

Collective molecular bands in ^{44}Ti within the dinuclear-system model

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The collective bands of ^{44}Ti are investigated within the dinuclear-system model by treating the nucleus as an $\alpha + ^{40}\text{Ca}^*$ molecular configuration. We examine whether the observed positive- and negative-parity sequences can be described as collective angular excitations of an α particle coupled to a superdeformed ^{40}Ca core. The radial and angular degrees of freedom are treated within an approximate adiabatic separation, and the fragment interaction is obtained from Coulomb and nuclear double-folding potentials. The orientation-dependent potential favors an equatorial arrangement of the fragments. The calculated spectrum reproduces the main ordering of the experimentally identified low-spin states and predicts higher-spin continuations of the proposed sequences. The calculated $B(E2)$ values agree with the available experimental data within their uncertainties and support the collective nature of these states. The results are consistent with a molecular interpretation of the observed bands and identify the relative fragment orientation as an important collective degree of freedom in ^{44}Ti .

Keywords: dinuclear-system model; α clustering; superdeformation; molecular bands; relative orientational motion

Introduction

Cluster degrees of freedom provide an important complementary description of nuclear structure, particularly in light and medium-mass nuclei close to the $N = Z$ line. In such systems, α -cluster configurations may coexist and mix with shell-model and mean-field structures, producing rotational bands, parity-doublet

sequences, and molecular resonances. General reviews of nuclear clustering and molecular configurations can be found in Refs. [1, 2].

The nucleus ^{44}Ti is a natural candidate for an $\alpha + ^{40}\text{Ca}$ description because the doubly magic ^{40}Ca nucleus provides a strongly bound core. Experimental α -transfer studies have revealed pronounced α -cluster components in ^{44}Ti [3], while resonating-group and local-potential calculations have described positive- and negative-parity rotational structures associated with the same partition [4–6]. Calculations that explicitly allow excitation of the ^{40}Ca core have further shown that core-excited α -cluster configurations are important for describing rotational bands over a broad excitation-energy range [7–9].

A superdeformed rotational sequence has also been identified experimentally in ^{44}Ti [10]. At the same time, the superdeformed band of ^{40}Ca is experimentally well established and is characterized by a large transition quadrupole moment [11, 12]. Microscopic antisymmetrized molecular-dynamics calculations predict the coexistence of superdeformed, triaxial, and $\alpha + ^{40}\text{Ca}$ cluster configurations in ^{44}Ti [13]. These observations motivate a description in which an α -particle moves relative to an excited and strongly deformed ^{40}Ca core.

In the present work, we apply the dinuclear-system (DNS) model to the $\alpha + ^{40}\text{Ca}^*$ configuration. The radial and angular degrees of freedom are treated within an approximate adiabatic separation, while the interaction between the fragments is calculated from Coulomb and nuclear double-folding potentials. The coupling between intrinsic core excitations and the relative motion is described by a multipole interaction. In addition, the angular dependence of the radial minimum generates an effective hexadecapole component in the orientation-dependent potential. We investigate the radial binding, the orientation-dependent potential, the moment of inertia, the excitation spectra, and the quadrupole transition strengths. Particular attention is paid to the energetically favored equatorial arrangement of the fragments and to the resulting collective spectra.

Methodology

To describe the molecular excitations of ^{44}Ti , we treat the nucleus as a DNS composed of an excited ^{40}Ca core and an α -particle in a touching configuration. Core-excited $^{40}\text{Ca} + \alpha$ configurations have previously been shown to provide a realistic description of cluster-type excitations in ^{44}Ti [8, 9]. The coexistence of cluster configurations and superdeformed structures in ^{44}Ti is also supported by microscopic calculations [13].

Here, we apply the DNS model developed in Refs. [14–16] to describe the radial and angular dynamics of the $^{40}\text{Ca} + \alpha$ molecular configuration. In the present approximation, the α -particle is treated as a spherical and structureless 0^+ fragment. Internal excitations of the α -particle, nucleon transfer between the fragments, and coupling to particle-decay channels are neglected. The intrinsic deformation of the ^{40}Ca core is assumed to remain unchanged during the angular motion of the DNS.

The Hamiltonian of the DNS is written as

$$\hat{H} = \hat{H}_{\text{Ca}} + \hat{H}_{\text{rel}} + \hat{V}_{\text{coup}}, \quad (1)$$

where $\hat{H}_{\text{Ca}}$ describes the intrinsic excitations of the ^{40}Ca core. The Hamiltonian of the relative motion is

$$\hat{H}_{\text{rel}} = -\frac{\hbar^2}{2\mu} \frac{1}{R^2} \frac{\partial}{\partial R} R^2 \frac{\partial}{\partial R} + \frac{\hbar^2 \hat{l}^2}{2\mu R^2}, \quad (2)$$

where μ is the reduced mass of the two fragments and R is their relative distance. The operator of the relative angular momentum is

$$\hat{l}^2 = -\left[\frac{1}{\sin \theta_R} \frac{\partial}{\partial \theta_R} \sin \theta_R \frac{\partial}{\partial \theta_R} + \frac{1}{\sin^2 \theta_R} \frac{\partial^2}{\partial \varphi_R^2} \right]. \quad (3)$$

The angles $\Omega_R = (\theta_R, \varphi_R)$ specify the orientation of the relative-coordinate vector $\mathbf{R}$ in the laboratory frame.

