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Shapes and Symmetries of Nuclei

A. Góźdź[1], **A. Pędrak**[1], **A. Dobrowolski**[1], **A. Szulerecka**[1]
A. Gusev[2], **S. Vinitsky**[2]

[1]Institute of Physics, Department of Mathematical Physics, University of Maria Curie-Skłodowska, 20 031 Lublin, Poland
[2]Joint Institute for Nuclear Research, Dubna, Russia

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Abstract. In this paper the notion of nuclear shape and its relation to the deformation parameters and symmetries is shortly discussed.

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1 Shapes

The notion of shape seems to be a natural notion for human thinking. However, a formal description of shapes is already not so obvious. The simplest, though not unique, is the description of geometric shapes, see e.g. [1], who writes: “In this paper ‘shape’ is used in the vulgar sense, and means what one would normally expect it to mean. [...] We here define ‘shape’ informally as ‘all the geometrical information that remains when location, scale[1] and rotational effects are filtered out from an object.’” In the case of nuclei this definition of shape is unsatisfactory. First of all, nuclei are quantum objects which cannot have a sharp boundary. Second, they are not rigid objects. Third, less fundamental but important, because of the very high nuclear incompressibility, uniformly scaled nuclei, though formally have the same geometrical shape, correspond to different energies and in fact they can have different intrinsic structures. The last feature confirms also the known property that geometric shapes and dynamics are related to each other.

As it was mentioned, nuclei are non-rigid objects. This problem has been already considered in respect to macroscopic objects, e.g. [2]. In this book, a concept of non-rigid shape similarity is introduced to answer the question: how to compare shapes that are susceptible to deformations? The idea is to search for deformation invariants. For example: movement of fingers in our hand, which is obviously a non-rigid object, is constrained by the length of bones. Thus in this case we can find a set of partial isometries, which in fact define the ’shape’

[1]scaling = uniform scaling only

of our hand. The second important problem in the case of non-rigid shapes is to find a quantitative measure of 'distance' between two shapes which allows us to define 'small' changes of shapes and, in fact, a continuous dynamics allowing for the description of shape evolution. Both problems, in the case of nuclei, are still open.

Nuclei are quantum objects, thus the corresponding 'quantum shape' should be a diffuse shape similar rather to a cloud without any sharp boundaries than to a geometric shape. This 'cloud' can be reproduced from the quantum wave function of the nucleus as the probability density plot represented by the square of the absolute value of the required wave function $|\Psi(x)|^2$. Having this wave function, we can calculate all nuclear properties, including the quantum shape. However, because of fundamental difficulties in using this straightforward description of quantum shapes, the geometric approach is very helpful, though one needs to keep in mind the quantum limitations of this notion.

1.1 Shapes and space of states

An interesting possibility allowing us to relate geometric shapes to the quantum world is to use the expansion of these shapes into an appropriate basis. Using such a basis one can parametrize geometric shapes uniquely.

For this purpose let us denote by q_1, q_2 and q_3 three continuous real functions of two real variables. These functions nearly always can be interpreted in R^3 as equations defining a surface described in terms of some curvilinear coordinates

$$q_k = q_k(u,v), \quad k = 1,2,3, \tag{1}$$

where $u, v \in S$, with $S \subset R^2$ being a compact subset.

Assume now that $q_k \in L^2_\rho(S)$, where $L^2_\rho(S)$ is the Hilbert space of complex square integrable functions with weight $\rho(u,v) \geq 0$, i.e. satisfying the following condition

$$\int_S dudv\rho(u,v)|q(u,v)|^2 < \infty. \tag{2}$$

The scalar product is defined using the above weight function

$$(f_1|f_2) = \int_S dudv\rho(u,v)f_1(u,v)^\star f_2(u,v). \tag{3}$$

The next step is to choose an appropriate orthonormal basis $\{e_n(u,v)\}$ in $L^2_\rho(S)$, which will allow for a clear physical/geometrical interpretation of the expansion coefficients $\alpha_{n,k}$ in the standard expansion

$$q_k(u,v) = \sum_n \alpha_{n,k}\, e_n(u,v). \tag{4}$$

To fulfil the last condition, one possibility is to introduce a set of commuting quantum observables for which the basis $\{e_n(u,v)\}$ will consist of eigenvectors of these observables. In this case these commuting quantum observables become the shape invariants mentioned above. Another possibility is to use some required symmetries and apply the bases of irreducible representations for the corresponding symmetry groups.

