Multiphonon \(\gamma\)-vibrational bands and the triaxial projected shell model

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We present a fully quantum-mechanical, microscopic, unified treatment of ground-state band and multiphonon \(\gamma\)-vibrational bands using shell model diagonalization with the triaxial projected shell model. The results, which agree very well with data on the \(g\)- and \(\gamma\)-band spectra in \(^{156-170}\)Er, as well as with recently measured \(4^+\) two-phonon \(\gamma\)-bandhead energies in \(^{166}\)Er and \(^{168}\)Er, are discussed in terms of the \(K\) mixing. Multiphonon \(\gamma\)-excitation energies are predicted.

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The atomic nucleus is a many-body system with pronounced shell effects that can have intrinsic deformation. In addition, it can, according to the semiclassical collective model, undergo dynamical oscillations around the equilibrium shape, resulting in various low-lying collective excitations. Ellipsoidal oscillation of the shape is commonly termed a \(\gamma\) vibration [1].

Thanks to advances in high-resolution \(\gamma\)-ray detectors, high quality measurements not only of high-spin states but also of low-spin states are now commonly available. As a consequence long-sought multiphonon \(\gamma\)-vibrational states have been discovered in a series of experiments over the last decade [2–7]. However, the status of unified theoretical descriptions for ground-state band (\(g\) band) and multiphonon \(\gamma\)-vibrational bands (\(\gamma\) band) is not so satisfactory. In the present work, we attempt a consistent description of these low-lying bands using an approach based on the projected shell model (PSM) [8].

In its original form, the PSM uses an axially deformed basis. The shell model diagonalization is carried out within the space spanned by the angular-momentum-projected quasiparticle (qp) vacuum, 2qp and 4qp states. In this sense, the PSM is a Tamm-Dancoff approach and one expects that the collectivity of low-lying states may be strongly affected by mixing many 2qp and 4qp states. Indeed, a multi-qp admixture can cause significant effects in band crossing regions [8].

However, in the low-spin region before any band crossings (\(I\leq10\)), the admixture is very weak and the calculated \(g\) band always exhibits the characteristics of an axially symmetric rotor. For example, the ordinary PSM fails to describe the steep increase of moment of inertia at low spins in transitional nuclei [8]. Quite recently, the restriction to an axially deformed basis in the PSM was removed by two of the present authors (J.A.S. and K.H.). It was shown that the observed steep increase of the moment of inertia for transitional nuclei can be well described if one introduces triaxiality in the deformed basis and performs three-dimensional angular momentum projection [9]. This approach is called the triaxial projected shell model (TPSM).

Another important issue is whether the PSM can describe bands built on collective vibrational states. The usual treatment of the \(\gamma\) band based on the Tamm-Dancoff or random phase approximation assumes different coupling constants for the \(\mu=0\) and \(\mu=\pm2\) parts of the \(QQ\) force, with the former related to the mean-field deformation and the latter adjusted to the \(\gamma\)-bandhead energy. In the PSM, as in the ordinary shell model, such an adjustment is not permitted because the Hamiltonian must be rotation invariant and thus these two coupling constants must be equal: One cannot simply fit the theoretical \(\gamma\) bandhead to the experimental one by modifying the \(QQ\) force in that manner.

On the other hand, one might hope that inclusion of many 2qp states could introduce a collective contribution that would produce the desired low-lying \(\gamma\) state. But such attempts have failed. Because of the large pairing gap, the energy of the lowest 2qp state is above 1.5 MeV and is much higher than the actual \(\gamma\)-bandhead energy, which typically lies between 0.5 and 1 MeV in rare-earth nuclei. The \(QQ\) force is too weak to lower the theoretical \(\gamma\)-band energy by such a large amount in a limited basis. Calculations including about 1000 2qp and 4qp states do not lead to low-lying excited states that look like the experimental \(\gamma\) band [10]. One therefore has to conclude that it is not practical to describe the \(\gamma\)-vibrational state in terms of multi-qp states in the framework of the axial PSM [11].

