Unified description of $2^+_1$ states within the deformed quasiparticle random-phase approximation

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We describe low-lying collective states in deformed even-even nuclei within a deformed quasiparticle random-phase approximation (dQRPA) by using a single-particle basis with good angular momentum. The statistical factors, accounting for the level occupancy, appear in the dQRPA in a natural way as rotation coefficients that take the intrinsic system to the laboratory system. We have used our model by performing a systematic analysis of E2 transitions from the first $2^+$ state to the ground state for all superfluid nuclei in the range $50 < Z \leq 100$ by using a common charge polarization parameter $\chi = 0.2$. In spite of its similarity to the QRPA, this method is able to describe in an unified way gross features of electromagnetic transitions from vibrational to rotational nuclei.

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I. INTRODUCTION

The many-body problem of deformed systems is a challenge for nuclear theory. In nuclear structure, the microscopic approaches dealing with deformed nuclei are based on the Nilsson model [1], describing single-particle (sp) dynamics in an intrinsic system of cylindrical symmetry. It provides a basis for the microscopic description of collective states in deformed systems. One of the most popular approaches to describe collective excitations is the quasiparticle random-phase approximation (QRPA) [2]. In deformed nuclei the calculations are performed in the intrinsic system of coordinates and therefore the physical states with good angular momentum are given by the projection procedure [3]. This method, called projection after variation, was widely used to describe a large variety of collective excitations, like the Gamow-Teller $1^+$ resonance in the context of double-beta-decay processes [4–7], low-lying states in neutron-rich nuclei [8–10], the linear response function [11], giant resonances [12–14], the pygmy resonance [15], and magnetic properties of nuclei [16]. Let us also mention in this context the pseudo-SU(3) model, used to describe the double-beta-decay process in deformed nuclei [17].

A more exact but much more complex method is to use projected wave functions before the variational procedure, as done for instance in the method of variation after mean-field projection in realistic model spaces (VAMPIR) [18]. This approach is able to describe very complex effects, like the shape coexistence phenomenon [19].

Special attention was paid to the analysis of the first-excited $2^+$ state in even-even nuclei by using the projected generator coordinate method [20,21].

Reference [22] proposed an alternative, relatively simple approach where the product between the spherical sp orbital and core wave function (described by a deformed coherent state), projected to a given angular momentum, is considered as a basis state for the many-body problem. In this way, many-particle–many-hole configurations are taken into account in an effective way due to the fact that the sp states are “dressed” by core wave functions. The resulting equations of motion have formally a similar form as the ones corresponding to a spherical system. Later on, this method was used to describe various collective excitations in deformed nuclei, like two-neutrino double beta decay [23–25], magnetic collective states [26], and collective excitations in atomic clusters [27].

The purpose of the present paper is to generalize the approach of Ref. [22] by using a particle-core wave function coupled to a given angular momentum. In the Sec. II we give the necessary theoretical background and in Sec. III we apply it to describe electromagnetic transitions from collective $2^+_1$ states for even-even vibrational, transitional, and rotational nuclei.

II. THEORETICAL BACKGROUND

In order to describe a deformed many-body system we will use an sp basis with good angular momentum:

$$a^\dag_{\tau n j m}(\Omega) = \sum_{Jk} X_{\tau jk}^J \left(D_{J^\tau K}^{\tau j m}(\Omega) \otimes c^\dag_{k m}\right)_{j m},$$

(2.1)

in terms of spherical orbitals $c^\dag_{k m}$, where $\tau$ is the isospin index, $k \rightarrow (\epsilon, l, k)$ has the meaning of sp energy $\epsilon$, angular momentum $l$, and total spin $k$. Notice that the angular momentum coupling of the Wigner function is performed over the first projection, denoted by a dot in the above relation. Here, $n$ denotes the eigenvalue index and the angular momentum coupling is considered over the laboratory projection $M$ of the normalized Wigner function $D_{J^\tau K}^{\tau j m}(\Omega)$, while the intrinsic projection is $K = 0$.

