omega \Omega_z) \sim \hbar \omega_0 (n + 1) + \frac{\hbar^2 \Lambda^2}{2 m R^2}. \] (2)

Fig. 1(a) gives the single-particle state energies as a function of $R/d$ for a toroidal nucleus with $I=0 \hbar$.

For a non-collectively rotating toroidal nucleus with aligned angular momentum, $I=I_z$, we use a Lagrange multiplier $\omega$ to describe the constraint $I_z = \langle \bar{J}_z \rangle = \sum_{\Omega_z} \Omega_z \rho_{\Omega_z}$. The constrained single-particle Hamiltonian becomes $\hat{H}^{\prime} = \hat{H} - \hbar \omega \bar{J}_z$, and the aligned angular momentum $I$ is a step-wise function of the Lagrange multiplier $\omega$ (12), with each $I$ spanning a small region of $\hbar \omega$. As the constrained Hamiltonian $\hat{H}^{\prime}$ is of the same form as that of a nucleus under an external cranking, the constraint can be effectively described as a cranking of the nucleus with an angular frequency $\omega$ (13) (14). The single-particle state energy of the $(n \Lambda \Omega \Omega_z)$ state, under the constraint of the non-collective aligned angular momentum $I$ is

\[ E(n \Lambda \Omega \Omega_z) \sim \hbar \omega_0 (n + 1) + \frac{\hbar^2 \Lambda^2}{2 m R^2} - \hbar \omega \Omega_z. \] (3)

Fig. 1(b) gives the single-particle state energies as a function of the constraining Lagrange multiplier $\hbar \omega_0$, for a toroidal nucleus with $R/d=4.5$, approximately the aspect ratio for many toroidal nuclei in this region. We can use Fig. 1(b) to determine $I=I_z$ as a function of $N$ and $\hbar \omega$. Specifically, for a given $N$ and $\hbar \omega$, the aligned $I_z$-component of the total angular momentum $I$ from the $N$ nucleons can be obtained by summing $\Omega_z$ over all states below the Fermi energy.

There are shell gaps for different $(N, I_z)$ configurations in Fig. 1. They represent configurations with relative stability for which additional shell corrections on top of the liquid-drop-type energy surface (13) (3) may enhance the stability for toroidal configurations. The energy scales of the $\hbar \omega_0$ and $E$ axes in Fig. 1(b) depend on $N$, $R/d$, $\langle \rho_{\text{torus}} \rangle/\langle \rho_0 \rangle$ which vary individually at different isomeric toroidal energy minima, but the structure of the $(N, I_z)$ shells and their relative positions in Fig. 1(b) remain approximately the same in this $A \approx 40$ mass region. We can use Fig. 1(b) as a qualitative guide to explore the landscape of the energy surface for different $(N, I_z)$ configurations, by employing a reliable microscopic model.

A microscopic theory that includes both the single-particle shell effects and the bulk properties of a nucleus is the Skyrme density energy functional approach in which we solve an equality-constrained problem:

\[
\begin{align*}
\min_{\bar{\rho}} & \ E^{\text{tot}}[\bar{\rho}] \\
\text{subject to} & \quad \langle \hat{N}_d \rangle = N_d, \\
& \quad \langle \hat{Q}_{\mu} \rangle = Q_{\mu}, \\
& \quad \langle \hat{J}_z \rangle = I_z,
\end{align*}
\] (4)
where an objective function, \( E_{\text{tot}}[\bar{p}] = \langle \hat{H}_{\text{Sk}} \rangle \), is the Skyrme energy density functional [16]. The constraint functions are defined by average values of the proton/neutron particle-number operator, \( \hat{N}_{p/n} \), the mass-multiple-moment operators, \( \hat{Q}_{\mu} \), and the components of the angular momentum vector \( \hat{J}_{\lambda} \), \( N_{p/n} = Z/N \) are the proton/neutron numbers, \( Q_{\mu} \) are the constraint values of the multiple-moments, and \( I_{\lambda} \) are the constraint components of the angular momentum vector.

