Conceptual Unfoundedness of Hybridization and the Nature of the Spherical Harmonics

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Abstract

The quantum mechanical concept of hybridization is based on mixing the "real" and "imaginary" parts of complex wave functions. The erroneousness of such an operation, resulted in the invention of electron configuration of atoms, is revealed in this paper. The true nature of spherical harmonics and important results originated from analyzing the above concept are presented here as well.

Key Words: Quantum mechanics, Quantum Chemistry, Hybridization, Electron configuration, Atomic orbitals, Wave functions, Complex functions, Imaginary number, Intra-atomic structure, Periodic table.

1. Introduction

1.1. The role and place of hybridization in atomic physics and chemistry.

The most of physicists and chemists are aware that quantum mechanics (QM) with the group-theory approach [1] to atomic systems elucidate theoretically atomic and molecular structure and the nature of Mendeleev's periodic law. This belief in reality of an image of an atom, imposed by the modern standard model of elementary particles, lies in the base of the above view.

Hitherto nobody has come into the question on the validity of a pure mathematical artificial manipulation with "real" and "imaginary" parts of spherical wave functions (atomic orbitals), consisted in making linear combinations of them (further mixing for short), which lay in the base of the construction of QM atomic model. The legality of linear combinations of wave functions is stated by one of the fundamental principles of QM – the superposition principle. This manipulation has promoted the development of quantum mechanics and quantum chemistry, and led to the invention of "*electron configuration*" of atoms.

The pure mathematical operation (linear combination) with real and imaginary parts was called *hybridization of atomic orbitals*. Quantum mechanics and quantum chemistry cannot do now without this notion, in spite of the obvious fact that the hybridization contradicts first of all to the main fundamental principle of QM on the probabilistic interpretation of wave functions. We will show this here.

Let us give at the beginning a few examples, taken from the world-wide university textbooks and monographs, which show how deeply hybridization took roots in the foundation of quantum mechanics and quantum chemistry. (The cited below is the present author's English translation of quotations taken from Russian versions of the reference works).

1. The authors, J.N. Murrell, S.F.A. Kettle, and J.M. Tedder, of the book "*Valence Theory*" [2] teach that the azimuth functions of the form $\exp(\pm im\varphi)$ have such an imperfection that *they cannot be presented in real space*. However, it is possible to obtain the real functions, which are solutions of the equation $\nabla^2\psi + \dfrac{8\pi^2 m}{h^2}\left(E + \dfrac{e^2}{r}\right)\psi = 0$, if one uses *linear combinations of*

spherical harmonics with the same quantum number *l*. Operating by this way, it is possible to obtain the functions as, for example,

$$\frac{1}{\sqrt{2}}(Y_{1+1} + Y_{1-1}) = \frac{\sqrt{3}}{2\sqrt{\pi}}\sin\theta\cos\varphi, \qquad (1.1)$$

where

$$Y_{1\pm1} = \frac{\sqrt{3}}{2\sqrt{2\pi}}\sin\theta\, e^{\pm i\varphi}. \qquad (1.2)$$

Further they state that since $\sin\theta\cos\varphi$ expresses an angular dependence of *x*-component of the radius-vector **r** (they mean the equalities: $x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$, and $z = r\cos\theta$), the linear combination (1.1) is termed the p_x-*atomic orbital*.

2. R.L. Flurry in "*Quantum Chemistry*" [3] writes that for the qualitative description of chemical bonds, it is convenient to express the wave functions $R_{nl}(r)\Theta_{lm}(\theta)e^{\pm im\varphi}$ in the *real form* if one takes linear combinations of degenerated functions, which correspond to the values $+ m$ and $- m$ of the magnetic quantum number *m*:

$$\psi_{nlm}^{(1)} = \frac{1}{2}(\psi_{nlm}^{+} + \psi_{nlm}^{-}) = R_{nl}(r)\Theta_{lm}(\theta)\cos m\varphi, \qquad (1.3)$$

$$\psi_{nlm}^{(2)} = \frac{1}{2i}(\psi_{nlm}^{+} - \psi_{nlm}^{-}) = R_{nl}(r)\Theta_{lm}(\theta)\sin m\varphi, \qquad (1.4)$$

where

$$\psi_{nlm}^{+} = R_{nl}(r)\Theta_{lm}(\theta)e^{im\varphi}, \qquad \psi_{nlm}^{-} = R_{nl}(r)\Theta_{lm}(\theta)e^{-im\varphi}. \quad (1.5)$$

The angular dependence of these functions, *e.g.*, for $|m| = 1$, shows that the function $\psi_{nlm}^{(1)}$ is directed along the *x*-axis and the function $\psi_{nlm}^{(2)}$ – along the *y*-axis in Cartesian coordinates. However, he notes that for these functions *m* is not already *the right quantum number* (although $|m|$ is the *right quantum number*) because every of these functions represents the combination of the functions with quantum numbers $+ m$ and $- m$.