The coupling interaction is represented by a separable multipole–multipole expansion. In its general form, the coupling Hamiltonian contains quadrupole and octupole core terms, and can be written as

$$\hat{V}_{\text{coup}} = V_0(R) + F_2(R) \left[\hat{Q}_2^{(\text{Ca})} \cdot Y_2(\Omega_R) \right] + F_3(R) \left[\hat{Q}_3^{(\text{Ca})} \cdot Y_3(\Omega_R) \right], \quad (4)$$

where $\hat{Q}_2^{(\text{Ca})}$ and $\hat{Q}_3^{(\text{Ca})}$ are the quadrupole and octupole operators of the ^{40}Ca core, respectively. The radial functions $F_\lambda(R)$, with $\lambda = 2, 3$, determine the corresponding radial dependence. The octupole term is retained only as part of the general formulation; it is inactive in the present positive-parity core space, as discussed below.

The scalar product of two spherical tensors is defined as

$$\left[\hat{Q}_\lambda^{(\text{Ca})} \cdot Y_\lambda(\Omega_R) \right] = \sum_{\mu=-\lambda}^{\lambda} (-1)^\mu \hat{Q}_{\lambda\mu}^{(\text{Ca})} Y_{\lambda,-\mu}(\Omega_R). \quad (5)$$

In principle, higher-order angular components may appear in the interaction. For example, a rank-four term can be constructed from the quadrupole operator as

$$\left[\left[\hat{Q}_2^{(\text{Ca})} \times \hat{Q}_2^{(\text{Ca})} \right]_4 \cdot Y_4(\Omega_R) \right]. \quad (6)$$

In the present calculation, however, no independent intrinsic hexadecapole operator is introduced. An effective rank-four contribution arises after the interaction is evaluated at the orientation-dependent position of the radial minimum.

The reduced matrix elements of the core multipole operators are related to the experimental electromagnetic transition probabilities through

$$B(E\lambda; nI_H \rightarrow n'I'_H) = \frac{1}{2I_H + 1} \left| \left\langle n'I'_H \left\| \hat{Q}_\lambda^{(\text{Ca})} \right\| nI_H \right\rangle \right|^2. \quad (7)$$

Here, the eigenstates of the ^{40}Ca core are denoted by $|nI_H\rangle$, where I_H is the angular momentum of the core and n represents the remaining quantum

numbers required to distinguish different core states with the same angular momentum. Accordingly, $|n'I_H'\rangle$ denotes the corresponding final core state, with angular momentum I_H' and additional quantum numbers n' . Experimental $B(E\lambda)$ values determine the magnitudes of the reduced matrix elements, while their relative signs must be fixed by a consistent phase convention or by an underlying model of the core states.

To determine the radial functions $F_\lambda(R)$, the interaction potential between the fragments is written as the sum of the Coulomb and nuclear contributions

$$V(R, \varepsilon) = V_C(R, \varepsilon) + V_N(R, \varepsilon), \quad (8)$$

where ε is the angle between the symmetry axis of the ^{40}Ca core and the relative-coordinate vector $\mathbf{R}$. The coordinate ε describes the relative orientation of the two fragments. Note that orientations with $\varepsilon \neq 0, \pi$ generally break the axial symmetry of the DNS configuration, while ε is a relative-orientation coordinate and should not be identified with the conventional Bohr triaxiality coordinate γ .

The Coulomb interaction is evaluated from the proton densities of the fragments as

$$V_C(R, \varepsilon) = e^2 \int \frac{\rho_p^{(\text{Ca})}(\mathbf{r}_1, \varepsilon) \rho_p^{(\alpha)}(\mathbf{r}_2)}{|\mathbf{R} + \mathbf{r}_2 - \mathbf{r}_1|} d^3r_1 d^3r_2. \quad (9)$$

The nuclear interaction is calculated using the double-folding expression

$$V_N(R, \varepsilon) = \int \rho^{(\text{Ca})}(\mathbf{r}_1, \varepsilon) \rho^{(\alpha)}(\mathbf{r}_2) \mathcal{F}(\mathbf{R} + \mathbf{r}_2 - \mathbf{r}_1) d^3r_1 d^3r_2, \quad (10)$$

where $\mathcal{F}$ is the density-dependent effective nucleon–nucleon interaction taken in the Migdal form [17, 18].

The fragment densities are approximated by Fermi distributions,

$$\rho_i(\mathbf{r}) = \frac{\rho_{0i}}{1 + \exp \left[\frac{r - R_i(\hat{\mathbf{r}})}{a_i} \right]}, \quad (11)$$

where ρ_{0i} is determined by the normalization condition. The radius parameters are taken as $r_{0,\text{Ca}} = 1.14$ fm, $r_{0,\alpha} = 1.00$ fm, and the diffuseness parameter is $a_{\text{Ca}} = a_\alpha = 0.55$ fm. In Eq. (11), $R_i(\hat{\mathbf{r}})$ denotes the nuclear radius in the direction of the unit vector $\hat{\mathbf{r}}$. The α -particle density is assumed to be spherical, whereas the density of the ^{40}Ca core contains the adopted static deformation.

