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Geometry of the shears mechanism in nuclei

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The geometry of the shears mechanism in nuclei is derived from the nuclear shell model. This is achieved by taking the limit of large angular momenta (classical limit) of shell-model matrix elements.

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A central theme in the study of quantum many-body systems is the understanding of its elementary modes of excitation. Of particular interest is the competition between single-particle and collective degrees of freedom. In general, single-particle motion gives rise to irregular level sequences, associated with the unique properties of the individual particles. Collective motion generates more regular structures, a typical example being that of rotational bands which follow closely a $J(J+1)$ sequence, characteristic of a quantum rotor.

In atomic nuclei, the energy scales of these modes are somewhat comparable, leading to a rich and complex structure [1]. ²⁰⁸Pb is considered a paradigm of a doubly-closed-shell nucleus with collective states based on an octupole phonon. Neighboring nuclei provided a wealth of important information for the shell model, on single-particle levels and residual interactions at the $Z = 82$, $N = 126$ shell closure, as well as on the role of particle-vibration coupling [2].

The observation in ¹⁹⁹Pb of a regular sequence of γ rays resembling, at first look, a rotational band came as a surprise [3–6]. A closer inspection of the data established that these transitions were of magnetic character, in contrast to the quadrupole nature in the well-known nuclear rotors [1]. The answer to this puzzle was provided by Frauendorf [7], who based on the Tilted Axis Cranking Model proposed the so-called “shears mechanism”. He showed that for a weakly deformed system, there exist low-energy configurations in which neutrons and protons combine into stretched structures (“blades”) and the angular momentum is generated by the re-coupling of these blades, resembling the closing of a pair of shears. As discussed in Ref. [8], the breaking of the rotational symmetry in this case originates in an anisotropic distribution of nucleonic current loops (rather than electric charge), and thus it is usually referred as magnetic rotation. Further experiments not only confirmed this picture in the lead region, but also established the mechanism in other regions of the Segré chart, near doubly-magic closures.

While an interpretation in terms of the shears mechanism provides an appealing, intuitive picture of these nuclear states, the question remains whether this geometric character is borne out by microscopic calculations. In numerical shell-model calculations Frauendorf *et al.* [9] showed that the shears picture is valid in the lead iso-

topes. A direct derivation of the geometry of the shears mechanism from the shell model has, however, to our knowledge never been given. Providing such a derivation by introducing a geometric interpretation of the shell-model matrix elements involved is the purpose of the present Letter.

Let us assume that two nucleons of one type (say neutrons) occupy particle-like orbits $j_{1\nu}$ and $j_{2\nu}$, while two nucleons of the other type (protons) occupy hole-like orbits $j_{1\pi}^{-1}$ and $j_{2\pi}^{-1}$ [10]. The neutrons and protons are coupled to angular momenta J_ν and J_π , respectively, which are close to stretched $J_\rho \approx j_{1\rho} + j_{2\rho}$ ($\rho = \nu, \pi$). The two-particle (2p) and two-hole (2h) states are represented as $|N\rangle = |j_{1\nu}j_{2\nu}; J_\nu\rangle$ and $|P^{-1}\rangle = |j_{1\pi}^{-1}j_{2\pi}^{-1}; J_\pi\rangle$, and we assume that the states are Pauli allowed, *i.e.*, that J_ρ is even if $j_{1\rho} = j_{2\rho}$. A shears band consists of the states $|NP^{-1}; J\rangle$ where J results from the coupling of J_ν and J_π .

We ask the following questions: How do the energies of the members of this band evolve as a function of J , and how does this evolution depends on the angular momenta of the single-particle orbits and the angular momenta of the blades? We answer these questions by adopting a shell-model hamiltonian of the generic form $H = H_\nu + H_\pi + V_{\nu\pi}$ and computing $\langle NP^{-1}; J | H | NP^{-1}; J \rangle$, which will be referred to as the (2p-2h) shears matrix element.

