Octupole-induced dipole moments of very deformed nuclei

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In order to estimate octupole-induced $E1$ strength in very deformed nuclei we calculate their intrinsic dipole moments within the shell correction method. We use the formula for the macroscopic part of the dipole moment derived by Dorso, Myers, and Swiatecki, however, without approximation limiting its validity to small deformations. We obtain rather large dipole moments in superdeformed Hg and Pb nuclei, in agreement with recent Hartree-Fock calculations. This points to the possibility that in these nuclei interband $E1$ transitions may be detectable in spite of enormous competition of superdeformed intraband $E2$ transitions. We give also estimates for dipole moments of even more deformed systems.

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I. INTRODUCTION

As is well known, the collective $E1$ transitions observed in some nuclei may result from dipole moments induced by the octupole or a more general reflection-asymmetric deformation. It has been suggested that octupole correlations are important in superdeformed (SD) nuclei, see, e.g., [1–7]. Such correlations, when sufficiently strong, could lead to a presence of low or moderately excited SD bands of parity opposite to that of the SD "ground state" (g.s.) band. This, in turn, opens a possibility that substantially enhanced $E1$ transitions between two opposite parity SD bands can be detected with new multidetector systems. The purpose of the present paper is to give an estimate of the octupole-induced $E1$ strength at superdeformed, and even at more deformed nuclear shapes.

In even-even nuclei, octupole correlations lead to a presence of a negative parity intrinsic excitation $\mid \pi-\rangle$ built of the local g.s. of positive parity, $\mid \pi+\rangle$. With the increasing correlation strength, $\mid \pi-\rangle$ changes its character from this of the octupole phonon built on the reflection symmetric shape to that of the negative parity combination of deformed intrinsic states, $\mid +\rangle$ and $\mid -\rangle$, corresponding to energy minima at $+\beta_3$ and $-\beta_3$.

Assuming axial symmetry of the local g.s. and following closely the rigid rotor model of [8] we have a formula for the $E1$ strength between two rotational bands built on $\mid \pi+\rangle$ and $\mid \pi-\rangle$:

$$B(E1; I_i, K_i \to I_f, K_f) = \frac{3}{4\pi} \mid \langle \pi- \mid \hat{D}_{K_f-K_i} \mid \pi+\rangle \mid^2 \times \langle I_i K_i 1 K_f - K_i \mid I_f K_f\rangle^2, \quad (1)$$

where $D_{K_f-K_i}$ is a spherical component of the nuclear dipole moment operator, $\mathbf{D} = e(\frac{N}{A}\sum_p \mathbf{r}_p - \frac{Z}{A}\sum_n \mathbf{r}_n)$. For simplicity, the signature-dependent term for $K_i = K_f = 1/2$ and the additional factor 2 for $K_f = 1, K_i = 0$ have been omitted. We will be interested in axial octupole correlations in even-even nuclei and therefore specialize to $K_i = K_f = 0$. We notice that one obtains from Eq. (1) the familiar formula for $E1$ transitions within the alternating parity $K = 0$ band using $\mid \pi\pm\rangle = \frac{1}{\sqrt{2}}(\mid +\rangle \pm \mid -\rangle)$, and $\langle + \mid -\rangle = \langle + \mid \hat{D}_0 \mid -\rangle = 0$, resulting in $\langle \pi- \mid \hat{D}_0 \mid \pi+\rangle = \langle + \mid \hat{D}_0 \mid +\rangle = -\langle - \mid \hat{D}_0 \mid -\rangle = D_0$. Thus, in an idealized case of noninteracting states $\mid \pm\rangle$ and degenerate states $\mid \pi\pm\rangle$, $E1$ transitions within the alternating parity rotational band are determined by the intrinsic dipole moment D_0.

In realistic cases, when the barrier between two degenerate intrinsic minima $\mid \pm\rangle$ is not very high or there is no reflection asymmetric minimum at all ($\mid \pi-\rangle$ is an octupole excitation) the magnitude of $E1$ rates between bands built on $\mid \pi\pm\rangle$ is determined by the transition dipole moment, $D_0^t = \langle \pi- \mid \hat{D}_0 \mid \pi+\rangle$, depending on two intrinsic states. One can expect that it is equal to D_0 of some octupole deformed state with deformation β_3 smaller than the mean deformation $\bar{\beta}_3$ of the state $\mid \pi-\rangle$, the latter being always nonzero. Therefore, knowing $D_0(\beta_3)$ and having some idea about deformation $\bar{\beta}_3$ one can estimate $E1$ rates also in the vibrational limit.

