

On the EPN-Resonance Mechanism of the Stabilization of Molecular Structures

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Over the three quarters of a century that have passed since the creation of quantum mechanics, enough results have been obtained to pose the question whether it is necessary to develop a theory that, under certain conditions, turns into quantum mechanics by analogy with quantum mechanics turning into Newtonian mechanics under well-known conditions. (By certain conditions, we mean, for example, large times, in which case a picosecond is a very long period.) One of these results is the detection of four-dimensional symmetries in electronic configurations of atoms as a function of the nucleus charge (the number of a chemical element in the periodic table) in the plane of the principal and orbital quantum numbers [1]:

$$\begin{aligned}
&5f \rightarrow 6d \rightarrow 7p \rightarrow 8s \\
&4f \rightarrow 5d \rightarrow 6p \rightarrow 7s \rightarrow \\
&\quad 4d \rightarrow 5p \rightarrow 6s \rightarrow \\
&3d \rightarrow 4p \rightarrow 5s \rightarrow \\
&\quad 3p \rightarrow 4s \rightarrow \\
&2p \rightarrow 3s \rightarrow \\
&\quad 2s \rightarrow \\
&1s \rightarrow
\end{aligned} \tag{1}$$

The shells and subshells in (1) have distinct symmetries in the horizontal and vertical and along both diagonals. This means that relations (1) are structured in two coordinate systems: in coordinates (n, l) and in coordinates $(n + l, n - l)$. Note that the structure of relations (1) viewed along the diagonals (i.e., in coordinates $(n + l, n - l)$), which is a pictorial representation of the solution to the multielectron problem of the order of filling electron subshells as a function of the element number, is formally related to the solution of the Schrödinger equation for the hydrogen atom (one-electron prob-

lem). In the plane of the principal and orbital quantum numbers, two pairs of coordinates (n, l) and $(n + l, n - l)$ are rotated by $\frac{\pi}{4}$ relative to each other. In coordinates (n, l) , the superposition of the set of electronic configurations [2] as a function of the element number in the periodic system [3] has the following structure [1, 4]:

$$\begin{array}{cccccccc}
 & & & \mathbf{5f} & 4f & & & \\
 & & & \mathbf{6d} & 5d & \mathbf{4d} & 3d & \\
 \boxed{8s} & \boxed{7p} & \boxed{6p} & \boxed{5p} & \boxed{4p} & \boxed{3p} & \boxed{2p} & \\
 & 7s & 6s & 5s & 4s & 3s & 2s & \boxed{1s}
 \end{array} \quad (2)$$

It was shown in [1] that relations (2) also have a four-dimensional structure. Moreover, the coordinates of the one-electron problem and of the valence properties of elements are the same (n, l), while the structure of filling electron shells as a function of the element number is rotated by $\frac{\pi}{4}$ relative to this coordinate system. Thus, the structural symmetries in coordinates (n, l) and ($n + l, n = l$) coexist in (1) and (2).

A fundamental question to ask is why there is symmetry between the one-electron problem (hydrogen-atom spectrum) and the multielectron problem (filling electron shells as a function of the nucleus charge) in the plane of the principal n and orbital l quantum numbers (moreover, in coordinate systems rotated by $\frac{\pi}{4}$) relative to each other). Another important question is about the conditions on the equations under which they generate symmetries that coexist as $t \rightarrow \infty$ (an example of such relations is given by (1) and (2)). The assertion that coexisting symmetries result from a certain semiempirical rule (as is customary to refer, for example, to Hund's rule [5, 6]) seems inadequate to the problem. In our view, the most constructive approach was proposed in [7], where these symmetries were regarded as a manifestation of special properties of Euclidean geometry and the Lorentz transformation in four

dimensions, since, in four and only four dimensions, a local Lie algebra can be decomposed into a direct sum of two simple algebras [8]. Thus, a natural conjecture is that the symmetries in (1) and (2) are generated by a pair of Hamiltonian-type operators. Such operators naturally arise in the presence of two commuting Lie algebras in a quantum system. The existence of symmetries generated by commuting simple Lie algebras implies the existence of a unique commuting pair of energy-type operators for localized quantum states. This result follows directly from the following theorem.