The potential energy of the DNS configuration, measured relative to the ground state of ^{44}Ti , is defined as

$$U(R, \varepsilon) = -Q_\alpha + E_{\text{SD}}^* + V(R, \varepsilon), \quad (12)$$

where $Q_\alpha = -5.1271$ MeV is the Q -value of the $^{44}\text{Ti} \rightarrow ^{40}\text{Ca} + \alpha$ channel [19]. Since this decay channel is energetically closed, $Q_\alpha < 0$, and therefore $-Q_\alpha$ is the corresponding α -separation energy. The quantity E_{SD}^* is the excitation energy of the superdeformed bandhead in ^{40}Ca . At large interfragment distances,

$$U(R \rightarrow \infty, \varepsilon) = -Q_\alpha + E_{\text{SD}}^*. \quad (13)$$

Thus, $-Q_\alpha + E_{\text{SD}}^*$ defines the $\alpha + {}^{40}\text{Ca}^*$ separation threshold relative to the ${}^{44}\text{Ti}$ ground state, while the radial energies quoted below are measured relative to this threshold.

The nuclear interaction decreases rapidly with increasing interfragment distance, and the molecular potential therefore becomes less attractive as the fragments move away from the touching configuration. At smaller distances, a strong overlap of the fragment densities is suppressed by the Pauli exclusion principle and would eventually destroy the α -cluster structure. The competition between these effects produces a potential minimum near the touching distance. A similar behavior is characteristic of phenomenological $\alpha + {}^{40}\text{Ca}$ potentials [5].

For each orientation ε , the position of the radial minimum is denoted by $R_m(\varepsilon)$. This distance is generally close to, but is not necessarily identical to, the geometrical touching distance of the two fragments. Since decay of the DNS configuration is not considered, the radial motion is assumed to remain localized near this minimum.

We employ an adiabatic approximation in which the radial and angular degrees of freedom are separated. The radial motion is restricted to its lowest state. The quantity E_{zpv} denotes the positive zero-point excitation measured upward from the minimum of the radial potential,

$$E_{\text{zpv}} = E_{r,0}^{(\text{eq})} - V_{\text{min}}^{(\text{eq})}, \quad (14)$$

where

$$V_{\text{min}}^{(\text{eq})} = V(R_m(\pi/2), \pi/2) \quad (15)$$

and $E_{r,0}^{(\text{eq})}$ is the lowest radial eigenenergy for the equatorial configuration.

In the relative rotational kinetic-energy term, the radial coordinate is fixed at the minimum of the equatorial radial potential, $R_0 = R_m(\pi/2) \simeq 4.8 \text{ fm}$. This same constant distance is used for all calculated angular states and is not treated as an adjustable parameter.

$$\hat{H}_{\text{eff}} = \hat{H}_{\text{Ca}} + \frac{\hbar^2 \hat{l}^2}{2\mu R_0^2} + E_{\text{zpv}} + \hat{V}_{\text{coup}}(R_m(\varepsilon), \Omega_R). \quad (16)$$

The constant threshold contribution $-Q_\alpha + E_{\text{SD}}^*$ fixes the absolute energy scale but does not affect the calculated angular level spacings.

The angular dependence of the coupling term in Eq. (16) is obtained from the same microscopic interaction $V(R, \varepsilon)$ introduced in Eq. (8). Within the adiabatic treatment, this interaction is evaluated along the orientation-dependent radial minimum, $R = R_m(\varepsilon)$, which defines the scalar orientation-dependent potential

$$V(\varepsilon) \equiv V(R_m(\varepsilon), \varepsilon). \quad (17)$$

Its angular dependence determines the effective multipole components entering $\hat{V}_{\text{coup}}$ and is represented by the Legendre expansion

$$V(\varepsilon) = \kappa_0 + \sum_{\lambda=2}^4 \kappa_\lambda P_\lambda(\cos \varepsilon). \quad (18)$$

The effective coefficients κ_λ are determined by fitting the calculated potential $V(R_m(\varepsilon), \varepsilon)$ over the full angular interval. For a reflection-symmetric configuration,

$$V(\varepsilon) = V(\pi - \varepsilon), \quad (19)$$

and therefore the odd coefficient vanishes,

$$\kappa_3 = 0. \quad (20)$$

The scalar potential consequently takes the form

$$V(\varepsilon) = \kappa_0 + \kappa_2 P_2(\cos \varepsilon) + \kappa_4 P_4(\cos \varepsilon). \quad (21)$$

The effective P_4 term originates predominantly from the orientation dependence of $R_m(\varepsilon)$ and does not represent an independently introduced intrinsic hexadecapole transition operator.

