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Lorentz Group and it's Role in the Non-Relativistic Atom Model

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In this article we discuss new symmetry in the atomic structure which was discovered by the second author. We also consider mathematical and physical arguments, which can potentially explain these symmetries.

Introduction

Let us first remind the description of the symmetry. As it was shown in [1], there is a symmetry between the order of completion of the electronic levels of different atoms [2] and the spectra of the hydrogen atom [3–7]. Let us consider the multielectron problem of the electronic shells and subshells structure as a function of atomic number. If one orders the electronic configuration in the coordinates $(n,\, l)$, e.g. in the same coordinates in which were ordered the energy levels of the hydrogen atom (relations (1)), the picture obtained does not reveal any structure or regularity. However, if the subshells are ordered differently, one gets clear-cut triangular structure. This ordering as a function of principal and orbital quantum numbers, might be restructured in the form [1].

$$
\begin{array}{c}
5f \to 6d \to 7p \to 8s \\
4f \to 5d \to 6p \to 7s \to \\
4d \to 5p \to 6s \to \\
3d \to 4p \to 5s \to \\
3p \to 4s \to \\
2p \to 3s \to \\
2s \to \\
1s \to
\end{array}
\tag{1}
$$

The shell and subshell structure in the relations (1) possesses a clear cut symmetry along both main and secondary diagonals, as well as along the horizontal line and the vertical one. This means that relations (1) are structured both in the coordinates $(n,\, l)$ and in the coordinates $(n+l,\, n-l)$. Note that odd line number $2k-1$ and even line $2k$, $k = 1,\, 2,\, 3,\, 4$ in (1) (counting bottom-up) have the same structure. The atoms (chemical elements), which constitute the pair of lines $2k-1$ and $2k$ in relations (1) have been called supercycle [1]. Hence there are four supercycles, consisting of 4, 16, 36 and 64 elements of the periodic table [8]. One should notice also the formal tie between relations (1) (which appear from the Schrödinger equation solution for the hydrogen atom [3–7]) and relations (1), which do represent the ordering of the electronic configuration of all atoms [9, 10]. In other words, one electron problem is structured in the coordinates $(n,\, l)$, while the multi electron problem (the electronic configurations of all atoms) becomes structured in the coordinates $(n+l,\, n-l)$. Two pairs of axes $(n,\, l)$ and $(n+l,\, n-l)$ are turned on the plane of the orbital and the principal quantum numbers by $\pi/4$ relative to each other [1]. Let's now compare the properties of the set of the electronic configurations of all atoms [9] with the periodically repeating properties of chemical elements [8] (how chemists call atoms, which are united with valence bonds [11, 12]). In order to do it, one must return from the coordinates $(n+l,\ n-l)$ to the coordinates $(n,\ l)$ in the relations (1), e.g. perform rotation by $\pi/4$ on the plane $(n,\ l)$. In the coordinates $(n,\ l)$ the superposition of the electronic configurations set with the periodic table, which describes chemical properties of atoms, gives the following subshell structure:

			5f	4f			
		6d	5d	**4d**	3d		
	7p	**6p**	5p	**4p**	3p	**2p**	
8s	7s	**6s**	5s	**4s**	3s	**2s**	**1s**

(2)

As has been demonstrated in [1], relations (2) also have a 4-dimensional symmetry related to the eigenvalues, which appear in the problem of the spectra of the hydrogen atom [13], by the rotation on the angle of $\pi/4$ [1]. Thus the structural symmetry between one-electron problem and multi-electron problem has been revealed. The symmetries, presented in relations (1) and (2), in particular, generate 4-dimensional pyramid of electronic configurations of atoms and periodically repeating properties of chemical elements (instead of 2-dimensional periodic tables [2]). The four-dimensional pyramid of atoms and elements of Magarshak is presented in [1].

1. Coexistence of the Symmetries and the Commutation

As has been shown in [3–5] the symmetries (1) and (2) are generated as symmetries of a pair of energy type operators, which naturally appear in the presence of two commuting Lie algebras of symmetries in the quantum system. Below we provide a mathematical observation, which supports this point of view.We show that the existence of commuting simple Lie algebras of symmetries in physical problem force the existence of unique commuting pair of energy type operators for the localized quantum states.