The shell-model hamiltonian is specified by the single-particle energies, the single-hole energies, the neutron-neutron and proton-proton (two-body) interaction matrix elements, and the neutron-proton (np) interaction matrix elements $V_{j_\nu j_\pi}^R \equiv \langle j_\nu j_\pi; R | V_{\nu\pi} | j_\nu j_\pi; R \rangle$. One finds that the contribution of H_ν and H_π to the energy is constant for all members of the shears band and that any J dependence originates from the np interaction $V_{\nu\pi}$. A multipole expansion of the latter interaction leads to the following expression for the shears matrix element:

$$\begin{aligned} & \langle NP^{-1}; J | V_{\nu\pi} | NP^{-1}; J \rangle \\ &= -\mathcal{P} \hat{J}_\nu \hat{J}_\pi \sum_R \hat{R} V_{j_{1\nu} j_{1\pi}}^R \begin{Bmatrix} j_{1\nu} & J_\nu & J_\pi & j_{1\pi} \\ j_{2\nu} & J & j_{2\pi} & R \\ j_{1\nu} & J_\nu & J_\pi & j_{1\pi} \end{Bmatrix}, \end{aligned} \quad (1)$$

where $\hat{x} \equiv 2x+1$ and $\mathcal{P} \equiv \mathcal{P}_\nu \mathcal{P}_\pi$ with \mathcal{P}_ρ an operator defined from $\mathcal{P}_\rho f(j_{1\rho}, j_{2\rho}) = f(j_{1\rho}, j_{2\rho}) + f(j_{2\rho}, j_{1\rho})$ for any function f . The object in curly brackets is a $12j$ symbol of the *first* kind, a quantity which is scalar under

rotations and depends on twelve angular momenta. The result (1) is obtained by expressing the shears matrix element as a sum over four $6j$ symbols, which can be related to a $12j$ symbol, see Eq. (19.1) of Ref. [11].

It is now a simple matter to introduce in the sum (1) values for the np interaction matrix elements and to derive the J dependence of the shears matrix element. For any reasonable nuclear interaction and for $J_\rho \approx j_{1\rho} + j_{2\rho}$, it is found that the sum (1) has an approximate parabolic behavior around its minimum around $J^2 \approx J_\nu^2 + J_\pi^2$.

To understand better this numerical finding, the geometry of the expression (1) can be studied by taking the limit of large angular momenta in the recoupling coefficients. Such limits are known since the seminal study of Wigner on the classical limit of $3j$ and $6j$ symbols (see chapter 27 of Ref. [12]), subsequently refined by Ponzano and Regge [13] whose work was put on a mathematically solid footing by Schulten and Gordon [14]. The classical limit of a $3j$ symbol is associated with the area of a (projected) triangle while that of a $6j$ symbol involves the volume of a tetrahedron, with the lengths of the sides determined by the angular momenta. Classical limits not only yield approximate expressions for (re)coupling coefficients but in addition provide an insight into their geometrical significance. The study of the classical limit of

$3nj$ symbols with $n > 2$ is still a topic of active research with ramifications in fields as diverse as quantum gravity and quantum computing (see, *e.g.* Refs. [15–17] and references therein), well beyond the standard applications in, for example, atomic or nuclear physics.

Since at this moment only partial results are known for $9j$ (let alone $12j$) symbols, a classical limit of the expression (1) for arbitrary interactions is difficult to obtain. We consider instead the surface delta interaction (SDI) [18], $V^{\text{SDI}}(i, j) = -4\pi a'_T \delta(\bar{r}_i - \bar{r}_j) \delta(r_i - R_0)$, which is known to be a reasonable approximation to the nucleon-nucleon interaction [19]. The np matrix element $V_{j_\nu j_\pi}^R$ of the SDI is [18]

$$-\frac{\hat{j}_\nu \hat{j}_\pi}{2} \left[a_{01} \begin{pmatrix} j_\nu & j_\pi & R \\ \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}^2 + a_0 \begin{pmatrix} j_\nu & j_\pi & R \\ \frac{1}{2} & \frac{1}{2} & -1 \end{pmatrix}^2 \right], \quad (2)$$

with $a_{01} = (a_0 + a_1)/2 - (-)^{\ell_\nu + \ell_\pi + R}(a_0 - a_1)/2$ in terms of the strengths $a_T = a'_T C(R_0)$, where $C(R_0)$ equals $R_{n_\nu \ell_\nu}^4(R_0) R_0^2 = R_{n_\pi \ell_\pi}^4(R_0) R_0^2$.

