On commuting operators related to asymptotic symmetries in the atomic theory

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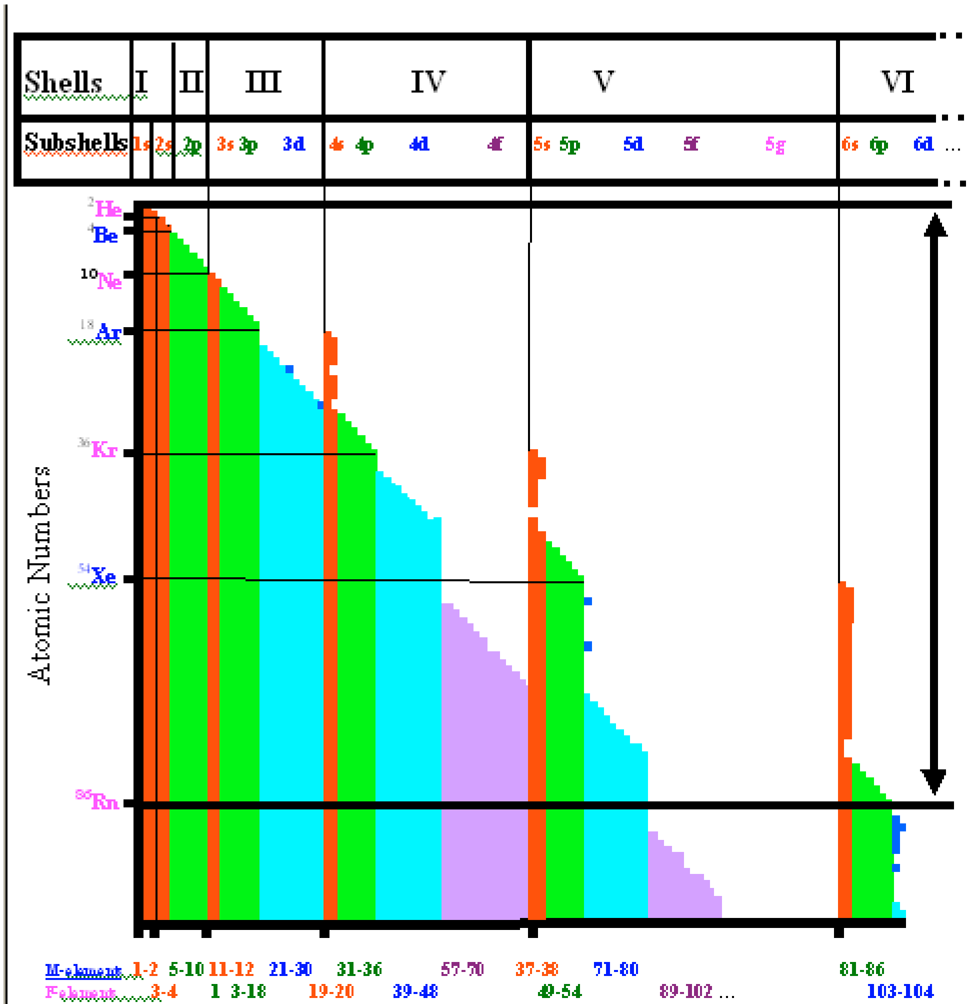
1.INTRODUCTION.

There are many situations in physics where two types of symmetries coexist asymptotically without interference. Let us bring up two examples of such a phenomena in the theory of atom. 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 [3,4]. 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 (Figure 1). However, if the subshells are ordered differently (Figure 2), one gets clear-cut triangular structure. This ordering as a function of principal and orbital quantum numbers, might be restructured in the form [1]:

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

The shell and subshell structure in the relations (2) 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 (2) are structured both in the coordinates (n , l) and in the coordinates (n + l , n - l). One should notice also the formal tie between relations (1) (which appear from the SchrÖdinger equation solution for the hydrogen atom [3,4]) and relations (1), which do represent the ordering of the electronic configuration of all atoms [5,6]. In other words, one electron problem is structured in the coordinates (n . l), as 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 /4 relative to each other [1].

