Microscopic aspects of $\gamma$-softness in atomic nuclei

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The microscopic origin of the $\gamma$-softness (fluctuations in the triaxiality parameter $\gamma$ of the nuclear shape) observed in atomic nuclei is studied in the framework of the triaxial projected shell model approach, which is based on a multi-quasiparticle configuration space generated from a deformed mean-field. It is demonstrated that the coupling to quasiparticle excitations drives the system from a $\gamma$-rigid to a $\gamma$-soft pattern. As an illustrative example for a $\gamma$-soft nucleus, a detailed study has been performed for the $^{104}$Ru nucleus. The experimental energies and a large sample of measured $E2$ matrix elements available for this nucleus are reproduced quite accurately. The shape invariant analysis of the calculated $E2$ matrix elements elucidates the $\gamma$-soft nature of $^{104}$Ru.

The emergence of collective phenomena from microscopic degrees of freedom is one of the challenging problems in quantum many-body physics. The collective features observed in condensed matter, atomic, molecular, nuclear and other systems are generally described using macroscopic approaches. In the case of atomic nuclei, the concept of a leptodermic droplet is employed and is the basis of the collective model introduced by Bohr and Mottelson [1]. This model parametrizes the spatial deformation of the nuclear density distribution in terms of a multipole expansion. For the interpretation of the low-energy properties, it is often sufficient to consider only the quadrupole terms in the multipole expansion, which are expressed in terms of the $\beta$- and $\gamma$-shape variables. These parameters are considered as "collective" dynamical variables, the motion of which are described by the Bohr Hamiltonian [1, 2]. The terminology of "rigid" and "soft" shape is based on its quantum eigenstates: rigid shape signifies small fluctuations around the equilibrium value and soft shape implies large fluctuations. As an alternative to the geometric Bohr Hamiltonian, the algebraic interacting boson method (IBM) [3, 4] accounts for the collective quadrupole degrees of freedom in the framework of a closed Lie algebra of boson operators with "rigid" and "soft" shapes defined in terms of group theoretical limits [5, 6].

The nucleons are in the ballistic regime, i.e., they travel quasi-free inside the nuclear surface and due to confinement, the motion is quantized. This generates the shell structure of the nucleonic states, like the shell structure of atoms, the electronic states of molecules or the band structure of the electrons in crystals. The quantization of the nucleonic motion governs the statics and dynamics of the nuclear shape, i.e., the nucleus may be viewed as a droplet of a fermionic liquid with long-range correlations, analogous to small metal clusters, He$_2$ droplets, Rydberg states in large atoms and ultracold fermionic atom gases.

A self-consistent description of the intertwined dynamics of the shape and single particle degrees of freedom is one of the major research themes in nuclear structure physics [2]. The adiabatic time-dependent mean-field (ATDMF) approach and the generator coordinate method (GCM) [7] have become the standard approaches to describe the collective dynamics [2, 8]. The advances in computer technology and the development of the new algorithms have made the spherical shell model (SSM) a viable approach to calculate the collective characteristics of the low-lying states [9–11].

In this work, we propose the triaxial projected shell model (TPSM) [12] as an alternative approach to elucidate the triaxial characteristics of atomic nuclei. In contrast to the SSM approach, the TPSM uses angular momentum projected quasi-particle configurations of a triaxial mean field that incorporates essential correlations, and the residual correlations are included through diagonalization of the Hamiltonian. This drastically reduces the numerical effort and simplifies the interpretation of the results. We think that such a novel approach may pave a way to describe other collective features in atomic nuclei, as well as in non-nuclear mesoscopic systems consisting of a few hundred particles.

