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SYMMETRY AND NANOPHYSICS - ESSENCE AND APPEARANCE

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A b s t r a c t. *Symmetry is among the deepest concepts of science and philosophy, as well as powerful technical tool. Together with symmetry breaking, defined in terms of symmetry, it gives insight to fundamental properties of the nature. General notions of symmetry and its breaking are analyzed and discussed in particular framework of nanotubes.*

1. *Introduction: symmetry and its breaking*

The aim of this contribution is to discuss the role of symmetry in nanoscience in quite simple way, understandable to wide audience. This also gives an opportunity to compare general physical, and in a sense philosophical principles, to particular problems and breakthroughs in nanoscience.

Symmetry is singled out from the ancient times. Aristotle concluded that "the chief forms of beauty are order and symmetry and definiteness, which the mathematical sciences demonstrate in a special degree". Of course, the context of the ancient period classified mathematical sciences as equivalent to contemporary (natural) sciences. From this metaphysical observation to modern physical definition and application of symmetry passed more than two millenniums. And nowadays the role of symmetry must be understood in the Eugene Wigner's manner, that it is the most important property, and that behavior of any system is determined either by symmetry or by breaking of symmetry.

To understand this I restrict consideration to pure geometry, starting by as much intuitive as broad definition of symmetry: assuming that two points of a geometrical object are *equal* when they have the same *impact* to the object *property*, the object symmetry is the set of the operations on the object (permutations of its points) which interchanges only mutually equal points. Its broadness makes this definition a bit fuzzy, demanding clarifications which themselves are fruitful as faithfully shape general symmetry based considerations.

Fig. 1: Two beautiful (meaning symmetric) faces and their joined halves

Firstly, it is clear that symmetry is contextual, depending on the property of the object. For different properties, the symmetries of the object will be different. In physics, the main property is usually total energy, as it governs the dynamics, but for clarity I begin with example of another intuitive property of the visual shape. Consider various pictures. The empty one, say completely monotonic blue paper, is the most symmetric, since all its points equally contribute to its homogeneous and isotropic shape. No message is emitted (even if it previously became a famous masterpiece of a post-surrealistic concept). However, even the single word, e.g. "symmetry" in the middle of the paper, breaking this absolute symmetry, gives a piece of information, sometimes very important (recall some transparent or advertisement). To summarize, the symmetry is related to the object and its property, while both the object and the property even exist (at least in the cognitive sense) due to the breaking of absolute symmetry. It appears, as I try to illustrate in the rest of this paper, that the interplay of these categories, object/property and symmetry/ breaking of symmetry is responsible for behavior of the systems.

Continuing this intuitive example, let me remind to frequent assertion that symmetrical faces of people are felt as beautiful (perhaps because of easier comprehending, if the story is true at all). Still, combining the two beauties, as two, now non-symmetric halves, can result in unexpected and surely disturbing effect (Figure 1), thus provoking dynamical reaction. The successive breakings lead to very non-symmetric objects, which are hardly comprehended, but finally may have a lot of hidden information, tracing the steps of the breaking process. Figure 2 obviously shows a brain, but the whole picture is unstable, making clear impression of illness, and hiding a portrait of the owner.

Fig.2. Martin Kippenberger: Portrait of Paul Schreber

2. *Line groups and symmetry of quasi one-dimensional systems and nanotubes*

Systems being along one direction (say along z-axis) much greater than in other two ones are called quasi one-dimensional. From the point of view of symmetry, particularly interesting are those with regular distribution of some elementary parts (monomers) along z-axis, i.e. quasi one-dimensional crystals.

The symmetry operations of such systems are gathered into infinitely many line groups, classified into 13 families. In fact, each line group operation is obtained combining one symmetry of monomer (these symmetries form axial point group), and a symmetry of their arrangement along z-axis (gathered into generalized translational group). Thus, each line group is product of one axial point group and one generalized translational group. There are 7 infinite (discrete) families of axial point groups and two types of generalized translations, helical axes (continuous family, including pure translations) and a glide plane. Combining these groups one obtains all line groups.