The question concerning the physical origin of two reference frames, generated by the relations (1), sounds natural. What differential equations set is able to cause the processes with two or more coexisting symmetries, neither of which suppresses the other at $t \to \infty$? The assumption, that such co-existing symmetries appear as a result of the implementation of certain « empiric rule» (as, for example, Hunds rule is often called [5,6 and others]) sounds inadequate. The equations, which solution possesses two coexisting symmetries, should be of a very special form. Our understanding is that in this particular case the appearance of additional symmetries is related to the special properties of Lorentz and Euclidian geometries in dimension four. In this dimension (and in this dimension only!) the Lie algebra of local rotations decomposes into a direct product of two simple algebras. This gives a pair of natural commuting energy type operators on any finite-dimensional complex representation of the group of four-dimensional rotations and of the Lorentz group related to this group by Wick's transformation. Remark that geometry and smooth topology in dimension 4 are substantially more rich and have much more refined structure than in other dimensions as it was shown during last twenty years and this fact is mostly due to the additional symmetry described above. Though this symmetry is present not in the Lorentz group but in its complexification, still the same effects hold for the Lorentz group in



Electronic Configurations
of elements from 1 to 104

Figure 1

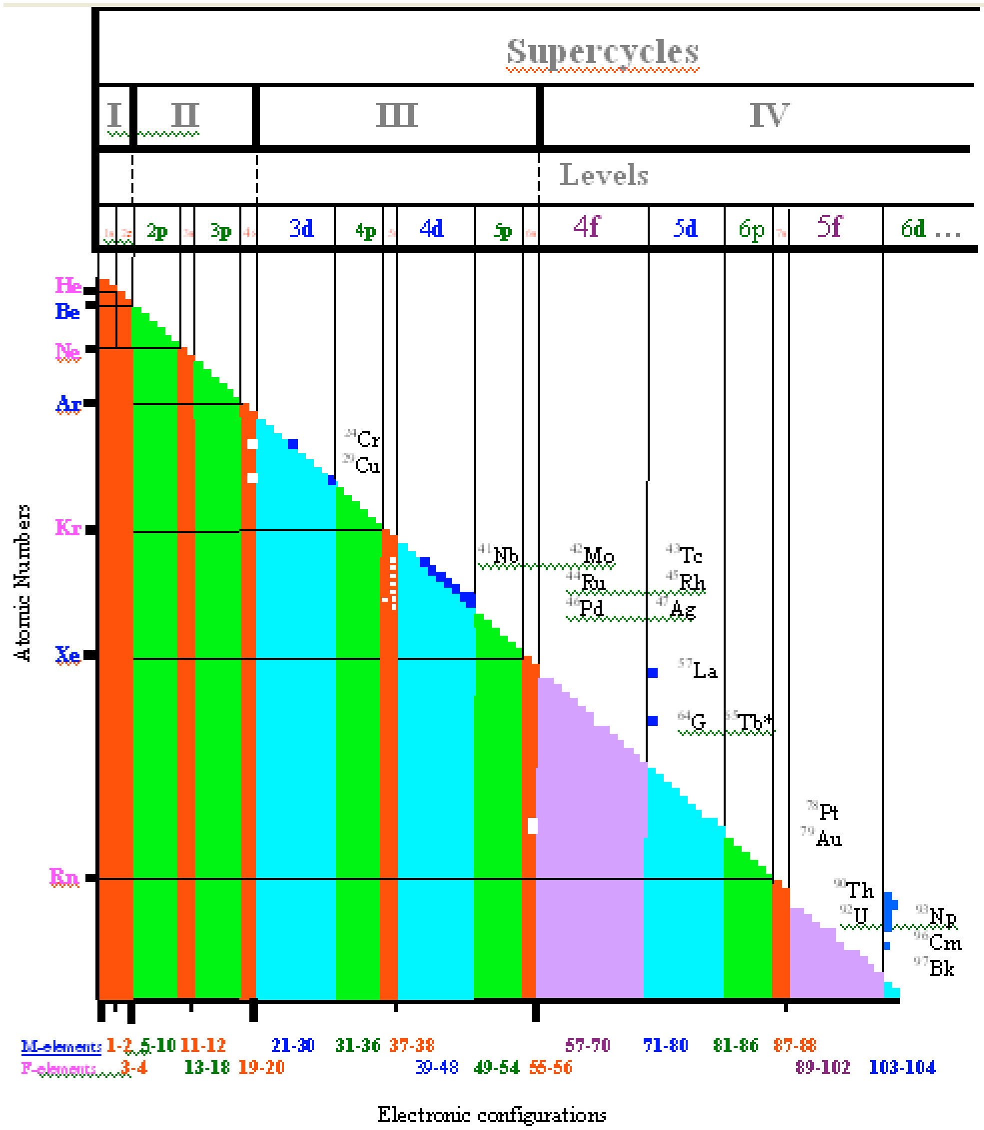

Supercycles
I
II
III
IV
Levels
2p
3p
3d
4p
4d
5p
4f
5d
6p
5f
6d ...
He
Be
Ne
Ar
Kr
Xe
Rn
Atomic Numbers
24Cr
29Cu
41Nb
42Mo
44Ru
46Pd
43Tc
45Rh
47Ag
57La
64G
65Tb*
78Pt
79Au
90Th
92U
93Np
96Cm
97Bk
M-elements 1-2 5-10 11-12 21-30 31-36 37-38 57-70 71-80 81-86 87-88
F-elements 3-4 13-18 19-20 39-48 49-54 55-56 89-102 103-104
Electronic configurations

Figure 2

the cases where the Wick's rotation is physically valid (spatially localized systems).Thus in this cases we can expect the same additional symmetries for the eigenspaces decomposition as in the euclidian case.

Let's now compare the properties of the set of the electronic configurations of all atoms [6] with the periodically repeating properties of chemical elements (how chemists call atoms, which are united with valence bonds) [7,8]. 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 [9], by the rotation on the angle of $\pi/4$.

II. COEXISTANCE OF THE SYMMETRIES AND THE COMMUTATION

We think that these symmetries 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 shows that the existence of commuting simple Lie algebras of symmetries in phisycal problem force the existence of unique commuting pair of energy type operators for the localized quantum states.

We consider finite-dimensional complex representations of products of semisimple Lie algebras. 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.

Theorem: Assume that $\mathbf{g}_1,\mathbf{g}_2$ 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 $\mathbf{g}_1,\mathbf{g}_2$ and have integer nonnegative eigenvalues on V.