The finite-dimensional complex representations of products of semisimple Lie algebras has been considered [3–5]. Any such representation V of $g_1 \times g_2$ decomposes into a sum of tensor products $V_k \times W_j$ where V_k are irreducible representations of g_1 and W_j are representations of g_2. The following theorem has been proved [3–5]:

Theorem 1. *Assume that g_1, g_2 are simple Lie algebras. Then there is a canonically defined pair of commuting operators Δ_1, Δ_2 such that both Δ_i, $i = 1, 2$ commute also with the action of g_1, g_2 and have integer nonnegative eigenvalues on V.*

Proof. It is a classical result. Consider Δ_i as the Casimir operator

$$\Delta_i = \sum ad\left(x_j^i\right)^2, \tag{2}$$

where x_j^i is an orthonormal basis of g_i with respect to the naturally defined Killing form B_{gi} [14]. It is well known that the operator Δ_i does not depend on the orthonormal basis in g_i and Δ_i is contained in the center of the enveloping algebra $U(g_i)$. Hence both operators commute with any element in both g_1, g_2. It is also a positive integer multiple of identity on any nontrivial irreducible representation V' of g_i. Thus the representation of $g_1 \times g_2$ is provided with a pair of canonically defined commuting operators with integer nonnegative eigenvalues on V. $\square$

2. Coexistence of Symmetries and Lorentz Group

Note that any element of the center of $U(g_i)$ has similar properties. If the algebra g_i has rank r (dimension of the Cartan subalgebra) then the central subalgebra is a polynomial algebra with r generators. If the rank of g_i is > 1 then we have other similarly defined canonical operators coming from g_i. However Casimir operator is the only operator in the center of $U(g_i)$, g_i — simple Lie algebra, which is equivalent to second order differential operator (Laplace operator) in natural representations of g_i. These representations appear on the spaces of special functions (or sections of vector bundles) over smooth manifolds with geometric action of the algebra g_i.

The above decomposition may exist in the compexification of the symmetry algebra and not in the algebra itself. Since complex finite-dimensional representations of the complexified Lie algebra are the same as of it's real form, the above decomposition holds anyway. In our application the complexification of both real algebras are isomorphic to $so(3, C) = sl(2, C)$ after a complexification and hence have rank 1. Thus there are two natural options:

1) both algebras are coming from the independent rotation invariance f both the nucleus and the electron envelope;
2) the local symmetry group is the Lorentz group $SO(3, 1)$ and though it's Lie algebra $so(3, 1)$ has no such a decomposition but the complexification $so(3, 1) \times C = sl(2, C) + sl(2, C)$. The actual Hamiltonian operator of the problem splits into a sum of two commuting energy time operators. In our opinion second case is physically more plausible since it opens a possibility to connect the problem with a Lorentz group and its nonramified double cover $Spin(3, 1)$ which are natural infinitesimal symmetry groups of general relativity.

It is a well established fact that one-electron problem is governed by the representations of the natural rotation group $Spin$ (2) and the corresponding level structure can be completely deduced from the representations theory of this group. In the multielectron problem we can see the presence of a similar but more complex structure. One of it's demonstrations is the natural decomposition of all possible types of atoms into groups which are naturally organized into supercycles [1]. The numerical structure of the latter reveals a connection with representation theory of the product of groups $Spin(3) \times Spin(3)/Z_2 = SO(4)$ with an additional symmetry between both $Spin(3)$-components and nontrivial representation on the center $Z_2 \subset Spin(3)$. Indeed, any supercycle has length $(2n)^2$ for $n = 1, 2, 3, 4$ and complex irreducible representation of $Spin(3)$, which are nontrivial on the center have even dimensions $2n$.

Thus the size of the supercycles corresponds to dimensions of first irreducible representations of $Spin(3) \times Spin(3)/Z_2$, which are symmetric with respect to both $Spin(3)$ components of the above group. This is hardly a simple coincidence and we would like to discuss possible physical and mathematical reasons for such a structure.

Note that symmetries (1) and (2) are observed within the set of atomic structures which are quantum objects. The appearance of complex valued Ψ-functions and complex representations of the symmetry groups identifies the spaces of complex (though not unitary!) representations of the groups $SO(4)$ and $SO(3, 1)$ where the latter is the Lorentz group of the relativity theory.