For a molecular state with total angular momentum I and its laboratory-frame projection M , the Hamiltonian (16) is diagonalized in the basis

$$|nI_H, I_R; IM\rangle = [\phi_{nI_H} \otimes Y_{I_R}(\Omega_R)]_{IM}, \quad (22)$$

where I_H is the angular momentum of the ^{40}Ca core, I_R is the relative angular momentum, and n denotes the remaining quantum numbers of ^{40}Ca core. The core states satisfy

$$\hat{H}_{\text{Ca}} \phi_{nI_H} = E_{nI_H} \phi_{nI_H}. \quad (23)$$

Since the intrinsic spin and parity of the α -particle are 0^+ , the parity of a basis state is

$$\pi = \pi_H (-1)^{I_R}, \quad (24)$$

where π_H is the parity of the corresponding ^{40}Ca core state. The angular momenta satisfy the triangular condition

$$|I_H - I_R| \leq I \leq I_H + I_R. \quad (25)$$

Consequently, coupling positive-parity core states to even and odd values of I_R generates positive- and negative-parity molecular states, respectively. The present core model space contains only the positive-parity members of the superdeformed rotational band of ^{40}Ca built on the 0^+ state at $E_{\text{SD}}^* = 5.213$ MeV [19]. Negative-parity core states are not included. Since the octupole operator has negative parity, its matrix elements between all core states retained in the calculation vanish. The octupole term in Eq. (4) is therefore present only in the general formulation and does not contribute to the calculated spectrum. Negative-parity molecular states are instead generated by coupling the positive-parity core states to odd values of the relative angular momentum I_R .

The relative angular momentum is included up to $I_R^{\text{max}} = 16$, which is sufficiently large to ensure convergence of the calculated low-lying spectrum. For each total angular momentum, the Hamiltonian is diagonalized in a 16×16 truncated basis. The coefficients of the effective Legendre expansion are obtained by fitting the calculated orientation-dependent interaction potential.

Results and Discussion

Core deformation and radial motion

For the numerical calculations, the DNS fragments are specified by $A_{\text{Ca}} = 40$, $Z_{\text{Ca}} = 20$, $A_{\alpha} = 4$, and $Z_{\alpha} = 2$. The ^{40}Ca core is assumed to occupy the experimentally established superdeformed rotational band [11, 12] built on the 0_3^+ state at

$$E_{\text{SD}}^* = 5.213 \text{ MeV}, \quad (26)$$

whereas the α -particle is treated as a spherical 0^+ fragment.

The deformation of the ^{40}Ca core is determined from the adopted experimental transition probability [19]

$$B(E2; 4_{\text{SD}}^+ \rightarrow 2_{\text{SD}}^+) = 170 \text{ W.u.} \quad (27)$$

For an axially symmetric $K = 0$ rotational band,

$$B(E2; I_i \rightarrow I_f) = \frac{5}{16\pi} Q_0^2 |\langle I_i 0 20 | I_f 0 \rangle|^2, \quad (28)$$

where Q_0 is the intrinsic quadrupole moment [20]. For a volume-conserving axially symmetric ellipsoid,

$$Q_0 = \frac{2}{5} Z_{\text{Ca}} e R_{\text{Ca}}^2 \left(b_{\text{ax}}^{4/3} - b_{\text{ax}}^{-2/3} \right), \quad (29)$$

where $b_{\text{ax}} = \frac{R_{\parallel}}{R_{\perp}}$ is the ratio of the major to minor semiaxes. The adopted transition strength gives

$$b_{\text{ax}} = 1.835. \quad (30)$$

Equating the intrinsic quadrupole moment of the volume-conserving ellipsoidal shape, parametrized by b_{ax} , to that of the standard axially symmetric spheroidal parametrization, we obtain the corresponding quadrupole deformation

$$\beta_0 \simeq 0.69. \quad (31)$$

The calculated radial interaction for the equatorial $\alpha + ^{40}\text{Ca}$ configuration at $\varepsilon = \pi/2$ is shown in Figure 1. The competition between the attractive nuclear interaction, the Coulomb repulsion, and the short-range repulsion associated with the Pauli exclusion principle produces a radial pocket near $R = R_m(\pi/2)$. Its minimum is denoted by

$$V_{\text{min}}^{(\text{eq})} = V(R_m(\pi/2), \pi/2) = -14.85 \text{ MeV}. \quad (32)$$

The equatorial radial potential, including the molecular pocket and the external-barrier region, is fitted by a Morse potential [21]. The corresponding Morse problem gives a lowest bound state at $E_{r,0}^{(\text{eq})} = -7.45 \text{ MeV}$ and a first excited state at $E_{r,1}^{(\text{eq})} \simeq 2.62 \text{ MeV}$. These energies are expressed relative to the physical $\alpha + ^{40}\text{Ca}^*$ separation threshold of the original interaction, for

