Theoretical Proof That Most Nuclei Must Have Positive Electric Quadrupole Moments

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Within a theory which unifies the nuclear collective and single-particle models and which is valid for arbitrary vibrational amplitudes, the average positiveness of the electric quadrupole moments follows from two requirements: (1) The nucleons have to stay within the range of nuclear forces for a strongly deformed nucleus; (2) the wave functions on the average do *not* show any preference for prolate or oblate shape.

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To the author's knowledge there is no simple theoretical explanation for the experimental fact that most nuclei have positive electric quadrupole moments. The shell-model values for these moments are by far too small and do not show a preference for positive values. The collective and the unified models do not offer a simple explanation either. All this is standard knowledge of theoretical nuclear physics and can be found in almost any book on this subject (see, e.g., Eisenberg and Greiner[1] and Hornyak[2]).

The reason for the failure of the collective model comes from its restriction to small nuclear deformations. The author has proposed a theory which is valid for arbitrary deformations. It starts from a transformation[3] which defines collective and new single-particle variables, and is brought into full agreement with the conventional unified model after the introduction of spin-orbit coupling and the restriction to small deformations.[4,5]

The latter restriction will not be used in this paper. It will be seen that deviations from the conventional unified theory (which is valid for small deformations only) are responsible for the large number of nuclei with positive electric quadrupole moments.

The transformation (Ref. 1) is defined by ($\mathbf{r}_n$ are space vectors of the nucleons in the center-of-mass system)

$$\mathbf{r}_n = s_{n1}\mathbf{y}_1 + s_{n2}\mathbf{y}_2 + s_{n3}\mathbf{y}_3, \quad (1)$$

with the constraints

$$\sum_{n=1}^{A} s_{nj} = 0, \quad (2)$$

$$\sum_{n=1}^{A} s_{nj} s_{nk} = \delta_{jk}, \quad (3)$$

$$\mathbf{y}_i \cdot \mathbf{y}_k = y_i^2 \delta_{ik}. \quad (4)$$

β and γ are defined as follows:

$$y_i = (y/\sqrt{3})[\cos\beta + \sqrt{2}\sin\beta\cos(\gamma - i2\pi/3)]. \quad (5)$$

The volume element is a product of two factors, the first depending solely on the collective coordinates, and the second on the s_{nj}. The latter is of no importance for the discussion of this paper. The collective part has the form

$$\{(y_1y_2y_3)^{A-4}|y_1^2 - y_2^2||y_2^2 - y_3^2||y_3^2 - y_1^2|\, dy_1\, dy_2\, dy_3\}\{\sin\theta\, d\theta\, d\phi\, d\psi\}. \quad (6)$$

Here ϕ, θ, and ψ are Euler angles defining the directions of the three orthogonal vectors $\mathbf{y}_i$ in the laboratory system. In terms of y, β, and γ the part of (6) depending on y_1, y_2, and y_3 is

$$(y^{3A-4}dy)\, g(A,\beta,\gamma)\, |\sin^3\beta \sin 3\gamma|\, d\beta\, d\gamma, \quad (7)$$

with

$$g(A,\beta,\gamma) = (\cos^3\beta - \tfrac{3}{2}\sin^2\beta\cos\beta + \tfrac{1}{2}\sqrt{2}\sin^3\beta\cos 3\gamma)^{A-4}(\cos^3\beta - \tfrac{3}{8}\sin^2\beta\cos\beta - \tfrac{1}{16}\sqrt{2}\sin^3\beta\cos 3\gamma). \quad (8)$$

The volume element in the theory of Bohr and Mottelson[6] is

$$d\tau_{\mathrm{BM}} = |\sin^3\beta\sin 3\gamma|\, d\beta\, d\gamma. \quad (9)$$

The consequences of the additional factors in (7) will be discussed under the assumption of axial symmetry, that is, $\gamma = n\pi/3$. Throughout the derivation wave functions will be used which have equal amplitudes for the prolate and the oblate shapes of nuclei. In the Bohr-Mottelson theory one would then have a vanishing collective quadrupole moment, while here it is positive because of the change of the volume element when going from prolate to oblate shape or vice versa, that is, when replacing $\gamma = n\pi/3$ by $\gamma = (n/3+1)\pi$.

To obtain axial symmetry it is assumed that the wave function Ψ has a very strong maximum at $\cos^2\gamma = 1$. The extreme case of a δ function is assumed for simplicity,

$$\Psi^*\Psi = [\delta(1-\cos\gamma) + \delta(1+\cos\gamma)]\chi^*\chi. \quad (10)$$

No γ dependence of χ is assumed, so that one has the announced complete symmetry of Ψ between oblate and prolate shapes. As $|\sin 3\gamma| d\gamma = \pm(4\cos^2\gamma - 1) d\cos\gamma$, integration over γ is readily carried out. One obtains with (7) and (8) (Q is the quadrupole moment operator, see below)

$$\int_0^{2\pi} \Psi^* Q(\gamma) \Psi g(A,\beta,\gamma) |\sin 3\gamma| d\gamma = 3\chi^*\chi[Q(0)g(A,\beta,0) + Q(\pi)g(A,\beta,\pi)]. \quad (11)$$

