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Electromagnetic transition strengths in soft deformed nuclei

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Spectroscopic observables such as electromagnetic transitions strengths can be related to the properties of the intrinsic mean-field wave function when the latter are strongly deformed, but the standard rotational formulas break down when the deformation decreases. Nevertheless there is a well-defined, non-zero, spherical limit that can be evaluated in terms of overlaps of mean-field intrinsic deformed wave functions. We examine the transition between the spherical limit and strongly deformed one for a range of nuclei comparing the two limiting formulas with exact projection results. We find a simple criterion for the validity of the rotational formula depending on $\langle \Delta J^2 \rangle$, the mean square fluctuation in the angular momentum of the intrinsic state. We also propose an interpolation formula which describes the transition strengths over the entire range of deformations, reducing to the two simple expressions in the appropriate limits.

I. INTRODUCTION

In mean-field theories, electromagnetic transition rates are often evaluated using the rotational formula [1] to relate them to the multipole moments of the mean-field wave functions. The formula is justified by factorizing the wave function as a product of a wave function for the orientation angles times an intrinsic wave function and assuming that the matrix elements between intrinsic states at different orientations vanish. From a more microscopic point of view, the formula can be obtained as the strong deformation limit of the transition probability computed with angular momentum projected wave functions [2, 3]. There are several studies in the literature investigating the validity of the rotational formula in well deformed nuclei [2, 4, 5]. However, as far as we know there has never been a systematic study of the validity and eventual breakdown of the rotational formula as the wave function approaches the spherical limit. A motivation for this study is the wide-spread use of this formula even outside of its domain of validity. For example, the increasing popularity of the Bohr Hamiltonian [6] as a tool to handle low energy vibrational and rotational properties in a mean-field framework calls for a careful analysis of the limitations of the rotational formula for $B(E2)$ transition strengths [7]. Often near-spherical configurations have a non-negligible amplitude in the wave functions and their contribution to the transition strengths needs to be handled with care. The purpose of this paper is to establish criteria for the use of rotational formulas, as well as to find useful approximations simpler than the full angular momentum projection to deal with moderate and soft deformations.

This paper is organized as follows. Sect. II below discusses the representation of the wave function at small deformations. Our main result, derived in Sect. III, is an expression for the transition strengths valid for small deformations Eq. (19) below. This expression gives a non-zero value in the limit of vanishing deformation, in contrast with the rotational formula, Eq. (3) below. In Sect. IV we examine the validity of the formulas by comparing with full projections from the intrinsic states, taking a number of representative examples including quadrupole and octupole transitions. The dividing line separating the small and large deformation limits is seen to be closely connected to the angular momentum content of the intrinsic wave function. This gives a simple criterion to identify the regions of validity of the rotational formula. We also find that the $B(E2)$ values can be simply parameterized as a function of the quadrupole deformation parameter, Eq. (26) below. Other transition strengths like the $B(E3, 3^- \rightarrow 0^+)$ will be discussed and we will see that similar considerations apply to them as well.

To set the notation, the multipole operators are defined as¹

$$\hat{Q}_{\lambda\mu} = \sqrt{\frac{4\pi}{2\lambda+1}} r^\lambda Y_{\lambda\mu} \quad (1)$$

and the corresponding electric operators as

$$\hat{Q}_{\lambda\mu}^e = e \frac{(1-2\tau_z)}{2} \hat{Q}_{\lambda\mu}. \quad (2)$$

The rotational formula for an axially symmetric intrinsic state is given by

$$B(EJ; J \rightarrow 0)_{\text{ROT}} = \frac{1}{4\pi} |\langle \phi | \hat{Q}_{J0}^e | \phi \rangle|^2. \quad (3)$$

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¹ Note that this differs by a factor of $\sqrt{\frac{2\lambda+1}{4\pi}}$ from the definition in [1].

II. MEAN FIELD WAVE FUNCTIONS NEAR SPHERICITY

The first step is the characterization of the intrinsic wave functions near sphericity. We will focus on quadrupole deformation because the generalization to other multiplicities is straightforward. We assume that the intrinsic wave functions are of the Hartree-Fock-Bogoliubov (HFB) mean-field type. The wave function $|\phi(q)\rangle$ is labeled by the components of the quadrupole moment $q_{2\mu} = \langle \phi | \hat{Q}_{2\mu} | \phi \rangle$ ($\mu = -2, \dots, 2$). The wave function can be expressed in terms of a suitable spherical reference state $|\phi(0)\rangle$ by means of the generalized Thouless theorem

$$|\phi(q)\rangle = \mathcal{N}_q \exp(i\hat{Z}(q))|\phi(0)\rangle. \quad (4)$$

Here $\hat{Z}(q)$ is a sum of 2-quasiparticle creation operators and \mathcal{N}_q is a normalization constant. Given the Bogoliubov amplitudes $U(q)$, $V(q)$ and $U(0)$, $V(0)$ defining $|\phi(q)\rangle$ and $|\phi(0)\rangle$ (see [3] for notation) the explicit form of $\hat{Z}(q)$ can be obtained [3, App. E.3]. However, we only need to assume for the formal development below that \hat{Z} can be expanded as a power series in q ,

$$\begin{aligned} \hat{Z}(q) = & \sum_{\mu} q_{2\mu} (-1)^{\mu} \hat{Z}_{2,-\mu} + \\ & \frac{1}{2} \sum_{\mu, \mu'} q_{2\mu} q_{2\mu'} (-1)^{\mu+\mu'} \hat{Z}'_{2,-\mu, -\mu'} + \dots \end{aligned} \quad (5)$$