The operators satisfy the following fermionic condition, written in the following form:

$$\langle \{a_{\tau n j m}, a^\dag_{\tau' n' j' m'}(\Omega)\} \rangle_C = \iint \langle a_{\tau n j m}(\Omega), a^\dag_{\tau' n' j' m'}(\Omega)\rangle d\Omega = \delta_{n n'}\delta_{\mu \mu'}\delta_{\nu \nu'}. $$

(2.2)

pointing out on the necessity to use the integration over Euler angles in deriving many-body equations. The expansion
coefficients \( X^{jk}_{\tau n j} \) are found by diagonalizing the multipole-multipole core-particle interaction \( r^2[Y_\lambda(\Omega) \otimes Y_\lambda(\hat{r})]_0 \).

In a simpler approach one supposes the adiabaticity, where the intrinsic spin \( sp \) projection \( v \) is conserved. In this case the amplitudes are given by (see Chapter 4.7 in Ref. [28])

\[
X^{jk}_{\tau n j v} = (-)^j + v \sqrt{2}(j; v; k - v|J0)X^{(e)}_{\xi \nu},
\]

in terms of Clebsch-Gordan coefficients and standard Nilsson amplitudes.

Next we will investigate \( 2^+_1 \) collective states within a deformed QRPA, by using the pairing plus quadrupole-quadrupole residual two-particle interaction and the deformed basis (2.1). We call this approach the dQRPA method. The dQRPA generalizes similar investigations performed by using the standard spherical QRPA code [29,30]. In this way it is possible to avoid the complicated problem of projecting out two-quasiparticle excitations of a deformed ground state. In our calculations we will consider the “yrast” Nilsson states with \( j = v \) in Eq. (2.3) by dropping the index \( v \) in our further notations.

Let us consider now the residual two-body interaction. The most general form, written in terms of the deformed basis (2.1), is given by

\[
H_{\text{int}} = \sum_{\tau \tau'} \sum_{\lambda \lambda'} \sum_{n\lambda} G^{(\lambda \lambda')_{\tau \tau'}}(n_1 j_1 n_2 j_2) \left\{ D^{(\lambda \lambda')}_{\tau \tau'} \otimes \left( Q_{\tau \lambda} \otimes Q_{\tau' \lambda'} \right)_{\lambda \lambda'} \right\} |0\rangle.
\]

The matrix elements are given by the integration of the product between the used two-body potential, single-particle wave functions, written in the representation (2.1), and the Wigner function. In our approach we will use a simplified separable form of the interaction, rewritten in the particle-hole representation as follows:

\[
H_{\text{int}} \rightarrow H \Phi = \sum_{\tau \tau'} \sum_{\lambda \lambda'} F^{(\lambda \lambda')_{\tau \tau'}}(n_1 j_1 n_2 j_2) \left\{ D^{(\lambda \lambda')}_{\tau \tau'} \otimes (Q_{\tau \lambda} \otimes Q_{\tau' \lambda'} \lambda \lambda') \right\} |0\rangle.
\]

The basic ingredients of our approach are the multipole operators, written in the deformed \((n \ j)\) representation as

\[
Q_{\tau \lambda \mu} = \sum_{12} \langle \tau n_1 j_1 | Q_\lambda | \tau n_2 j_2 \rangle C (a^\dagger_{\tau n_1 j_1} \otimes a_{\tau n_2 j_2})_{\lambda \mu},
\]

where the index \( C \) denotes the integration over the core Euler angles \( \Omega \), similar to Eq. (2.2). By using Eq. (2.1), one obtains the reduced matrix element of this operator in terms of standard spherical reduced matrix elements as follows:

\[
\langle \tau n_1 j_1 | Q_\lambda | \tau n_2 j_2 \rangle C = \hat{J}_{j_1 j_2} \sum_{Jk_{12}} X^{Jk_{12}}_{\tau n_1 j_1} X^{Jk_{12}}_{\tau n_2 j_2} \langle -^k_1 j_1 j_2 + j_2 \rangle \times W(j_1 k_{12} j_2 k_{12}; J\lambda) \langle \lambda k_{12} | Q_\lambda | \tau k_{12} \rangle,
\]

where \( \hat{J} = \sqrt{2J + 1} \) and \( W \) is the standard Racah symbol. In the case of monopole operators the above relation for the band head \( J = 0 \) and \( k = j \) can be written in terms of the largest Nilsson component and has a simple form

\[
\langle \tau n_1 j_1 | Q_\lambda | \tau n_2 j_2 \rangle C = \delta_{12} \frac{2(v_{n_1 j_1})^2}{2j_1 + 1} \langle \tau j_1 | Q_\lambda | \tau j_1 \rangle.
\]

