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Orbital 1^+ strengths from self-consistent deformed mean field calculations

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We present results for summed orbital 1^+ strengths in Sm and Nd isotopes obtained from deformed Hartree-Fock +BCS calculations, using a microscopic formulation of the scissors mode (the PHFB model) that excludes spurious contributions. It is found that the calculated 1^+ strengths for the two chains of isotopes are proportional to δ^2 and that the summed strengths up to 4 MeV are in fair agreement with experimental data. It is also found that when pairing is neglected the total scissors mode strength is proportional to δ rather than to δ^2. Analytical expressions are given for the explicit dependence on the deformation parameter with and without pairing, valid for the anisotropic harmonic oscillator model.

In 1984, the first observations of low-lying 1^+ excitations in even-even deformed nuclei were reported [1]. Since then, much work has been devoted to understanding their nature, not only in rare-earth nuclei [1, 2] but also in the s, d and p, f shells [3], and the uranium region [4]. A variety of experimental probes have been used (electrons, protons, γ's) and many theoretical models have been applied, as reviewed in Ref. [5]. The distinctive feature of these excitations is that they are seen in electron but not in proton scattering, so they are primarily of orbital rather than spin-flip type. Since both the rigid rotor model [6] and interacting boson model (IBA) [7] had predicted the existence of a scissors mode, these 1^+ excitations were interpreted as examples of such a mode.

In Ref. [8] a doorway state

$$|\Phi_1 >= \frac{1}{\mathcal{N}} \left[< J_\nu^2 > J_+^\pi - < J_\pi^2 > J_+^\nu \right] |\Phi_0 > \qquad (1)$$

was proposed as the microscopic formulation of the scissors mode predicted by the two-rotor model [6]. In Eq. (1) $|\Phi_0 >$ represents the deformed ground-state Hartree-Fock-Bogolyubov (HFB) wave function, and $|\Phi_1 >$ is constructed to be normalized to one and orthogonal to the spurious state $|\Phi_1^S >=< J^2 >^{-1/2} \; J_+|\Phi_0 >$. Assuming a pure orbital mode the $M1$ strength is given by [8]

$$B(M1)\!\uparrow_{\rm sc.} = \frac{3}{4\pi} \frac{< J_\pi^2 >< J_\nu^2 >}{< J^2 >} \, \mu_N^2 \qquad (2)$$

with $< J^2 > \left(=< J_\pi^2 > + < J_\nu^2 >\right)$ the mean value of the total angular momentum operator squared in the intrinsic ground state Φ_0,

$$< J_\rho^2 > = 2 \sum_{\alpha\,\beta} (u_\alpha v_\beta - v_\alpha u_\beta)^2 \, | < \alpha | \, j_x^\rho \, | \beta > |^2$$
$$\equiv 2 \sum_{\alpha\,\beta} \Phi_{\alpha\beta} | < \alpha | \, j_x^\rho \, | \beta > |^2 \; , \qquad (3)$$

where v_α^2 is the occupation of the single particle state α in the deformed HFB mean field, ($u_\alpha^2 = 1 - v_\alpha^2$), and the sum over $\alpha\beta$ extends over all two-quasiparticle states for neutrons ($\rho = \nu$) or for protons ($\rho = \pi$).

As in Ref. [8] we refer to this model as the PHFB model because it is inspired by — and makes use of — the angular momentum projected HF (or HFB) formalism [9].

In Ref. [8], it was found that this model predicts a much larger 1^+ strength for ^{156}Gd than had been experimentally observed. The $B(M1)\!\uparrow_{\rm sc.}$ value obtained for ^{156}Gd was $7\mu_N^2$, similar to the values obtained by Hilton [10] from QRPA calculations, while the reported experimental $M1$ strength $\sim 1.3\ \mu_N^2$ [1] was closer to the IBA prediction ($2.8\ \mu_N^2$) [7]. It was therefore suggested that the scissors mode may be fragmented over a rather extensive energy region.