In the present paper, the TPSM extension of the PSM and the computer code developed in [9] are used to study multiphonon \(\gamma\) bands. (Although the present theory is not based on a vibrational phonon excitation mechanism as in other models [12], we shall use the conventional vibrational terminology in our discussion.) We shall show the following: (1) For well-deformed nuclei, the introduction of triaxiality in the basis does not destroy the good agreement for the \(g\) bands obtained previously in axial PSM calculations (for example, those presented in Ref. [8]). (2) However, it produces new excited states (\(\gamma\) bands) at the correct energies that do

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not occur in the axial PSM. (3) For transitional nuclei, use of a basis of fixed triaxiality improves the \( g \)-band moments of inertia, as already shown in [9], and at the same time produces realistic \( \gamma \) bands. (4) By a single diagonalization of the Hamiltonian (with the same parameters in the deformed basis), we obtain not only the \( g \) and \( \gamma \) bands, but also higher excited bands that can be identified as the multiphonon \( \gamma \) bands, and these compare very well with recently measured \( 4^+ \) two-phonon \( \gamma \) bands. (5) Finally, we make predictions for the two- and three-phonon \( \gamma \) bands (referred to as \( 2 \gamma \) and \( 3 \gamma \) bands hereafter) of those Er isotopes treated here for which no measurement has yet been reported.

Since an extensive review of the PSM exists (see Ref. [8] and references cited therein), we shall describe the model only briefly. The PSM (TPSM) closely follows the shell model philosophy and is, in fact, a shell model truncated in a deformed basis. One uses a Nilsson potential having axial (triaxial) deformation to generate the deformed single-particle states. The Nilsson spin-orbit force parameters \( \kappa \) and \( \mu \) are essential in reproducing correct shell fillings. For rare-earth nuclei, we use the early compilation of Nilsson et al. [13] without modification. For the axial deformation parameter \( \epsilon \) in the Nilsson model, we take the values given in Ref. [14]. Thus, for the TPSM, the triaxial deformation \( \epsilon' \) is the single adjustable parameter. The static pairing correlations are treated by the usual BCS approximation to establish the Nilsson+BCS basis. The three-dimensional angular momentum projection is then carried out on the Nilsson+BCSqp states to obtain the many-body basis, and the Hamiltonian is diagonalized in this projected basis.

In the present work, we consider only low-spin states where no band crossing with any multi-qp band occurs in the yrast region. Thus, the many-body basis may be restricted to the projected triaxial qp vacuum state:

\[
\{\hat{P}^I_{MK}|\Phi\}, \quad 0 \leq K \leq I, \tag{1}
\]

where \( |\Phi\rangle \) represents the triaxial qp vacuum state. This is the simplest possible configuration space for an even-even nucleus. Note that only one state is possible for spin \( I=0 \) (the ground state). Thus, multi-qp components have to be taken into account if one wants to describe \( I=0 \) excited states (see further discussion below). The diagonalization is performed over a chain of Er isotopes up to spin \( I=10 \).

As in the usual PSM calculations, we use the Hamiltonian [8]

\[
\hat{H} = \hat{H}_0 - \frac{1}{2} \sum_\mu \hat{Q}_\mu \hat{Q}_\mu - G_M \hat{P}^1 \hat{P} - G_Q \sum_\mu \hat{P}^1_\mu \hat{P}_\mu, \tag{2}
\]

so that the corresponding Nilsson Hamiltonian (with triaxiality) is given by

\[
\hat{H}_N = \hat{H}_0 - \frac{2}{3} \hbar \omega \left( \epsilon \hat{Q}_0 + \epsilon^2 \frac{\hat{Q}_2+\hat{Q}_{-2}}{\sqrt{2}} \right). \tag{3}
\]

Here \( \hat{H}_0 \) is the spherical single-particle Hamiltonian, which contains a proper spin-orbit force as mentioned before, while the interaction strengths are taken as follows. The \( QQ \)-force strength \( \chi \) is adjusted such that the physical quadrupole deformation \( \epsilon \) is obtained as a result of the self-consistent mean-field [Hartree-Fock-Bogoliubov (HFB)] calculation [8]. The monopole pairing strength \( G_M \) is of the standard form \( G_M = 21.24 \pm 13.86(N-Z)/A \), with "-" for neutrons and "+" for protons, which approximately reproduces the observed odd-even mass differences in this mass region. This choice of \( G_M \) is appropriate for the single-particle space employed in the PSM, where three major shells are used for each type of nucleon \((N=4,5,6 \) for neutrons and \( N=3,4,5 \) for protons). The quadrupole pairing strength \( G_Q \) is assumed to be proportional to \( G_M \), the proportionality constant being fixed as usual to be in the range 0.16–0.18. These interaction strengths are consistent with those used previously for the same mass region [8,9].