The phases are introduced for consistency with the following properties of the deformation parameters $q_{2\mu} = \langle \hat{Q}_{2\mu} \rangle = \langle \hat{Q}_{2\mu} \rangle^* = (-1)^{\mu} \langle \hat{Q}_{2,-\mu} \rangle = (-1)^{\mu} q_{2,-\mu}$. It also implies that $\hat{Z}_{2,\mu}^{(1)+} = (-1)^{\mu} \hat{Z}_{2,-\mu}$ and $\hat{Z}_{2,\mu,\mu'}^{(2)+} = (-1)^{\mu+\mu'} \hat{Z}'_{2,-\mu, -\mu'}$. The tensor character of the multipole operators implies that the deformation parameters of the rotated wave function $|\phi(q'_{2\mu})\rangle = \hat{R}(\Omega)|\phi(q_{2\mu})\rangle$ also behave as the components of a spherical tensor $q'_{2\mu} = \sum_{\mu'} \mathcal{D}_{\mu\mu'}^*(\Omega) q_{2\mu'}$. To be consistent with this property, the operator $\hat{Z}_{2,\mu}$ must transform under rotations as

$$\hat{R} \hat{Z}_{2\mu} \hat{R}^+ = \sum_{\mu'} \mathcal{D}_{\mu\mu'}^2(\Omega) \hat{Z}_{2\mu'}. \quad (6)$$

The corresponding transformation properties of the operators $\hat{Z}'_{2,-\mu, -\mu'}$ are given by

$$\hat{R} \hat{Z}'_{2,\mu, \mu'} \hat{R}^+ = \sum_{\nu\nu'} \mathcal{D}_{\nu\mu}^2(\Omega) \mathcal{D}_{\nu'\mu'}^2(\Omega) \hat{Z}'_{2,\nu, \nu'} \quad (7)$$

This property makes it possible to decompose the operator as the direct sum of spherical tensors

$$\hat{Z}'_{2,\mu, \mu'} = \sum_{JM} \langle 2\mu 2\mu' | JM \rangle \hat{Z}'_{JM} \quad (8)$$

In the present example the range of the spherical tensors \hat{Z}'_{JM} is $J = 0, \dots, 4$. Using the same kind of arguments

it is easy to show that the \hat{Z} and \hat{Z}' operators must be even under parity. The generalization to an arbitrary multiplicity λ is straightforward; we consider the case $\lambda = 3$ in more detail below.

III. TRANSITION STRENGTHS IN THE SPHERICAL LIMIT

Close to the spherical limit, the deformation parameters of the intrinsic wave function are small and we can expand $|\phi(q)\rangle$ to second order in $q_{2\mu}$. The wave function is then projected on good angular momentum using the projection operator

$$\hat{P}_{MK}^J = \frac{2J+1}{8\pi^2} \int d\Omega \mathcal{D}_{MK}^J(\Omega) \hat{R}_{\Omega} \quad (9)$$

and the transformation properties of the Z operators. The ground state $|0^+\rangle$ is obtained by projecting with \hat{P}_{00}^0 . It is given up to second order in $q_{2\mu}$ by

$$|0^+\rangle = \mathcal{N}_0 \left\{ |\phi(0)\rangle + q_2^2 \left([\hat{Z} \otimes \hat{Z}]_0^0 + \frac{1}{2} \hat{Z}_{00}' \right) |\phi(0)\rangle + \dots \right\} \quad (10)$$

Here we have introduced the notation

$$q_2^2 = \frac{1}{\sqrt{5}} \sum_{\mu} q_{2\mu} q_{2-\mu} (-1)^{2-\mu} \quad (11)$$

and

$$[\hat{Z} \otimes \hat{Z}]_M^J = \sum_{\mu, \mu'} \langle 2\mu 2\mu' | JM \rangle \hat{Z}_{2,\mu} \hat{Z}_{2,\mu'} \quad (12)$$

Only the first term in Eq. (10), zeroth order in $q_{2\mu}$, will be required in the derivations below. The projection on $J = 2$ with the operator \hat{P}_{MM}^2 gives the excited $|2^+M\rangle$ state as

$$|2^+M\rangle = \mathcal{N}_{2M} \left\{ (-1)^M q_{2-M} \hat{Z}_{2M} |\phi(0)\rangle + O(q_{2M}^2) \right\} \quad (13)$$

with a normalization factor \mathcal{N}_{2M} given by

$$1 = |\mathcal{N}_{2M}|^2 \left(q_{2-M}^2 \langle \phi(0) | \hat{Z}_{2M}^+ \hat{Z}_{2M} | \phi(0) \rangle + O(q_{2M}^3) \right). \quad (14)$$

Since $|\phi(0)\rangle$ is a spherical wave function, the state $\hat{Z}_{2M} |\phi(0)\rangle$ has angular momentum 2 and the mean value on the right hand side of the above equation is independent of M . It will be written as $\langle ||\hat{Z}_2^+ \hat{Z}_2|| \rangle$ which is a notation reminiscent of the reduced matrix elements of the Wigner-Eckart theorem. With this definition we finally obtain the expression for the normalized excited state wave function

$$|2^+M\rangle = \frac{\hat{Z}_{2M}}{\langle ||\hat{Z}_2^+ \hat{Z}_2|| \rangle^{1/2}} |\phi(0)\rangle + O(q_{2M}) \quad (15)$$

The wave function $|2^+M\rangle$ is well defined in the $q_{2\mu} \rightarrow 0$ limit and is a linear combination of 2-quasiparticle excitations of the spherical state. The expressions in Eqs.