3. E. Cartwell and G.W.A. Fowels write (in "*Valency and Molecular Structure*", Sect 4.6. *Angular functions* $Y(\theta, \varphi)$" [4]) that mathematical expressions for solutions of the wave equation contain complex functions which cannot be easy presented in a graphical form. This is why, and *in order*

to deal with the real solutions, *chemists prefer linear combinations of these functions* presented in the form of "polar" diagrams (which are permissible solutions to the wave equation as well). Although, it is impossible to ascribe to the functions, obtained in that way, the definite values of *m*.

4. In the book "*Molecular Structure and Dynamics*" [5] by W.H. Flagare, we find the following instructions: because of impossibility to present orbitals in the complex space, one should realize "*the transition from the complex basis into the real one by the following formulas of matrix transformation*":

$$\left(p_x\, p_y\, p_z\right) = \left(Y_{1-1}\, Y_{11}\, Y_{10}\right)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i & 0 \\ 1 & i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}, \qquad (1.6)$$

$$\left(d_{xy}\, d_{x^2-y^2}\, d_{xz}\, d_{yz}\, d_{z^2}\right) = \left(Y_{2-2}\, Y_{22}\, Y_{2-1}\, Y_{21}\, Y_{20}\right)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & i & 0 & 0 & 0 \\ 1 & -i & 0 & 0 & 0 \\ 0 & 0 & +1 & i & 0 \\ 0 & 0 & -1 & i & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2} \end{pmatrix}" \quad (1.6a)$$

5. The "*angular parts of the wave function Y_{lm} of the hydrogen atom*", presented in the explicit form with the corresponding linear combinations (on the right) in "*The Molecular Structure Theory*" by V.I. Minkin, B.Ya. Simkin, and R.M. Minaev [6], have the form:

$$s \quad \rightarrow \quad Y_{00} = \frac{1}{\sqrt{4\pi}} \; ; \qquad\qquad (1.7)$$

$$p_z \quad \rightarrow \quad Y_{10} = \frac{\sqrt{6}}{2\sqrt{2\pi}}\cos\theta \, ;$$

$$p_y \quad \rightarrow \quad Y_{1-\bar{1}} = \frac{\sqrt{6}}{2\sqrt{2\pi}}\sin\theta\sin\varphi \, , \qquad \frac{1}{i\sqrt{2}}(Y_{11} - Y_{1\bar{1}}) \, ;$$

$$p_x \quad \rightarrow \quad Y_{1+1} = \frac{\sqrt{6}}{2\sqrt{2\pi}}\sin\theta\cos\varphi \, , \qquad \frac{1}{\sqrt{2}}(Y_{11} + Y_{1\bar{1}}) \, ;$$

$$d_{z^2} \quad \rightarrow \quad Y_{20} = \frac{\sqrt{10}}{4\sqrt{\pi}}(3\cos^2\theta - 1) \, ;$$

$$d_{xz} \rightarrow Y_{2+1} = \frac{\sqrt{15}}{2\sqrt{\pi}} \sin\theta\cos\theta\cos\varphi, \qquad \frac{1}{\sqrt{2}}(Y_{21} + Y_{2\bar{1}}) ;$$

$$d_{yz} \rightarrow Y_{2-\bar{1}} = \frac{\sqrt{15}}{2\sqrt{\pi}} \sin\theta\cos\theta\sin\varphi, \qquad \frac{1}{i\sqrt{2}}(Y_{21} - Y_{2\bar{1}}) ;$$

$$d_{x^2-y^2} \rightarrow Y_{2+2} = \frac{\sqrt{15}}{4\sqrt{\pi}} \sin^2\theta\cos 2\varphi, \qquad \frac{1}{\sqrt{2}}(Y_{22} + Y_{2\bar{2}}) ;$$

$$d_{xy} \rightarrow Y_{2-\bar{2}} = \frac{\sqrt{15}}{4\sqrt{\pi}} \sin^2\theta\sin 2\varphi, \qquad \frac{1}{i\sqrt{2}}(Y_{22} - Y_{2\bar{2}}) ''$$

Let us gain an insight into the meaning of the above cited texts.