To demonstrate how $\gamma$-softness arises from the TPSM picture, we have chosen $^{104}$Ru nucleus as an example because a detailed Coulomb excitation (COULEX) experiment has been performed for this nucleus with the measurement of twenty-eight $E2$ and three $M1$ matrix elements [13] among the low-lying states. From the analysis of the shape invariants [14, 15], derived from the set of $E2$ matrix elements, it was deduced [13] that $^{104}$Ru is "$\gamma$-soft", i.e., the $\gamma$-degree of freedom is distributed over a wide range between prolate ($\gamma = 0^\circ$) and oblate ($\gamma = 60^\circ$) shapes. The authors of Ref. [13] compared the observed data with a variant of the ATDMF approach [16], referred to as the quadrupole collective Bohr Hamiltonian (QCBH). These calculations reproduced the matrix elements from the COULEX experiment with a good accuracy. In particular, the dispersions of the shape invariants indicated that $^{104}$Ru nucleus is $\gamma$-soft, which is consistent with the shallow potential of their QCBH.
In the present work, we demonstrate that experimental energies and the COULEX matrix elements are accurately reproduced in the framework of the TPSM approach [12]. The results turn out to be quite similar to the ones obtained using the QCBH approach, tabulated in Ref. [13] as the "dynamic" (dyn.) variant. In particular, the important features of γ-softness are obtained without considering a collective Hamiltonian, instead they emerge directly by mixing multi-quasiparticle configurations with a fixed deformation.

It was demonstrated in Ref. [17], for a large set of nuclei, that TPSM approach reproduces the experimental staggering parameter

$$S(I) = \frac{[E(I) - E(I - 1)] - [E(I - 1) - E(I - 2)]}{E(2^+)}$$  \hspace{1cm} (1)

of the γ-bands, which allowed to classify the studied nuclei as γ-soft or γ-rigid. In this work, we demonstrate for the first time that the TPSM reproduces the more direct criteria for γ-softness by means of the shape invariants deduced from the E2 transition matrix elements. This method has also been used to extract the collective quadrupole characteristics from large-scale SSM calculations [11].

The basic methodology of the TPSM approach is similar to the SSM with the exception that angular-momentum projected deformed basis is employed to diagonalize the shell model Hamiltonian [18]. The Hamiltonian consists of monopole deformed basis is employed to diagonalize the shell model Hamiltonian [18]. The Hamiltonian consists of monopole pairing $(\hat{P}^\dagger \hat{P})$, quadrupole pairing $(\hat{Q}^\dagger \hat{Q})$, and quadrupole-quadrupole $(\hat{Q}^\dagger \mu \hat{Q}^\dagger \mu)$ interaction terms within the configuration space of three major oscillator shells ($N = 3, 4, 5$ for neutrons and $N = 2, 3, 4$ for protons) :

$$\hat{H} = \hat{H}_0 - \frac{1}{2} \chi \sum_\mu \hat{Q}^\dagger \mu \hat{Q}^\dagger \mu - G_M \hat{P}^\dagger \hat{P} - G_Q \sum_\mu \hat{P}^\dagger \mu \hat{P}^\dagger \mu,$$  \hspace{1cm} (2)

where $\hat{H}_0$ is the spherical single-particle potential [19]. The pairing parameters are taken from our earlier work [20] with $G_M$ chosen such that the overall observed odd-even mass differences are reproduced for nuclei in this region, and the quadrupole pairing strength $G_Q$ is assumed to be 0.18 times $G_M$. The QQ-force strength $\chi$ is fixed by the self-consistency relation between the input deformation and the quadrupole mean field (see Ref. [18]).

The shell model Hamiltonian of Eq. (2) is diagonalized in the space of angular-momentum projected multi-quasiparticle states. In the present work, the basis is composed of the 0-qu vacuum, the two-quasiproton, the two-quasineutron and the combined four-quasiparticle configurations

$$\hat{P}^\dagger_{MK} | \Phi >, \hat{P}^\dagger_{MK} a^\dagger_{p1} a^\dagger_{p2} | \Phi >, \hat{P}^\dagger_{MK} a^\dagger_{n1} a^\dagger_{n2} | \Phi >,$$

$$\hat{P}^\dagger_{MK} a^\dagger_{p1} a^\dagger_{p2} a^\dagger_{n1} a^\dagger_{n2} | \Phi >,$$  \hspace{1cm} (3)

respectively, where $a^\dagger$ is the quasiparticle creation operator, "p" labels the quasiproton and "n" the quasineutron states, $P^\dagger_{MK}$ is the standard three-dimensional angular-momentum projection operator [7], and $| \Phi >$ represents the triaxially-deformed quasiparticle vacuum state.