The expansion coefficients $\alpha_{n,k}$ are expressed in terms of the scalar product in $L^2_\rho(S)$ as

$$\alpha_{n,k} = \int_S dudv\, \rho(u,v)\, e_n(u,v)^\star q_k(u,v), \tag{5}$$

and they can be considered as new deformation parameters describing a family of surfaces.

The best known example of this idea consists of spherical tensors obtained in the following way. We choose three functions q_k, so that the first function $q_1 = r$ is interpreted as the radial variable in R^3, while the remaining two functions $q_2 = \theta$ and $q_3 = \phi$ are interpreted as the spherical angles θ, ϕ which, in turn, are identified with the parameters $u = \theta$, $v = \phi$ of our construction.

In this case, the natural choice of the basis $\{e_n(u,v)\}$ is related to the angular momentum operators $\hat{J}^2$ and $\hat{J}_z$, thus the basis is identified with the spherical harmonic functions $\{e_n(u,v)\} \to \{Y_{lm}(\theta,\phi)\}$. The expansion (4) can now be written in the traditional form as follows

$$r = R(\theta,\phi) = R_0 \left(1 + \sum_{\lambda,\mu} \alpha^{(lab)\star}_{\lambda\mu} Y_{\lambda\mu}(\theta,\phi) \right). \tag{6}$$

The other two expansions are not needed, because $q_2 = \theta$ and $q_3 = \phi$ are dependent variables.

This parametrization of nuclear shapes is often used in nuclear single particle/collective models. A set of commuting operators can be used in any quantum mechanical model of a "particle" moving in a two dimensional compact space, e.g. motion in a two dimensional potential well. Choosing, in addition, the appropriate set of the curvilinear coordinates $\{q_k\}$ in order to get a closed surface, one can get a useful parametrization of this surface.

To summarize, one needs to notice a few important problems.

- What are the invariants of nuclear deformations?
- What is the "distance" between nuclear shapes? Maybe the difference of some characteristic energies related to these shapes?

These problems are still unsolved.

In addition, there is a set of difficulties related to this method. Two of them are mentioned here.

- The problem of ”monster shapes”. Sometimes it happens that a given parametrization of geometric shapes leads to shapes which correspond to unphysical nuclear configurations. This is in general a problem of the relation between the geometric definition of the deformation parameters and the ”shapes” related to quantum states.
- The center of mass is strongly correlated with any parametrization of a shape. To work in the center of mass one needs to impose the appropriate three constraints on the deformation parameters.

1.2 Examples of ”monster shapes”

The first problem, i.e. the problem of ”monster shapes” is less recognized till now. The second one, i.e. the problem of the center of mass, leads to some complications but it has been solved.

Let us consider shortly the first problem of ”monster shapes” in the case of the nuclear surfaces considered above

$$R(\alpha;\theta,\phi) = R_0 \left(1 + \sum_{\lambda,\mu} \alpha^{(lab)\star}_{\lambda\mu} Y_{\lambda\mu}(\theta,\phi) \right) . \tag{7}$$

For large deformations one can observe unrealistic shapes. In Figure 1 a few examples of monster shapes have been plotted. If the deformation parameters