A very interesting observation is that in the Sm isotopes, the total $M1$ strength up to 4 MeV is measured to be proportional to the square of the deformation parameter [11]. In this paper we will demonstrate that such a dependence can be explained by the PHFB model. We will first show this by detailed calculations, and then interpret these results in the framework of the anisotropic oscillator model.

(1) Table I contains our results for Sm and Nd isotopes, from HF+BCS calculations using the Skyrme III interaction and constant gap parameters. We show the total scissors mode strength [as given by Eq. (2)] as well as the strengths obtained when the sum over two-quasiparticle excitations in Eq. (3) is restricted to energies up to 4 MeV ($E^* \leq 4$) and up to 6 MeV ($E^* \leq 6$). Also shown in the table are the observed strengths from Ref. [11]. Our calculated quadrupole moments and mass quadrupole deformation parameters β are shown in columns 4 and 5. The experimental quadrupole moments from Ref. [12] are shown in column 6. As can be seen in the table, the results for quadrupole moments are in good agreement with experiment except for the spherical isotopes

TABLE I. Pairing gap parameters and results for Sm and Nd isotopes for mass quadrupole deformation parameters β, charge quadrupole moments, mean values of the angular momentum squared for protons and neutrons and $M1$ strengths (see text). Experimental quadrupole moments are from Ref. [12] and experimental summed $M1$ strengths are from Ref. [11].

	Δ_π MeV	Δ_ν MeV	β	$Q_0^{\text{th.}}$ fm^2	$Q_0^{\text{exp.}}$ fm^2	$< J_\pi^2 >$	$< J_\nu^2 >$	$B(M1)\uparrow_{\text{sc.}}$ Total	$E^* \leq 6$	$E^* \leq 4$	$\Sigma B(M1)\uparrow_{\text{exp}}$	$B(M1)\uparrow_{\text{sc.}\ \Delta=0}$
^{144}Sm	1.19	1.38	0.005	9.9	163.5(2.4)	0.064	0.051	0.01	0.00	0.00	0.28 ± 0.10	0.01
^{148}Sm	1.35	1.06	0.138	290	269(6)	12.08	18.12	1.73	1.17	0.86	0.51 ± 0.08	5.39
^{150}Sm	1.44	1.19	0.202	428	368.4(4.1)	23.65	32.91	3.29	2.03	1.25	0.97 ± 0.06	6.59
^{152}Sm	1.12	1.20	0.269	578	588.1(3.4)	43.47	57.73	5.92	3.63	2.53	2.35 ± 0.11	9.72
^{154}Sm	0.88	0.98	0.304	654	662.0(3.8)	56.22	79.87	7.88	5.07	3.41	2.65 ± 0.15	10.44
^{142}Nd	1.23	1.39	0.015	32.2	164.8(2.4)	0.365	0.228	0.03	0.00	0.00	0.02 ± 0.01	0.05
^{146}Nd	1.33	1.05	0.145	293	276(5)	12.66	18.80	1.81	1.21	0.94	0.72 ± 0.06	5.68
^{148}Nd	1.44	1.12	0.192	388	372.5(4.0)	20.22	30.59	2.91	1.84	1.06	1.12 ± 0.09	6.45
^{150}Nd	1.22	1.05	0.249	511	525.8(3.8)	35.56	53.17	5.09	3.21	2.33	2.12 ± 0.11	9.73

^{144}Sm and ^{142}Nd for which the procedure used in Ref. [12] for extracting intrinsic quadrupole moments from $B(E2)$ strengths is questionable. In addition we also show in the last column of the table the results obtained for the total scissors mode strength when pairing is neglected $[B(M1)\uparrow_{\text{sc.}\ \Delta=0}]$.