The electromagnetic transition matrix elements are calculated using the electric quadrupole tensor $\mathcal{M}(E2)_\mu$ with the effective charge of 1.5e for protons and 0.5e for neutrons, and the magnetic dipole operator $\mathcal{M}(M1)_\mu$ with the spin g factors reduced by a factor of 0.75 [21]. The deformed basis states are generated from a mean-field Nilsson Hamiltonian with fixed deformation parameters $\epsilon = 0.258$ and $\epsilon' = 0.150$, which corresponds to a triaxiality parameter of $\gamma = \arctan(\epsilon'/\epsilon) = 30.2^\circ$. As in our earlier studies [17, 21, 22], these two parameters were adjusted to reproduce the $B(E2,2^+_1 \rightarrow 0^+_1)$ value [23] and the energy $E(2^+_2)$ of the γ-band of $^{104}$Ru. Moreover, the pairing strength was reduced by a factor of 0.5 for the bands built on the excited $0^+_2$ and $0^+_3$ states.

Fig. 1 compares the TPSM energies with the experimental data and also with the corresponding energies obtained in the QCBH approach. It is evident from the figure that the TPSM reproduces the experimental energies quite well. Fig. 2 displays the staggering parameter $S(I)$ obtained from the corresponding energies of the γ-band. The relation between staggering pattern of γ softness were reviewed in Ref. [2]. The experimental $S(I)$ depicts the even-I-down pattern of a γ-soft nucleus, which is very well reproduced by the TPSM calculations that include the quasiparticle admixtures. The TPSM results with the vacuum configuration only show the odd-I-down pattern of a γ-rigid nucleus. The feature of the γ-softness is, therefore, generated by the quasiparticle admixtures. The QCBH values indicate γ-softness as well, however, overestimate the amplitude of $S(I)$.

![FIG. 1. Comparison of the measured energy levels of $^{104}$Ru nucleus with the results of TPSM and QCBH calculations. The QCBH energies are taken from Fig. 6 of Ref. [13] level sequence QCBH(dyn).](image)

Tables I and II compare the experimental reduced $E2$ matrix elements with the ones calculated using the TPSM wavefunctions. The corresponding values of the QCBH calculations are given in the Tables 1-3 of Ref. [13]. We adopted the
FIG. 2. (Color online) Staggering parameter $S(I)$ for the $\gamma$-band in $^{104}$Ru. The criterion for $\gamma$-softness is $S(I_{even}) < S(I_{odd})$ and $\gamma$-rigidity is $S(I_{odd}) < S(I_{even})$. The observed values (Exp.) are compared with the TPSM values including the quasiparticle excitations (Full), the TPSM with vacuum configuration only (Vacu. only), the QCBH (dyn.) values, the Davydov Filippov (DF) and the Wilets Jean (WJ) limits. The QCBH (dyn.), DF and WJ staggering values have been calculated from the energies of the respective models, shown in Fig. 6 of Ref. [13].

TABLE I. Comparison of all known experimental reduced $E2$ diagonal, in-band and inter-band matrix elements $\langle I_f | E2 | I_i \rangle$ (e.b.), (associated errors in parenthesis) and calculated ones for yrast- and $\gamma$-band of $^{104}$Ru.