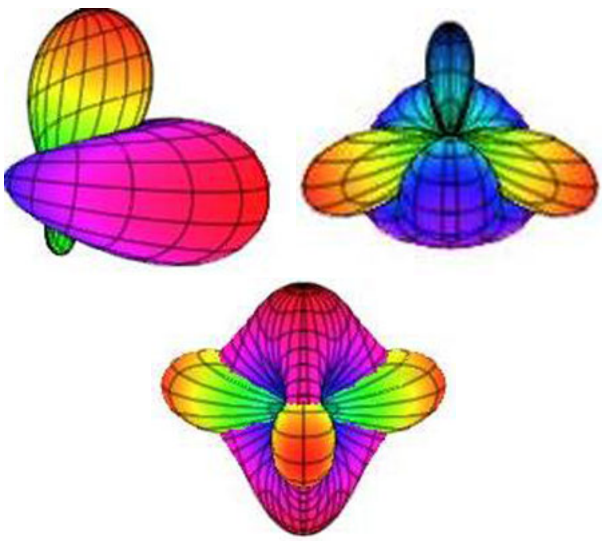

Figure 1. (Color online) The monster dipole, quadrupole and quadrupole-octupole shapes obtained for large values of the deformation parameters.

are used as parameters and not as variables, as for example in not-self-consistent mean-field approaches, one can always omit undesired configurations by hand. However, if the deformation parameters are used as collective variables, then the monster shapes cannot be omitted because integration in the scalar product runs over the whole domain of deformations. The only thing we can do is to hope that the monster shapes will have only very small contributions to the collective wave functions. In most cases, the wave function should be strongly damped for large values of these collective variables.

1.3 Hamiltonian and shapes

In many nuclear models one uses Hamiltonians parametrized by some parameters which are often called "deformation parameters". One of the first examples is the well known single particle Nilsson Hamiltonian [3]

$$H = \frac{-\hbar^2}{2m}\triangle + \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right). \tag{8}$$

The frequencies of this harmonic oscillator Hamiltonian are considered as deformation parameters because the equipotential energy surfaces are represented by ellipsoids with axes parameters $\{a_i\}$ related to the frequencies $\{\omega_i\}$, $i = x, y, z$, by

$$\omega_i = \omega_0 \frac{r_0}{a_i}, \quad \omega_x \omega_y \omega_z = \omega_0^3, \text{ volume conservation.}, \tag{9}$$

where $r_0 \sim 1.2A^{1/3}$ is the nuclear radius for equivalent spherical nucleus. Nuclear 'shapes' in this model are identified with these ellipsoids.

One assumes the same interpretation of nuclear "shapes" for Hamiltonians in which the equipotential energy surfaces are identified with $r = R(\alpha; \theta, \phi)$, as seen in Eq. (6). In this case the single particle Hamiltonian can be written, in general form, as

$$H = \frac{-\hbar^2}{2m}\triangle + V(\mathrm{dist}(\vec{r} - R(\alpha; \theta, \phi))), \tag{10}$$

where the dist function measures the distance between the position of the particle represented by the radius vector $\vec{r}$ and the surface $r = R(\alpha; \theta, \phi)$.

Another situation occurs when deformation parameters become collective variables, as it happens in nuclear collective models. In this case the collective variables are quantum observables represented by the appropriate "position" operators. For the deformation parameters, which are only numbers, this is not the case. In nuclear collective models one needs to distinguish between static and dynamic deformation. Static deformations, by analogy to classical mechanics, occur at the points in which the potential energy has minima (sometimes it happens that more than one minima exist). The simplest example of such a deformation is the shifted harmonic oscillator in the collective variable ξ

$$H = \frac{-\hbar^2}{2m}\triangle + \frac{m}{2}\omega_0^2(\xi - \xi_0)^2. \tag{11}$$

In usual language the case with $\xi_0 = 0$ is called the "spherical" oscillator, while the case with $\xi_0 \neq 0$ is called a deformed oscillator. However, one needs to notice that even in the case in which each value of the collective variable ξ corresponds to a given geometric shape, the collective wave function $\psi(\xi)$ as well as any nucleus in this state, do not represent any fixed shape. It only represents the probability density $|\psi(\xi)|^2$ that this nucleus has a shape corresponding to the value ξ. Obviously, using such a wave function one can calculate the average shape $< \xi >= \langle\psi|\xi|\psi\rangle$ as well as the distribution of shapes (variance) $\langle\psi|(\xi- < \xi >)^2|\psi\rangle$ around this average shape which is sometimes called the dynamic deformation. In this context, in general, it is difficult to speak about shapes in many collective models. One needs to explicitly define the notion of shape for the particular model.