Our objective is to locate local toroidal figures of equilibrium, if any, in the multi-dimensional search space of \((A, Q_{20}, I)\). We first map out the energy landscape for axially-symmetric toroidal shapes under these \( Q_{20} \) and \( I \) constraints, with fine grids in \( Q_{20} \) and all allowed non-collective rotations in \( 0 \leq I \leq 120 \hbar \) for different \( A \). If the topographical landscape reveals a local energy minimum then the quadrupole constraint is removed at that minimum and free-convergence is tested to ensure that the non-collectively rotating toroid nucleus is indeed a figure of equilibrium.

For the case of \( I=0 \), as shown in Fig. 2, the Skyrme-Hartree-Fock-Bogoliubov (HFB) calculations for \( N=Z \) with \( 24 \leq A \leq 48 \) reveal that as the quadrupole moment constraint, \( Q_{20} \), decreases to become more negative, the density configurations with sphere-like geometry (open circular points) turn into those of an axially-symmetric torus (solid bullet points), as would be expected from the single-particle state diagrams of Fig. 1(a). The energies of axially-symmetric toroidal configurations as a function of \( Q_{20} \) lie on a slope. This indicates that even though the shell effects cause the density to become toroidal when there is a quadrupole constraint, the magnitudes of the shell corrections are not sufficient to stabilize the tori against the bulk tendency to return to sphere-like geometry.

We next extend our Skyrme-HFB calculations further to include both the quadrupole moment \( Q_{20} \) constraint and the angular momentum constraint, \( I=I_{\lambda} \). The pairing energies are smaller for toroidal nuclei than with a spherical geometry, for a case of \( I=0 \), additionally pairing interaction is suppressed as the two degenerate \( \pm \Omega \) states split apart under the constraining \( h\omega \) when \( I\neq0 \). We shall carry out the cranking calculations without the pairing interaction, using a Skyrme-HF approach. The results of such calculations for \( 28 \leq A \leq 48 \) are presented in Fig. 3 where we plot the excitation energy of the high-spin toroidal states relative to the spherical ground state energy, \( E^* = E_{\text{tot}}(I) - E_{\text{tot}}(0) \), as a function of the constrained \( Q_{20} \), for different quantized \( I \). For each point \((Q_{20}, I)\) on an \( I \) curve for a fixed \( A \), it was necessary to adjust \( h\omega \) judiciously within a range to ensure that the total aligned angular momentum of all nucleons in the occupied states gives the quantized \( I \) value of interest. The energy curves in Fig. 3 become flatter as \( I \) increases, similar to the energy curves in the liquid-drop model as the angular momentum increases [7].

With our systematic method outlined above, we are...
able to locate many high-spin toroidal isomeric states: $^{28}$Si($I=44$ h), $^{32}$Si($I=48$, 66 h), $^{36}$Ar($I=56$, 72, 92 h), $^{40}$Ca($I=60$, 82 h), $^{44}$Ti($I=68$, 88, 112 h), and $^{48}$Cr($I=72$, 98, 120 h), as shown in Fig. 3 and listed in Table I. Note that with a fixed initial shape of a ring of 10 alpha particles, the earlier result of [11] finds only a single case of $^{40}$Ca($I=60$ h) as an isomeric toroidal figure of equilibrium. However, with the help of Fig. 1(b) and the fine grids in the large multi-dimensional space of ($A$, $Q_{20}$, $I$), we find a large number of isomers, demonstrating the general occurrence of toroidal high-spin states. The $A$ and $I$ values have their correspondences in the $(N, I)$ shells in Fig. 1(b). The equilibrium configurations at the energy minima have been tested and found to be self-consistently free-converging after the removal of the quadrupole moment $Q_{20}$ constraint.

Table I gives the properties of the high-spin toroidal isomers in $28 \leq A \leq 48$: their $Q_{20}$, $h\omega$, and excitation energy $E^*$ values, obtained with the Skyrme SkM* interaction. The excitation energy is of order 140-270 MeV. The toroidal density can be parametrized as a Gaussian function, $\rho(r, z) = \rho_{max} \exp[-(r^2 + z^2)/(d^2/\ln 2)]$, where $R$, $d$, and $\rho_{max}$ for isomeric states are listed. While the major radius $R$ and $R/d$ increase with increasing $A$, the minor radius $d$ remains to be approximately the same.