The structure of irreducible finite-dimensional representations of the group of real matrices $Spin(3, 1)$ and it's Lie algebra is the same as for the Lie algebras $sl(2, C) + sl(2, C)$ (or $so(3) + so(3)$) only if we consider finite-dimensional representations. Physically this is the case of the interactions for ensembles localized within small spatial domains like atom. However the class of infinite-dimensional irreducible unitary representations of the group $Spin(3, 1)$ is substantially bigger then the class of representations of $so(3) + so(3)$. Thus the additional symmetry appears only in the description of *a priori* localized systems of particles where the whole interaction process is restricted to such a domain and space were quantum effects are dominating. The representations of $Spin(3, 1)$ which appear on the corresponding system are of finite dimension. However this effect does not appear when we consider nonlocal interaction problem. Corresponding irreducible representations of $Spin(3,1)$ are infinite dimensional. In particular, this symmetry would not show up on the quasi-classical level. The important detail is that the action of the Lorentz group is mixing the electric and magnetic components. Namely both components constitute a tensor represented by skewsymmetric form on four-dimensional space with a standard representation of $SO(3,1)$. The action of both commuting Lie algebras $so(3,R)$ of pseudosymmetry on the complexification of the above representations does the same. It exactly corresponds to the coordinate change $(n,\, l)$ to $(n+l,\, n-l)$ on the set of quantum states so that electric n and magnetic l components are mixing via the symmetry transform. The group $so(3)$ acts on the space of the tensors of the electromagnetic field: in $\Lambda^2 R^4$ and $so(3)_\Delta$ acts splits $\Lambda^2 R^4 = \Lambda^2 R^3$ (magnetic) $+R^3$ electric charge. The group $so(3)_L$ acts on complexified space $\Lambda^2 C^4 = \Lambda^2 S^+ \times S^-$. The algebra $so(3)_L$ acts as $su(2)$ on $S^{\{+\}}$ and identically on $S^{\{-\}}$. Thus $so(3)_L$ acts as $S^{\{+\}} \times S^{\{+\}} + C^2 = C^3_S + C^3_I$. The representation $S \times S^+ = C^3_S + C$ of $so(3)_L$ coincides with C^4-complexification of the space-time R^4 and rotates "complexified" tensors of magnetic and electric fields. Thus the group $Spin(3) \times Spin(3) Z_2 = SO(4)$ is not the real symmetry group of the problem but a shadow of Lorentz group $SO(3,1)$ with a given spatial subgroup $SO(3)$.

3. *I*-Particle

How could such a symmetry appear in reality? Currently the standard answer to such question is symmetry break. Namely the existence of symmetry [15] within an ensemble of different particles is usually explained by considering them as different states of an "ideal object" with the above symmetry so that the particles are degenerate states of the above object where the symmetry is broken due to some process of natural degeneration.

If we try to apply similar explanation we are brought to the idea to view the atom as one of the possible states of an ideal particle which we will be denoting as I-particle. This particle has Lorentz symmetry algebra within a bigger algebra of local symmetries and supersymmetries corresponding to other potential fields. The I-particle exists in this ideal state only 0-time which in practice means a very short time depending on the total energy of the I-particle according to the "uncertainty principle". While degenerating the I-particle creates an avalanche of intermediate particles which retain only pieces of the initial symmetry but previous symmetry is manifested in the set of possible degenerate states.

Note that due to the short time existence of I-particle it is more relevant to speak about the Lie algebra of symmetry and not of the group in this case. The process of the symmetry breaking can be put into phases. Namely one of the first symmetries to be broken is the symmetry between all possible space-type three-dimensional subspaces.

Thus the first break occurs on the level of space definition. It corresponds to the appearance of the selected space subgroup — subalgebra $so(3)_\Delta \subset sl(2,C)$ which is contained within a product of two commuting algebras: $so(3) \times so(3)$ in the complexification $sl(2,C) \times sl(2,C)$ of the Lorentz algebra $so(3,1)$.