Thus, the factor multiplying the spherical reduced matrix element in Eq. (2.7) automatically contains the “statistical factors,” which become \( \frac{2j_1 + 1}{2j_1} \) for the monopole case. This factor, well known in proton emission [see Eq. (4.66) in Ref. [28]], was introduced in Ref. [22] ad hoc by using purely statistical reasoning. Here, we suppose the validity of the adiabatic assumption, due to the fact that the core states have low angular momenta. This condition keeps valid the intrinsic pairing condition, but seen in the laboratory system of coordinates. We will restrict ourselves to a monopole pairing Hamiltonian with constant strengths for protons and neutrons, respectively, by recoupling \( pp \) components with higher multipolarity into the corresponding \( \pi \pi \) terms. Thus, the pairing Hamiltonian can be approximated by the following ansatz in the deformed \((n \ j)\) representation

\[
H_P \rightarrow \sum_{\tau} \sum_{n j} (e_{\tau nj} - \Lambda_{\tau}) \frac{2}{2j + 1} N_{\tau nj} - \frac{1}{4} \sum_{n j n' j'} \sum_{n jn' j'} G_{\tau n j n} \frac{2}{2j + 1} P_{\tau nj n'} \frac{2}{2j' + 1} P_{\tau n' j n' j},
\]

where

\[
e_{\tau nj} = e_{\tau j} (n_{\tau j}^{(n)} \rangle^{2}), \quad G_{\tau n j n'} = G_{\tau j} (\langle n_{\tau j}^{(n)} \rangle^{(n') \rangle}.\]

Here \( N_{n l} \) denotes the particle-number operator and the monopole pairing operator is given by \( P_{\tau nj} = \sqrt{2j + 1} (a^\dagger_{\tau nj} \otimes a_{\tau nj}) \). One can easily see that in the case of a common value of the Nilsson amplitude, one obtains the standard Hamiltonian with shifted \( sp \) energies and a renormalized constant pairing strength. Indeed, this is approximately true for a given deformation concerning the orbitals around the Fermi level, which play the leading role in determining the pairing gap. In our calculations we will use this approximation.

It is worth mentioning that Eq. (4.5) of Ref. [22] has a similar ansatz with our Eq. (2.9), but the paired states are spherical orbitals “dressed” by core states. In our case the paired states are deformed Nilsson orbitals in the laboratory system, dressed by the core states. Thus, it becomes possible to use the replacement \( 2j + 1 \rightarrow 2 \) in spherical BCS equations in order to obtain the same relations as for the deformed case. In the quasiparticle representation

\[
a^\dagger_{\tau nj} = u_{\tau nj} a^\dagger_{\tau nj} + v_{\tau nj} a_{\tau nj - m} (-)^{j - m},
\]

the multipole operator becomes

\[
Q_{\tau \lambda \mu} = \sum_{n j_1 j_2} \hat{\xi}_{n j_1 j_2} \left[ A^\dagger_{\lambda \mu}(\tau j_1) + (-)^{\lambda - \mu} A_{\lambda - \mu}(\tau j_1) \right],
\]

in terms of the normalized pair quasiparticle operator

\[
A^\dagger_{jm}(\tau j_1) = \frac{1}{\sqrt{1 + \delta_{n j_1 j_2} \delta_{\lambda \mu}}} (a^\dagger_{\tau n j_1} \otimes a_{\tau n j_2})_{jm},
\]

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where we used the short-hand notation \( \tau_{12} = (\tau_{11}, n_{1} j_{1} n_{2} j_{2}) \) and 
\[
\xi_{\lambda \tau_{12}} = \frac{\langle \tau_{11}, n_{1} j_{1} | Q_{\lambda} | \tau_{12} j_{2} \rangle}{\sqrt{(2\lambda + 1)(1 + \delta_{n_{1} n_{2}} \delta_{j_{1} j_{2}})}} \times (u_{\tau_{n_{1} j_{1}} v_{\tau_{n_{2} j_{2}}} + v_{\tau_{n_{1} j_{1}} u_{\tau_{n_{2} j_{2}}}}).
\]