To evaluate dipole moments one can use a microscopic approach, like the Hartree-Fock method [9,10,7], or a more phenomenological shell-correction approach, introduced in Ref. [11]. In the latter, the dipole moment is decomposed into a macroscopic part, D_0^{macr}, smoothly varying with N and Z, and a fluctuating shell-correction term D_0^{shell}:

$$D_0 = D_0^{\text{macr}} + D_0^{\text{shell}}. \quad (2)$$

The shell-correction term is calculated as $D_0^{\text{shell}} = \langle \hat{D}_0\rangle - \langle \tilde{\hat{D}}_0\rangle$, where $\langle \hat{D}_0\rangle$ is the expectation value of the operator $e(\frac{N}{A}\sum_p \hat{z}_p - \frac{Z}{A}\sum_n \hat{z}_n)$ on the g.s. wave function constructed using a phenomenological single-particle potential and including pairing correlations at the BCS level, and $\langle \tilde{\hat{D}}_0\rangle$ is the same quantity smoothed according to the Strutinsky prescription. This smoothing reduces to the replacement of the BCS occupation numbers $n_i = 2v_i^2$ in $\langle \hat{z}\rangle = \sum_i 2v_i^2\langle i \mid \hat{z} \mid i\rangle$ by smoothed occupation numbers $\tilde{n}_i$ [11]. One has also to take into account the reduction of the effective charge due to the particle-vibration coupling with the $E1$ giant resonance, $e^{\rm eff} = e(1+\chi)$, where the polarizability coefficient χ has been estimated to fall within the range $-0.72 < \chi < -0.59$ [11,8,12].

Concerning macroscopic contribution, a formula for the dipole moment is necessary. Such a formula has been derived by Dorso, Myers, and Swiatecki [13] from the droplet model [14]. Since it was meant to apply primarily to weakly or moderately deformed nuclei, it has been worked out in a form valid up to the second order in deformation parameters describing distortions of a sphere. The comparison between dipole moments calculated with the aid of this formula within the shell correction scheme and the experimental data in light Ra-Th and heavy Xe-Ba regions is contained in Ref. [15].

It is rather obvious that calculating dipole moments of very deformed nuclei one has to reject the confinement to the lowest order in deformations in the formula [13]. The calculation of $D^{\rm shell}$ at the SD local minimum is analogous to that at normal deformation. There is a number of corrections which come from rotation and, in principle, should be considered. We will neglect some, like a modification of $D^{\rm macr}$ caused by rotation, assuming it is small, and comment on others, like a change of the polarizability coefficient χ or a dependence of $D^{\rm shell}$ on the rotational frequency, in Sec. IV.

The plan of the paper is as follows: In the next section, we recall the formula for the macroscopic dipole moment [13], then, in Sec. III, discuss modifications introduced by the exact calculation with respect to the second-order approximation used up to now. In Sec. IV we present results for SD nuclei and in Sec. V, for more deformed systems. In Sec. VI we give conclusions and some technical aspects of our calculations are mentioned in the Appendix.

II. MACROSCOPIC DIPOLE MOMENTS

The macroscopic dipole moment induced by a reflection asymmetric deformation consists of two parts [13] arising from the charge redistribution and neutron skin effects, respectively:

$$\mathbf{D} = \mathbf{D}_{\rm red} + \mathbf{D}_{\rm skin}. \qquad (3)$$

For a nucleus with Z protons and N neutrons, $A = N + Z, I = (N-Z)/A$, one obtains from the droplet model the following expressions for both components [13]:

$$\mathbf{D}_{\rm red} = \frac{AZe^2}{8}\left(\frac{1}{J} + \frac{6LI}{KJ}\right)(\langle v\rangle_V \langle \boldsymbol{\zeta}\rangle_V - \langle v\boldsymbol{\zeta}\rangle_V), \qquad (4)$$

$$\mathbf{D}_{\rm skin} = \frac{2NZ}{A}(I-\bar{\delta})R_0(\langle \boldsymbol{\zeta}\rangle_V - \langle \boldsymbol{\zeta}\rangle_S) + \frac{9}{32}\frac{ZA^{2/3}e^2}{Q}B_S(\langle v\rangle_S\langle \boldsymbol{\zeta}\rangle_S - \langle v\boldsymbol{\zeta}\rangle_S). \qquad (5)$$