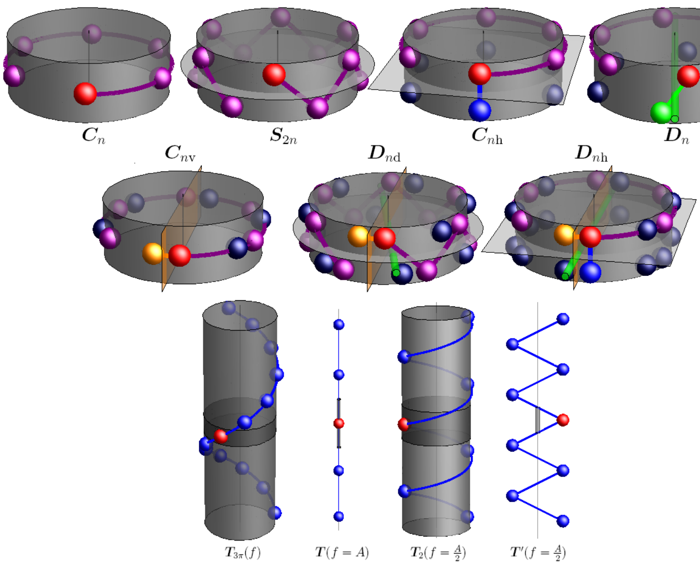

Fig. 3. Seven axial point groups families (upper panel) and two types of generalized translations (bottom panel; the first tree examples are helical systems, with general and two special helical groups, and the last one is glide plane)

Carbon nanotubes, being one of the focuses of modern physics and other sciences and technology are among these quasi one-dimensional systems. Nanotube is a stripe of grapheme, two-dimensional layer of graphite, rolled up in a tube. Obviously, the stripes can be of different wideness, resulting in the nanotubes of different diameters. Also, the stripes differ by the direction (chiral angle) in the graphene, which gives nanotubes of different chirality.

Thus, there is infinite variety of different nanotubes, parameterized by diameter and chiral angle. Each of them has ymmetry group belonging to the 5^{th} family, except in the cases of so called zig-zag and armchair nanotubes, with doubled symmetry belonging to the 13^{th} family.

It is important to note that the acting by the symmetry operation on an arbitrary atom, the whole nanotube is generated. This means that nanotubes are maximally symmetric objects, i.e. that all their properties are derived from properties of a single atom (including here the interaction of this atom with all other ingredients of the considered physical problem) and symmetry. Another important observation is that these large symmetry groups are mutually incompatible, i.e. that for two different nanotubes the intersection of their symmetry groups is unexpectedly small. These two observations have far reaching physical consequences.

3. *Symmetry determines properties*

The fact that arbitrary atom generates whole nanotube by the symmetry group operations enables to reduce all the calculations to single atom, which immediately contributes to the efficiency of the applied procedures. This is particularly important for numerical algorithms, indispensable in nanoscience. However, the benefits in the deep insight to the phenomena are even more important.

At first, application of full symmetry directly gives eigenenergies and the corresponding quantum eigenfunctions assigned by the symmetry based, meaning conserved during the time, quantum numbers. This includes also the classical picture of eigenenergies grouped into the energy bands along the one dimensional Brillouine zone (its points correspond to the quantum number of the helical momentum), each of them carrying the quantum numbers of angular momentum. Besides these two, there are also parity quantum numbers related to rotations around horizontal axis and reflections in the vertical mirror planes appear.

Having the eigenenergies of phonons and electrons (or other quasi particles) in nanotubes assigned by the conserved quantum numbers, one can study all possible processes using these quantities. Indeed, the physical processes are induced by some external perturbation, causing transitions between the eigenstates. However, the external perturbation is also characterized by particular values of the same set of quantum numbers (helical and angular momenta and parities). And only transitions in which the sum of the initial state quantum numbers and quantum numbers of the perturbation equals the quantum numbers of the final states are physically possible. This is a very precise and maximally generalized form of the well-known laws of conservation of energy or momenta. Accordingly, the analysis of the process is reduced to calculation of these *selection rules*. As the quantum numbers themselves are symmetry based, one concludes that all the processes are governed by symmetry.

Typical example is optical absorption. It is important for technology in various ways, but also determines visual color of the object. To find it, it is necessary to start with electronic energies. They have band like structure, manifesting helical periodicity (Figure 4). Each band is assigned by the angular momentum quantum number. On the other hand, photon has negligible momentum, and angular momentum 1 or -1. Therefore, the allowed transitions are vertical (conservation of momentum), but for the light polarized along the tube or perpendicularly to it angular momentum selection rules are different, which results in very different absorption of the light of the two polarizations.

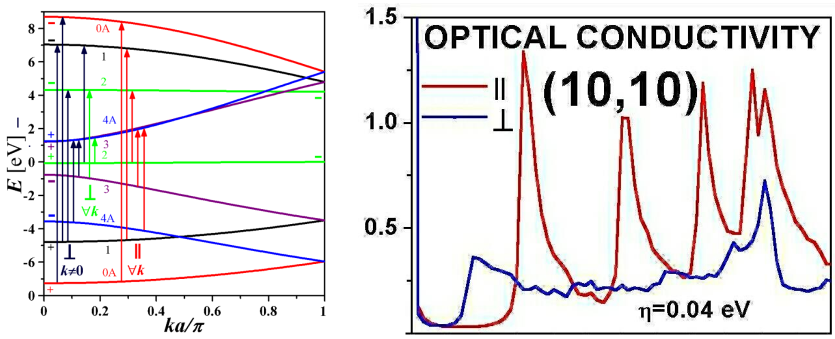

Fig. 4. Left: Electronic energy bands assigned by quantum numbers of angular momentum and arrows denoting allowed transitions of electrons which absorbed quant of light. Right: resulting absorption for the two polarizations

This way we are able to predict properties of nanotubes and their behavior in various situations. During the past two decades many of these properties are considered theoretically and measured experimentally. Just the fact that there are many different nanotubes with different properties opens possibility to choose suitable one for possible applications. And this is the reason that the nanotubes initialized the age of nanotechnology.