(10) and (15) can be now used in the defining formula for the $B(E2)$ transition strength

$$B(E2, 0^+ \rightarrow 2^+) = \frac{5}{4\pi} \sum_{M\mu} |\langle 2^+ M | \hat{Q}_{2\mu}^e | 0^+ \rangle|^2 \quad (16)$$

where $\hat{Q}_{\lambda\mu}^e$ is the standard electric multipole operator of rank λ . Taking the expressions for the wave functions in the small deformation limit, the matrix element becomes

$$\langle \phi(0) | (\hat{Z}_{2M})^+ \hat{Q}_{2\mu}^e | \phi(0) \rangle = \delta_{\mu M} \langle ||\hat{Z}_2^+ \hat{Q}_2^e|| \rangle \quad (17)$$

The final expression for the $B(E2)$ is

$$B(E2, 0^+ \rightarrow 2^+)_{\text{Sph}} = 5 \frac{5}{4\pi} \frac{|\langle ||\hat{Z}_2^+ \hat{Q}_2^e|| \rangle|^2}{\langle ||\hat{Z}_2^+ \hat{Z}_2|| \rangle} \quad (18)$$

The generalization to arbitrary multipolarity λ is

$$B(E\lambda, 0^+ \rightarrow \lambda^{\pi\lambda})_{\text{Sph}} = (2\lambda + 1) \frac{2\lambda + 1}{4\pi} \frac{|\langle ||\hat{Z}_\lambda^+ \hat{Q}_\lambda^e|| \rangle|^2}{\langle ||\hat{Z}_\lambda^+ \hat{Z}_\lambda|| \rangle}. \quad (19)$$

In contrast to the rotational formula, Eq. (18) is nonzero in the spherical limit. This is a clear indication of the inadequacy of the rotational formula for the evaluation of transition strengths near sphericity.

The quantities entering Eqs. (18) and (19) can be calculated in linear response theory, but it is rather easy to calculate them using the intrinsic states of the HFB theory. The only additional computational capability needed is the evaluation of matrix elements between different intrinsic states. In particular, we make use of the matrix element of quadrupole operator between deformed and spherical states given by

$$\langle \phi(q_{2\mu}) | \hat{Q}_{2\nu}^e | \phi(0) \rangle = -iq_{2\nu} \langle ||\hat{Z}_2^+ \hat{Q}_2^e|| \rangle + O(q_{2\nu}^2). \quad (20)$$

To get the normalization in Eq. (18), we make use of the derivatives of the overlap function. The second derivative of the overlap between two intrinsic wave functions satisfies

$$\gamma = \frac{\partial^2}{\partial q_{2\nu} \partial q'_{2\nu}} \langle \phi(q_{2\nu}) | \phi(q'_{2\nu}) \rangle_{q_2 q'_2 \rightarrow 0} = \langle ||\hat{Z}_2^+ \hat{Z}_2|| \rangle \delta_{\nu\nu'}. \quad (21)$$

The second derivative can be approximated by a finite difference formula in the limit $q_{2\nu} \rightarrow 0$

$$\gamma = \lim_{q_{2\nu} \rightarrow 0} \frac{(\langle \phi(q_{2\nu}) | - \langle \phi(-q_{2\nu}) |) (\langle \phi(q_{2\nu}) \rangle - \langle \phi(-q_{2\nu}) \rangle)}{4q_{2\nu}^2}. \quad (22)$$

Using this result and Eq. (20) we obtain the following result for the $B(E2)$ in the spherical limit,

$$B(E2, 0^+ \rightarrow 2^+)_{\text{Sph}} = 5 \frac{5}{4\pi} \lim_{q_{2\nu} \rightarrow 0} \frac{|\langle \phi(q_{2\mu}) | \hat{Q}_{2\nu}^e | \phi(0) \rangle|^2}{\frac{1}{4} (2 - \langle \phi(q_{2\nu}) | \phi(-q_{2\nu}) \rangle - \langle \phi(-q_{2\nu}) | \phi(q_{2\nu}) \rangle)}. \quad (23)$$

It is worth remarking that this derivation is valid for any value of ν and therefore the axial case corresponding to $\nu = 0$ can be used as well. This formula could be easily implemented in Wood-Saxon codes to obtain a quick estimate of the spherical transition strength.