1.2. Briefly about conceptual flaws of hybridization.

First, it is not so difficult to find that the concept of mixing (hybridization) adopted in QM through the superposition principle is not in concordance with the primary principle of QM on the probabilistic interpretation of the wave functions. Actually, all presented above manipulations express an elementary simple thing, just *usage and mixing of real and imaginary terms* of the space factor $\hat{\psi}$ of the wave function $\hat{\Psi} = \hat{\psi}(r,\theta,\varphi)e^{i\omega t}$:

$$\mathrm{Re}\,\psi_{nlm} = R_{nl}(r)\Theta_{lm}(\theta)\cos m\varphi, \qquad (1.8)$$

$$\mathrm{Im}\,\psi_{nlm} = R_{nl}(r)\Theta_{lm}(\theta)\sin m\varphi. \qquad (1.9)$$

While the hypothetical electron density, determined in quantum mechanics as $e|\psi_{nlm}|^2$, excludes from the probabilistic analysis $\mathrm{Re}\,\psi_{nlm}$ and $\mathrm{Im}\,\psi_{nlm}$. Recognizing a difficulty in the interpretation of complex quantities, quantum mechanics assumes that the *physical sense has only the modulus squared of the wave function*

$$\psi_{nlm}\psi_{nlm}^* = \mathrm{Re}^2\,\psi_{nlm} + \mathrm{Im}^2\,\psi_{nlm} = R_{nl}(r)^2\Theta_{lm}(\theta)^2. \qquad (1.10)$$

This operation has cost one dear – it made away with the azimuth component $\Phi_m(\varphi)$ from the wave function $\psi_{nlm} = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\varphi)$ [7]. In spite of this, simultaneously, QM tacitly accepted (under the term the atomic orbitals

with "*incorrect magnetic numbers*") to use for the "qualitative" analysis the squares of $\mathrm{Re}^2\,\psi_{nlm}$ and $\mathrm{Im}^2\,\psi_{nlm}$.

Thus, the phrase "*the transition from the complex basis into the real one…*" [5] is the curious one. It means that, in essence, it costs nothing to easily leave the world of imaginary shades and to enter in the real world. It is very strange because it contradicts the basic concept of quantum mechanics on the *probabilistic interpretation* of the wave function Ψ, introduced in order to get rid of unreal ("imaginary") components.

Second, a statement about orientation of the functions $\psi_{nlm}^{(1)} = R_{nl}(r)\Theta_{lm}(\theta)\cos m\varphi$ and $\psi_{nlm}^{(+)} = R_{nl}(r)\Theta_{lm}(\theta)\sin m\varphi$ along the *x*- and *y*-axes, respectively [2], is incorrect as well because any atomic system in spherical polar coordinates has the only axis of symmetry, namely the polar *z*-axis.

Third, "real" functions $\Theta_{11}(\theta)\cos\varphi$ and $\Theta_{11}(\theta)\sin\varphi$ (p_x- and p_y-orbitals, see Fig. 1.1) are linear combinations of complex functions $\Theta_{11}(\theta)e^{\pm im\varphi}$. The mixing of these complex functions, contained "real" and "imaginary" quantities, together, as it has been done in quantum mechanics, is inadmissible, just like *it is impossible*, *e.g.*, *to mix together the electric and magnetic fields* and then to ascribe to the obtained mixture the properties inherent only in the electric field (or, *vice versa*, only in magnetic). Thus, hybridization as a *mathematical mixing* of qualitatively opposite properties is *physically* impossible and hence unreal. It is merely a mathematical trick used by creators of QM at the earliest stage of its building because of the ignorance of the physical sense of complex wave functions.
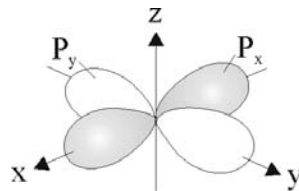

Fig. 1.1. The $p_x -$ and $p_y -$ orbitals of quantum mechanics.

The above statements require the convincing clarification that is the goal of this paper. We will show here the inadmissibility of the aforementioned mixing of the real and imaginary terms from the physical and philosophical

standpoints. We rest mainly on the comprehensive analysis carried out by the authors of the work [8]. At the end of this paper we will show the important results originated from analyzing hybridization.