In these formulas, J, K, Q, and L are the following droplet model parameters: the volume symmetry-energy coefficient, the nuclear matter compressibility, the effective neutron skin stiffness, and the density symmetry coefficient, respectively. The other DM parameters are the nuclear radius, $R_0 = r_0 A^{1/3}$, where $r_0 = 1.16$ fm, and the equilibrium value of the average relative neutron excess, $\bar{\delta} = [I + (9e^2/80r_0Q)ZA^{-2/3}]/[1+(9J/4Q)A^{-1/3}]$, related to the average value of the neutron-skin thickness $\bar{t}$ via the expression $\bar{t} = (2/3)(I-\bar{\delta})R_0$. Nuclear shape enters the formulas (4) and (5) through its integral properties: the B_S constant, being the ratio of the nuclear surface area to that of the sphere of the same volume, and the volume and surface integrals of the Coulomb potential v (in units of Ze/R_0), and of the scaled radius vector $\zeta = \mathbf{r}/R_0$. These integrals are taken over the nuclear surface and the volume enclosed by it and are defined as follows: $\langle f\rangle_V = \frac{1}{V}\int_V f$ and $\langle f\rangle_S = \frac{1}{S}\int_S f$.

The part of the dipole moment coming from the neutron skin may be also expressed as [13]

$$\mathbf{D}_{\rm skin} = (NZ/A)(\Delta/V)(\mathbf{r}_A - \mathbf{r}_t), \qquad (6)$$

where $\mathbf{r}_A$ and $\mathbf{r}_t$ are the centers of mass of the whole nucleus and the neutron-skin layer, respectively, and Δ is the neutron-skin layer volume. It turns out that this expression, and more precisely, its first component in Eq. (5), has a sign opposite to that of the $\mathbf{D}_{\rm red}$, thus reducing the total macroscopic dipole moment. This has been found necessary to reproduce experimental data within the shell-correction method simultaneously in Ra-Th and Xe-Ba regions [15]. One can mention that the formulas (4) and (5), and the presence of the negative contribution in particular, have been questioned in [16], and recently in [17]. Since we think that the main points of this criticism are not well founded (see [18]), we rely in what follows on the formulas (4) and (5).

In the present paper we parametrize the nuclear surface by means of spherical harmonics and deformation parameters $\beta_{\lambda\mu}$:

$$R(\theta,\phi) = R_0 c(\beta)\left(1 + \sum_{\lambda\mu}\beta_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi)\right). \qquad (7)$$

The radius vector in Eqs. (4) and (5) is attached to the origin of coordinates in which the nuclear surface is defined.

III. RELATION BETWEEN THE EXACT AND THE SECOND-ORDER FORMULA

Up to now, macroscopic dipole moments have been calculated using the second-order formula of [13]. To assess the correctness of the latter we have first recalculated dipole moments in Ra-Th and Xe-Ba regions using the full expression of Eqs. (4) and (5). Deformations of g.s. octupole minima and the whole microscopic part of our calculations is in fact identical with [15] since we are using the same deformed Woods-Saxon single particle model. Consequently, we have the same pairing strengths, averaging procedure, and the polarizability coefficient, $\chi = -0.66$. Numerical details of calculations of

$D^{\rm macr}$ are given in the Appendix. The DM parameters are J=32.5 MeV, K=240 MeV, Q=50 MeV, and L=100 MeV, as in [15].

Since $D^{\rm macr}$, containing the whole difference between our results and those of [15], varies smoothly with Z and N, and in each of the two regions equilibrium deformations are similar, the overall change in D can be easily summarized giving its average increase. In the heavy Ba region, where $D^{\rm macr}$ are small, they increase roughly by 0.02 e fm, hence the use of the exact formula has rather insignificant effect. In Ra and Th nuclei, $D^{\rm macr}$ increases by 0.08–0.11 e fm, which improves agreement with experimental data for N = 132–134 but ruins the agreement with experimentally observed cancellation of D in ^{224}Ra.

In order to show modifications resulting from the exact formula in more detail we compare in Fig. 1 $D^{\rm macr}$ of weakly deformed ^{224}Ra nucleus calculated using the exact integration (continuous lines) and the second-order formula of [13] (dashed lines). Deformation has been imposed in two ways, in both cases keeping the relative ratios of $\beta_{\lambda 0}$ fixed. Therefore, only one of deformation parameter, e.g., β_2 as in our Fig. 1, has to be specified. The relative ratios we have chosen correspond to (1) the ground state as found in [19], and (2) all $\beta_{\lambda 0} = 0$ except for $\lambda = 2, 3$, which are taken again from [19] [curves labeled (3)]. The end point in β_2 is its equilibrium value. The exact evaluation of integrals leads in both cases to larger dipole moments. When only low multipolarities occur (two lower curves), the difference between the exact and the second-order formula is small, as expected. When higher multipolarities are present (up to β_8), the second-order result is close to the exact one (two upper curves) only for very small deformations and then diverges rather quickly, being nearly two times smaller at the equilibrium deformation of ^{224}Ra. Since the higher multipolarity deformations (at least $\lambda = 4, 5$) are important in ground states of "octupole" nuclei from actinides and heavy Ba regions, it follows that the second-order formula for the macroscopic dipole moment works in fact much worse than expected from the magnitudes of typical equilibrium deformations.