2 Geometry versus Symmetry

One can expect that quantum shapes, considered as a kind of "cloud" consisting of nuclear matter, possibly have some intrinsic symmetry which influences not only the dynamics but also the Hamiltonian symmetry of this nuclear system.

To show this property we apply the Generator Coordinate Method with the Gaussian Overlap Approximation to the rigid rotor [4–6].

The generating function of the rigid rotor can always be written as

$$|\Omega\rangle = \hat{R}(\Omega)|\alpha\rangle, \tag{12}$$

where $\hat{R}(\Omega)$ denotes the rotation operator in the many-body nucleon space and $|\alpha\rangle$ is the intrinsic many-nucleon generator function representing a deformed nucleus. The parameter α is a static deformation parameter (no vibrations are supposed to occur).

As a first example let us consider the axially symmetric intrinsic generator function $|\alpha\rangle$ and the axially symmetric intrinsic deformed Hamiltonian $H(\alpha)$. We assume that the Hamiltonian has this form at the "moment" when both the laboratory and the intrinsic frames coincide. At any other "moment" the Hamiltonian is rotated

$$H' = \hat{R}(\Omega)H(\alpha)\hat{R}(\Omega)^\dagger = \hat{R}(\Omega_1, \Omega_2, 0)H(\alpha)\hat{R}(\Omega_1, \Omega_2, 0)^\dagger.. \tag{13}$$

The third angle is equal to 0 ($\Omega_3 = 0$), because of axial symmetry.

The calculated GCM+GOA metric tensor has the non-vanishing components

$$\begin{aligned} g_{11} &= \sin(\Omega_2) < \alpha|(I_x)^2|\alpha >, \\ g_{22} &=< \alpha|(I_x)^2|\alpha >, \end{aligned} \tag{14}$$

where $\hat{I}_k$ are components of the angular momentum operator in the nucleon space.

Similarly, the inverse mass tensor is diagonal

$$(M^{-1})_{11} = \sin(\Omega_2)^2 (M^{-1})_{22}, \\ (M^{-1})_{22} = (M^{-1})_{22}(\alpha), \tag{15}$$

i.e. $(M^{-1})_{22}$ is a constant dependent here only on the static deformation.

The corresponding inertia parameter can thus be written as

$$\mathcal{J}^{-1} = \frac{(M^{-1})_{22}(\alpha)}{< \alpha|(I_x)^2|\alpha >^2}, \tag{16}$$

being a function only of the deformation parameter α, as it should be.

It turns out that the rotor Hamiltonian H_{rot} generated by the GCM+GOA method has higher symmetry than both the intrinsic generating function, which describes the quantum shape of the rotating body (as a ”cloud”), and the generating Hamiltonian. The rotor Hamiltonian is spherically symmetric

$$H_{rot} = \frac{1}{2}\mathcal{J}^{-1}(\alpha)\hat{J}^2 + V(\alpha). \tag{17}$$

The corresponding eigenenergies and eigenfunctions are

$$E_{rot;J} = \frac{1}{2}\mathcal{J}(\alpha)^{-1}\, J(J+1), \\ r^J_{M,K=0}(\Omega) = \sqrt{2J+1}D^{J\star}_{M0}(\Omega). \tag{18}$$

As we see, the axially symmetric shape of a nucleus allows only for $K = 0$, where K is the quantum number representing the third component of the angular momentum operator. In this case the Hamiltonian of this rotor, H_{rot}, is rotationally invariant with respect to both the laboratory and intrinsic rotations. One needs to notice that the resulting Hamiltonian has higher symmetry than the initial Hamiltonian and the intrinsic generating function.