If this reasoning is applied to the octupole case, the $|3^- M\rangle$ wave function is given by the expression

$$|3^- M\rangle = \frac{\hat{Z}_{3M}}{\langle ||\hat{Z}_3^+ \hat{Z}_3|| \rangle^{1/2}} |\phi(0)\rangle + O(q_{3M}). \quad (24)$$

This coincides with the negative parity projected wave function $|\Psi_-(q_{3\mu})\rangle = \mathcal{N}_-(1 - \hat{\Pi})|\phi(q_{3\mu})\rangle$ up to order $q_{3\mu}$. On the other hand, the $|0^+\rangle$ wave function is given by the positive parity projected wave function $|\Psi_+(q_{3\mu})\rangle = \mathcal{N}_+(1 + \hat{\Pi})|\phi(q_{3\mu})\rangle = |\phi(0)\rangle + O(q_{3\mu}^2)$. Taking into account these quantities in the general definition of Eq. (19) we arrive at the formula

$$B(E3, 0^+ \rightarrow 3^-)_{\text{Sph}} \approx 7 \frac{7}{4\pi} |\langle \Psi_-(q_{30}) | \hat{Q}_{30}^e | \Psi_+(0) \rangle|^2 \quad (25)$$

Use of this formula of course requires that the q_{30} in the negative parity wave function is small enough so that this wave function is well approximated by Eq. (24). We used this formula recently in a global study of octupole correlations [8] to understand some discrepancies observed in the comparison with experimental data.

We finish this section by mentioning that the previous methodology can also be used with scalar operators like the Hamiltonian. It is possible to obtain in this way formulas for the energies of $J \neq 0$ states in the spherical limit. This is briefly discussed in the appendix.

IV. COMPARISON WITH EXACT PROJECTED TRANSITION STRENGTHS

A. Validity of rotational formula

In this section we compare the transition strengths computed with exact angular momentum projection with the rotational formula and our spherical limit. The mean-field wave functions were calculated in the Hartree-Fock-Bogoliubov approximation assuming axial symmetry and obtaining a range of deformations by including an external quadrupole field in the Hamiltonian. The range of deformations β_2 spans the interval -0.3 to 0.4 in steps of 0.02 and a finer mesh with a step size of 0.01 is used in the -0.1 to 0.1 interval². For those intrinsic wave functions the $B(E2, 2^+ \rightarrow 0)$ transition strength has been computed with the rotational formula and exact angular

² We use the standard practical definition of β_2 , related to the mass quadrupole moment Q_2 by $Q_2 = \sqrt{\frac{4\pi}{5}} \frac{3}{4\pi} AR_0^2 \beta_2$ with $R_0 = 1.2A^{1/3}$ fm.

momentum projection with $|\phi(\beta_2)\rangle$ as the intrinsic states (see [9] for the relevant formulas). In Fig. 1 the ratio $B(E2)_{\text{ROT}}/B(E2)_{\text{PROJ}}$ is plotted as a function of β_2 for a sample of nuclei spanning a wide range of masses. As expected, the ratio increases toward one as β_2 becomes large. However, the limit is only reached in medium and heavy nuclei within our range of β_2 values. For small values of β_2 the ratio is smaller than one and approaches zero as $\beta_2 \rightarrow 0$. One can see that the β_2 value by itself does not provide a good indicator of the region of validity of the rotational formula. To get a more robust criterion, we go back to the basic assumption in deriving the rotational formula, that the intrinsic states have vanishing overlaps under finite rotations of the orientations. This requires a large angular momentum content of the intrinsic states. The mean square angular momentum of the intrinsic state $\langle \Delta \vec{J}^2 \rangle$ can be easily computed from the HFB wave function, so we may consider that quantity as a practical indicator. We note that overlap between rotated wave functions approaches a Gaussian of width $1/\langle \Delta \vec{J}^2 \rangle$ [3]. This result suggests that the validity of the rotational formula could be linked to specific values of $\langle \Delta \vec{J}^2 \rangle$. To explore this possibility we have determined the value of $\langle \Delta \vec{J}^2 \rangle$ for the intrinsic configuration that satisfies $B(E2)_{\text{PROJ}}/B(E2)_{\text{ROT}} \approx 3/4$ (a value we have chosen to establish the limits of validity of the rotational formula) in each of the nuclei of our calculation. The values are shown as a histogram in Fig. 2. We see that the values are strongly peaked around $\langle \Delta \vec{J}^2 \rangle \approx 10\hbar^2$. This remarkable fact gives us an easily computed estimator of the validity of the rotational formula for the $B(E2)$ transition strength for any nucleus in the Chart of Nuclides.

B. Selected isotope and isotone chains

The behavior of the spherical $B(E2)$ transition strengths as a function of proton and neutron numbers is analyzed next. In panel (a) of Fig. 3 the spherical transition strengths of Eq. (18) are plotted as a function of neutron number for several isotopic chains. They have been computed using the exact angular momentum projected transition strengths for a deformation of the intrinsic state of $\beta_2 = 0.005$. The values of those spherical transition strengths are smaller than the typical values of well deformed nuclei that can reach a few hundreds of W.u. for heavy nuclei. The decrease with neutron number is rather weak except around magic neutron numbers where a marked peak is observed. This is probably a consequence of the lowering of the level density near magic numbers. Surprisingly, a peak at the non-magic number $N = 40$ is also seen. This behavior is not observed when the quantity is plotted as a function of proton number (see panel (b)). First the spherical transition strength increases with increasing Z values and a reduction at those values of Z corresponding to magic numbers is observed, specially at $Z=82$. The values of $B(E2)_{\text{Sph}}$ expressed in

W.u. follow a trend with Z that is consistent with the expected linear behavior in Z based on the scaling of the mean value of proton's quadrupole moment (remember that W.u. scale like nuclear radius squared). A least square fit to the computed values for over two hundred nuclei yields the rule $B(E2, 2 \rightarrow 0)_{\text{Sph}} = 0.85 Z$ (W.u.).