How relevant is this finding for theoretical estimates of $E1$ collectivity performed so far? As inspection of Eqs. (4) and (5) shows one can compensate to the large extent for the difference between the exact and the second-order formula changing droplet model parameters. Two least determined of them are L and Q. In [15], they have been assumed equal to 100 and 50 MeV, respectively, and their change by 50% is quite consistent with the present level of uncertainty. We have checked that the decrease of L from 100 to 50 MeV, with other constants kept as before, allows for a very similar agreement with experimental data using the exact formula as the one achieved in [15] with the use of the second-order formula.

Since the DM parameters were in fact fitted in [15] to obtain satisfactory agreement with data, the relevance of our more exact calculation is that *a priori* it determines more correctly the droplet model constants. Unfortunately, as discussed above, it is difficult to say which L value is really better. We therefore proceed to evaluate dipole moments for super- and more deformed states with L=100 MeV, and comment on modifications arising from the use of L=50 MeV, where necessary.

The differences between the exact and the second-order formula at large deformations are illustrated in Figs. 2 and 3. In Fig. 2, we show the macroscopic dipole moment vs octupole deformation, $D^{\rm macr}(\beta_3)$ for SD ^{192}Hg. Deformations β_2 and β_4 have been kept constant, β_2=0.47, β_4=0.06, typical of the Hg-Pb region, see e.g., [20]. As in Fig. 1, the presence of odd multipolarity deformation with $\lambda > 3$, $\beta_5 = \frac{1}{2}\beta_3$, substantially increases the exact value of $D^{\rm macr}$ (full line) as compared to the purely octupole shape [full line labeled (3)]. For the latter, $D^{\rm macr}$ is very similar to the second-order result [dashed line with the label (3)], and to the second-order result with $\beta_5 = \frac{1}{2}\beta_3$ (dashed line). Thus, the second-order formula

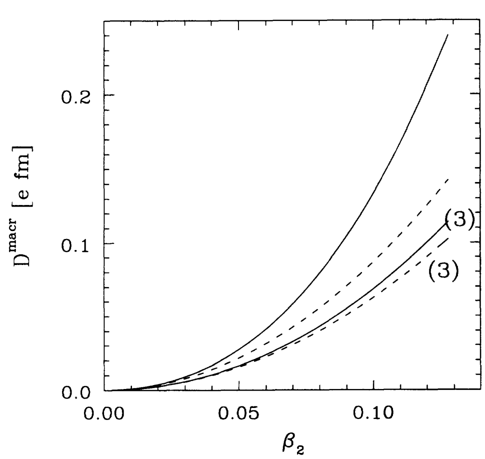

FIG. 1. Macroscopic dipole moments of ^{224}Ra calculated by means of the exact (full lines) and the second-order formula (dashed lines) vs deformation: lower curves include only β_2,β_3, upper curves involve the whole $\{\beta_{\lambda 0}\}$ set, as in realistic calculations.

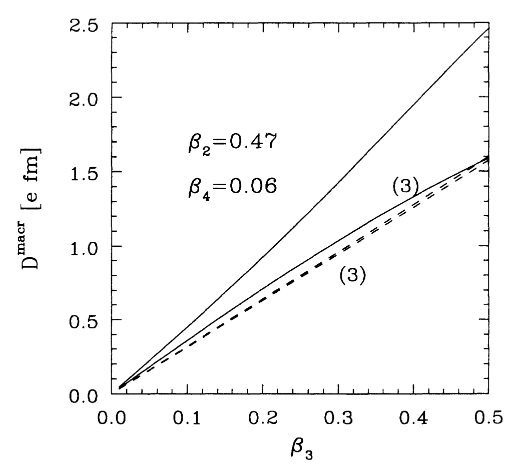

FIG. 2. Macroscopic dipole moments vs octupole deformation, $D^{\rm macr}(\beta_3)$, at the SD minimum in ^{192}Hg. Lines labeled (3) correspond to pure octupole distortions; those without label have been obtained using relation $\beta_5 = \frac{1}{2}\beta_3$. Continuous lines correspond to the exact formula, dashed ones to the second-order approximation.