As a result of the deformation, the residual Hamiltonian (2.5) couples QRPA phonons of multipole \( \lambda \)
\[
\Gamma_{\lambda \mu}^{\uparrow}(v) = \sum_{\tau} \sum_{n_{1} j_{1} \leq n_{2} j_{2}} \left[ \lambda_{\lambda}^{(v)}(\tau_{12}) \bar{A}_{\lambda \mu}(\tau_{12}) - \lambda_{\lambda}^{(v)}(\tau_{12}) \bar{A}_{\lambda - \mu}(\tau_{12})(-\lambda^{2} - \mu^{2}) \right],
\]
with phonons of other multipoles leading to the general phonon 
\[
D_{\lambda \mu}^{(v)}(v) = \sum_{\lambda \lambda'} Z_{\lambda \lambda'}^{(v)}[(\lambda_{\lambda}^{(v)}(\tau_{12}) + \lambda_{\lambda}^{(v)}(\tau_{12}))],
\]
In this work we will restrict ourselves to the lowest term with \( \lambda_{0} = 0 \) and \( \lambda = \lambda' \). Thus, we will use the pairing plus multipole-multipole Hamiltonian 
\[
H = H_{p} - H_{0} = H_{p} - \frac{1}{2} \sum_{\lambda} \sum_{\tau \tau'} F_{\tau \tau'}^{(2)} \sqrt{2\lambda + 1} (Q_{\tau \lambda} \otimes Q_{\tau' \lambda})_{0},
\]
and the QRPA equations become decoupled. We further assume that a similar averaged rule (2.2) can also be applied to the commutator of quasiparticle pair operators (2.14). By minimizing the functional 
\[
E_{\lambda}(v) = \frac{\langle \Gamma_{\lambda}(v), H, \Gamma_{\lambda}^{\dagger}(v) \rangle_{C}}{\langle \Gamma_{\lambda}(v), \Gamma_{\lambda}^{\dagger}(v) \rangle_{C}},
\]
where the expectation values include the integration over \( \Omega \), the QRPA amplitudes are given by (the dQRPA) equations of motions which are formally similar to those of the spherical version: 
\[
\begin{pmatrix}
A_{\lambda} & B_{\lambda} \\
-B_{\lambda} & -A_{\lambda}
\end{pmatrix}
\begin{pmatrix}
\lambda_{\lambda}^{(v)} \\
\lambda_{\lambda}^{(v)}
\end{pmatrix}
= E_{\lambda}(v)
\begin{pmatrix}
\lambda_{\lambda}^{(v)} \\
\lambda_{\lambda}^{(v)}
\end{pmatrix}.
\]
The dQRPA matrix elements are given by the following symmetric double commutators: 
\[
A_{\lambda}(\tau_{12} \tau'_{12}) = \langle [\bar{A}_{\lambda \mu}(\tau_{12}), H, \bar{A}_{\lambda \mu}^{\dagger}(\tau'_{12})] \rangle_{C}
\]
\[
= \delta_{\tau_{12} \tau'_{12}} E_{\lambda} + E_{\lambda} E_{\lambda} - F_{\tau \tau'}^{(2)} \xi_{\tau_{12}}^{(v)^{2}}
\]
\[
B_{\lambda}(\tau_{12} \tau'_{12}) = -\langle [\bar{A}_{\lambda \mu}(\tau_{12}), H, \bar{A}_{\lambda - \mu}(\tau'_{12}(-\lambda^{2} - \mu^{2}))] \rangle_{C}
\]
\[
= -F_{\tau \tau'}^{(2)} \xi_{\tau_{12}}^{(v)^{2}}
\]
and they contain quasiparticle energies \( E_{\lambda} \), labeled by the eigenvalue index \( n \), and the factors \( \xi_{\tau}^{(v)^{2}} \) (2.14) featuring the deformed matrix elements. As we will show latter, in spite of the similarity to the spherical QRPA, this formalism is more general. It is able to describe in an unified way low-lying excitations not only in spherical but also in deformed systems.

