Symmetries, Selection Rules

and

Why Dinosaurs had Small Heads

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What an imperfect world it would be if every

symmetry was perfect

Abstract

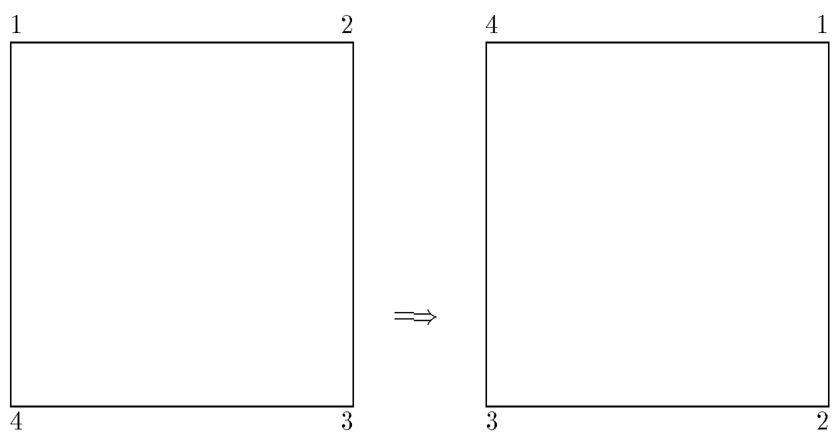
A lecture for students of quantum mechanics on the role of symmetry in physics with a particular emphasis on examples. The consequences of changes of scale as it affects the dimensions of animals is outlined. The relationship of symmetry considerations to selection rules and the observation of forbidden transitions is discussed.

■ Introduction

Symmetry plays a major role in modern physics and in this lecture I propose start by giving some examples of symmetries and mention their relevance to the familiar conservation laws. Considerations of scaling lead to a simple discussion of why dinosaurs had small heads. I shall then give a brief discussion of angular momentum selection rules and the way symmetry considerations lead to selection rules. Methods of breaking symmetry selection rules in atomic are reviewed and the distinction between rotations through 2π and 4π illustrated by some demonstration experiments. After consideration of forbidden transitions in gaseous nebulae, induced by nuclear magnetic moment interactions we conclude by considering the breaking of selection rules in crystals containing trivalent holmium ions by a similar process.

■ Examples of Symmetry

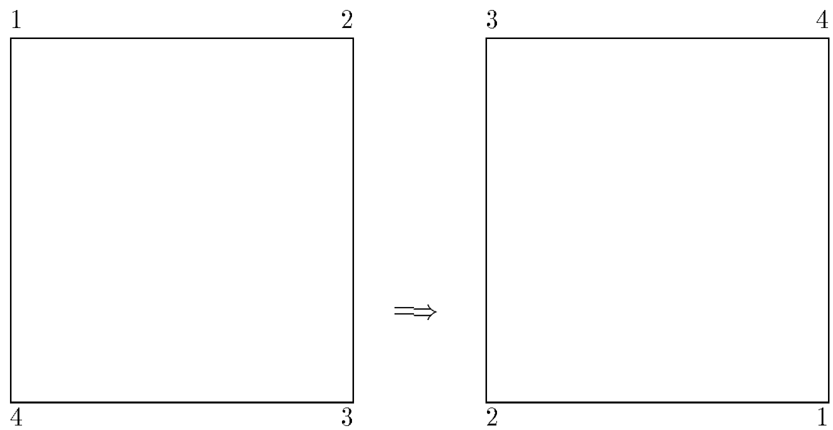
Symmetry and invariance are closely related. Symmetries are usually associated with an operation on a system that transforms it into itself in such a manner that the system after the transformation is indistinguishable from its initial state. If the symmetry is perfect, which is rarely the case, then it should be experimentally impossible to distinguish any change in the system after carrying out the symmetry transformation. A simple example is the case of a square lying on a plane surface. If the square is rotated through an angle of 90^o about its centre it should be indistinguishable from the original unrotated square. If that is the case then the square is said to be symmetric with respect to a rotation through a finite angle of 90^o about its centre. The properties of the square are said to be *invariant* with respect to such a rotation. In picturing such a transformation it is useful to attach the integers $1, 2, 3, 4$ to the vertices of the original square and to display the rotated square displaced from the original square as below