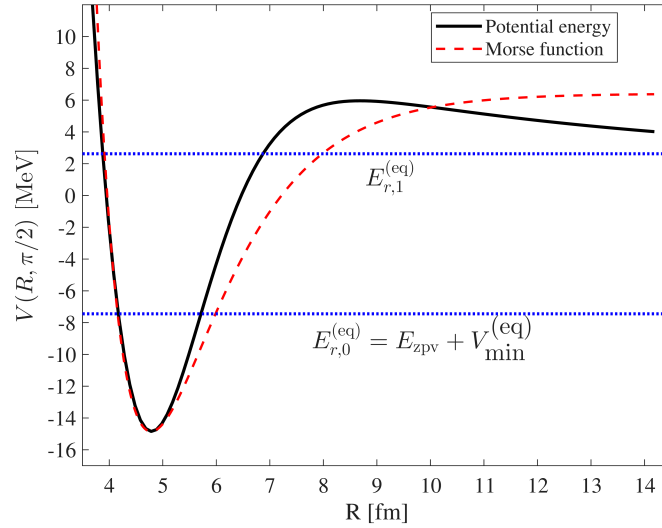


Figure 1. Calculated radial interaction potential for the equatorial $\alpha + {}^{40}\text{Ca}$ configuration, $\varepsilon = \pi/2$, and its fit by a Morse potential. The horizontal lines indicate the lowest radial state, $E_{r,0}^{(\text{eq})} = -7.45$ MeV, and the first excited Morse state, $E_{r,1}^{(\text{eq})} \simeq 2.62$ MeV, measured relative to the separated-fragment threshold. The latter is bound in the Morse fit but corresponds to a quasibound pocket state of the original interaction potential. Their spacing, used as the characteristic internal radial scale $\hbar\omega_R$, is approximately 10.07 MeV.

which $V(R \rightarrow \infty) = 0$. The first excited state remains bound in the fitted Morse potential, but lies above the physical separation threshold and therefore corresponds to a quasibound pocket state of the original interaction. Radial decay through the external barrier is not included in the present treatment. The radial zero-point excitation is $E_{zpv} = E_{r,0}^{(\text{eq})} - V_{\min}^{(\text{eq})} = 7.4$ MeV. The spacing $\Delta E_r = E_{r,1}^{(\text{eq})} - E_{r,0}^{(\text{eq})} \simeq 10.07$ MeV is used as the characteristic internal radial scale, $\hbar\omega_R \equiv \Delta E_r$. Only the lowest radial state is retained in the subsequent angular calculation.

Using the radial zero-point excitation obtained for the equatorial configuration, the absolute theoretical energy of the molecular bandhead relative to the ${}^{44}\text{Ti}$ ground state is

$$\begin{aligned} E_{\text{bh}}^{\text{th}} &= -Q_\alpha + E_{\text{SD}}^* + V_{\min}^{(\text{eq})} + E_{zpv} \\ &= 2.89 \text{ MeV}. \end{aligned} \quad (33)$$

The calculated value is about 0.99 MeV above the experimental energy $E_{\text{bh}}^{\text{exp}} = 1.904$ MeV of the excited 0^+ state in ${}^{44}\text{Ti}$ [19]. Given the simplified treatment of the radial binding, this proximity supports associating the low-lying collective sequence with the $\alpha + {}^{40}\text{Ca}^*$ DNS configuration and suggests that this molecular degree of freedom may contribute significantly to the structure of the 1.904-MeV 0^+ state.

Orientation-dependent potential

The angular dynamics is governed primarily by the orientation-dependent potential and the moments of inertia of the DNS. For each value of ε , the radial coordinate is fixed at the corresponding radial-minimum distance $R_m(\varepsilon)$. The resulting orientation-dependent potential is shown in Figure 2.

The potential exhibits local minima near $\varepsilon = 0$, $\pi/2$, and π , separated by pronounced barriers. The deepest minimum occurs at $\varepsilon = \pi/2$, in contrast to heavier α -cluster DNS configurations, for which the energetically favored configurations are generally located near $\varepsilon = 0$ and π [15]. A similar shift towards the equatorial configuration has previously been found in light asymmetric DNS configurations and is associated with the relatively weak Coulomb repulsion and the Pauli exclusion principle [22].

The calculated angular dependence is accurately parametrized as

$$V(\varepsilon) = V_{\text{pole}} + a_\varepsilon \sin^2 \varepsilon + b_\varepsilon \sin^2(2\varepsilon), \quad (34)$$

where

$$V_{\text{pole}} = V(R_m(0), 0), \quad (35)$$

and $a_\varepsilon = -0.50$ MeV, $b_\varepsilon = 2.36$ MeV.

To estimate the characteristic time scale of small-amplitude orientational motion, we expand the potential locally around the equatorial minimum. With $x = \varepsilon - \pi/2$,

$$V(\varepsilon) = V_{\text{min}}^{(\text{eq})} + \frac{1}{2}C_\varepsilon x^2 + \mathcal{O}(x^4), \quad C_\varepsilon = -2a_\varepsilon + 8b_\varepsilon = 19.88 \text{ MeV}. \quad (36)$$

The inertia associated with the relative reorientation of the two fragments is the reduced orientational moment of inertia [16]

$$\mathcal{J}_\varepsilon = \frac{\mathcal{J}_{\text{Ca}} \mu R_m^2(\pi/2)}{\mathcal{J}_{\text{Ca}} + \mu R_m^2(\pi/2)} \simeq 1.56 \hbar^2 \text{MeV}^{-1}, \quad (37)$$

which gives the local harmonic orientational scale

$$\hbar\omega_\varepsilon^{(\text{harm})} = \sqrt{\frac{C_\varepsilon}{\mathcal{J}_\varepsilon/\hbar^2}} \simeq 3.6 \text{ MeV}. \quad (38)$$

For the calculated lowest 0^+ molecular state, the angular wave function can be represented as a function of ε alone. For $I = 0$, the coupled angular functions enter through scalar products of spherical harmonics, which can be rewritten in terms of Legendre polynomials $P_{I_R}(\cos \varepsilon)$. We denote this angular representation of the wave function of the lowest 0^+ state by $\psi_0(\varepsilon)$. Its probability density is defined as

$$P_0(\varepsilon) = \sin \varepsilon |\psi_0(\varepsilon)|^2, \quad \int_0^\pi P_0(\varepsilon) d\varepsilon = 1, \quad (39)$$

where $\psi_0(\varepsilon)$ is normalized with the angular measure $\sin \varepsilon d\varepsilon$. The corresponding probability density is shown by the dashed curve in Figure 2.