![Figure 3: (Colour online.) The excitation energy of high-spin toroidal states ($E^*$) of $^{28}$Si, $^{32}$Si, $^{36}$Ar, $^{40}$Ca, $^{44}$Ti, and $^{48}$Cr as a function of $Q_{20}$ for different angular momentum along the symmetry axis, $I=I$. The density distributions and locations of isomeric toroidal energy minima are indicated by the star symbols.](image)

![Figure 4: (Colour online.) The density distributions of the toroidal configurations of $^{40}$Ca with $I=60$ h as a cut in the radial $x$-direction for different $Q_{20}$. One notes that the average density for $^{40}$Ca($I=60$ h) at the toroidal energy minimum of $Q_{20} = -15$ b (thick solid curve) is only 0.64 of the average nuclear density for a spherical $^{40}$Ca (dash-dot curve). This is a general phenomenon for light toroidal nuclei, as the nuclear density is affected by the presence of all forces [22].](image)
collective rotational motion, we determine an effective moment of inertia $\mathcal{I}_{\text{eff}}$ for toroidal $^{40}\text{Ca}$ from the total energy of the system as a function of \(I\) as $E^{\text{tot}}(I) = E^{\text{tot}}(0) + I(I + 1)/2\mathcal{I}_{\text{eff}}$. Using the results in Fig. 3, we find in Fig. 5(a) that such a linear dependence between $E^{\text{tot}}(I) - E^{\text{tot}}(0)$ and $I(I + 1)/\mathcal{I}_{\text{eff}}$ holds for different $Q_{20}$. An effective moment of inertia $\mathcal{I}_{\text{eff}}$ can be extracted as a function of $Q_{20}$. On the other hand, for different $Q_{20}$, one can calculate the rigid-body moment of inertia $\mathcal{I}_{\text{rigid}} = mN2\pi^{2}R^{2}/ln2\pi^{2}/(2ln2)\pi^{2}$ from the density distributions in Fig. 4. The comparison of $\mathcal{I}_{\text{eff}}$ and $\mathcal{I}_{\text{rigid}}$ in Fig. 5(b) indicates the approximate equality of $\mathcal{I}_{\text{eff}}$ and $\mathcal{I}_{\text{rigid}}$. This is in agreement with the result of Bohr and Mottelson who showed that the moment of inertia associated with the alignment of single-particle orbits along an axis of symmetry is equal to the rigid-body moment of inertia. Figure 5: (Color online) (a) The total energy difference $E^{\text{tot}}(I) - E^{\text{tot}}(0)$ as a function of $I(I + 1)$ for toroidal $^{40}\text{Ca}$ at different $Q_{20}$. The inverses of the slopes of different lines give the effective moments of inertia $\mathcal{I}_{\text{eff}}$. (b) The effective moments of inertia $\mathcal{I}_{\text{eff}}$ and the rigid body moments of inertia $\mathcal{I}_{\text{rigid}}$ as a function of $Q_{20}$ for toroidal $^{40}\text{Ca}$.

It is clear from Fig. 5(b) that large shell effects are expected for some odd $N$ and $Z$ at various $I$ values, and for combining different $(N, I_N)$ with $(Z, I_Z)$ at the same $\hbar\omega$. Hence light toroidal nuclei with odd-$N$, odd-$Z$, and $N\neq Z$ may be possible. The large shell gaps for $(N, I) = (58, 58\ h)$, $(64, 32\ h)$, and $(64, 96\ h)$ calls for future exploration of high-spin toroidal isomers in the mass region of $A \sim 120$.

In conclusion, under the considerations of the aligned single-particle angular momentum and the bulk behaviour, the constrained self-consistent Skyrme-Hartree-Fock model calculations reveal that high-spin toroidal isomers may have general occurrences in the mass region of $28 \leq A \leq 48$. Experimental search for these nuclei may allow the extraction of the bulk properties of this new type of nuclear fluid and its possible utilization as a source of energy.

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