rotation

Note that our rotation could be regarded as equivalent to a permutation of the vertices of the square such that $1 \to 2, 2 \to 3, 3 \to 4, 4 \to 1$. It is not difficult to see that there are eight distinct permutations that leave our square invariant and each of these permutations can be associated with either a rotation about the centre of the square or a reflection about the diagonals or bisectors of the square. This gives an example of a *finite symmetry* characterized by a finite number of symmetry operations which form the elements of a *finite group.*

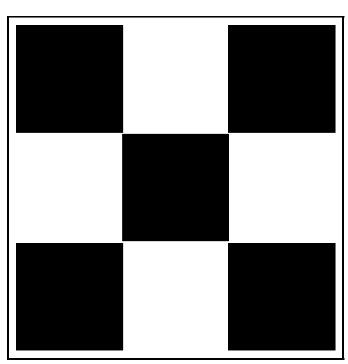
Our square is also symmetric with respect to an inversion through its centre. In that case the inversion symmetry is equivalent to a rotation through 180^o about the centre as seen below



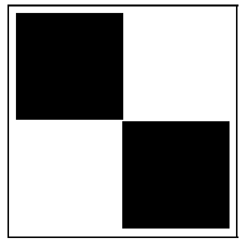
inversion

The Platonic solids, the cube, octahedron, dodecahedron and icosahedron all posssess a centre of inversion which, however, can not be made equivalent to any set of rotations.

We could decorate our square and still leave a square that has the full symmetry of the plain square as shown, for example, below

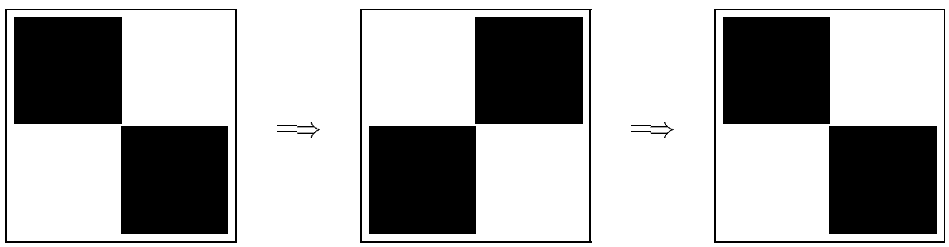


The figure below clearly no longer possesses the symmetry of the plain square as clearly it does not go into itself under a simple rotation of 90^o about its centre.



However, we could extend our symmetry by introducing a more complicated transformation - first carry out the rotation and then a counterchange operation that turns black into white and white into black.

This two step process is illustrated below.



rotation **counterchange**

This is an example of a black and white symmetry beautifully outlined in four articles published by H.J. Woods in the British Journal of the Textile Institute in the early 1930's, the counterchange operation arising naturally in the production of textiles. These Black and White groups are commonly referred to as Shubnikov groups though it is clear that Woods work preceded that of Shubnikov. It was Landau who supplied the interpretation in the physics of magnetism by regarding the counterchange operation as the equivalent of flipping a spin.

Permutational symmetry is important in considering the interchange of identical objects. A diatomic molecule with each atom being of the same isotope will exhibit permutational symmetry - interchange of the two atoms leaves the molecule in position indistinguishable from its former position. If the two atoms involve different isotopes then the permutational invariance is broken.

The preceding examples all involve finite symmetry transformations. Other examples can involve *continuous transformations*. Thus a blank coin will exhibit cylindrical symmetry with respect to any rotation about an axis perpendicular to its centre. A sphere devoid of any markings and perfectly regular may be rotated into itself by any rotation about any axis that passes through its centre. An atom sitting in free space exhibits spherical symmetry. Since there is no preferred direction in space there is no preferred direction to align the angular momentum of the atom with the result that the $2J+1$ states $|JM\rangle$ are degenerate. Break the spherical symmetry by placing the atom in a magnetic field which destroys the spherical symmetry locally and the degeneracy is lifted as in the Zeeman effect.