As seen in Figure 2, the calculated $P_0(\varepsilon)$ is strongly localized around $\varepsilon = \pi/2$ thus confirming the relevance of the local harmonic scale for this state. Comparison with $\hbar\omega_R \simeq 10.07$ MeV gives $\omega_R/\omega_\varepsilon^{(\text{harm})} \simeq 2.8$. The resulting time-scale separation is moderate, but supports the approximate lowest-radial-channel treatment adopted for the low-lying spectrum.

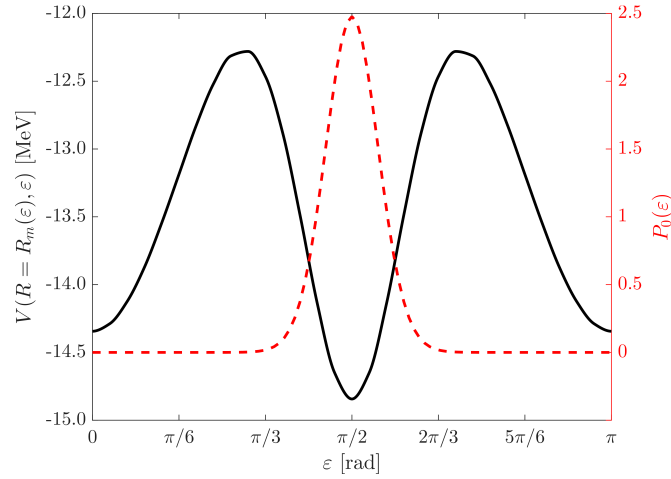


Figure 2. Calculated interaction potential $V(R_m(\varepsilon), \varepsilon)$ as a function of the angle ε between the symmetry axis of the ^{40}Ca core and the relative-coordinate vector $\mathbf{R}$. The normalized angular probability density $P_0(\varepsilon)$ of the calculated lowest 0^+ molecular state is shown by the dashed curve and refers to the right-hand scale.

In terms of Legendre polynomials, Eq. (34) becomes

$$V(\varepsilon) = V_{\text{pole}} + \frac{2a_\varepsilon}{3} + \frac{8b_\varepsilon}{15} + \left(-\frac{2a_\varepsilon}{3} + \frac{8b_\varepsilon}{21} \right) P_2(\cos \varepsilon) - \frac{32b_\varepsilon}{35} P_4(\cos \varepsilon). \quad (40)$$

Comparison with Eq. (21) gives

$$\begin{aligned} \kappa_0 &= V_{\text{pole}} + \frac{2a_\varepsilon}{3} + \frac{8b_\varepsilon}{15}, \\ \kappa_2 &= -\frac{2a_\varepsilon}{3} + \frac{8b_\varepsilon}{21}, \\ \kappa_4 &= -\frac{32b_\varepsilon}{35}. \end{aligned} \quad (41)$$

Thus, the effective hexadecapole coefficient is generated by the angular dependence of the radial minimum and is obtained directly from the fit to the calculated scalar potential. The appearance of both P_2 and P_4 terms is consistent with the effective quadrupole and hexadecapole components in Eq. (21).

The deepest minimum at $\varepsilon = \pi/2$ therefore describes an energetically preferred equatorial fragment orientation. Because ε is distinct from the Bohr coordinate γ , this minimum is not interpreted as a static triaxial deformation.

Moment of inertia

The moment of inertia of the superdeformed ^{40}Ca core is calculated in the Inglis–Belyaev approximation using single-particle states generated by the Nilsson Hamiltonian. The standard Nilsson oscillator, spin–orbit parameters and the oscillator-shell conventions are taken from Ref. [23] and are not readjusted here. Neutron and proton pairing correlations are treated within the BCS approximation. Because ^{40}Ca is doubly magic, three-point odd–even mass differences

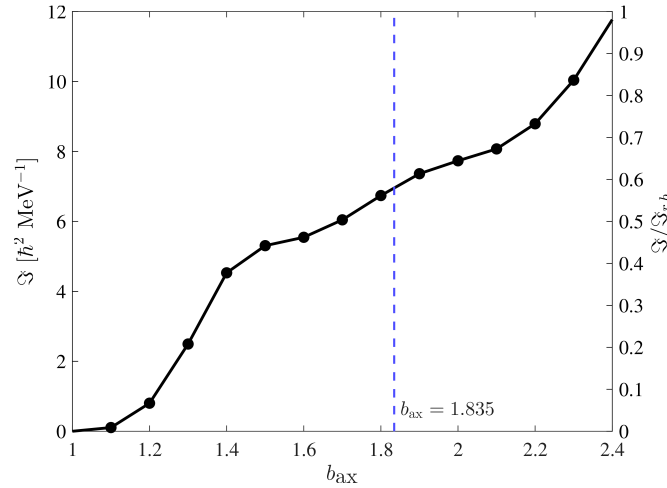


Figure 3. Calculated moment of inertia $\mathcal{J}$ of the ^{40}Ca core as a function of the ellipsoidal axis ratio b_{ax} . The right-hand scale shows the ratio $\mathcal{J}/\mathcal{J}_{r.b.}$. The dashed line marks the adopted value $b_{ax} = 1.835$, corresponding to $\beta_0 \simeq 0.69$.