2. The groundlessness of mixing the real and imaginary terms

It is not so difficult to come to the conclusion that all above mentioned theoretical curvilinear steps are directed to the one goal, namely implicitly to legalize the probabilities

$$dw_r = (\operatorname{Re}\psi)^2 dV \qquad \text{and} \qquad dw_i = (\operatorname{Im}\psi)^2 dV ; \qquad (2.1)$$

whereas, from the beginning, QM distinguishes the only differential of probability expressed by the equality

$$dw = |\psi|^2 dV . \qquad (2.2)$$

As a result, we have an interesting relation, which has never been discussed and which nobody has tried to notice:

$$dw = |\psi|^2 dV = dw_r + dw_i . \qquad (2.3)$$

The question arises: what do the probabilities dw_r and dw_i (and their bond with the originally postulated probability dw) mean?

The mathematical operations, given rise to s-, p-, and d-orbitals, were directed to an implicit usage not only real but also "imaginary" components of complex wave functions $\hat{\psi} = \psi_r + i\psi_i$. At that, constant factors of the functions are determined on the basis of the following normalization conditions:

$$\int_0^\pi \Theta_{l,m}^2 \sin\theta d\theta = 1, \qquad \int_0^{2\pi} \psi_{r,m}^2 d\varphi = 1; \qquad \int_0^{2\pi} \psi_{i,m}^2 d\varphi = 1 . \qquad (2.4)$$

Since Max Born introduced the probabilistic interpretation of the wave function [9], till now the "imaginary" parts, regarded as unreal quantities, do not have a firm physical interpretation. Let us cite Born's explanation: "*The reason for taking the square of the modulus is that the wave function itself (because of the imaginary coefficient of the time derivative in the differential*

equation) *is a complex quantity, while quantities susceptible of physical interpretation must of course be real*" [9, p.142].

Before "piling up" the "real" and "imaginary" parts of the complex wave function, it is necessary to think about how they are related. What does it mean imaginary? Already their names, "real" and "imaginary", say that we deal with the *qualitatively opposite properties* of wave fields and objects. Such properties are unquestioned at the description of all other physical processes and phenomena.

Actually, nobody will add a potential function (*e.g.*, potential energy) to the corresponding kinetic function (kinetic energy) and then call the resulting sum the potential function (potential energy). It is nonsensical. But why similar operations are the norm in QM (and, hence, in quantum chemistry)?

For example, a complex resistance of the *RLC* electric circuit has the following form

$$Z = R + i(X_L + X_C) = R + i\left(L\omega - 1/C\omega\right). \qquad (2.5)$$

It is impossible to imagine that someone could regard the "imaginary resistances", iX_L and iX_c, as unreal quantities. Naturally, the "real" and "imaginary" resistances are qualitatively opposite but *real* features. Such is the dialectics of electric circuits. The complex resistance by itself is contradictory just like other phenomena of nature.

The "real" resistance" R is an element of the dispersion of energy at the atomic level, whereas the "imaginary" resistances, positive iX_L and negative iX_c, are the elements accumulating, correspondingly, kinetic and potential energies of the subatomic level (of "electromagnetic field").

When we are interested in an amplitude value of current, the relation between current and amplitude of voltage is determined by means of the modulus of the total resistance:

$$I_m = U_m / |Z| = U_m / \sqrt{R^2 + \left(L\omega - 1/C\omega\right)^2} \ . \qquad (2.6)$$

And the modulus of power of the dispersion of energy depends on the modulus squared of the total resistance:

$$N_m = I_m^2 R = \frac{U_m^2 R}{|Z|^2} = \frac{U_m^2 R}{R^2 + \left(L\omega - 1/C\omega\right)^2} \ . \qquad (2.7)$$

Of course, the description of the wave field of *H*-atom on the basis of complex numbers is more complicated than the description of the simplest circuits. However, one should understand that the "real" and "imaginary" components of the polar-azimuth function express *qualitatively different wave states* of atoms and their structural units (like the active and reactive resistances in electric circuits or like the "electric" (longitudinal) and "magnetic" (transversal) fields, *etc*.). Unfortunately, it was not realized in quantum mechanics. As a result, the "real" and "imaginary" terms of the Ψ-function are regarded in QM erroneously as qualitatively similar. Accordingly, the complicated orbitals built on the basis of mixture of the "real" and "imaginary" components (*i.e*., mathematical mixture of physically immiscible) became the basis for the construction of QM models of atoms and molecules.