Theorem. *Assuming that g_1 and g_2 are semisimple Lie algebras, there is a canonical pair of commuting operators Δ_1 and Δ_2 that both commute with the action of g_1 and g_2 and have nonnegative integer eigenvalues on V .*

A theorem on the necessity of the existence of commuting operators for the coexistence of two or more symmetries was formulated and proved in [7]. Thus, any representation $g_1 \times g_2$ has a canonically defined pair of commuting energy-type operators with nonnegative integer eigenvalues. We apply this result to atomic theory, specifically, to the symmetries in (1) and (2). One of the commuting operators required for the generation of these symmetries is well known: this is the Schrödinger equation. The question arises as to what the second operator is. Since an atom consists of an electron shell and a nucleus, the only possible generator of the second operator can be the field interaction between the electrons of the shell and the nucleus. The most natural implementation of this requirement is a Hamiltonian operator that splits into a sum of two commuting operators possessing the Lorentz group symmetry [7]. Note that, in this case, the Lorentz group arises in a nonrelativistic setting as the most natural implementation of the theorem's requirement that there must be two commuting Hamiltonian operators, in particular, as applied to hidden four-dimensional structures in the electron shells of a collection of atoms (see (1) and (2)). For a set of particles, such situations are usually viewed as the various states of an ideal object possessing a high symmetry, while commuting operators are obtained by splitting this state.

Thus, in view of (1) and (2), we arrive at the natural idea of a collection of atoms (arranged in ascending order of nucleus charges) viewed as the states of a certain superatom, an object that was called an I-particle in [7] (from Ideal particle).

The I-particle exists for a very short time with its lower bound estimated in order of magnitude as lying between 10^{-21} and 10^{-20} s [9]. Note that this value is close in order of magnitude to the characteristic time

$$\tau_{C(e)} = \frac{\lambda_{C(e)}}{c} \cong 3 \times 10^{-21} \text{ s},$$

which is required for the transition of an electron to a state in which the quantum mechanical uncertainty of the momentum and energy is larger than or equal to

$\geq mc$ and $\geq mc^2$, respectively. Here, $\lambda_{C(e)} \approx 3.86 \times 10^{-13}$ m is the Compton wavelength of the electron:

$$\lambda_{C(e)} = \frac{\hbar}{mc}.$$

For $t < \tau$, it is senseless to treat the particle as a point object, since pairs of particle-antiparticle begin to be created. Instead, it has to be viewed as an object of quantum field theory with an infinite number of degrees of freedom.

The physical nature of the I-particle, which is capable of generating symmetries (1) and (2) and a canonical pair of commuting operators, was not discussed in [7]. A quantum field mechanism representing the most natural implementation of the requirements of the theorem on the existence of two commuting Hamiltonian operators as applied to atoms was proposed in [9].

RESONANCE MODEL OF AN ATOM

Postulate 1. Atoms are formed due to the resonance between the following two resonance processes:

(I) reversible interaction between the electrons of the shell and the protons of the nucleus

$$e + p \leftrightarrow n + \text{neutrino (epn-resonance)},$$

(II) the resonance between an electron localized in the nucleus (and involved in epn-resonance with a proton and a neutron) and its location in the space surrounding the shell according to its Ψ -function ($\beta\Psi$ -resonance).

Postulate 2. The space in the neighborhood of a nucleus is a resonator in which the energies of the electrons and their Ψ -functions are determined by the Schrödinger equation. The transition of the electron from the state localized in the nucleus by epn-resonance to the "wave" delocalized state corresponding to its Ψ -function due to $\beta\Psi$ resonance is possible at these and only these energies.

Thus, we propose a super-resonance model of an atom that involves two fundamental resonances (epn and $\beta\Psi$) that are in resonance with each other. Higher-level resonances (such as resonance valence bonds in the benzene molecule) are determined by the fundamental resonances. Moreover, according to the super-resonance model, resonances, the interaction between resonances, and the hierarchy of resonances are universal mechanisms determining the structure of atoms and molecules.

SUPER-RESONANT NATURE OF VALENCE BONDS

Postulate 1. In the valence interaction between the atoms in a molecule, an electron that is on the shell of one of the atoms is involved in the super-resonant interaction with a proton in the nucleus of another atom.

Postulate 2. A valence bond is formed due to jumps of an electron of the shell between the nuclei connected by the valence bond, and each of the jumps to a certain nucleus has a super-resonance nature and is the resonance between epn- and $\beta\Psi$ -resonances.

Postulate 3. In molecules consisting of more than two atoms, resonances between resonances can occur that determining the valence bonds. The number of hierarchical levels of resonances in nature is unlimited.

Thus, according to the super-resonance model, the physical nature of valence bonds is the same as the nature of atoms: it is super-resonance that is resonance between two fundamental resonances. The time required for the atoms move away from each other at a distance at which no valence bond can be formed is of the same order as the period of oscillations of atoms in molecules (10^{-12} – 10^{-15} s). If $\beta\Psi$ resonance occurs several orders faster than the upper bound for this range, the electron has enough time to form valence bonds that hold the atoms together. Molecules of any size are formed in a similar manner, i.e., due to super-resonance interactions between the electrons of the shell of all the atoms in a molecule and the nuclei connected with them by valence bonds.