are not used directly as pairing gaps: at $N = Z = 20$ they contain a substantial shell-gap contribution [24, 25]. We instead adopt

$$\Delta_n = \Delta_p = 0.45 \text{ MeV}, \quad (42)$$

consistent with the reduced pairing correlations expected near closed shells in microscopic Lipkin–Nogami calculations [24]. At the ground-state deformation these gaps give $G_n = 0.1319 \text{ MeV}$ and $G_p = 0.1290 \text{ MeV}$. The same pairing strengths are used at all other deformations, while the corresponding gaps are obtained from the BCS equations. The pairing calculation retains 300 single-particle states for each nucleon species. The calculated deformation dependence of the Inglis–Belyaev moment of inertia is shown in Figure 3. At the adopted deformation $b_{ax} = 1.835$, the resulting moment of inertia is $\mathcal{J}_{Ca} \simeq 6.97 \hbar^2 \text{MeV}^{-1}$, corresponding to approximately $0.70 \mathcal{J}_{r.b.}$. The calculated ratio is close to the experimental estimate $\mathcal{J}_{exp} \simeq 0.74 \mathcal{J}_{r.b.}$ deduced from the superdeformed rotational sequence in ^{40}Ca .

Excitation spectra and electromagnetic transitions

The calculated excitation spectra of the $\alpha + ^{40}\text{Ca}^*$ DNS are compared with the experimental data from Ref. [19] in Figure 4. For convenience, the three sequences considered in the comparison are denoted as bands A, B, and C. These labels are used only to distinguish the different calculated and experimental sequences. They do not imply a definite value of the intrinsic projection K , since the calculated eigenstates contain mixtures of several K components. The experimental information for the superdeformed sequence includes the nonyrast high-spin states reported in Ref. [10]. A common energy offset is applied to the calculated levels to align the theoretical and experimental bandheads of band A. This shift does not affect the calculated level spacings or electromagnetic transition probabilities. The absolute bandhead energy discussed above provides an independent test of the radial binding, whereas the common offset used

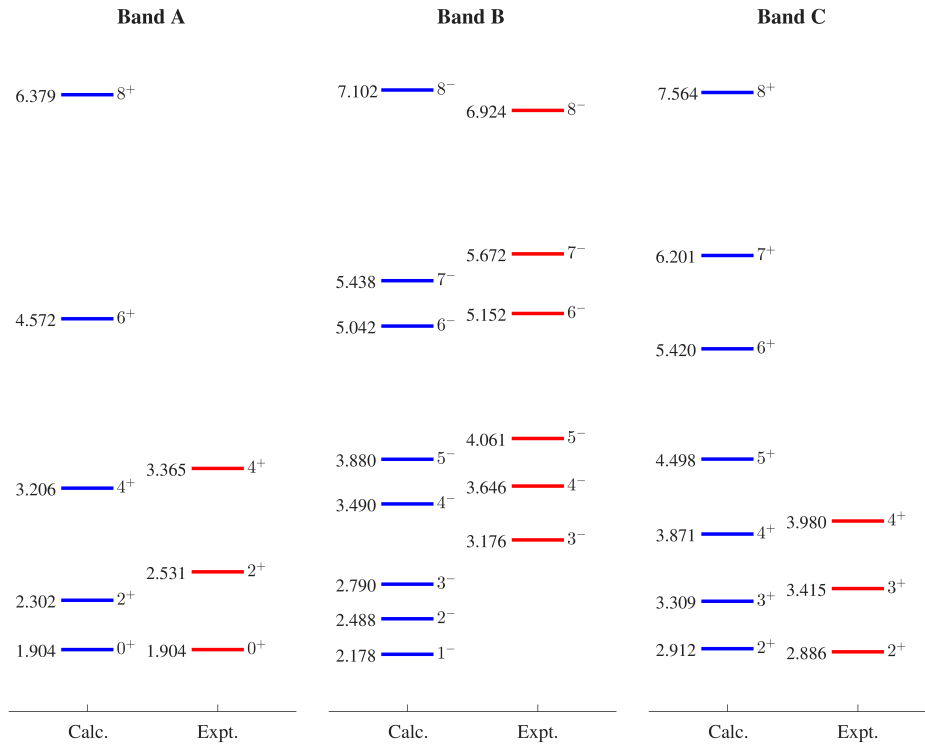


Figure 4. Calculated and experimental excitation spectra of bands A, B, and C in ^{44}Ti . The calculated levels are shown in blue and the experimental levels in red. A common energy offset has been applied to the calculated spectrum to align the bandhead of band A. For band C, the experimental states included in the comparison are presently limited to the 2^+ , 3^+ , and 4^+ states, while its higher-spin continuation is a prediction of the model. The experimental data are taken from Ref. [19].

in Figure 4 is introduced only to compare relative rotational spacings. No independent energy adjustment is made for the individual bands.