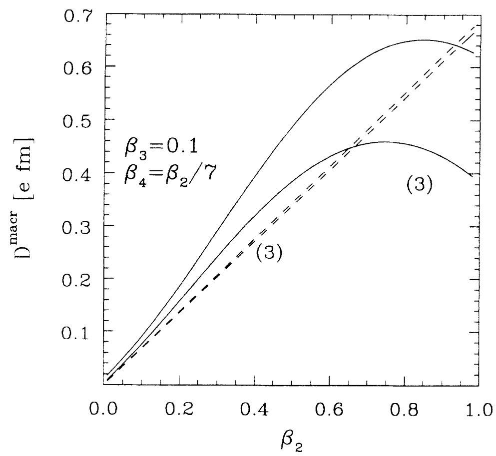

FIG. 3. Macroscopic dipole moments of ^{192}Hg vs quadrupole deformation, $D^{\rm macr}(\beta_2)$, at fixed β_3=0.10 (3), and β_3=0.10, β_5=0.05 (without label). The linear relation $\beta_4 = \frac{1}{7}\beta_2$ has been imposed. Continuous and dashed lines as in Fig. 2.

is quite insensitive to β_5, in contrast to the exact formula.

Quite similar observations follow from the Fig. 3 where $D^{\rm macr}$ of the same ^{192}Hg is displayed vs β_2 at fixed β_3=0.10, with or without [curves labeled (3)] β_5=0.05. The hexadecapole deformation varies according to $\beta_4 = \frac{1}{7}\beta_2$ so that the deformation path goes through the calculated SD minimum. Again, the second-order formula is quite insensitive to β_5 (dashed curves) in contrast to the exact one (full curves). With the pure octupole distortion the agreement between the exact and the second-order formulas is closer than for the β_5=0.05 shape. One additional remarkable feature in Fig. 3 is the saturation and subsequent fall of $D^{\rm macr}(\beta_2)$ (at fixed $\beta_{3(5)}$) for large β_2 predicted by the exact formula as opposed to the linear increase given by the second-order formula. It turns out that this effect comes from the reduction of the charge redistribution term for very elongated shapes. This effect is, of course, of consequence for predictions at very large quadrupole deformations.

IV. DIPOLE MOMENTS OF SUPERDEFORMED NUCLEI

Octupole correlations at SD shape in Gd-Dy and Hg-Pb regions studied so far in various theoretical models [1–7] do not seem to be strong enough to produce deep energy (Routhian) minima. Therefore one anticipates rather a vibration scenario, perhaps, reaching an intermediate situation of a very shallow reflection asymmetric minimum at higher spins. In such a case, an estimate of the $E1$ strength between the SD excited octupole band and the SD g.s. band must be based on (1) intrinsic dipole moments $D(\beta_3)$ in a range of β_3 typical of vibrations and on (2) some knowledge of the effective octupole deformation $\bar{\beta}_3$ of the octupole band.

We have calculated $D(\beta_3)$ for a number of Gd, Dy, Hg, and Pb nuclei at β_3=0.05, 0.10, 0.15—values typical of octupole vibrations on SD shapes in the Hg-Pb region [7]. Quadrupole and hexadecapole deformations have been fixed at typical values resulting from cranking calculations [22,20]: $\beta_2 = 0.61, \beta_4 = 0.11$ in Gd and Dy nuclei, and $\beta_2 = 0.47, \beta_4 = 0.06$ in the Hg-Pb region. We have also studied the dipole moment sensitivity to small changes of deformation, in particular, led by the results described in the previous section, to the effect of including the next odd multipolarity deformation β_5.

Since in both regions SD minima are experimentally known at high spins one should, in principle, account for the dependence of $D^{\rm macr}$ and $D^{\rm shell}$ on the rotational frequency ω. As indicated in the Introduction we have neglected the former. Concerning the latter, one can remark that in [11,15] it was confined to the term $\langle\hat{D}\rangle$ whereas the smeared quantity was always calculated at spin zero. Relatively small sensitivity of $\langle\hat{D}\rangle$ to ω in Ra-Th nuclei at normal deformation has been already found in [11] where it has been remarked that the main effect of rotation on dipole moments comes through shape changes. Results of cranking calculations [22,21] show that in even-even nuclei from both Gd-Dy and Hg-Pb regions SD bands correspond to fairly fixed shapes and configurations in the experimentally interesting spin range. As we have checked, the expectation value $\langle\hat{D}\rangle$ is modestly sensitive to ω in the Gd-Dy region, e.g., in ^{152}Dy, it changes from -0.99 e fm at ω=0 to -1.2 e fm at $\hbar\omega$=0.6 MeV ($I \approx 60\hbar$), and quite insensitive in the Hg-Pb region. Based on this, we consider $D^{\rm macr}(\omega = 0) + D^{\rm shell}(\omega = 0)$ as a reasonable estimate of $D(\omega)$ and neglect, as it was done in [11,15], the rotation effect on $\langle\tilde{\hat{D}}\rangle$, postponing tedious (and involving rough approximations) calculation of this quantity.