C. An interpolating formula

Even better than a criterion for the validity of Eq. (3) would be an interpolating formula that would also capture the transition region between spherical and strongly deformed nuclei. To this end we consider parameterizing the $B(E2)$ by the function

$$B(E2, 2^+ \rightarrow 0)_{\text{Int}} = \frac{C_0}{1 - \exp[-(\beta_2/\beta_2^{(0)})^2]} \beta_2^2 \quad (26)$$

The parameter C_0 is set to $C_0 = (9e^2)/(80\pi^2)Z^2R_0^4$ to recover the rotational formula at large deformation. The parameter $\beta_2^{(0)}$ is set to a value that reproduces the spherical limit,

$$\beta_2^{(0)2} = \frac{1}{C_0} B(E2, 2^+ \rightarrow 0^+)_{\text{Sph}}. \quad (27)$$

The results obtained with Eq. (26) are plotted as dashed lines in Fig. 1. Remarkably, for most of the cases and for almost the whole range of β_2 values both the exact and the approximate results are indistinguishable. It seems that our model can be used with confidence to compute $B(E2)$ values provided that the parameter $\beta_2^{(0)}$ can be obtained.

D. Computing the spherical limit

An alternative formula for the evaluation of $B(E2)_{\text{Sph}}$ was obtained in Eq. (23) in terms of simple overlaps with the wave functions $|\phi(q_{2\nu})\rangle$. To test its applicability we have performed calculations with our axially symmetric wave functions as a function of β_2 and some representative results are given and compared to the exact results in Fig. 4. From the comparison we conclude that the formula is accurate enough for β_2 values up to 0.05 for light nuclei and up to 0.01 for heavy ones and therefore can be used for a computationally inexpensive estimation of $B(E2)_{\text{Sph}}$ to be used in the model of Eq. (26) to compute the $\beta_2^{(0)}$ parameter as $\beta_2^{(0)} = (B(E2)_{\text{Sph}}/C_0)^{1/2}$.

E. Octupole transitions

Another interesting case to study is the one of the $B(E3, 3^- \rightarrow 0)$ transition strengths. They are associated to the octupole degree of freedom, parameterized in