■ Continuous and Discrete Symmetries

The above examples of symmetries may be divided into two classes, *continuous* and *discrete*. Discrete symmetries such as reflections, inversions, permutations and finite rotations are associated with *multiplicative quantum numbers* whereas continuous symmetries are associated with *additive quantum numbers* such as, for example, angular momentum addition.

■ Changes of Scale

There is a class of transformations that amount to simply a change of scale as seen for example in the Russian $1Rb$ and $100Rb$ coins. (After 1 January 1995 it will be possible to substitute Polish coins for this example!). The circular shape of the coins is preserved but there size is increased. This is an example of a *dilation* though some may refer to it as an inflation. In the period of gold coinage the size of the coin often accurately reflected its value.

The concept of scale and changes of scale plays an important role in physics and the failure to appreciate this concept can lead to catastrophic consequences. It has been known since Greek times, at least, that the area, $A_\circ$, enclosed by a circle of radius r is given by

$$A_\circ = \pi r^2$$

while the surface area, A_{sphere}, was

$$A_{sphere} = 4\pi r^2$$

The volume, V_{sphere}, of a sphere of radius r was known to be

$$V_{sphere} = \frac{4}{3}\pi r^3$$

From the above three elementary results can follow profound conclusions.

It is a familiar observation that small animals maintain a much higher activity than large animals and must metabolise food more rapidly than larger animals. Let us with the usual physicists licence model an animal as a sphere. Consider a small sphere and a large sphere both at a temperature T. The total heat content of a sphere will be proportional to the *cube* of its radius while the heat radiated from a sphere will be proportional to its surface area and hence to the *square* of its radius. Thus

$$\frac{\text{Heat lost by sphere}}{\text{Heat content of sphere}} \propto \frac{1}{r}$$

Thus the ratio depends on the inverse of the radius of the sphere. The larger the sphere the smaller is the ratio. This leads us to expect that small animals will lose heat, in relationship to their size, faster than large animals and hence will need to metabolise food more rapidly than large animals as observed. By the same reasoning we expect babies to be more susceptible to temperature changes than adults which is why they are provided with better insulating clothes than adults. Now to

- **Why do Dinosaurs have small heads?**

Let us model a small dinosaur by small sphere (the head) connected by a cylindrical rod (the neck) to a larger sphere (the body). What happens if the dinosaur grows and each characteristic radius is simply scaled? The head and body would grow as the *cube* of the radii but the *strength* of the neck will be proportional to its cross-sectional area *consider muscles* and hence as the *square* of its radius. Thus if the head grows in proportion to the body of the dinosaur it will rapidly outgrow the strength of its neck. Such a characteristic can be seen in most animals. The head of the infant relative to its body is significantly larger than for the adult animal.

It was Galileo who first pointed out that scaling lead to limits of the size of animals. In the case of whales the head scales and there is no neck. There the bouyancy of the water overcomes the force of gravity experienced by the land dwelling animals and of course whales become helpless out of water.

■ Lessons from Scaling

Failure to appreciate the significance of scaling effects has been the source of repeated industrial problems and failures. A pilot plant is designed and found to work and then it has been simply scaled for industrial production and often found not to work. When we change the scale of objects often new properties arise that are not noted on the small scale.

Gravitational forces are extremely weak, indeed the weakest of all known forces. In describing the properties of a small object they can be wholly neglected but for large objects such as the sun or in super novae they can become overwhelming.

A cubic cm of ^{239}Pu weighs about 19grams and can be safely carried in the pocket if enclosed in a plastic bag. A 400 cubic centimeter sphere, of diameter about 9cm becomes a fearsome object.