The strength of an electric transition, connecting the dQRPA eigenstate \( v \) to the ground state, is characterized by the \( B(E\lambda) \) value defined by 
\[
B(E\lambda : v \rightarrow 0) = \frac{1}{2\lambda + 1} |\langle 0 | \bar{T}_{\lambda} | v \rangle|^{2},
\]
with the reduced matrix element 
\[
\langle 0 | \bar{T}_{\lambda} | v \rangle_{C} = \sqrt{2\lambda + 1} \sum_{n_{1} j_{1} \leq n_{2} j_{2}} e_{\tau} \xi_{\tau_{12}}^{(v)^{2}} \lambda_{\lambda}^{(v)}(\tau_{12}) + \lambda_{\lambda}^{(v)}(\tau_{12})],
\]
where \( e_{\tau} \) are the effective charges 
\[
e_{\tau} = e(1 + \chi), \quad e_{v} = \chi,
\]
expressed in terms of the polarization parameter \( \chi \).

**III. NUMERICAL APPLICATION**

We have applied the dQRPA approach to describe the \( B(E2) \) values of decays from the \( 2^{+} \) collective state to the ground state in superfluid vibrational, transitional, and rotational nuclei. Nilsson states in the intrinsic system of coordinates were provided by diagonalizing the axially symmetric quadrupole interaction \( Bm_{n}m_{f}^{2}Y_{20}(\theta') \). As a basis we used the eigenstates of the spherical Woods-Saxon potential with a universal set of parameters [31] plus a Coulomb interaction for protons. The deformation parameters were taken from Ref. [32] and the experimental pairing gaps were estimated by using binding-energy data [32] of neighboring nuclei. The pairing gaps \( G_{r} \), in Eq. (2.10) were automatically determined. The quadrupole-quadrupole coupling strengths \( F_{r r'}^{(2)} \), defined by Eq. (2.17), were considered equal, as in the classical Ref. [29]. The common value was determined from the experimental \( 2^{+} \) energy [33] for each nucleus by using the standard dispersion-relation technique for separable interactions. For the polarization parameter in Eq. (2.23) we adopted the (universal) value \( \chi = 0.2 \).

For the spherical \( sp \) basis we used five orbitals below and five above the Fermi level giving about 50 QRPA pairs, while for the deformed one we used an equivalent space provided by 15 levels below and 15 above the Fermi level, i.e., about 350 pairs in the dQRPA basis. As a test we analyzed the energy-weighted strength function, defined by the product 
\[
EWSF = E(v) B(E2 : v \rightarrow 0),
\]
as a function of the QRPA eigenvalues \( E(v) \). The result for the vibrational nucleus \( ^{130}Te \), given by the standard spherical QRPA code, is plotted in Fig. 1(a). The similar result, but provided by the deformed QRPA code, with the deformation parameter \( \beta = 0 \), is given in Fig. 1(b). One sees that the two results practically coincide, proving the validity of the key ingredient of dQRPA, which is the reduced matrix element in the deformed basis, given by Eq. (2.7). As a reference, we give in Figs. 1(c) and 1(d) the same plots, but for the rotational nucleus \( ^{240}Pu \). Here, the deformation parameter \( \beta = 0.22 \) was used in the dQRPA calculation. As is well visible the results of the spherical QRPA and dQRPA are completely different.

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FIG. 1. Energy-weighted strength function (3.1) for (a) the spherical QRPA and (b) dQRPA in the case of the vibrational nucleus $^{130}\text{Te}$. Similar plots are given in panels (c) and (d) for the rotational nucleus $^{240}\text{Pu}$, by using the deformation parameter of the deformed field from Ref. [32].

Notice that the strength corresponding to the $2^+_1$ state becomes significantly larger.

In order to analyze the differences between the spherical and deformed approaches, we have investigated the E2 decay properties of the $2^+_1$ states in superfluid even-even nuclei for the region $50 < Z \leq 100$. We have divided the data into two sets separated by the magic number $Z = 82$.

In Fig. 2(a) we give by the open symbols the experimental $B(E2)$ values [33] in the region $50 \leq Z \leq 82$ (111 values), while by the filled symbols we indicate the $B(E2)$ values for $82 < Z \leq 100$ (27 values). The correspondence between the charge number of the isotopic chains we analyzed, the associated neutron numbers and the interval of the index values $n$ is given in Table I.