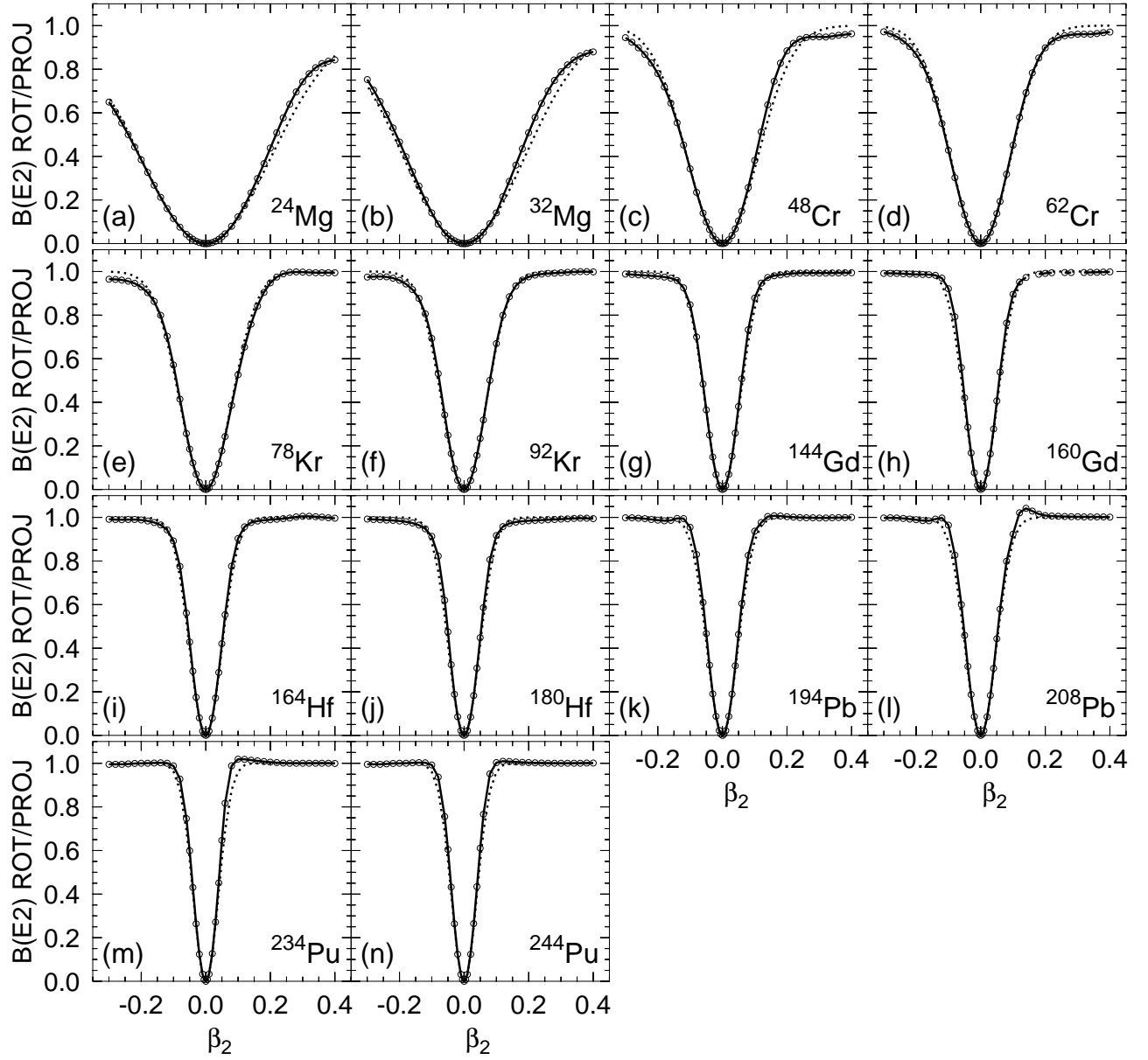


Figure 1: The ratio $B(E2)_{\text{ROT}}/B(E2)_{\text{PROJ}}$ is plotted as a function of the deformation parameter β_2 for a range of nuclei. The solid line connects calculated values. The dashed line is calculated from the interpolating formula, Eq. (26) and (27).

terms of the octupole moments $q_{3\mu}$. The rotational formula, valid in the strong quadrupole deformation limit, reads in this case $B(E3, 3^- \rightarrow 0) = \frac{1}{4\pi} |\langle Q_3^e \rangle|^2$. Contrary to the quadrupole deformation case, there is no spontaneous parity symmetry breaking in most of the nuclei of the Nuclide chart with the exception of a few light Ra and Th isotopes and some rare earth nuclei like neutron poor Ba isotopes. Therefore the mean value of the octupole operator in the intrinsic state is zero. As a consequence, theories dealing with dynamical correlations are required in order to describe octupole correlations and the associated $B(E3)$. In those theories the intrinsic octupole deformed state for the 0^+ is different from the one of the 3^- . A typical example is that of

parity projection with restricted variation of the intrinsic state [8], that assigns the intrinsic states of the 0^+ and 3^- states to the ones producing the lowest parity projected energies $E_{\pm}(q_3)$ computed for axially symmetric octupole constrained intrinsic states with octupole deformation q_{30} . In this theory, the rotational formula restricted to axially symmetric configurations becomes $B(E3, 3^- \rightarrow 0^+)_{\text{ROT}} = \frac{1}{4\pi} |\langle \Psi_-(q_{30}^{(-)}) | \hat{Q}_{30}^e | \Psi_+(q_{30}^{(+)}) \rangle|^2$ where now $|\Psi_{\pm}(q_{30})\rangle$ are parity projected wave functions obtained from an intrinsic state with octupole deformation q_{30} . In order to study the validity of this formula in the spherical limit, calculations as a function of the quadrupole moment should be carried out. The difficulty

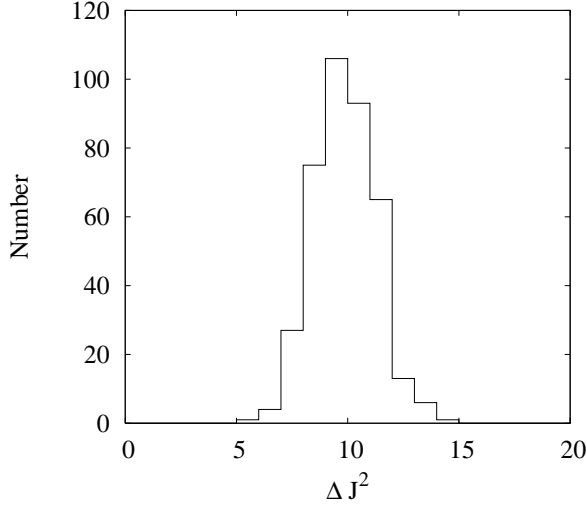


Figure 2: Lowest $\langle \Delta J^2 \rangle$ values of intrinsic wave functions that meet our criterion for using the rotational formula (see text).

here is that there are two intrinsic states that potentially have different quadrupole deformations and therefore a study in terms of four variables (the quadrupole and octupole moment of the positive and negative parity intrinsic states) should be carried out for a series of isotopes. Instead of this long calculation we have just taken the intrinsic states for positive and negative parity from the results of [8] and computed the corresponding transition strengths with angular momentum projected wave functions. The ratio $B(E3, 3^- \rightarrow 0^+)_{\text{PROJ}}/B(E3, 3^- \rightarrow 0^+)_{\text{ROT}}$ is plotted in Fig. 5 as a function of the $\beta_2(+)$ deformation parameter of the positive parity intrinsic state. Values corresponding to nuclei where the negative parity quadrupole deformation parameter $\beta_2(-)$ differs significantly from $\beta_2(+)$ (by ± 0.1) have not been included in the plot. This includes nuclei with strong shape coexistence where the ground state is, for instance, prolate and the negative parity state is oblate. As a consequence of the mismatch in quadrupole deformations the overlap between the wave functions is very small and the corresponding $B(E3)$ are much smaller (and therefore more dependent on little details) than for intrinsic states with similar quadrupole deformation parameters.