■ Symmetry, Conservation Laws and Impossible Experiments

The existence of a symmetry is always tentative and experiments are required to determine the limits of applicability of a given symmetry. No symmetry can be considered as a perfect symmetry. The object of much of fundamental physics is the establishment of the limits of particular symmetries and where a symmetry is broken to explain the nature of the symmetry breaking mechanism. One cannot overemphasize the connection between symmetry and experiment. In 1905 Emmy Nöether made the remarkable observation the conservation laws in physics are associated with particular symmetries. Thus conservation of linear momentum was associated with invariance with respect to spatial translations, angular momentum with spatial rotations etc. Parity conservation was associated with the equivalence of the mirror image of an interaction and the real interaction. Every symmetry can be considered as a statement that a certain experiment is impossible. If the experiment is possible then the symmetry must at least be broken. Thus for the parity conservation the impossible experiment would be to detect a difference between the mirror image of a real process and the process itself. If you could detect such a difference then the symmetry is broken and parity is not conserved. Indeed, Madame Wu succeeded in 1956 in making a $\beta-$decay experiment that showed an asymmetry with respect to parity and hence parity conservation was broken by weak interactions. Still more subtle was the demonstration, in 1964 by Fitch and Cronin, of CP violation for K mesons .

■ **Symmetry and Selection Rules**

The existence of a symmetry usually implies that certain processes are not possible. If they were possible then the symmetry would be broken. Part of the application of symmetry considerations is to determine selection rules and to determine the conditions under which these selection rules are broken. Thus in the case of transition matrix elements those that satisfy the selection rules are said to correspond to *allowed* transitions and those that violate the selection rules are termed *forbidden* transitions. In the case of electric dipole transitions in atoms there are the well-known angular momentum selection rules

$$\Delta S = 0 \quad \Delta L = 0, \pm 1 \quad \Delta J = 0, \pm 1$$

and in each case $NOT\ 0 \leftrightarrow 0$. These selection rules arise directly from the fact that the electric dipole operator is spin-independent and transforms like a vector with repect to the group of angular rotations SO_3. The electric dipole operator has *odd* parity so can only connect states of opposite parity.

As a consequence of the above selection rules we would expect electric dipole transitions involving ${}^1S_0 \leftrightarrow {}^3P_0$ to be strongly forbidden. Nevertheless such transitions are observed in gaseous nebulae. The selection rules on the quantum numbers S and L can be broken by the spin-orbit interaction but it cannot break the $NOT\ J = 0 \leftrightarrow J = 0$ selection rule.

■ **Resolution of the $^1S_0 \leftrightarrow ^3P_0$ Puzzle**

To understand the origin of these seemingly highly forbidden transitions we need to first ask "What is the total angular momentum of an atom?". The quantum number J represents the total *electronic* angular momentum of the atom. But the atom has a nucleus that also has a total *nuclear* angular momentum I so that the total angular momentum of the atom F is

$$\mathbf{F} = \mathbf{I} + \mathbf{J}$$

I will be an integer (or half-integer) if the number of protons plus neutrons is *even* (or *odd*) while J will be an integer (or half-integer) if the number of electrons is *even* (or *odd*). If J is an integer and I is a half-integer then F will be a half-integer. If $I \geq \frac{1}{2}$ then the nucleus may possess a nuclear magnetic moment that can couple to the electronic moments leading to a mixing of states of different electronic angular momentum J leading to a breakdown of the $\Delta J = 0\ NOT\ 0 \leftrightarrow 0$ selection rule as occurs for example in the transition array associated with the $3s^2 \leftrightarrow 3s3p$ transition array.

■ **Integer and Half-Integer Angular Momenta**

The basic particles of the universe can be divided into two distinct classes

> **Fermions** which have half-integer spin such as the electron, nucleon, neutrinos quarks etc all of which follow Fermi-Dirac statistics and involve antisymmetric states,
>
> **Bosons** which have integer spin such as the mesons, photon, gluons, graviton etc all of which follow Bose-Einstein statistics and involve symmetric states.