The model reproduces the general ordering and rotational evolution of the experimentally identified low-spin states. It generates the positive-parity sequence of band A, the negative-parity sequence of band B, and an additional positive-parity sequence containing both even- and odd-angular-momentum states, denoted band C. Band C is used only as a sequence label; no more specific structural classification is assigned.

The present results may be compared with earlier $\alpha + ^{40}\text{Ca}$ calculations. Within the resonating-group method, Wada and Horiuchi obtained positive-parity rotational states associated with the $\alpha + ^{40}\text{Ca}$ configuration and predicted a corresponding negative-parity band [4]. Local-potential calculations likewise described positive- and negative-parity α -cluster structures in ^{44}Ti [5]. A comprehensive discussion of the local-potential approach to α -nucleus interactions and its applications to cluster states is given in Ref. [6] and the references therein. Furthermore, the core-excited double-folding calculation of Ref. [9] showed that rotational bands over a broad range of excitation energies can be described by explicitly including excited configurations of the ^{40}Ca core. The present DNS calculation supports this general cluster interpretation, while treating the angular motion of the α -particle relative to the deformed core as a collective degree of freedom. This makes it possible to describe the positive- and negative-parity sequences associated with bands A, B, and C within a common collective Hamil-

tonian.

A complementary microscopic description was obtained using deformed-basis antisymmetrized molecular dynamics [13]. That calculation predicts strongly deformed positive-parity structures together with a negative-parity band possessing a pronounced $\alpha + {}^{40}\text{Ca}$ cluster component. Although the microscopic and DNS approaches are conceptually different, these results provide complementary support for the coexistence and relevance of strongly deformed and cluster degrees of freedom in ${}^{44}\text{Ti}$.

The reduced quadrupole transition probabilities are calculated using the quadrupole operator introduced in Ref. [15]. To account phenomenologically for core polarization and configurations outside the truncated collective model space, we use $e_{\text{eff}} = 1.5e$ for all transitions. This is of the conventional magnitude used in pf -shell calculations [26, 27]. Since $B(E2) \propto e_{\text{eff}}^2$, changing e_{eff} from $1.5e$ to $1.4e$ or $1.6e$ changes the calculated strengths by -12.9% or $+13.8\%$, respectively, without changing their relative pattern.

Selected calculated and experimental transition probabilities are listed in Table 1.

Table 1.

Comparison of selected experimental and calculated reduced quadrupole transition probabilities in band A and band C of ${}^{44}\text{Ti}$. The experimental data are taken from Ref. [19]. All values are given in Weisskopf units.

Band	Transition	Experiment	Calculation
A	$2_A^+ \rightarrow 0_A^+$	22 ± 6	26.11
A	$4_A^+ \rightarrow 2_A^+$	20_{-8}^{+10}	29.18
C	$4_C^+ \rightarrow 2_C^+$	28_{-9}^{+18}	20.0

The calculated values are consistent with the experimental uncertainties and demonstrate strong collective quadrupole transitions. They support the collective character of the states included in the comparison and are consistent with their interpretation as angular excitations of the $\alpha + {}^{40}\text{Ca}^*$ DNS.

Conclusion

The collective excitations of ${}^{44}\text{Ti}$ have been studied by treating the nucleus as an $\alpha + {}^{40}\text{Ca}^*$ DNS in which the ${}^{40}\text{Ca}$ core occupies its superdeformed rotational band. The fragment interaction is obtained from Coulomb and nuclear double-folding potentials. Within the adopted positive-parity core space, the present numerical calculation contains the quadrupole core coupling, while negative-parity molecular states are generated by odd values of the relative angular momentum I_R .

The radial interaction develops a molecular pocket near the touching configuration. For the equatorial configuration, the zero-point excitation measured upward from the minimum is $E_{\text{zpv}} = 7.4 \text{ MeV}$, giving the absolute bandhead estimate

$$E_{\text{bh}}^{\text{th}} = 2.89 \text{ MeV}. \quad (43)$$

The spacing to the first quasibound pocket excitation gives a characteristic radial scale $\hbar\omega_R \simeq 10.07$ MeV, compared with the local orientational scale $\hbar\omega_\varepsilon^{(\text{harm})} \simeq 3.6$ MeV. The resulting ratio $\omega_R/\omega_\varepsilon^{(\text{harm})} \simeq 2.8$ supports the approximate lowest-radial-channel treatment.

The orientation-dependent potential has its deepest minimum near $\varepsilon = \pi/2$, indicating a preferred equatorial fragment orientation. Angular vibrations about this minimum generate dynamical nonaxiality, rather than implying a static triaxial deformation.

The calculated spectrum reproduces the general ordering and rotational evolution of the experimentally identified low-spin states, while the higher-spin continuations of the proposed sequences are predictions of the model. The calculated in-band $B(E2)$ values agree with the available experimental data within their uncertainties and support the collective character of the states included in the comparison. Overall, the results support the relevance of the $\alpha + {}^{40}\text{Ca}^*$ molecular degree of freedom for the collective structure of ${}^{44}\text{Ti}$.

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