Several interesting features are seen in this Table: (i) $B(M1)\uparrow_{\text{sc.}}$ is considerably reduced when one takes into account only low energy two-quasiparticle excitations, getting very close to the experimental $M1$ strengths for $E^* \leq 4$ MeV. (ii) The total scissors mode strengths as well as $B(M1)\uparrow_{\text{sc.}}$ for $E^* \leq 6$ MeV or $E^* \leq 4$ MeV are proportional to β^2. (iii) When pairing is neglected, the total $B(M1)\uparrow_{\text{sc.}}$ strengths are considerably larger and are no longer proportional to β^2 but tend to be proportional to β. These results are further illustrated in Fig. 1 where we also plot the available experimental data, and in Fig. 2 where we compare the total scissors mode strengths with and without pairing.

The large difference (roughly a factor 2) between the calculated total scissors mode strength and $B(M1)\uparrow_{\text{sc.}}$ for $E^* \leq 4$ MeV, is due to the fact that there are many small contributions to Eq. (3) from two-quasiparticle $\alpha\beta$ states at higher excitation energies (up to $E^* \sim 25$ MeV). For the deformed isotopes the stronger contributions to $< J^2 >$ occur always in the range 2 MeV $< E^* <$ 4 MeV. Results for orbital and spin strengths of each individual $\alpha\beta$ contribution as well as their spectral distributions and form factors will be presented and discussed elsewhere [13]. However it is also interesting to see that the main features mentioned above, that result from involved calculations, can be understood in the light of a simpler model. To this end we discuss in what follows the results for the anisotropic harmonic oscillator (HO) model.

(2) In the *anisotropic HO* the single-particle states α are characterized by the cartesian quantum numbers (n_x, n_y, n_z), with $N_\alpha = n_x^\alpha + n_y^\alpha + n_z^\alpha$ the major shell quantum number of the state α. We assume axial symme-

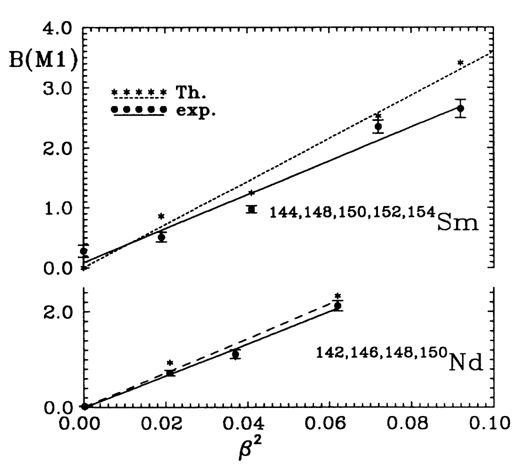

FIG. 1. Experimental and theoretical summed 1^+ strengths up to 4 MeV for Sm and Nd isotopes plotted versus β^2. The straight lines are least-square fits.

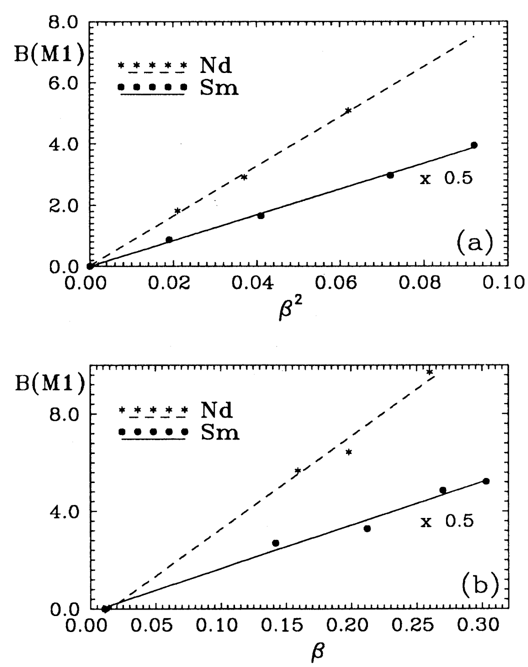

FIG. 2. Theoretical total scissors mode strengths with (a) and without (b) pairing versus deformation (see text). Strengths for Sm isotopes are divided by two.

try ($\omega_x = \omega_y \neq \omega_z$) and pair filling, i.e., each $(n_x^\alpha, n_y^\alpha, n_z^\alpha)$ level is equally occupied by two (spin up and down) nucleons.