The polarizability coefficient χ for high spin SD states is assumed equal to that at spin zero and normal deformation. It is known that properties of the giant dipole resonance (GDR) are mainly determined by deformation, the effect of rotation being smaller. The simplest estimate for χ, $\chi(\omega) \approx (1 + \frac{2\kappa Q^2_{\rm GDR}\omega_{\rm GDR}}{\omega_0^2-\omega^2})^{-1}$ [8], reduces to $\chi \approx (\frac{\omega_0}{\omega_{\rm GDR}})^2$ at the transition frequency $\omega = 0$. Thus, χ is indeed much less deformation dependent than the energy distance between major shells $\hbar\omega_0$ and the GDR energy $\hbar\omega_{\rm GDR}$, which are very much reduced for the $K = 0$ mode built on the SD shape as compared to the spherical case.

In the Gd-Dy region, the shell correction contributions $D^{\rm shell}$ are negative and tend to cancel the macroscopic part. In ^{152}Dy, at β_3=0.10, $D^{\rm shell}$ = -0.55 e fm, $D^{\rm macr}$=0.29 e fm, and the resulting D = -0.26 e fm; in ^{150}Gd, $D^{\rm shell}$ = -0.46 e fm, $D^{\rm macr}$=0.27 e fm, and D = -0.19 e fm. The use of the DM parameter value L=50 MeV instead of L=100 MeV reduces $D^{\rm macr}$ by roughly 20% and one obtains e.g., D = -0.30 e fm for ^{152}Dy. Unfortunately, the uncertainty in higher odd-multipolarity deformations is more serious. Assuming β_5=0.05 in addition to β_3=0.10 in ^{152}Dy leads to a serious reduction in magnitude of $D^{\rm shell}$ to -0.34 e fm, and increase in $D^{\rm macr}$ to 0.39 e fm resulting in D=+0.05 e fm. This sensitivity of D to β_5 is typical of SD nuclei in the Gd-Dy region and obtained dipole moments range from sizable negative to small positive. This prevents us from making predictions for Gd-Dy region except that we do not expect very large dipole moments there.

Fortunately, the situation is different in the Hg-Pb region where both $D^{\rm shell}$ and $D^{\rm macr}$ have positive signs. Moreover, the macroscopic contributions are on average larger than in the Gd-Dy region, e.g., $D^{\rm macr} \approx 0.36$ e fm at β_3=0.10. Dipole moments calculated assuming pure octupole deformation at SD minima are given in Table I. It is remarkable that these results are very similar to those obtained within the self-consistent Hartree-Fock calculations [7]. If we accept the mean deformation of the octupole phonon state $\mid \pi- \rangle$, $\bar{\beta}_3 \approx 0.12$, and the relation between corresponding intrinsic dipole moment $D_0(\bar{\beta}_3)$ and the transition dipole moment $\langle \pi- \mid \hat{D}_0 \mid \pi+ \rangle$ from [7], we can read from Table I the transition dipole moments as little less than $D(\beta_3 = 0.10)$. It is important that the results of Table I are less sensitive to the assumed deformation β_5 than those for the Gd-Dy region, e.g., adding β_5=0.05 to β_3=0.10 reduces D for ^{192}Hg from 0.79 to 0.54 e fm. Small changes in even-multipolarity deformations $\beta_2, \beta_4, \beta_6$ in the range predicted in [20] cause much smaller changes in D, less than 10%. Finally, a change of the DM parameter L from 100 to 50 MeV reduces $D^{\rm macr}$ by $\approx$ 20% which means 10% reduction of the total D. Therefore, one can hope that our calculations provide a reasonable estimate of dipole moments $D(\beta_3)$ in SD Hg and Pb nuclei.