4. *Double wall nanotubes: symmetry breaking*

The graphene layers in graphite are spaced by 3.44 Angstroms. Analogously, very frequently nanotubes are synthesized as coaxial double layers with radii mutually differing by the same amount; this structure is called double-wall carbon nanotube. Recalling the incompatibility of their symmetries, it is clear that the symmetry of such nanotube is greatly reduced with respect to the symmetry of isolated walls.

The interaction between the walls is simply the sum of the pairwise interactions of the atoms from interior and outer wall; this interaction depends on the mutual distance of the atoms. To find this sum, we firstly find the interaction potential created by the interior wall in the arbitrary point of the space: this is the sum of the potentials created in that point by the atoms of the interior tube. As the symmetry operations of the interior wall only permute the atoms, the sum is invariant, i.e. symmetric with respect to the interior wall line group symmetry. In other words, despite each atom emits spherical potential, the symmetry acts as a sort of filter, and outside the tube outgoes only symmetric part of the potential (indeed, if this was not the case, some detector would notice object of different symmetry). Analogously, independently of the type of the outer potential, interaction energy of the outer tube is the sum of the values of this potential taken in the positions of atoms of the outer wall. Again, this sum is symmetric with respect to the outer wall line group. Again, the symmetry acts as a filter admitting only symmetric part of the outer potential. It follows that the mutual interaction of the walls doubly filtered. Only the part having symmetry of the interior wall is emitted, and from this part only the part having the symmetry of the second wall is accepted. Taking in the account that the two symmetries are incompatible, it follows that the interaction is highly reduced, i.e. that the walls hardly have mutual friction. Note that no concrete form of the pairwise potential is précised, meaning that the conclusion on the weak interaction of the walls is universal consequence of the symmetry only. This effect of super-slippery walls is experimentally verified, and serves as one of the most important principles in constructing of the nanomachines. Let me stress out that this dynamical effect is a manifestation of the symmetry breaking caused by the incompatibility of the symmetries of the walls (in pparticle physics the same effect is known as the Goldstone mode).

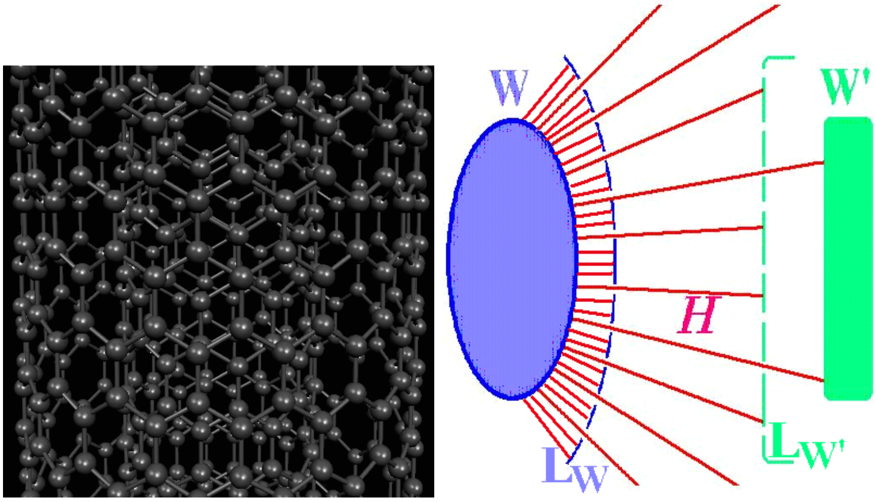

Fig. 5. Double-wall nanotube and the scheme of the interaction between walls.

6. *Conclusions*

From the ancient times considered as an important constituent of the beauty, particularly characterizing science, symmetry evolved to the cornerstone of the contemporary physics, having deep implications and manifestations in each subfield of the physics. The notion of symmetry today includes also breaking of symmetry as complementary, but by no means opposed. Namely, the broken symmetry is dynamically reestablished through the energy free degrees of motion induced by breaking process, known as Goldstone modes.

Quasi one-dimensional systems, especially carbon nanotubes, are the most prominent objects of nanoscience. Their symmetry is described by line groups. All the general principles invoked by symmetry refer to this case, and thorough analysis reveals number of new phenomena characteristic for the reduced dimensionality and specific symmetries.

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