It should be stressed that the characteristic times of higher-order resonances can be several orders of magnitude shorter than the fundamental epn-resonances. In particular, they can be comparable with the oscillation frequencies of the atoms and, thus, can influence the structure of the molecule and its chemical activity.

The approaches developed in [7, 9] have a common conceptual and mathematical foundation. Since an electron that is in a wave state is part of epn-resonance, which is regarded in [9] as a process determining the structure of atoms and molecules, the word “particle” in the name of the I-particle proposed in [7] does not seem very good. On the other hand, the volume of the states in which an electron and proton are localized in the nucleus is at least 10^{10} times less than the volume occupied by the wave function of an electron in the atomic shell, which sharply distinguishes this hypothetical process from all known resonances of elementary particles. Therefore, the physical nature of the phenomenon is only in part determined by the term “resonance.”

The terminological problem is associated with the fact that epn-resonance in the I-particle (according to the hypothesis) is a special state of substance in the form of particles, waves, and resonances between the particles that exist simultaneously. The term “halo”¹ for this state of substance seems the most suitable. Thus, according to the halo hypothesis, the substance in atoms and molecules (atoms connected by valence bonds) is in the halo state of matter. According to the halo hypothesis, the existence of stable atoms in the universe and the existence of properties of atoms that interact with each other to form molecules are caused

by interaction processes between protons, neutrons, and electrons strictly determined by atomic nuclei. Valence bonds (ionic, polar, or covalent) in molecules are determined not by shifts of electron clouds, as is postulated in the standard model [10], which is now generally accepted [11, 2], but rather by the halo and electrons drifting between nuclei in the neighborhood of a nucleus or in the internuclear space (in the case of molecules), which are generated by epn-resonances.

Discussion. The halo structure of atoms and molecules generated by epn-interactions between the electrons of the shell and the protons of the nucleus can explain a number of experimental facts and theoretical statements that are difficult to explain in terms of quantum mechanics.

1. INCREASE IN ENTROPY AND ENERGY DISSIPATION IN HALO SYSTEMS

Entropy in closed quantum mechanical systems cannot increase (von Neumann’s theorem), whereas all actual processes in atomic and molecular physics, in particular, the thermodynamic interaction of atoms and the formation of molecules, are dissipative. The problem of energy dissipation in quantum mechanics as based on Hamiltonian formalism was discussed in numerous studies but no conclusive solution was proposed. In the halo model, energy dissipation and entropy increase are consequences of the field interaction between the electrons of the shell and the nucleons of the nucleus.

In statistical mechanics, the entropy of atomic nuclei is generally not taken into account, since it is assumed that there is an infinite potential hill between the motion of nucleons in nuclei and the motion of atoms as a whole in the sense that the motion of elementary particles in nuclei makes no contribution to the entropy of gases, liquids, or solids. In the halo model, on the contrary, the electrons of the shell and the nucleus are in constant field interactions that determine the structure and dynamics of atoms and molecules. The same is true of the interaction between the electrons of the shell in one atom and the nucleus of another atom. If this interaction is not sufficiently strong to hold the atoms together, the atoms move apart. In this case, time reversibility (which follows from both Newtonian and Hamiltonian formalism) no longer occurs. Energy exchange between atoms in the epn-halo interaction is possible. As in the computation of entropy, in the halo model it is necessary to take into account the total entropy of a polyatomic system, including the entropy of the nucleus. Recall that the velocity of atoms at room temperature is 10^2 – 10^3 m/s, while the velocity of nucleons in nuclei comprises tens of percent of the velocity of light; i.e., it is higher by at least four orders of magnitude [12]. Thus, in a closed halo system, there is no time reversibility; the entropy of a collection of atoms increases; and energy dissipates, turning into heat, which is observed in reality. Note that, in the halo

¹ By analogy with the halo of galaxies.

model, entropy increase in a closed system of atoms (with allowance for the entropy of the nuclei) occurs without assuming the existence of phase trajectories generating instability in the system.

2. ORIGIN OF ATOMS FROM LITTLE BANGS

Why is the total number of positively charged particles in the universe equal to the number negative particles and, thus, the universe is neutral on the whole? According to the halo hypothesis of the atomic and molecular structure, this phenomenon can be explained by the origin of neutrons preceding the origin of protons and electrons. In this case, in contrast to what is now accepted, atoms did not appear from the union of protons, neutrons, and electrons but emerged as soon as there were conditions for epn-resonances in the neighborhood of a "crystallization center" of an atom. In the halo model, an atom is unfolded from a neutron predecessor of the nucleus like a parachute (which is reverse to the collapse of atomic nuclei and shell electrons in the formation of a neutron star). As a result of each atomic little bang, protons and electrons are formed from neutrons in equal numbers (their total charge is zero). Atoms, the neutron complexes generating them (according to the hypothesis), and the universe as a whole remain neutral before and after every little bang (epn-explosion). Since neutrons have no charges, they can approach each other to form multineutron proatom centers without overcoming the potential hill (which is extremely great in the case of protons approaching each other).