When the SDI np matrix elements (2) are introduced in the shears matrix element (1), one encounters sums of the type

$$\sigma_n^{(\lambda)} \equiv (2J_\nu + 1)(2J_\pi + 1) \sum_R (-)^\lambda (2R + 1) \begin{pmatrix} j_{1\nu} & j_{1\pi} & R \\ \frac{1}{2} & n - \frac{1}{2} & -n \end{pmatrix}^2 \begin{Bmatrix} j_{1\nu} & J_\nu & J_\pi & j_{1\pi} \\ j_{2\nu} & J & j_{2\pi} & R \\ j_{1\nu} & J_\nu & J_\pi & j_{1\pi} \end{Bmatrix}, \quad (3)$$

for $(\lambda, n) = (0, 0)$, $(0, 1)$ and $(1, 0)$. These reduce to simple expressions in the classical limit. For example, for $\lambda = 0$, the sum can be exactly rewritten as

$$\sigma_n^{(0)} = (2J_\nu + 1)(2J_\pi + 1) \sum_{\substack{m_\nu, M_\nu \\ m_\pi, M_\pi}} \begin{pmatrix} j_{1\nu} & j_{2\nu} & J_\nu \\ \frac{1}{2} & m_\nu & M_\nu \end{pmatrix}^2 \begin{pmatrix} j_{1\pi} & j_{2\pi} & J_\pi \\ -n + \frac{1}{2} & m_\pi & M_\pi \end{pmatrix}^2 \begin{pmatrix} J_\nu & J_\pi & J \\ M_\nu & M_\pi & m_\nu + m_\pi - n + 1 \end{pmatrix}^2. \quad (4)$$

The classical approximation consists of replacing the last $3j$ symbol in Eq. (4) according to [12]

$$\begin{pmatrix} J_\nu & J_\pi & J \\ M_\nu & M_\pi & M \end{pmatrix}^2 \mapsto \left(4\pi A_{M_\nu M_\pi M}^{J_\nu J_\pi J} \right)^{-1}, \quad (5)$$

where $A_{M_\nu M_\pi M}^{J_\nu J_\pi J}$ is related to the Caley determinant,

$$\left(A_{M_\nu M_\pi M}^{J_\nu J_\pi J} \right)^2 = -\frac{1}{16} \begin{vmatrix} 0 & a_{J_\nu M_\nu} & a_{J_\pi M_\pi} & 1 \\ a_{J_\nu M_\nu} & 0 & a_{JM} & 1 \\ a_{J_\pi M_\pi} & a_{JM} & 0 & 1 \\ 1 & 1 & 1 & 0 \end{vmatrix}, \quad (6)$$

with $a_{JM} \equiv (J + \frac{1}{2})^2 - M^2$. While the $3j$ symbol in Eq. (5) usually is a rapidly oscillating function of M_ν and M_π , its classical approximation is smooth. Many oscillations occur except when J is close to its minimum or

maximum value, $J = |J_\nu - J_\pi|$ or $J = J_\nu + J_\pi$, respectively. The approximation (5) in the sum (4), therefore, can be expected to be reasonable in most cases, in particular in the region of physics interest where $J^2 \approx J_\nu^2 + J_\pi^2$. Since $J_\rho \approx j_{1\rho} + j_{2\rho}$, a classical approximation cannot be made for the first two $3j$ symbols in Eq. (4). From the explicit expressions for the $3j$ symbols one can show that the sum over M_ν and M_π can be restricted to the region around $M_\nu = M_\pi = 0$. Since the classical approximation (5) is nearly constant for small values of M_ν and M_π , the classical limit for the $3j$ symbols with zero projections on the z axis can be taken, to obtain