The expected $E1$ strength between opposite parity SD bands may be expressed in a practical way using the standard formula:

$$\frac{T(E1)_{I\to I-1}}{T(E2)_{I\to I-2}} = 1.303 \frac{E_\gamma^3(E1)}{E_\gamma^5(E2)} \frac{8}{5} \frac{(2I-1)(I-1)}{(I-1)^2 - K^2} \left(\frac{D_0^t}{Q_0} \right)^2 , \tag{8}$$

where transition energies are expressed in MeV, the transition dipole moment D_0^t in e fm and electric quadrupole moment in 1000 fm^2. Taking experimental values of $E_\gamma(E2)$ =0.6 MeV at $I \approx 36$ and Q_0=18 b, and assuming D_0^t=0.7 e fm and $K = 0$ we obtain $T(E1)/T(E2) = 8.11 E_\gamma^3(E1)$. Therefore, for $E_\gamma(E1)$ =0.5 MeV we obtain $T(E1)/T(E2)$ ratio equal to unity, i.e., the competition between interband $E1$ and intraband $E2$ transitions. In [7], the predicted excitation of a negative parity state at spin zero was 1.5–2.0 MeV. However, other calculations suggested that this excitation energy would decrease with spin. In such a case, $E1$ transitions could be indeed detectable in experimentally observed spin range. We notice that for large I, the explicit I dependence in Eq. (8) becomes very weak [though $T(E1)/T(E2)$ is still strongly I dependent], while large K values favor $E1$ transitions.

TABLE I. For nuclei indicated in the first column the calculated intrinsic dipole moments at SD shape are given in e fm as a function of octupole deformation β_3.

Nucleus	β_3 =0.05	β_3 =0.10	β_3 =0.15
^{190}Hg	0.43	0.83	1.16
^{192}Hg	0.41	0.79	1.08
^{194}Hg	0.39	0.73	0.99
^{192}Pb	0.47	0.90	1.23
^{194}Pb	0.45	0.85	1.14
^{196}Pb	0.43	0.80	1.03

V. DIPOLE MOMENTS AT VERY LARGE DEFORMATIONS

There have been a number of calculations predicting very deformed energy minima corresponding to quadrupole deformation $\beta_2 \approx 1.0$, i.e., the ellipsoid axis ratio 3:1, recently named hyperdeformed (HD). The third minima around ^{232}Th is the best experimentally documented case. The analysis of neutron-induced fission cross sections for ^{230}Th(n,f) and ^{232}Th(n,f) [23,24] led to conclusion that their fine details can be understood assuming the presence of two rotational bands with the same K and opposite parities. Rotational parameter derived from the data, $\frac{\hbar^2}{2\mathcal{J}} \approx 2.0$ keV, suggests a HD shape, and the positive-negative parity splitting of $\approx$10 keV suggests static octupole deformation. Together it is evidence for the presence of a third well in the fission barrier of these nuclei, corresponding to an octupole deformed, very elongated shape. Recent calculations [25] predict for this excited minimum in ^{232}Th the set of deformations: β_2=0.86, β_3=0.34, β_4=0.18, and β_5=0.056. Since we deal here with the static reflection-asymmetric minimum, we expect the alternating parity rotational band with the $E1$ transitions determined by the intrinsic dipole moment corresponding exactly to the local equilibrium shape. Our calculations give D_0=2.19 e fm, being predominantly the macroscopic effect: $D^{\rm macr}$=2.38 e fm. Thus, assuming parity degeneracy and the electric quadrupole moment of 50 b we obtain from Eq. (8) for I=4 the $T(E1)/T(E2)$ ratio around 200. This would mean a complete dominance of $E1$ transitions. We note that the calculated value of D is not very much sensitive to deformation β_5 in this case, e.g., we obtain 1.84 e fm when we assume $\beta_5 = 0$ in the third minimum.

The second example is the HD minimum in ^{146}Gd predicted at very high spin, $I = (60-80)\hbar$, by Åberg [26]. Its deformations are ϵ=0.93, ϵ_3=0.12, ϵ_4=0.13, and $\epsilon_5 = -0.056$, so it has also a static octupole deformation. Since a full minimization has not been attempted in [26], and a relation between shape parameters ϵ, characteristic of the Nilsson potential, and β, used in our Woods-Saxon model, is not a simple one [27], we have calculated dipole moments of ^{146}Gd for a number of deformations: β_2=0.9, 1.0, 1.1, β_4 =0.2, 0.3, and octupole deformations β_3=0.1, 0.2, 0.3. It turns out that due to equal signs of $D^{\rm macr}$ and $D^{\rm shell}$ we obtain quite sizable dipole moments D=1–2 e fm, for β_2=0.9, 1.0. The inclusion of $\beta_5 = \beta_3/2$ still increases D. However, a firm prediction of D is impossible since at β_2=1.1 dipole moments can be very drastically reduced for β_4=0.3, where due to the change in sign of the proton contribution the total dipole moment vanishes. One has to mention that modifications of $D^{\rm shell}$ by rotation are non-negligible in the present case; we have found an increase of $D^{\rm shell}$ with rotational frequency, which can be as large as 0.7 e fm at

$\hbar\omega$=0.65 MeV, corresponding to spin $I \approx 80\hbar$. Similar dipole moments are obtained for the HD configuration in ^{152}Dy.