Bosons and fermions behave differently under particle interchange or a rotation through 2π.

■ **Examples of 2π and 4π Rotations**

Our intutitive expectation is that if we rotate a system through 2π or if we circumnavigate a system once we will return to the initial state. I now give you three demonstrations where the niave expectation does not hold.

The Möbius Strip

We can readily make ourselves a Möbius strip by taking a longish narrow strip of paper and rotating one end through 180^o and then bringing the two ends together and sticking them together with glue. Now place a reference mark on the strip and from that mark draw a line along the middle of the strip continuing until you return to the reference mark. You will note that in doing this you have traversed the strip *twice!*.

Cup and Saucer

Place a cup on a saucer and hold it in the palm of your hand. Now turn the cup and saucer by rotating your hand through 2π. This leaves your hand twisted. To return to the original untwisted configuration rotate through a further 2π. To do that you will need to move your hand over your head to complete the total rotation through 4π and return to the original position. This is more dramatic if the cup is partially filled with water - this makes the cup more stable though your students are likely to find the failure of the experiment memorable.

Rotation of a Triangle

Make an equilateral triangle with distinguishable sides. Make a hole in each vertex and attach to each hole a differently coloured tape, e.g. red, green and blue. Attach the loose ends to fixed points. Now rotate the triangle through 2π by turning it over twice so as to develop a twist in two of the tapes. At this stage it is impossible to undo the twist without reversing the rotation or cutting the tapes. Now rotate the triangle through a further 2π so that the two twisted tapes are further twisted. I now assert that the twist can be removed while keeping the triangle in a fixed position and not untying any of the tapes. Indeed the twists incurred by any rotation through an even multiple of 2π may be undone but not for odd multiples of 2π. An illustration of the relevant steps in undoing the twist is shown in the Appendix.

■ Forbidden Transitions in Crystals

Nuclear hyperfine interaction in crystal fields can lead to a breakdown in the usual selection rules for transitions among Stark levels in crystals containing Ho^{3+}. The existence of such a possibility was given by the author over three decades ago. Recently very high-resolution spectroscopic studies in Moscow have supplied a rich source of experimental information. The analysis of these spectra gives an interesting display of the interplay of point groups and their double groups and of crystal field and nuclear hyperfine interactions.

Forbidden transitions were observed in paramagnetic resonance studies of holmium salts in the late 1950's and a complicated mechanism based on the Jahn-Teller effect invoked. The alternative possibility of interaction between different crystal field levels via the nuclear magnetic moment was suggested by the author. Hyperfine structure was observed in the optical spectra of salts containing Pr^{3+} and Ho^{3+} in the early sixties but at relatively low resolution. Subsequent technological developments culimnating in the Fast Fourier Transform spectrometers in the mid-eighties led to resolutions of $0.01cm^{-1}$ permitting for the first time detailed observation of complete fully resolved patterns together with accurate intensities for single crystals of $LiYF_4 : Ho^{3+}$ were made in Moscow by Popova and her associates .

Holmium occurs in nature as a single stable isotope with nuclear angular momentum $I = \frac{7}{2}$ and being a deformed nucleus has both a nuclear magnetic dipole moment and an electric quadrupole moment. The dominant hyperfine structure comes from the interaction of the nuclear magnetic moment with the electron spin and orbital magnetic moments. In the particular case of $LiYF_4 : Ho^{3+}$ the Ho^{3+} ion substitutes into a site whose point group symmetry is S_4 (not to be confused with the symmetric group which is also designated as S_4).

The low lying states of the Ho^{3+} ion occur in the $4f^{10}$ electron configuration and hence the number of electrons is even and the angular momentum J will be integral. Since the nuclear angular momentum is half-integer the total angular momentum F will be half-integer. As a consequence, just as in the case of the gaseous nebulae it is possible for the nuclear magnetic moment to mix states of different J making possible the observation of "forbidden transitions". The presence of the nuclear hyperfine interaction changes the electric dipole selection rules.

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