$$\sigma_0^{(0)} \approx \sigma_1^{(0)} \approx \frac{(2J_\nu + 1)(2J_\pi + 1)}{4\pi(2j_{1\nu} + 1)(2j_{1\pi} + 1)A}, \quad (7)$$

where $A \equiv A_{000}^{J_\nu J_\pi J}$ is the area of a triangle with sides of

lengths $J_\nu + \frac{1}{2}$, $J_\pi + \frac{1}{2}$, and $J + \frac{1}{2}$ [20]. We may alternatively express this sum in terms of the shears angle,

$$\theta_{\nu\pi} = \arccos \frac{J(J+1) - J_\nu(J_\nu+1) - J_\pi(J_\pi+1)}{2\sqrt{J_\nu(J_\nu+1)J_\pi(J_\pi+1)}}, \quad (8)$$

leading to

$$\sigma_0^{(0)} \approx \sigma_1^{(0)} \approx \frac{2}{\pi(2j_{1\nu}+1)(2j_{1\pi}+1)\sin\theta_{\nu\pi}}. \quad (9)$$

A similar derivation yields the classical approximation

$$\sigma_0^{(1)} \approx -(-)^{j_\nu+j_\pi} \frac{2}{\pi(2j_{1\nu}+1)(2j_{1\pi}+1)\tan\theta_{\nu\pi}}. \quad (10)$$

Introducing the preceding approximations into the expression for the shears matrix element (1), we obtain

$$\langle NP^{-1}; J | V_{\nu\pi}^{\text{SDI}} | NP^{-1}; J \rangle \approx \frac{s_2}{2\pi \sin\theta_{\nu\pi}} + \frac{t_2}{2\pi \tan\theta_{\nu\pi}}, \quad (11)$$

where

$$\begin{aligned} s_2 &= 4(3a_0 + a_1), & t_2 &= \varphi(a_0 - a_1), \\ \varphi &= \mathcal{P}(-)^{\ell_{1\nu}+j_{1\nu}+\ell_{1\pi}+j_{1\pi}}. \end{aligned} \quad (12)$$

The classical limit of the shears matrix element for the SDI does not depend on the individual single-particle angular momenta but only on the shears angle, which is defined by the angular momenta J_ν and J_π of the blades and the total angular momentum J .

In Fig. 1 the exact shears matrix elements of the SDI are compared with their classical approximation for the neutron and proton angular momenta of the blades $J_\nu = J_\pi = 20$. The approximation is good for the stretched case, $J_\rho = j_{1\rho} + j_{2\rho}$, but deteriorates rapidly as J_ρ diminishes. However, in the region of interest, where the two angular momenta J_ν and J_π are close to orthogonal, $J^2 \approx J_\nu^2 + J_\pi^2$, the classical approximation is good, also for $J_\rho = j_{1\rho} + j_{2\rho} - 1$, and the geometric picture underlying the shears mechanism remains valid.

This analysis also reveals the limits of the validity of this geometric picture, as is illustrated in Fig. 2 which shows the shears matrix element of the SDI for the neutron and proton angular momenta $J_\nu = J_\pi = 12$. In one case these arise from aligned single-particle angular momenta ($j_{1\rho} = \frac{11}{2}$ and $j_{2\rho} = \frac{13}{2}$) and the classical approximation is seen to be reasonable. In the second case the single-particle angular momenta are larger ($j_{1\rho} = j_{2\rho} = \frac{21}{2}$) and they are not aligned ($J_\rho = j_{1\rho} + j_{2\rho} - 9$), leading to a breakdown of the shears interpretation. The alignment of the particles in high- j orbits, introduced here by hand, is in a more realistic shell-model calculation due to their interaction with particles in low- j orbits [9].