To simplify the discussion we assume equal prolate deformations for neutrons and protons and define the deformation parameter $\delta = 3Q_0/(4 < R^2 >)$. Using $< R_i^2 >= \hbar\sigma_i/M\omega_i$ together with the self-consistency condition [14] $\sigma_x\omega_x = \sigma_y\omega_y = \sigma_z\omega_z = \sigma_0\omega_0$, where $\sigma_i = \sum_\alpha v_\alpha^2 (n_i^\alpha + \frac{1}{2})$ $(i = x, y, z)$, gives at the equilibrium deformation δ for the ground state $|\Phi_0>$

$$\sigma_z^2 = \sigma_0^2 \left(1 + \tfrac{4}{3}\delta\right) \ , \ \sigma_y^2 = \sigma_0^2 \left(1 - \tfrac{2}{3}\delta\right) \ , \qquad (4)$$

$$\omega_z^2 = \omega_0^2 \left(1 + \tfrac{4}{3}\delta\right)^{-1} \ , \ \omega_y^2 = \omega_0^2 \left(1 - \tfrac{2}{3}\delta\right)^{-1} \ .$$

For $N = Z$ we have $< J^2 > = 2 < J_\nu^2 > = 2 < J_\pi^2 >$ and the scissors mode strength in Eq. (2) is simply given by $B(M1)\uparrow_{\rm sc.} = (3/16\pi) < J^2 >$. Then to analyze the properties of the scissors mode we have only to study the behavior of $< J^2 >$. In this simplified model the nonzero matrix elements contributing to Eq. (3) are

$$< n_x \ n_z - 1 \ n_y + 1 | \ \ell_x \ | n_x \ n_z \ n_y >= \frac{\beta^+}{2i} \left[n_z(n_y+1)\right]^{1/2} \ , \qquad (5)$$

$$< n_x \ n_z + 1 \ n_y + 1 | \ \ell_x \ | n_x \ n_z \ n_y > = \frac{\beta^-}{2i} \left[(n_z+1)(n_y+1)\right]^{1/2} \qquad (6)$$

and their Hermitian conjugates, with $\beta^\pm = \sqrt{\omega_y/\omega_z} \pm \sqrt{\omega_z/\omega_y}$.

Hence we see that there are two types of contributions to $< J^2 >$: (i) Contributions from single-particle states $\alpha\beta$ with equal major shell quantum numbers $(N_\alpha = N_\beta)$. These contributions are proportional to $(\beta^+)^2$ and involve single-particle excitations $|\epsilon_\alpha - \epsilon_\beta| = \hbar(\omega_y - \omega_z)$. (ii) Contributions from single-particle states $\alpha\beta$ with major shell quantum numbers differing by two units $(N_\beta = N_\alpha \pm 2)$. These contributions are proportional to $(\beta^-)^2$ and involve single-particle excitations $|\epsilon_\alpha - \epsilon_\beta| = \hbar(\omega_y + \omega_z)$. We therefore write $< J^2 > = < J^2 >_1 + < J^2 >_2$ with

$$< J^2 >_1 = 2 \sum_{\substack{\alpha\beta \\ (N_\alpha = N_\beta)}} \Phi_{\alpha\beta} | < \beta | \ \ell_x \ | \alpha > |^2 ,$$
$$< J^2 >_2 = 2 \sum_{\substack{\alpha\beta \\ (N_\alpha = N_\beta \pm 2)}} \Phi_{\alpha\beta} | < \beta | \ \ell_x \ | \alpha > |^2 . \qquad (7)$$