The first noteworthy observation is that the transition strengths computed with the projected angular momentum wave functions are always greater or equal the values obtained with the rotational formula. The results show that for $\beta_2(+)$ values greater than 0.15 the rotational formula works reasonably well within a factor of 2. Around $\beta_2(+)=0$ the ratio lies in between 3 and 8 in good agreement with the results of Eq. (25) that predict a factor 7 difference with the rotational formula in the spherical limit. The main conclusion is that for quadrupole deformations smaller than $\beta_2 \approx 0.15$ the rotational formula should not be trusted and its use avoided in relating tran-

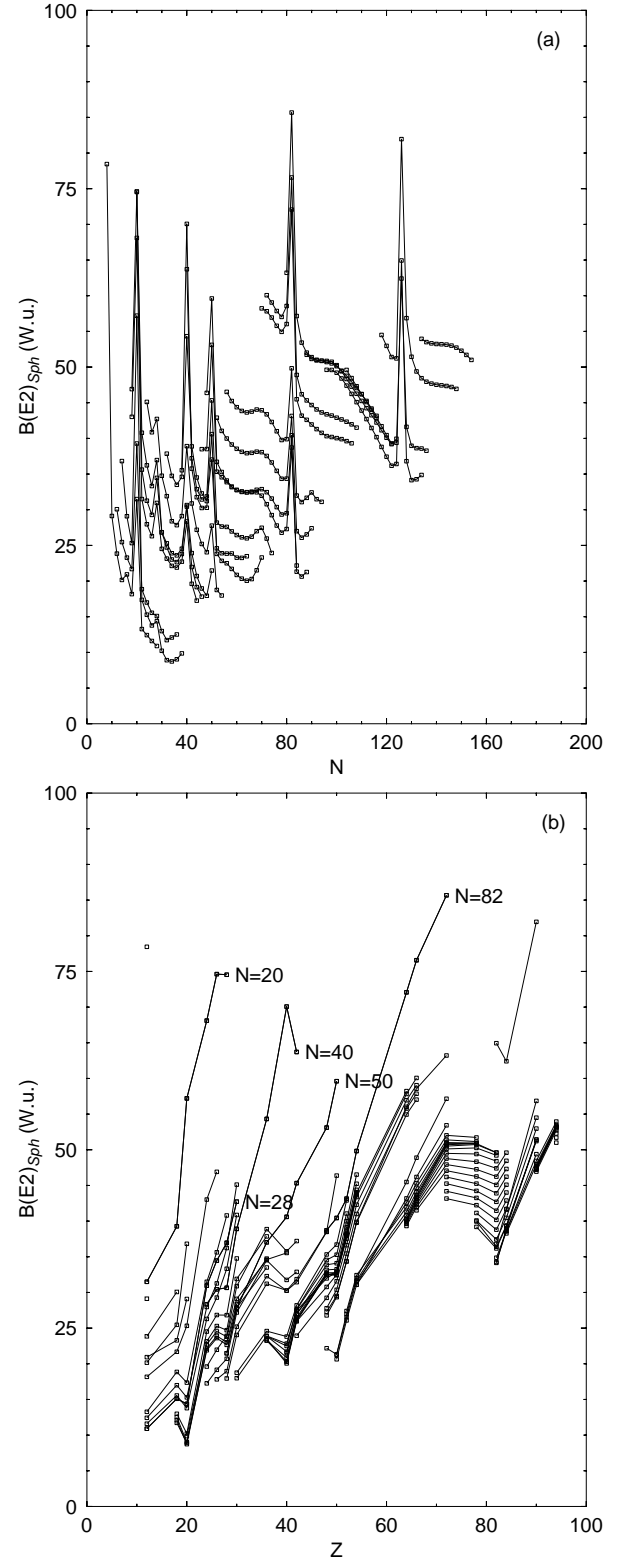


Figure 3: The spherical-limit transition strengths of Eq. (18) are displayed for several isotopic chains as a function of neutron number N in panel (a) and as a function of Z in panel (b). The isotopic chains correspond to Z values between 12 and 94 in steps of 6 units. Strengths are given in Weisskopf units, $1 \text{ W.u.} = 5.94 \times 10^{-6} A^{4/3} e^2 b^2$.

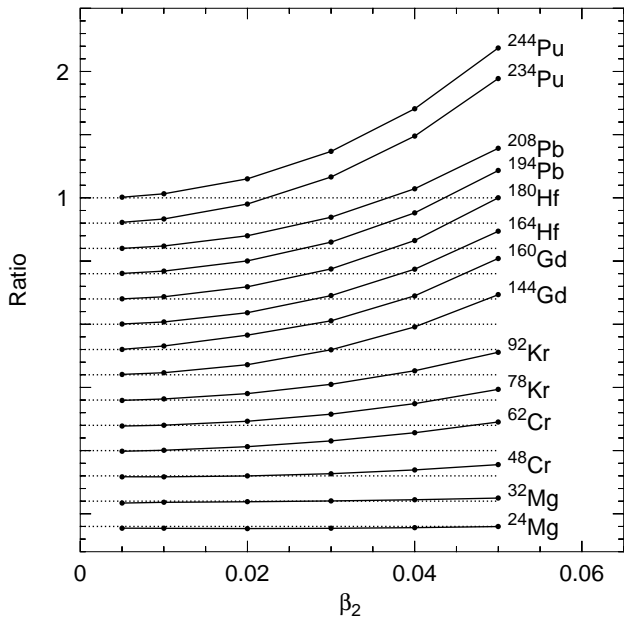


Figure 4: Accuracy of Eq. (23) to calculate $B(E2)$ values in the spherical limit. Plotted is the ratio of the $B(E2)$ from Eq. (23) to the value obtained by a full projection of the wave functions at $\beta_2 = 0.005$. The horizontal scale gives the β_2 values used in Eq. (23). The ratios are offset for clarity, with the dotted lines indicating equal values.