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

$$\Delta_i = \sum ad(x^i_j)^2 \tag{3}$$

where x^i_j is an orthonormal basis of $\mathbf{g_i}$ with respect to the naturally defined Killing form [10]. It is well B_{gi} known that the operator Δ_i does not depend on the orthonormal basis in $\mathbf{g_i}$ and Δ_i is contained in the center of the enveloping algebra U($\mathbf{g_i}$).Hence both operators commute with any element in both $\mathbf{g_1}$,$\mathbf{g_2}$. It is also a positive integer multiple of identity on any nontrivial irreducible representation V' of g_i. Thus the representation of $\mathbf{g_1} \times \mathbf{g_2}$ is provided with a pair of canonically defined commuting operators with integer nonnegative eigenvalues on V.

III. DISCUSSION

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

Remark 2. Note that the above decomposition may exist in the compexification of the symmetry algebra and not in the algebra itself. Since finite-dimensional representations of the complexified Lie algebra are the same as of it's real form and the above decomposition holds anyway. In our application the complexification of both real algebras are presumably isomoprhic 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 of 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 decompostion but the complexification ***so***(3,1) × C = ***sl***(2,C) + ***sl***(2,C). The actual Hamiltonian operator of the problem splits into a sum of two commuting energy time operators.

Remark 3. 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 infintesimal symmetry groups of general relativity. The structure of irreducible finite-dimensional representations of **Spin**(3,1)=SL(2C) 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. Here we also treat as unitary also representations with nondegenerate, but not positively defined Hermitian forms. 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 apriory 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. Corresponing reducible representations of **Spin**(3,1) are infinite dimensional. In particular it would not show up on the quasi-classical level.

Remark 4. Note 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 represetations does the same. It exactly corresponds to the coordinate change (n + l, n – l) on the set of quantum states so that elektric n and magnetic l components are mixed.

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The results of the present contribution can be applied on any system with two coexisting symmetries. They might be useful in solid state physics and chemistry [11], femtophysics and femtochemistry [12], material science [13] and other areas.

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Figure Captions

Figure 1. Electronic configurations of the first 104 atoms of the periodic system, ordered in the following lrder: Shell -> Subshell -. Elements constituting a subshell

Figure 2. Electronic configurations of the first 104 atoms of the periodic system, ordered in the following order: Supercycle -> Cycle -> Subshell -> Elements Constituting a Subshell