The classical expression (11) is reminiscent of the interpretation of nuclear matrix elements in terms of the angle between the vectors of the single-particle angular momenta, as proposed by Schiffer [21] and developed in more detail by Molinari *et al.* [22]. In fact, it can be

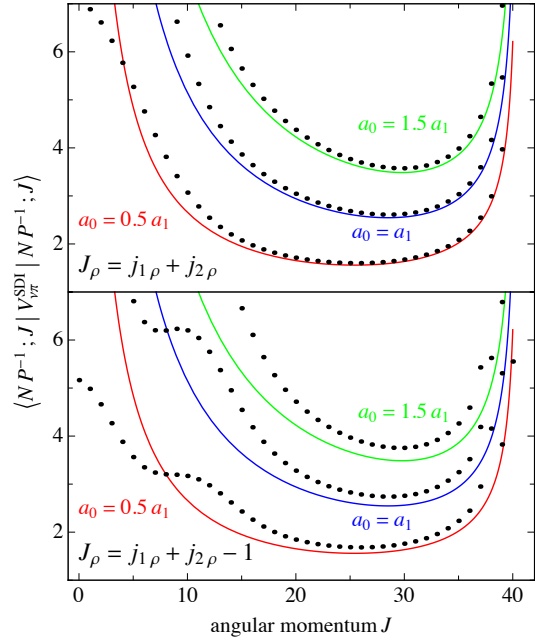


FIG. 1: The exact expression (1) for the 2p-2h shears matrix element of the SDI (dots) compared with its classical approximation (11) (lines) for neutron and proton angular momenta $J_\nu = J_\pi = 20$. The single-particle angular momenta are $j_{1\rho} = \frac{19}{2}$ and $j_{2\rho} = \frac{21}{2}$ (top), and $j_{1\rho} = j_{2\rho} = \frac{21}{2}$ (bottom). Results are shown for three choices of the ratio a_0/a_1 . The matrix element is in units a_1 .

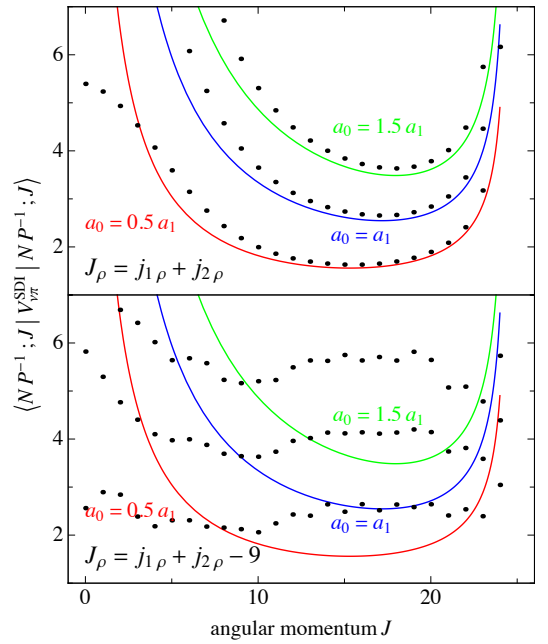


FIG. 2: Same as Fig. 1 for neutron and proton angular momenta $J_\nu = J_\pi = 12$ and single-particle angular momenta $j_{1\rho} = \frac{11}{2}$ and $j_{2\rho} = \frac{13}{2}$ (top), and $j_{1\rho} = j_{2\rho} = \frac{21}{2}$ (bottom).