| $I_i \rightarrow I_f$ | Exp. | TPSM (Full) | TPSM (Vac.) | $I_i \rightarrow I_f$ | Exp. | TPSM (Full) | TPSM (Vac.) |
|----------------------|------|-------------|-------------|----------------------|------|-------------|-------------|
| $2_1 \rightarrow 2_1$ | -0.71(11) | -0.817 | -0.634 | $4_2 \rightarrow 3_1$ | ±0.68 (5) | -0.787 | -0.597 |
| $4_1 \rightarrow 4_1$ | -0.79(15) | -0.906 | -0.437 | $5_1 \rightarrow 3_1$ | 1.22(4) | 1.184 | 0.697 |
| $6_1 \rightarrow 6_1$ | -0.76(30) | -0.868 | -0.342 | $6_2 \rightarrow 4_2$ | 1.52 (2) | 1.521 | 0.682 |
| $8_1 \rightarrow 8_1$ | -0.66(26) | -0.855 | -0.297 | $8_2 \rightarrow 6_2$ | 2.02 (4) | 2.056 | 0.747 |
| $2_2 \rightarrow 2_2$ | 0.62 (8) | 0.634 | 0.633 | $2_2 \rightarrow 0_2$ | -0.156 (2) | -0.141 | -0.225 |
| $4_2 \rightarrow 4_2$ | -0.58 (18) | -0.749 | -0.534 | $2_2 \rightarrow 2_2$ | -0.75 (4) | -0.722 | -0.612 |
| $6_2 \rightarrow 6_2$ | ±1.06 (3) | -1.105 | -0.763 | $2_2 \rightarrow 4_2$ | ±0.6 (0.1) | -0.090 | -0.001 |
| $2_1 \rightarrow 0_1$ | 0.917 (25) | 0.973 | 0.901 | $3_1 \rightarrow 1_1$ | 0.22 (60) | 0.254 | 0.302 |
| $4_1 \rightarrow 2_1$ | 1.43 (4) | 1.591 | 1.456 | $3_1 \rightarrow 4_1$ | -0.57 | -0.517 | -0.559 |
| $6_1 \rightarrow 4_1$ | 2.04 (8) | 2.081 | 1.830 | $4_2 \rightarrow 2_2$ | -0.107 (8) | -0.113 | -0.054 |
| $8_1 \rightarrow 6_1$ | 2.59 (24) | 2.486 | 1.902 | $4_2 \rightarrow 4_2$ | -0.83 (5) | -0.840 | -0.505 |
| $10_1 \rightarrow 8_1$ | 2.7 (6) | 2.668 | 1.623 | $4_2 \rightarrow 4_2$ | -0.22 (12) | -0.230 | -0.682 |
| $3_2 \rightarrow 2_2$ | -1.22 (10) | -1.241 | -0.955 | $6_2 \rightarrow 6_2$ | >-0.84 | >-0.947 | >-0.411 |
| $4_2 \rightarrow 2_2$ | 1.12 (5) | 1.095 | 0.510 |

phase convention of Ref. [13] (Section 6). The agreement of the TPSM results with the COULEX data and QCBH calculations is remarkable, because the $E2$ matrix elements provide the most direct information on the statics and dynamics of the collective quadrupole modes. Comparing with the matrix elements Vacu. shows that the quasiparticle admixtures generate the substantial shifts needed for the good agreement with the experiment. Table III presents TPSM reduced $M1$ matrix elements, which also reproduce the known experimental values quite well.

TABLE II. Comparison of all known experimental reduced $E2$ matrix elements $\langle I_f | E2 | I_i \rangle$ (e.b.), diagonal, in-band and inter-band values (associated errors in parenthesis) and calculated ones for excited $0^+$ bands of $^{104}$Ru.

| $I_i \rightarrow I_f$ | Exp. | TPSM (Full) | TPSM (Vac.) | $I_i \rightarrow I_f$ | Exp. | TPSM (Full) | TPSM (Vac.) |
|----------------------|------|-------------|-------------|----------------------|------|-------------|-------------|
| $2_1 \rightarrow 2_2$ | 0.71(4) | 0.682 | -0.370 (4) | $2_3 \rightarrow 2_1$ | 0.613 | ±0.22 (22) | -0.237 |
| $4_1 \rightarrow 2_1$ | 0.75 (25) | 0.613 | 2.12 | $2_1 \rightarrow 2_2$ | 0.21 | 0.318 (13) | 0.221 |
| $0_2 \rightarrow 2 _1$ | -0.266 (8) | -0.221 | 0.318 (13) | $2_1 \rightarrow 4_2$ | 0.53 (32) | 0.481 |
| $2_1 \rightarrow 0_1$ | 0.08 (3) | 0.099 | 0.048 | $2_1 \rightarrow 2_2$ | -0.071 (3) | -0.048 | >-0.1 |
| $2_1 \rightarrow 2_2$ | ±0.07 (3) | ±0.031 | ±0.08 (12) | $2_3 \rightarrow 2_3$ | -0.631 |