Let us first consider a well-deformed nucleus \( ^{168}\text{Er} \), which is generally considered to be axially symmetric. In fact, previous (axial) PSM calculation for this nucleus gave an excellent description of the yrast band up to a very high spin [8]. Figure 1(a) shows the calculated energies as functions of the triaxiality parameter \( \epsilon' \) for angular momenta up to \( I=10 \). In addition to the usual \( g \) band with spins \( I=0,2,4, \ldots \), a new set of rotational states with spins \( I=2,3,4, \ldots \) appears. This figure looks similar to the one shown by Davydov and Filipov [15], but now obtained in terms of a fully microscopic theory. Unlike the irrotational flow model, the PSM spectrum depends not only on the deformation parameters but also on the shell filling of the nucleus in question. We see that, for the \( g \) band of \( ^{168}\text{Er} \), the energies as functions of triaxiality are nearly flat and their values remain close to those at zero triaxiality. Thus, the triaxial basis has no significant effect on the \( g \) band for a well-deformed nucleus and does not destroy the good \( g \) band result obtained with an axially deformed basis.

However, it has a drastic effect on new excited bands (second and higher excited bands are not shown in the figure). Their excitation energies are indeed very high for axial symmetry, but come down quickly as the triaxiality in the basis increases. At \( \epsilon' = 0.13 \), the first excited band reproduces the observed \( \gamma \) band in \( ^{168}\text{Er} \) (while preserving the good \( g \)-band agreement). It should be noted that the excited bands studied in this paper are obtained by introducing a \( \gamma \) degree of freedom in the basis (quasiparticle vacuum). They are collective excitations, but not quasiparticle excitations. We may thus identify the first excited band as the \( \gamma \) band, the second excited band as the \( 2 \gamma \) band, the third excited band as the \( 3 \gamma \) band, etc.

The above results can be understood by studying the \( K \)-mixing coefficients for each projected \( K \) state [see Eq. (1)] in the total wave functions. It is found that for this well-deformed, axially symmetric nucleus, \( K \) mixing is negligibly small. States in the \( g \) band are essentially the projected \( K = 0 \) state for any \( \epsilon' \). That is why the basis triaxiality does not destroy the result obtained with an axially deformed basis. The excited bands are also built by rather pure projected \( K \) states. For example, the first excited band with the bandhead spin \( I=2 \) is mainly the projected \( K=2 \) state and the second excited band with the bandhead spin \( I=4 \) is the projected \( K=4 \) state. A small amount of \( K \) mixing can be seen only for
states with higher total spin if triaxiality in the basis is sufficiently large.

Figure 1 illustrates another example, the transitional nucleus $^{156}$Er. We see that the energies for the $g$ band are no longer constant, but clearly vary as functions of triaxiality. This feature is expected for a $g$-soft nucleus. For the excited bands, triaxiality in the basis has a similar effect as we have seen for well-deformed nuclei: it drastically lowers their energies to those of the observed $g$ band.

A rather different picture of $K$ mixing is observed for this $g$-soft nucleus. The states are no longer pure projected $K$ states, but highly mixed. For example, the two $I=2$ states [the one in the $g$ band and the other one being the bandhead of the first excited band (the $\gamma$ band)] are mixed from the projected $K=0$ and $K=2$ states. At $\epsilon'=0.13$, the $I=2$ state of the $g$ band is contaminated by the projected $K=2$ state with a weight of about $1/4$, and the $I=2$ state of the first excited band contains the projected $K=0$ state with a weight of about $1/4$. Stronger $K$ mixing is seen for states with higher total spin and larger basis triaxiality.

Figure 2 presents results for a chain of Er isotopes with neutron numbers from $N=88$ to 102. This covers both transitional ($N\approx 90$) and well-deformed ($N\approx 98$) nuclei. The theoretical results are compared with available data for both $g$ and $\gamma$ bands up to $I=10$. The axial and triaxial deformation parameters used in the present calculations are listed in Table I. The triaxial parameter $\epsilon'=0.13$ giving the correct position of the $g$ band for $^{168}$Er and $^{156}$Er corresponds to $\gamma=25.5^\circ$ in terms of the usual gamma parameter, if one uses as a very rough estimate $\gamma=\tan^{-1}(\epsilon'/\epsilon)$.