Let us now break the axial symmetry of the intrinsic generating function to the dihedral group D_2. In this case the generating function has formally the same shape

$$|\Omega\rangle = \hat{R}(\Omega)|\alpha\rangle, \tag{19}$$

but the intrinsic generating function is now invariant only in respect to rotations about the x, y, z axes by an angle π

$$|\alpha\rangle = e^{-i\pi\hat{I}_k}|\alpha\rangle, \tag{20}$$

where the correspondence among indices $(k = 1) \to x$, $(k = 2) \to y$, $(k = 3) \to z$ has been used. In other words, the intrinsic generating function is D_2

invariant. As in the previous example, we assume that the intrinsic generating Hamiltonian $H(\alpha)$ is D_2 symmetric (at the "moment" when both the laboratory and the intrinsic frames coincide). At any other "moment" the Hamiltonian is

$$H' = \hat{R}(\Omega)H(\alpha)\hat{R}(\Omega)^{\dagger}. \tag{21}$$

In this case one gets the full metric tensor

$$g_{kk'} = \sum_{l=1}^{3} b_{kl}(\Omega)b_{k'l}(\Omega) < \alpha|(I_l)^2|\alpha >, \tag{22}$$

where the matrix b is

$$b(\Omega) = \begin{bmatrix} -\sin(\Omega_2)\cos(\Omega_3) & \sin(\Omega_2)\sin(\Omega_3) & \cos(\Omega_3) \\ \sin(\Omega_3) & \cos(\Omega_3) & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{23}$$

Thus in this case all three moments of inertia are fixed non-zero numbers (dependent only on the deformation parameter α).

As a result one gets that the corresponding rotor Hamiltonian, derived from the GCM+GOA approach, represents a general rigid quantum rotor

$$H_{rot} = \frac{1}{2}\sum_{k=1}^{3} \mathcal{J}_k^{-1}(\alpha)(\hat{J}_k)^2. \tag{24}$$

In the case in which two inertia parameters are equal, $\mathcal{J}_x(\alpha) = \mathcal{J}_y(\alpha)$, one gets the axially symmetric rotor, which is widely used in nuclear physics. The eigenenergies of the axially symmetric rotor are

$$E_{rot;JK} = \frac{1}{2}\left[\frac{J(J+1)-K^2}{\mathcal{J}_x(\alpha)} + \frac{K^2}{\mathcal{J}_z(\alpha)}\right]. \tag{25}$$

In this case one obtains non-zero values of the K quantum number, as it is commonly expected for an axially symmetric rotor. The corresponding eigenfunctions for $K \neq 0$ can be now written as

$$r^{(\pm)J}_{M,K}(\Omega) = \frac{1}{\sqrt{2}}\left[r^J_{MK}(\Omega) \pm r^J_{M,-K}(\Omega)\right]. \tag{26}$$

For $K = 0$ the eigenenergies and eigenvectors are the same as for the symmetric top, given in Eq. (18).

It is important to observe that the quantum shape of this rotor, represented by the intrinsic generating function (the appropriate mass density distribution), is different from the "macroscopic" axial symmetry which is implied by the quantum number $K \geq 0$. In addition, in this axial case the rotor Hamiltonian H_{rot} has axial symmetry, although the generating Hamiltonian has only dihedral symmetry.

As we see, the intrinsic symmetry represented by the intrinsic generating function and the microscopic Hamiltonian does not always coincide with the resulting symmetry of the collective Hamiltonian.

3 Conclusions

In this paper the notion of shape, as it is used in nuclear physics, has been shortly reviewed. The standard definition of geometric shapes treats them as invariants under three transformations: translations, rotations, and scaling. However, in the case of nuclear physics, scaling leads to a breathing mode which, due to high nuclear incompressibility, is related to rather high excitation energy, implying that a nucleus excited in this way should rather be treated as a different physical object, though having the same geometric shape. As a consequence, the nuclear geometric shape should be rather defined as the feature of the mass distribution of the nucleus which is invariant with respect to translations and rotations. In this analysis we neglected the fermionic nature of nucleons in nuclei, which requires some fine tuning of the geometrical structure of the nuclear shape.

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