Indeed $so(3)_\Delta \subset sl(2,C)$ is contained in the unique product $so(3)_L \times so(3)_R \subset sl(2,C) \times sl(2,C)$. Note that $so(3)_L \times so(3)_R$ appear symmetrically which explains why the atomic structures are distributed via representations belonging to the tensor product of equivalent representations of $so(3)_L$ and $so(3)_R$.

However this process proceeds with a different speed in different regions and atomic nuclei [16] can be considered as a domain where this process stalls at some moment. To visualize the picture we can view the I-particle as a cluster of vortices (or oscillators) rotating with different speeds comparable with the speed of light which makes impossible to fix a spatial direction. Thus it opens up the possibility for the existence of the Lorentz symmetry if we assume an equisitrubition of the angles of the rotating vortices. The absence of a preferred space and time directions within the I-particle brings naturally Lorentz group in the picture. It is certainly a very simple model which only hints the possibility of such an effect.

The process of degeneration of an I-particle is inhomogeneous and involves the creation of radiation and some elementary particles. At the same time it goes much slower in some domains and stalls in the intermediate state in some minuscule domains insulated by surrounding clouds of electrons. This is the process which leads to the creation of big atoms.

Thus the nuclei (at least sufficiently big ones) can be considered as cooled down states of the I-particle and the electronic envelope consists of the cloud of emanated electrons which compensate the electric charge of the nuclei. There is a supporting evidence for this picture in recent experimental data which shows the existence of sublight velocities in some processes within the nuclei [16].

This general picture provides with a potential explanation of the structure and symmetries within the set of existing atoms. It also indicates the role of the electronic envelope of the atom. Being a relatively stable degenerate state of an I-particle the atom is electrically neutral and it's stability is sustained by the interaction between the nucleus and the electronic cloud. Some recent experimental data which show that sublight velocities of processes within the nucleus points in this direction [16].

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References

1. *Magarshak Y.* Four-Dimensional Pyramidal Structure of the Periodic Properties of Atoms and Chemical Elements // Sci. Isr. Technol. Adv. — Vol. 7, No 1, 2. — 2006. — Pp. 134–150.
2. *Magarshak Y., Malinsky J.* A Three-Dimensional Periodic Table // Nature. — Vol. 360. — 1992. — Pp. 114–115.
3. *Schrödinger E.* // Annalen der Physik. Leipzig. — Vol. 79. — 1926. — P. 361.
4. *Schrödinger E.* // Annalen der Physik. Leipzig. — Vol. 79. — 1926. — P. 489.
5. *Schrödinger E.* // Annalen der Physik. Leipzig. — Vol. 79. — 1926. — P. 734.
6. *Schrödinger E.* // Annalen der Physik. Leipzig. — Vol. 80. — 1926. — P. 437.
7. *Schrödinger E.* // Annalen der Physik. Leipzig. — Vol. 81. — 1926. — P. 109.
8. *Mendelejeff D.* On the Relationship of the Properties of the Elements to their Atomic Weights // Zeitschrift für Chemie. — Vol. 12. — 1869. — Pp. 405–406.
9. *Cowan R. D.* The Theory of Atomic Structure and Spectra. — Science, 1981.
10. *Messiah A.* Quantum Mechanics. — Courier Dover Publications, 2000.
11. *Pauling L.* The Nature of the Chemical Bond. — Cornell Univ. Press, 1939.
12. *Pauling L.* Chemistry. — San Francisco: W.H.Freeman Publishing House, 1978.
13. *Levine I.* Quantum Chemistry. — 5th edition edition. — Prentice Hall, 1999.
14. *Fulton W.* J.Harris Representation Theory. — Springer, 1991.
15. *Murray Gell-Mann.* Symmetry Properties of Fields // Proceedings of Solvay Congress. — 1961.
16. *Niyazov R. A., Weinstein L. B. et al.* Two-Nucleon Momentum Distributions Measured in $^3He(e, e'pp)n$ // Phys. Rev. Lett. — Vol. 92. — 2004. — P. 052303.

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Группа Лоренца и ее роль в нерелятивистской модели атома

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В работе мы обсуждаем новые симметрии атомных структур, недавно открытых вторым соавтором. Мы также обсуждаем математические и физические аспекты возможного объяснения этих симметрий.