Let us first consider the case of no pairing ($\Delta = 0$). In this case $\Phi_{\alpha\beta}$ is zero when α and β are both above (below) the Fermi level (λ), and $\Phi_{\alpha\beta} = 1$ for α below and β above the Fermi level (or vice versa). This gives for $< J^2 >_1$ and $< J^2 >_2$

$$< J^2 >_{1(\Delta=0)} = (\beta^+)^2 \sum_\alpha v_\alpha^2 \left(n_z^\alpha - n_y^\alpha\right) = (\beta^+)^2 \left(\sigma_z - \sigma_y\right) \simeq 4\sigma_0\delta \left(1 - \frac{\delta}{6}\right) \ , \qquad (8)$$

$$< J^2 >_{2(\Delta=0)} = (\beta^-)^2 \sum_\alpha v_\alpha^2 \left(n_z^\alpha + n_y^\alpha + 1\right) = (\beta^-)^2 \left(\sigma_z + \sigma_y\right) \simeq 2\sigma_0\delta^2 \ . \qquad (9)$$

In this limit the total $M1$ strength is proportional to δ, to lowest order in the deformation parameter. In addition one can see in this simplified model that the total PHF strength will be fragmented in two peaks: (i) A low energy peak at $E_1^* \simeq \hbar\omega_0\delta$ (~ 3 MeV, for typical values of $\hbar\omega_0$ and δ) with strength proportional to δ, $B(M1)\uparrow_{\rm sc.} = (3/16\pi) < J^2 >_1 \simeq (3/4\pi)\sigma_0\delta$, which is analogous to that considered in Ref. [15], and is built from degenerate 1p-1h states with $|\epsilon_\alpha - \epsilon_\beta| = E_1^*$. (ii) A high energy peak at $E_2^* \simeq 2\hbar\omega_0$ (~ 20 MeV) with strength proportional to δ^2, $B(M1)\uparrow_{\rm sc.} = (3/16\pi) < J^2 >_2 \simeq (3/8\pi)\sigma_0\delta^2$, which is built up from degenerate 1p-1h with $|\epsilon_\alpha - \epsilon_\beta| = E_2^*$.

Hence this model is useful to understand the fragmentation of the scissors mode into low energy and high energy modes [16]. It is also useful to understand the dependence on δ observed in Fig. 2(b) when pairing is neglected.

To understand the dependence on δ^2 observed in Figs. 1 and 2(a) we have to take pairing into account. To see that, we write the occupation coefficients $\Phi_{\alpha\beta}$ as

$$\Phi_{\alpha\beta} = \frac{\left(\epsilon_\alpha - \epsilon_\beta\right)^2}{4E_\alpha E_\beta} \left(1 - P_{\alpha\beta}\right) \ , \qquad (10)$$

where $E_\alpha = \sqrt{\left(\epsilon_\alpha - \lambda\right)^2 + \Delta^2}$ and

$$P_{\alpha\beta} = \frac{\left(E_\alpha - E_\beta\right)^2}{\left(\epsilon_\alpha - \epsilon_\beta\right)^2} = \frac{\epsilon_{\alpha\beta}^2}{\epsilon_{\alpha\beta}^2 + E^2 + \Delta^2} \left[1 + \frac{E^2\epsilon_{\alpha\beta}^2}{\left(\epsilon_{\alpha\beta}^2 + E^2 + \Delta^2\right)^2} + \cdots\right] \qquad (11)$$

with $\epsilon_{\alpha\beta} = \frac{1}{2}\left(\epsilon_\alpha + \epsilon_\beta\right) - \lambda$ and $E = \frac{1}{2}\left(\epsilon_\alpha - \epsilon_\beta\right)$. We notice that $0 \leq P_{\alpha\beta} \leq 1$ and that for fixed E and Δ the dominant contributions to $< J^2 >$ come from terms for which $\epsilon_{\alpha\beta} = 0$ $[P_{\alpha\beta} = 0, \Phi_{\alpha\beta} = E^2/(E^2 + \Delta^2)]$, i.e., from single-particle levels α and β that are equidistant from the Fermi level.