In the Bohr-Mottelson theory one would have $g=1$ and the collective part of Q would yield a vanishing result from Eq. (11). Here a positive collective quadrupole moment is found because of the additional factors g, which behave unsymmetrically when going from prolate to oblate shape. One may say this in more plausible words: The available configuration space is larger for the prolate phase than for the oblate phase; because, given a certain interval $\Delta\beta$, the probability to find the nucleus within this interval and with the prolate shape is proportional to $\chi^*\chi g(A,\beta,0)\Delta\beta$, while the probability for the oblate shape is $\chi^*\chi g(A,\beta,\pi)\Delta\beta$. The latter is smaller. The reader may easily check this for all $A > 4$ and the known deformations β:

$$g(A,\beta,0) > g(A,\beta,\pi). \quad (12)$$

For large A the left-hand side in (12) is large compared to the right-hand side. So the probability for prolate shape is in any case larger, and in most cases large compared to the probability for oblate shape.

The effect is enhanced by the y-dependent factor in (7). y is defined by

$$y^2 = \sum_{i=1}^{A} r_i^2. \quad (13)$$

Requiring that the distances of the nucleons to their nearest neighbors do not change when deforming the nucleus, one can show that y^2 must increase with $|\beta|$, but more strongly for the prolate than for the oblate shape. Therefore, qualitatively it has the same effect as that of g, Eq. (8), but a numerical check showed that the effect of g is much stronger. Hence, in the following it is assumed that the expectation value of y^2 for given β is the same for prolate and oblate shapes.

The quadrupole moment operator has the following form for the case of axial symmetry,[5] with the sum running over the protons:

$$Q \approx \sum_{n=1}^{Z} s_n^2 y^2 \left\{ (\sqrt{2}/3) D_{00}^2 \sin 2\beta \cos\gamma + \tfrac{4}{15}(5\pi)^{1/2} \sum_K (-)^K D_{0K}^2 y_{2K} \right\}. \quad (14)$$

Nuclei near closed shells are not considered, because only nuclei between closed shells have the large and predominantly positive quadrupole moments. Their wave functions are well described in the strong-coupling approximation and are proportional to

$$D_{JJ}^j \chi_{jJ} + (-)^{J+j} D_{J,-J}^j \chi_{j,-J}. \quad (15)$$

Here χ_{jJ} is the wave function in the body-fixed frame of reference and depends on the s_{nj} and the spins only. j is the total internal angular momentum and J its projection on the symmetry axis, which is equal to the total angular momentum. For the dependence of the wave function Ψ on the collective coordinates it is assumed that there are strong maxima for special values of y_0 and β_0; again δ functions are assumed for simplicity:

$$\chi^*\chi = N^2 \delta(y-y_0)\delta(\beta-\beta_0)\frac{2J+1}{16\pi^2}|D_{JJ}^j \chi_{jJ} + (-)^{J+j} D_{J,-J}^j \chi_{j,-J}|^2. \quad (16)$$

Here N^2 is the squared normalization factor. With (14) and (16) one finds for the collective part q_c of the quadrupole moment [that is, the expectation value of the first term in (14)]

$$q_c \approx \frac{3}{5}\sqrt{2}\frac{Z}{A}\rho^2 A^{5/3} \frac{J(2J-1)}{(J+1)(2J+3)} f(A,\beta_0). \quad (17)$$

Here

$$f(A,\beta_0) = \sin 2\beta_0 \frac{g(A,\beta_0,0) - g(A,\beta_0,\pi)}{g(A,\beta_0,0) + g(A,\beta_0,\pi)}, \quad (18)$$

$$y_0^2 = \tfrac{3}{5} A^{5/3} \rho^2, \quad (19)$$

$$\rho \approx 1.2 \times 10^{-13}\ \text{fm}. \quad (20)$$

The factor $f(A,\beta_0)$ is always positive although the wave function does not show any preference for prolate or oblate shape. Numerical values of (18) are given in Table I for $\beta = 0.25$ and $J=2$: It is seen that these quadrupole moments have the order of magnitude of the experimental values.

In reality the wave functions will show preferences for either oblate or prolate shape. That means, for Eq. (10), that the two δ functions will have different factors. The collective quadrupole moments will then be either above or below the average values, which are roughly those of Table I.

In conclusion it can be said that the many-particle

TABLE I. Collective quadrupole moments for wave functions which show no preference for oblate or prolate shape.

Z	A	q_c (b)
24	50	0.4
44	100	1.6
63	150	3.2
80	200	5.1

coordinates[4] have helped to find the simple reason for the mostly positive electric quadrupole moments of nuclei. It is the change of the volume element when going from prolate to oblate shape, or—in other words—the difference in the available configuration space between prolate and oblate shapes.

Shell-model calculations including many nucleons show the preference of nuclei for the prolate shape.[7] But as these calculations use ordinary single-particle coordinates and are performed on a computer, the simple reason for that property could not be seen.

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