A microscopic description of transitional nuclei has always been challenging. The nuclei discussed here with neutron number around 90 have $g$ bands that are quasirotational but with considerable vibrational character. The ground-state energy surface of a transitional nucleus was shown to have a shallow minimum at a finite $g$ deformation in HFB calculations [16]. It has been demonstrated that such a shallow minimum becomes a prominent minimum when projected onto spin $I=0$ [17]. The necessity of introducing triaxiality in the PSM basis to describe the observed $g$-band moment of inertia in transitional nuclei was demonstrated in Ref. [9]. We now see that, with the same triaxiality, the first excited TPSM band reproduces also the observed $\gamma$ band. By adjust-
ing a single parameter $\epsilon'$ in the TPSM, the spectra of both the $g$ and $g'$ bands are described simultaneously and consistently by the Hamiltonian (2) diagonalized within the Hilbert space (1).

Next, let us turn to a discussion of multiphonon $\gamma$ bands. In Fig. 3, we plot all the states for spins $I \leq 10$ obtained after diagonalization within our projected triaxial basis for two nuclei in which a $2\gamma$ band has been reported. For $^{168}$Er, the second excited theoretical band agrees beautifully with the new $4^+\gamma$ band reported in Ref. [7]. For $^{166}$Er, the observed $4^+\gamma$ bandhead [4] is also well reproduced. Since our theory agrees very well with the $g$ band and the (one-phonon) $\gamma$ band observed in these nuclei, the present results support strongly the interpretation of these data as $2\gamma$ bands.

To our knowledge, no $3\gamma$ band has yet been seen experimentally. According to our calculations, they should appear between 3 and 3.6 MeV. In Table I, we list the theoretical values for the $2^+\gamma$, $4^+2\gamma$, and $6^+3\gamma$-bandhead energies. As Table I shows, the predicted $\gamma$-vibrational spectra are quite anharmonic. Anharmonic $\gamma$ vibrations have been discussed by several authors [18–20]. This anharmonicity is a straightforward consequence of the present microscopic theory. This may be contrasted with earlier models that found it necessary to introduce explicit anharmonicities to reproduce the $\gamma$-band spacings [18].

Finally, we mention briefly the $0^+$ excited states. Unlike the usual collective models based on phonon excitations, a $0^+$ collective excited state does not exist in the present calculation. Excited $0^+$ states can occur if we include multi-qp states on top of the present vacuum configuration. However, since the states constructed in this way are mainly qp in character, the collectivity of such a $0^+$ excited state is generally expected to be much weaker than that of a two-phonon $\gamma$ state, which should have a large $E2$-decay probability to a one-phonon $\gamma$ state. Furthermore, such states should depend strongly on the shell fillings. Therefore, the nature of the $4^+$ two-phonon excited state discussed in the present paper is kinematical while the $0^+$ two-phonon excited state is dynamical. There has been one experiment reporting a $0^+$ excited state in $^{168}$Er [5]; the measured $B(E2:0^+\rightarrow2^+_2)$ is enhanced, suggesting that this $0^+$ excited state is of two-phonon nature. At present, this is a single observed example of the $0^+$ two-phonon excited state. Whether this observation can be reproduced by the TPSM with inclusion of qp states remains to be seen.

To summarize, we have applied the triaxial projected shell model to some Er isotopes to investigate multiphonon $\gamma$ vibrational bands. The shell model diagonalization is not carried out in a spherical basis as for a conventional shell model, but in a deformed basis with triaxiality. It is found that this simultaneously improves the description of the $g$ bands in transitional nuclei and leads to a consistent description of multiphonon $\gamma$ bands in both transitional and well-deformed nuclei. The newly observed $4^+\gamma$ bands are reproduced by the same calculation, thus supporting their experimental assignment, and the bandhead energies of as yet unobserved $6^+\gamma$ bands are predicted.

Thus, our unified view of the $g$ and multiphonon $\gamma$ bands agrees surprisingly well with the existing data, even though we have used the simplest possible configuration space. The physics of the $\gamma$ bands is discussed in terms of the $K$ mixing, suggesting a microscopic connection between the $\gamma$-excited states and the nuclear ground state properties.

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