TABLE III. Comparison of all known experimental reduced $M1$ matrix elements $\langle I_f | M1 | I_i \rangle$ (µN), in-band and inter-band values (associated errors in parenthesis) and calculated ones for $^{104}$Ru.

| $I_i \rightarrow I_f$ | Exp. | TPSM (Full) | TPSM (Vac.) | $I_i \rightarrow I_f$ | Exp. | TPSM (Full) | TPSM (Vac.) |
|----------------------|------|-------------|-------------|----------------------|------|-------------|-------------|
| $2_1 \rightarrow 3_1$ | -0.054 (4) | -0.044 | 0.82 (10) | $2_1 \rightarrow 2_1$ | 0.82 (10) | 0.791 |
| $2_1 \rightarrow 2_2$ | <0.02 | <0.038 | 0.15 (5) | $2_1 \rightarrow 2_1$ | -0.136 |

Fig. 3 depicts the quadrupole shape invariants and their dispersions calculated from the reduced $E2$ matrix elements. The pertaining expressions are given in Refs. [13–15]. The invariant $\langle I_n^9 | Q^2 | I_n^9 \rangle$ measures the average intrinsic deformation of a state $I_n^9$. The invariant $\langle I_n^9 | \cos 3\delta | I_n^9 \rangle$ contains the information about the triaxiality of the intrinsic shape, where $\delta = \arctan \langle I_n^9 | \cos 3\delta | I_n^9 \rangle$. The parameters $Q$ and $\delta$ can be related to the effective deformation parameters $\beta$ and $\gamma$ of the liquid drop model [1]. The relevant formulae for ellipsoidal shape are given in the appendix of Ref. [13]. Evaluating them, we found $\delta < \gamma$ with $|\delta - \gamma| < 2.5^\circ$.

The TPSM values $\langle Q^2 \rangle = 1.00(2b)^2$ for the ground-band are nearly constant in agreement with the experimental data. The corresponding effective deformation of $\beta = 0.28$ is the input in the TPSM. The TPSM values of $\langle Q^2 \rangle = 0.7$ corresponding to $\beta = 0.27$ indicate a smaller deformation for the $\gamma$-band, which is again consistent with the experiment.

For the ground-band, the TPSM values of $\langle \cos 3\delta \rangle$ signify a substantial triaxiality with preference for prolate shape. The value of $0.6$ corresponds to $\delta = 18^\circ$. For $I = 2$, the experimental data shows a shift towards prolate shape, which is seen in the TPSM values as well. The TPSM dispersion $\sigma < \cos 3\delta \rangle > 0.3$ signifies large fluctuations of the triaxiality parameter with $70\%$ of the distribution within the range $9^\circ < \delta < 24^\circ$. This indicates that $^{104}$Ru is $\gamma$-soft in accordance with the staggering parameter $S(I)$ of Fig. 2. The QCBH dispersion of $\sigma < \cos 3\delta > 0.4$ corresponds to a distribution with $70\%$ in the larger range $0^\circ < \delta < 26^\circ$. The QCBH values seem to overestimate the $\gamma$-softness, which is consistent with the QCBH values for $S(I)$ being larger than the TPSM and the experimental values.

For the $\gamma$-band, the TPSM values of $\langle \cos 3\delta \rangle$ for $I = 2, 3$ and 4 indicate a shift towards prolate shape, which is in accordance with the experimental values. This shift is also
In the TPSM diagonalization, the most important quasiparticle admixtures to the γ-band are the K = 1 state projected from the \( h_{\frac{11}{2}} \) two-quasineutron configuration and the K = 1, 3 states, projected from the \( g_{\frac{9}{2}} \) two-quasiproton configuration. Their admixtures increase with I and are about 20% for the I = 7 state. As noted from Fig. 4, these quasiparticle band structures show a pronounced even-I low staggering.