Let us first consider $< J^2 >_2$. In this case $2E = |\epsilon_\beta - \epsilon_\alpha| = E_2^* \simeq 2\hbar\omega_0$ and neglecting terms of the order $(\Delta\delta/\hbar\omega_0)^2$ we find that $\Phi_{\alpha\beta} \simeq 1$ for $\epsilon_\alpha < \lambda, \epsilon_\beta > \lambda$ (or vice versa) and $\Phi_{\alpha\beta} \simeq 0$ otherwise. Therefore for

$< J^2 >_2$ we recover the result in Eq. (9) up to terms of the order $(\Delta\delta/\hbar\omega_0)^2$, and $< J^2 >_2$ is again proportional to δ^2.

We now consider $< J^2 >_1$, for which $2E = |\epsilon_\alpha - \epsilon_\beta| = E_1^* \simeq \hbar\omega_0\delta$, and substitution of Eqs. (10) and (5) into Eq. (7) gives

$$< J^2 >_1 = \delta^2 \sum_{\alpha\beta}(1 - P_{\alpha\beta})\frac{(\hbar\omega_z n_z^\alpha)(\hbar\omega_y n_y^\beta)}{E_\alpha E_\beta}. \quad (12)$$

Here the sum is restricted to $\alpha\beta$ states with $N_\beta = N_\alpha$, $n_z^\beta = n_z^\alpha - 1$, $n_y^\beta = n_y^\alpha + 1$. In Eq. (12) we clearly see that $< J^2 >_1$ is now proportional to δ^2 too. Indeed the term under the sum decreases as $\epsilon_{\alpha\beta}$ increases and has only a weak dependence on δ. This can be easily seen from the fact that as $\epsilon_{\alpha\beta}$ increases, $P_{\alpha\beta}$ goes to 1 and $E_\alpha E_\beta$ increases as $\epsilon_{\alpha\beta}^2$.

Hence when pairing is taken into account each two-quasiparticle $\alpha\beta$ contribution is proportional to δ^2, and so are the total or partial summed strengths obtained from Eq. (2). In addition the two peaks at E_1^* and E_2^*, found for the case of no pairing, are further fragmented because now each $\alpha\beta$ pair contributing to $< J^2 >_1$ or $< J^2 >_2$ occurs at a different energy $E_{\alpha\beta}^* = E_\alpha + E_\beta$, and one can expect to see fragmentation in the low energy region too.

In *conclusion* we have found that the PHFB model with effective Skyrme interactions gives for Sm and Nd isotopes $B(M1)\uparrow_{\rm sc.}$ strengths that are proportional to the square of the deformation parameter, and that are in fair agreement with the observed summed strengths for two-quasiparticle excitations up to 4 MeV. Fair agreement with experiment is also found for quadrupole moments. Though spin-orbit effects are important in these realistic calculations, the main features of the results can be qualitatively understood with a simple anisotropic harmonic oscillator model without spin-orbit. With this simplified HO model one can see analytically how $B(M1)\uparrow_{\rm sc.}$ depends on deformation. One can also see analytically the important role that pairing plays, particularly in the fragmentation and δ^2 dependence of the strength at low energy. The detailed energy distribution of the total $M1$ strength is modified when spin-orbit and residual interactions are taken into account [13, 16, 17]; however, the trend found for the HO of dependence on δ^2 when pairing is taken into account (or on δ when there is no pairing) persists in realistic calculations of total or partial summed orbital strengths, as seen from the results shown in Figs. 1 and 2. Since in our description this feature appears to be a general property of deformed nuclei, it would be interesting to test experimentally whether this behavior is also observed in other isotopic chains.

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