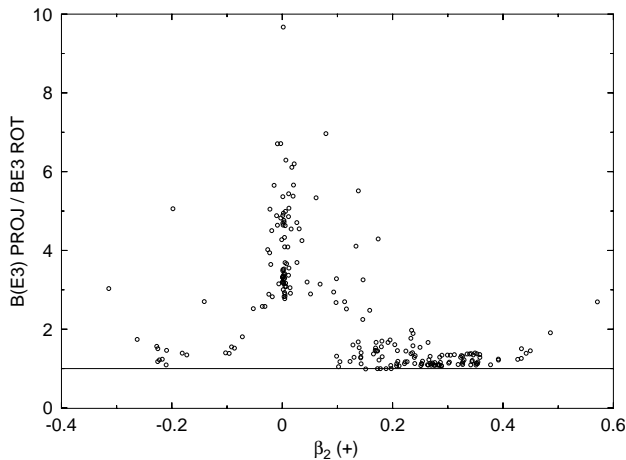


Figure 5: The ratio $B(E3, 3^- \rightarrow 0^+)_{\text{PROJ}}/B(E3, 3^- \rightarrow 0^+)_{\text{ROT}}$ is plotted as a function of the $\beta_2(+)$ quadrupole deformation parameter of the positive parity intrinsic state.

sition strengths to intrinsic octupole deformation parameters. A typical example illustrating the general trend is that of ^{208}Pb where the rotational formula predicts a $B(E3)$ value of 7.1 W.u. whereas the transition strength with the angular momentum projected wave functions is 23.1 W.u. which is in much better agreement with the experimental value of 34 W.u.. Such enhancement of the $B(E3)$ transition probabilities for near spherical configurations as compared to the rotational formula was already noticed in [10, 11] for some spherical or near spherical nu-

clei.

V. CONCLUSIONS

The validity of the rotational formula for multipole transition strengths is questioned for near spherical configurations. A general formula to compute those transitions in terms of intrinsic mean values and/or overlaps is derived by exploiting the simple structure of angular momentum projected wave functions in the spherical limit. An enhancement factor of $2\lambda + 1$ for transitions of order λ is obtained. Thorough numerical calculations of $B(E2)$ and $B(E3)$ transition strengths show the validity of the formulas obtained and establish criteria of validity for the rotational approximation. For quadrupole transitions, we proposed a simple model to compute the $B(E2)$ and found that it is quite accurate over the entire range of deformation. The model contains two parameters that are fixed from the calculated transition strengths at the two limits, Eqs. (3) and (18). We have also established a criteria to determine the validity of the rotational formula that only requires the evaluation of a mean field quantity: the fluctuation $\langle \Delta \bar{J}^2 \rangle$ should be larger than ~ 10 for the rotational formula to be useful; it becomes quite accurate above $\langle \Delta \bar{J}^2 \rangle > 15$. For octupole transition strengths $B(E3)$, the quadrupole deformation parameter β_2 of the ground state has to be larger than 0.15 for the rotational formula to be valid and precautions are in order for those cases of shape coexistence where the quadrupole deformation parameters of positive and negative parity states differ considerably. For spherical configurations the $B(E3)$ can be up to a factor of 8 larger than the values provided by the rotational formula.

A table is provided, as supplementary material, with the spherical $B(E2)$ strengths and the $\beta_2^{(0)}$ parameters for 818 even-even nuclei computed with the Gogny D1S interaction [12].

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Appendix A: Projected energies in the spherical limit

The same arguments used in the previous section can be used to compute the energy of the $|2^+ M\rangle$ as given by

Eq. (15) in the spherical limit

$$E(2^+)_{\text{Sph}} = \frac{\langle ||\hat{Z}_2^+ \hat{H} \hat{Z}_2|| \rangle}{\langle ||\hat{Z}_2^+ \hat{Z}_2|| \rangle} + O(q_{2\mu}^2). \quad (\text{A1})$$

Defining

$$\begin{aligned} h_{qq'} &= \frac{\partial^2}{\partial q_{2\nu} \partial q'_{2\nu'}} \langle \phi(q_{2\mu}) | \hat{H} | \phi(q'_{2\mu'}) \rangle_{|q_2 q'_2 \rightarrow 0} \quad (\text{A2}) \\ &= \langle ||\hat{Z}_2^+ \hat{H} \hat{Z}_2|| \rangle \delta_{\nu\nu'} \end{aligned}$$

as using Eq. (21) the excitation energy can be written as

$$E(2^+)_{\text{Sph}} = \frac{h_{qq'}}{\gamma} \quad (\text{A3})$$

an expression that coincides with twice the zero point energy correction obtained in the Generator Coordinate Method (GCM) for the quadrupole coordinate in the harmonic limit of the Gaussian Overlap Approximation (GOA) (See Eq. (10.136) of [3]). The energy of the 2^+ state in the spherical limit is not given in calculations with angular momentum projection as its evaluation involves the ratio of two very small quantities which are difficult to compute with the required accuracy [9].

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 - [12] See Supplemental Material at [URL will be inserted by published] for a table of the spherical $B(E2)$ strengths and the $\beta_2^{(0)}$ parameters for 818 even-even nuclei computed with the Gogny D1S interaction.