In order to probe the microscopic origin of the appearance of γ-soft characteristics, the energies of the angular momentum projected quasiparticle configurations are depicted in Fig. 4. The K = 0, 2, 4, ... states, projected from the quasiparticle vacuum configuration, have an increasing content of the angular momentum oriented along the long-axis with the smallest moment of inertia. For K = 0, there are only even-I states. When the TPSM Hamiltonian is diagonalized with vacuum configuration only, it mostly couples the K = 0 with the K = 2 states. The coupling pushes up the even-I states of the γ-band above the mean energy of the adjacent K = 2 states with odd I, which are not shifted because they do not have a partner in the ground-band. This results in the odd-I low pattern of the staggering parameter S(I).

In the TPSM diagonalization, the most important quasiparticle admixtures to the γ-band are the K = 1 state projected from the \( h_{\frac{11}{2}} \) two-quasineutron configuration and the K = 1, 3 states, projected from the \( g_{\frac{9}{2}} \) two-quasiproton configuration. Their admixtures increase with I and are about 20% for the I = 7 state. As noted from Fig. 4, these quasiparticle band structures show a pronounced even-I low staggering.

The coupling pushes the states with even I further down than the states with odd I, and the coupling is strong enough to reverse the staggering pattern of the γ-band into the even-I low pattern of a γ-soft nucleus. The high-j orbitals \( h_{\frac{11}{2}} \) and \( g_{\frac{9}{2}} \) have large quadrupole moments, and a moderate admixture of these states modifies the E2 matrix elements such that the pattern of a γ-soft nucleus emerges from the γ-rigid pattern of the vacuum configuration only. The superposition of configura-
tions with different triaxiality increases the shape fluctuations as seen in Fig. 3.

A further indication for γ-softness is the appearance of a $\Delta I = 2$ band built on an excited $0^+_2$ state which is connected by collective $E2$ transitions with the $\gamma$-band. In terms of the collective Bohr Hamiltonian, it represents a pulsation of the triaxial surface that carries no angular momentum (see Fig. 6 of the review [2]). The limiting cases are the $K = 0$ double $\gamma$ vibration about the axially symmetric equilibrium shape [1] and the $0^+_2$ state in the $\gamma$-independent potential, where it represents the oscillation between prolate and oblate shapes through a triaxial path. The COULEX experiment observed $0^+_2$ and $0^+_2$ states of this type [13]. As seen in Fig. 1 and Table II, the TPSM calculations account well for the experimental data. For the $0^+_2$ state, the shape invariant $\langle \cos 3\delta \rangle$ in Fig. 5 indicates strong triaxiality of $\delta = 26^\circ$, which decreases towards the prolate value of zero with $I$. For the $0^+_2$ state, weak triaxiality is noted that increases to the maximal value with $I$. The dispersions indicate large fluctuations in $\delta$. The $0^+_2$ state contains a 60% component of the $K = 0$ two $h_{11/2}$ quasineutron configuration (2$\nu$, 0, 2.06 in Fig. 4), which decreases to 20% for the $6^+_1$ state by admixing many small components. The $0^+_2$ state contains a 95% component of the $K = 0$ two $g_{9/2}$ quasiproton configuration (2$\pi$, 0, 1.63 in Fig. 4), which decreases to 40% for the $6^+_1$ state by admixing many small components.

The dominating two-quasiparticle character of the $0^+_2$ states justifies the reduction of the pairing strength in the TPSM calculation, which lie too high in the excitation energy with full strength (see Fig. 4). The QCBH calculations [13] also point to a change of the pair correlations.

To conclude, we have shown that TPSM approach reproduces the extended set of collective $E2$ matrix elements measured in the COULEX experiment with a remarkable accuracy. The shape invariant quantities deduced from these matrix elements capture the features of a $\gamma$-soft nucleus with the mean value of the triaxiality parameter of $\delta \sim 20^\circ$, and fluctuations within the range $0^\circ < \delta < 26^\circ$. The important inference drawn from the present analysis is that admixtures of quasiparticle states into the collective vacuum configuration can transform the pattern of the energies and $E2$ matrix elements from $\gamma$-rigid to that of $\gamma$-soft character. The spherical shell model calculations with a sufficiently large basis set should also capture the discussed collective features [9–11]. However, the small number of quasiparticle configurations in the present deformed shell model approach provides another perspective on the nature of $\gamma$-softness in atomic nuclei: it represents the superposition of a few configurations with different triaxiality.

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