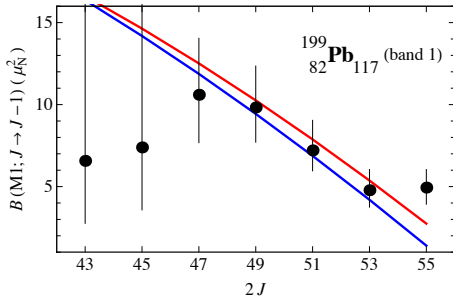


FIG. 3: Experimental (points) and calculated (lines) $B(M1)$ values for band 1 in ^{199}Pb as a function of twice the angular momentum J . The red line is the exact shell-model expression and the blue line is its classical limit (13).

shown that the classical limit of the 1p-1h matrix element $\langle j_\nu j_\pi^{-1}; J | V_{\nu\pi}^{\text{SDI}} | j_\nu j_\pi^{-1}; J \rangle$ leads to the same dependence on the angle $\theta_{\nu\pi}$ as in Eq. (11) but with coefficients s_1 and t_1 that depend differently on the strengths a_T of the interaction.

The present results make contact with the semi-classical analysis [5, 6] in terms of an interaction $V_0 + V_2 P_2(\cos \theta_{\nu\pi})$, assumed to exist between the blades of the shears bands. In line with the intuitive picture one has of the shears mechanism, this interaction necessarily implies a shears-band head with $\cos \theta_{\nu\pi}^0 \approx 0$ or, alternatively, a minimum energy for $J^2 \approx J_\nu^2 + J_\pi^2$ when the angular momentum vectors \vec{J}_ν and \vec{J}_π are orthogonal. Our analysis shows that this is not generally valid since a minimum energy is obtained from Eq. (11) for $\cos \theta_{\nu\pi}^0 \approx -t_2/s_2 = \varphi(a_1 - a_0)/4(3a_0 + a_1)$. Therefore, if the isoscalar and isovector interaction strengths are different, a minimum energy is found for a *non-orthogonal* configuration.

Shears bands are characterized by strong M1 transitions that decrease with increasing angular momentum J . For a general configuration $|NP^{-1}; J\rangle$, where $|N\rangle$ is an m -particle neutron and $|P^{-1}\rangle$ an m' -hole proton configuration with angular momenta J_ν and J_π , respectively, standard recoupling techniques [23] lead to the following

classical expression for the $B(M1)$ values:

$$B(M1; J \rightarrow J - 1) \approx \frac{3}{4\pi} (g_\nu - g_\pi)^2 \frac{(2J_\nu + 1)^2 (2J_\pi + 1)^2}{16J(2J + 1)} \sin^2 \theta_{\nu\pi}, \quad (13)$$

where g_ν and g_π are the g factors of the neutron and proton configurations $|N\rangle$ and $|P^{-1}\rangle$, respectively. This result agrees with that obtained from a schematic vector-coupling model [24]. The expression (13) can be tested in ^{199}Pb where lifetimes of some shears-band levels have been measured [25]. In particular, the states in band 1 with $\frac{43}{2} < J < \frac{55}{2}$ have the suggested [26] configuration $\nu(1i_{13/2}^{-3})_{33/2} \times \pi(1h_{9/2}1i_{13/2})_{11}$, from where the g factors can be obtained, $g_\nu = -0.29 \mu_N$ and $g_\pi = 1.03 \mu_N$. (Similar configurations are confirmed from measured dipole and quadrupole moments in neighboring lead isotopes [27, 28].) Application of Eq. (13) with $J_\nu = \frac{33}{2}$ and $J_\pi = 11$ leads to the result shown in Fig. 3 (in blue), which is seen to be close to the exact result (in red). In the spin region $\frac{47}{2} \leq J \leq \frac{53}{2}$, where the above configuration is thought to apply, agreement is obtained.

The data on M1 transitions indicate that fixed neutron and proton configurations do not apply to an entire but only to part of a shears band. For this reason it will be difficult to use energy formulas like Eq. (11) with constant coefficients s_2 and t_2 for an entire band. The present analysis suggests however that, under certain conditions of angular-momentum alignment, the generic form of the expression (11) is approximately valid with coefficients s_i and t_i depending on the structure of the neutron and proton configurations that apply to certain ranges of the total angular momentum J . This problem is currently under study.

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