To have a rough idea about $T(E1)/T(E2)$ ratio for the hypothetical HD alternating parity band in ^{146}Gd we assume the intrinsic dipole moment D_0 of 1 e fm, the electric quadrupole moment of 35 b [26], the $E_\gamma(E2)$ of 1.0 MeV (corresponding to $I \approx 60\hbar$) and $E_\gamma(E1) = \frac{1}{2}E_\gamma(E2)$. We obtain from these $T(E1)/T(E2)$=0.042. Thus, the $E1$ transitions are hardly expected to compete with $E2$'s in this case. Note that the striking difference in $T(E1)/T(E2)$ ratios predicted for HD alternating parity bands in ^{146}Gd and ^{232}Th comes mainly from the great difference in $E2$ transition energies.

VI. CONCLUSIONS

In this work we aimed at predicting intrinsic or transition dipole moments of reflection-asymmetric SD and more deformed nuclear states. Both in the vibrational limit and in the static deformation limit these quantities determine $E1$ strength between the excited octupole band and the local g.s. band. We have adopted the shell correction method of [11] which, however, required a refinement of the macroscopic contribution for large nuclear deformations.

At first, we discussed the formula for the macroscopic dipole moment freed from the approximation used so far, which was valid only up to the second order in distortions of a sphere. Our calculation shows that even for weakly deformed nuclei from the Ra-Th region the second-order approximation is not numerically correct in the presence of higher multipole deformations.

Assuming small octupole distortions, we have calculated intrinsic dipole moments of SD states in the Gd-Dy and Hg-Pb regions. We have found a partial cancellation of macroscopic and shell correction terms in the Gd-Dy region which leads to very small or at most moderate dipole moments. Large sensitivity to the deformation β_5 prevents us from giving more firm conclusions in this case. In contrast, equal signs of both contributions in the Hg-Pb region result in sizable dipole moments. Their values found in the present work agree very well with the self-consistent Hartree-Fock results obtained in [7].

We have also obtained large dipole moments for theoretically predicted very deformed states like the third minimum in ^{232}Th and the HD minimum in ^{146}Gd, predicted at spin $I = (60 - 80)\hbar$. However, experimentally detectable consequences of a large dipole moment, in particular the large $T(E1)/T(E2)$ ratio, are foreseen only for heavy nuclei with HD rotational bands at low spin, due to much smaller $E2$ transition energies.

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APPENDIX: NUMERICAL PROCEDURES

In the actual calculation, the double volume integrals are converted by means of the divergence theorem to the double surface integrals, which reduce further to the three-dimensional integrals for axially symmetric shapes. In particular, the volume integrals involving Coulomb potential v may be transformed into one of the following:

$$\int_V \xi v dV = -\frac{1}{2}\int_S\int_{S'} dS\, dS' \mathbf{n}\cdot\mathbf{n}'\xi \mid \mathbf{r}-\mathbf{r}' \mid$$
$$= -\frac{1}{6}\int_S\int_{S'} dS\, dS' \frac{\xi[\mathbf{n}\cdot(\mathbf{r}-\mathbf{r}')][\mathbf{n}'\cdot(\mathbf{r}-\mathbf{r}')]}{\mid \mathbf{r}-\mathbf{r}' \mid}, \tag{A1}$$

where ξ may be 1 or z. Surface integrals of v are transformed using $\nabla \cdot \frac{\mathbf{r}}{r} = \frac{2}{r}$.

The three-dimensional (four-dimensional, without axial symmetry) integrals are calculated numerically by means of threefold (fourfold) Gauss-Legendre procedures, so the question of accuracy appears immediately. To get a confidence in our numerical method we have used it in one nontrivial case which can be calculated (nearly) analytically. This is the case of a half sphere of a radius r_2 connected to the spherical section of a radius $r_1 > r_2$, obtained by removing the spherical cup determined by a polar angle α, so that the matching condition, $r_2 = r_1 \cos\alpha$, is fulfilled. For this one-parameter family of axially symmetric shapes all integrals determining macroscopic dipole moment can be worked out in a form of a finite expression or a quickly convergent series. As we have checked for few values of α, the results of numerical integration agree to the satisfactory accuracy with those of the analytic calculation.

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