According to the little bang hypothesis, the formation of atoms took place simultaneously with the separation of neutrons into protons and electrons. The separation of charges into positive and negative ones also occurred in the formation of atoms from little bangs. However, only some rather than all neutrons of a crystallization center (from which an atom is created) are split into electrons in the shell and protons remaining in the nucleus (which was created from the little bang of this atom), while the remaining neutrons remain neutrons localized in the nucleus. The question as to why it is so lies beyond the scope of the qualitative consideration performed in this paper.

Conditions suitable for a little bang (accompanied by the emergence of divided charges from neutral matter and by the unfolding of an "atomic parachute") can arise, in particular, with a sharp decrease in temperature and/or pressure, for example, after the explosion of a supernova. It seems rather interesting to determine processes (except for explosions of supernovas) in which chemical elements can be created and, in particular, determine whether suitable conditions for little bangs could arise at a certain stage of the Big Bang.

This section offers an independent hypothesis whose correctness or incorrectness does not influence the remaining content of this paper.

3. APPLICABILITY OF THE SUPER-RESONANCE VALENCE MODEL TO DIABATIC PROBLEMS

It was shown by Gribov [13] that, in diabatic problems, in which the computation of electron shells cannot be separated from the motion of nuclei, the Schrödinger equation gives average and only average values of physical quantities (in particular, energy), while additional considerations and/or equations are required for deriving exact nonaveraged values. Gribov also showed that the matrix approach is applicable to many chemistry and biochemistry problems even when the operator approach fails; i.e., in contrast to a popular belief, the Heisenberg and Schrödinger approaches are not always equivalent [14]. An example of processes that functionally involves both the motion of nuclei and the dynamics of electronic configurations, which cannot be separated from each other, is photosynthesis, in which the motion of an electron depending on the conformations of molecules can now be traced in real time on pico- and sometimes femtosecond scales [14]. The presence of epn (halo) interactions in atoms naturally explains molecular processes in which electronic configurations depend on coordinates directly rather than in an averaged manner.

We are not interested in the question whether there are limits of applicability of quantum mechanics: of course, they are (for example, at times less than the Compton limit). The question is whether there are effects in atoms and molecules happening at times larger (or larger by several orders of magnitude) than the Compton time that cannot be explained in terms of quantum mechanics and require the application of a more general theory, in particular, quantum field theory.

However, the modern views of atoms are based on processes occurring at lower levels of the organization of matter than atoms and only at such levels. Computational problems related to the analytical calculation of atoms with a more complex structure than hydrogen (not to mention the direct derivation of fundamental laws of chemistry, such as the periodic system and molecular orbitals, by solving the Schrödinger equation) are viewed as temporal difficulties associated with the insufficient efficiency of modern computing techniques. The above physical dependences are called semiempirical, like Hund's rule, because we fail to deduce them from the fundamental principles of quantum mechanics. The use of pejorative terms is a verbal attempt to hide the shortcomings of the theory and the obvious fact that the modern fundamental pattern of the world explaining processes from bottom to top (quarks $\rightarrow$ elementary particles $\rightarrow$ nucleus $\rightarrow$ atoms $\rightarrow$ molecules $\rightarrow$ biomolecules $\rightarrow$ biomolecular complexes, etc.) has a gap between physics on the one hand and chemistry, biochemistry, and molecular biology on the other hand. Despite much effort over 80 years after the creation of quantum mechanics, this gap has not been narrower but has become even wider. In fact, the semiempirical dependences are laws of matter struc-

ture, and they are as fundamental as other laws of nature.

Evidence for the hypothesis of epn (halo) interactions determining the structure of atoms is that the origin of resonances and numerous symmetries in chemistry and material science (including Hund's rule and hidden symmetries in electronic configurations of chemical elements, which follow from the periodic law but are not deduced from the basic postulates) correlates with the principle underlying the theory. Other (equally important) evidence is that two commuting operators (one of which is Schrödinger) are necessary to exist in order to explain hidden four-dimensional structures contained in electronic configurations of atoms, which were discussed in Section 1. Anyway, it is intriguing and important to answer the question whether some processes in atoms and molecules happening at times several orders of magnitude longer than the Compton limit are determined by field rather than quantum mechanical effects.

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