In Fig. 2(b) are plotted the results given by the spherical QRPA code. They reproduce the order of magnitude of the $B(E2)$s in the region $50 \leq Z \leq 82$ (open symbols), containing mostly vibrational and transitional nuclei. The relative mean square error in this region is about 30%. In the region $82 < Z \leq 100$ (filled symbols), where most nuclei have small $2^+_1$ energies and rotational spectra, the computed $B(E2)$ values are by a factor 2 to 3 lower, the mean-square error being about 100%. So, as expected, the spherical QRPA fails in reproducing the $B(E2)$ values for rotational nuclei. On the contrary, in Fig. 2(b) this region is much better reproduced by the dQRPA (filled symbols). Indeed, the mean-square error decreases down to 25%. In order to enable a clear comparison, in Fig. 2(d) we show again the experimental values. The better agreement of the dQRPA results with the data can be explained by the summation over core states $J$ in the reduced matrix element given by Eq. (2.7). Indeed, by considering only the lowest yrast core state the $B(E2)$ results become lower, comparable to the spherical method. Thus, the core states play an important role in describing well deformed nuclei. In Fig. 3(a) we plotted the same data, but versus the quadrupole deformation parameter $\beta$. One notices different slopes for the two mentioned regions. This feature cannot be explained by the spherical QRPA given in Fig. 3(b), but it is nicely reproduced by dQRPA in Fig. 3(c).

Finally, in Fig. 4 we give the quadrupole-quadrupole coupling strength $F_{ττ'}^2$ as a function of the mass number for the spherical case by filled symbols and deformed case by open symbols. The values are close to each other, especially in the region above $Z > 82$. Their bulk features can be approximated by the corresponding power laws, given in Fig. 4. An interesting observation, notice that the strength of the deformed

### Table I

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<th>$Z$</th>
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interaction follows better a quadratic law in the region below the double-magic nucleus $^{208}$Pb.

It is not the purpose of this paper to analyze the higher $2^+_k$ states, predicted by QRPA eigenvalues. Anyway, let us mention that this approach is able to describe their gross features. In order to illustrate this fact, we plotted by open symbols in Fig. 5(a) spherical $2^+_k$ QRPA eigenvalues, corresponding to $k = 2, 3, 4$, for the region $Z > 82$. This region contains mainly well-deformed nuclei. As a comparison, there are given the corresponding available experimental values by filled symbols. One sees that the theoretical values display the same clustering features as the experimental ones ($k = 2, 3, 4$ eigenvalues are close to each other for each isotope), but they are higher, especially for $Z = 88$ and 90 isotopes. On the other hand, the corresponding dQRPA eigenvalues in Fig. 5(b) improve the situation. The electric transitions connecting these states to the ground state are much smaller in comparison to $2^+_1$ states, i.e., between 0.1 and 0.4 W.u. (Weisskopf units) (depending on the excitation energy), thus reproducing the experimental order of magnitude. One has to keep in mind that we used a very simple approach by considering that all $QQ$ strengths in Eq. (2.17) are equal. By using different coupling strengths it is of course possible to improve the agreement of higher $2^+_k$ states with experiment.

IV. CONCLUSIONS

In conclusion, we described the quadrupole collective excitations in even-even nuclei within a common formalism, called the deformed QRPA (dQRPA), by using an $sp$ basis with good angular momentum provided by the Nilsson states rotated into the laboratory frame of coordinates. Thus, the physical collective states are directly determined, without any additional projection procedure. The statistical factors, taking into account the level occupancy in the laboratory system, appear in a natural way within the dQRPA as rotation coefficients of the wave function when taking it from the
intrinsic to the laboratory system. We analyzed E2 transitions from the collective $2^+_1$ state to the ground state for superfluid nuclei in the charge-number range $50 < Z \leq 100$ by using a single value $\chi = 0.2$ for the polarization charge. It turned out that, as expected, the standard spherical QRPA approach fails in describing rotational nuclei with $E_2 < 100$ keV. On the other hand, the dQRPA improves dramatically the description of the E2 transitions for these nuclei. Therefore the assumed adiabaticity seems to be a reasonable assumption in describing low-lying collective states. This relatively simple approach seems to be very promising in analyzing any kind of spin-multipole interaction, including magnetic type of excitations and intraband transitions in deformed nuclei within the multipole-coupled approach given by Eq. (2.16). Further applications of the dQRPA are under way.

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