Let us consider the above stated from the pure philosophical point of view.

3. Logical bases of two different physical models of Nature

The spirit of extreme abstraction, based on ideology of chance and indeterminacy, wanders in quantum mechanics. It does not favor uncovering the real spatial structure of microobjects. This abstract approach does not endure the rigorous critique. In his time Hegel has noted that scientific abstraction must be the beginning and the elements, from which the concrete images of phenomena and states of nature must be developed; in opposite case we deal with abstractionism, which is far from the true science.

In Nature chance and necessity, definiteness and indeterminacy form symmetrical pairs of polar opposite properties of the Universe. Therefore, description of phenomena in microworld must not be reduced only to probability and indeterminacy.

In accordance with dialectical logic, foundation of which was laid by Hegel, to every affirmative judgment Yes, *e.g*., chance, possibility, definiteness, concreteness, discreteness, symmetry, *etc*., corresponds the symmetrical polar opposite judgment No: necessity, reality, indeterminacy, abstractiveness, continuity, asymmetry, *etc*.

The symmetry of polar properties, expressed by the binary dialectical judgment Yes – No, is the base of *dialectical model* of the Universe, which rests on the basic law of dialectical logic, namely the law of affirmation-negation (the Yes – No law) [10]. With this, there is no clear boundary

between Yes and No: properties Yes continuously and discontinuously (discretely) turn to opposite properties No.

Dialectical symmetry of polar properties of the Universe is a result of the formation of the Universe as Being from Non-Being with the zero measure. From the metaphysical point of view Non-Being is merely a mathematical emptiness, whereas from dialectical point of view Non-Being is another existence of Being in the uttermost unstable state of the highest degree of continuity, which transients into its opposition – Being. With that, the zero measure of Non-Being remains the same measure for Being. This is why to an arbitrary set Yes always corresponds, in the whole, the equal and opposite quantity No. From this it originates the symmetry of opposite properties of the Universe as Being. Being and Non-Being always go alongside, their fields-spaces intersect.

By virtue of the above stated it is obvious that we should speak with the Universe on the language of dialectical symmetry of oppositions.

For example, following Einstein, only relative motion exists. But, simultaneously, his theory operates with the speed of light, which remains the same in all systems of coordinates independently of the relative motions of sources and detectors. The last statement means, in the accurate language of dialectical logic, that the relativity theory simultaneously implicitly rests on the absolute motion of electromagnetic waves and the absolute speed of light. Absoluteness of properties means their independence of frames of references.

The aforementioned logical manipulations are not needed for dialectical model of Nature. In dialectical model any motion in the World is regarded as the complicated symmetrical complex of absolute-relative motion, Yes – No, in which the law of conservation and transformation of absolute-relative motion acts. So that to the property of motion Yes = *relative* responds the symmetrical property No = *absolute* [11].

Aristotle's *formal logic*, the logic of only Yes or only No, is unable of principle to overcome the one-sided view about Nature and therefore cannot correctly describe Nature, whereas Hegel's *dialectical logic* with the law Yes – No is able to do it.

The formal logic excludes the joining of Yes and No. This is why the modern physics is *forced* to operate by the law of dialectical logic Yes – No in implicit form.

Symmetrical opposite properties of processes and objects of Nature demand for their description an introduction of the numerical field of the symmetrical structure Yes – No as well, *i.e.*, with the opposite algebraic

properties, because only such a numerical field is able to express exactly the dialectical judgment Yes – No [12, 13].

Thus if for the formal logic and metaphysics it is sufficient the common (mono) numerical field, for the dialectical logic and dialectical philosophy (the philosophy of symmetrical structure of the Universe) it is necessary the symmetrical (binary) numerical field. The essential principles of the binary numerical field are the following.

Obviously, affirmation of affirmation is affirmation; therefore, the unit of affirmation 1 follows the algebra of affirmation (Yes-algebra):

$$(\pm 1)(\pm 1) = +1, \qquad (\pm 1)(\mp 1) = -1. \qquad (3.1)$$

It is natural as well that negation of negation is some affirmation. Therefore, the unit of negation $\bar{1}$ follows the algebra of negation (No-algebra), which is characterized by the opposite algebra of signs with respect to the Yes-algebra of signs:

$$(\pm \bar{1})(\pm \bar{1}) = -1, \qquad (\pm \bar{1})(\mp \bar{1}) = +1. \qquad (3.2)$$

It is convenient to present the unit of negation $\bar{1}$ by the letter i (imaginary number in complex numbers is designated by the same letter), then No-algebra takes the form

$$(\pm i)(\pm i) = -1, \qquad (\pm i)(\mp i) = +1. \qquad (3.2a)$$

Obviously, in the field of numbers with negative algebra of signs (3.2a), it is possible to extract the square root of negative unit $\sqrt{-1}$ and impossible of the positive unit $\sqrt{+1}$.

The equalities (3.1) and (3.2a) express the basic axioms of dialectical judgments and binary numerical field of *dialectics* (*dialectical philosophy and logic*).

The units of affirmation and negation give an adequate description of symmetrical (polar) properties of the Universe on the basis of dialectical functions-judgments $\hat{\Psi}$ of the logical structure Yes – No:

$$\hat{\Psi} = Yes \cdot 1 + No \cdot \bar{1}$$

or briefly

$$\hat{\Psi} = Yes + iNo.$$

The similar description of opposite properties Yes – No is impossible in formal logic if we will strictly follow its common rules of only Yes or only No.

Here is an example of realization of Yes-algebra. The identical (in sign) two charges repeal (the sign "+" in the left equality of (3.1) expresses it) and the opposite charges attract (the sign "–" in the right equality of (3.1) reflects it). Such is an objective algebra of *central*, *longitudinal* fields of interaction (exchange of matter-space-time).

The next example manifests the realization of No-algebra. Currents of the same sign (*i.e.*, the same direction) $\pm i$ and $\pm i$ attract through their magnetic (*transversal*) fields. The attraction (just like the repulsion) has the central character, so that the negative unit of the longitudinal field –1 reflects it. Currents of opposite signs, $\pm i$ and $\mp i$, repeal that is expressed by the measure +1.

Euler's famous formula $\exp(i\varphi) = \cos\varphi + i\sin\varphi$ is valid for the symmetrical dialectical numerical field. Therefore, if judgments Yes and No vary in course of time with the cyclic frequency ω, then an elementary symmetrical alternating dialectical judgment takes the form

$$\hat{\Psi} = \Psi_m(\cos\omega t + i\sin\omega t) \tag{3.3}$$

where

$$\Psi_m = \sqrt{Yes^2 + No^2}$$

is the modulus of the binary judgment Yes – No.

The geometry of dialectical judgments (3.3) repeats the geometry of those processes and phenomena, which these judgments represent. In other words, dialectical judgments, as against the formal logical judgments, present by themselves the "logical pictures" of an object of study, which are similar, to a definite extent, to art images.

The symmetry of polar opposite properties is reflected in the binary (complex) representation of the properties. This concerns also potential and kinetic features of physical phenomena (or processes). Let us proceed now to consider these features, because they have the direct relation to complex wave function Ψ.

4. Symmetry of potential and kinetic fields

Symmetrical potential and kinetic parameters form the binary parameters of potential-kinetic fields of every level of matter-space-time [14, 15]. In particular, a simple comparison of potential and kinetic energies of harmonic oscillations of a material point enables to write them in the symmetrical form

$$W_p = kx^2/2 = m\upsilon_p^2/2, \qquad W_k = ky^2/2 = m\upsilon_k^2/2. \qquad (4.1)$$

The symmetrical parameters of harmonic oscillations, used here, are the *potential displacement*

$$x = a\cos\omega t, \qquad (4.2)$$

along with the kinetic displacement

$$y = -\upsilon_k\sqrt{m/k} = a\sin\omega t, \qquad (4.3)$$

and the *potential speed*

$$\upsilon_p = x\sqrt{k/m} = \omega x, \qquad (4.4)$$

along with the kinetic speed

$$\upsilon_k = \upsilon = -\omega a\sin\omega t = -\omega y. \qquad (4.4a)$$

If the kinetic speed (and the kinetic displacement) is the measure of intensity of motion and of kinetic energy, then the potential speed (and the potential displacement) is the measure of intensity of rest and of potential energy.

The potential and kinetic displacements in an *oscillating process* [14] form the total potential-kinetic displacement $\hat{\Psi}$ of the form

$$\hat{\Psi} = x + iy = a(\cos\omega t + i\sin\omega t) = ae^{i\omega t}. \qquad (4.5)$$

The potential-kinetic displacement in the harmonic *wave field* [15], including intra-atomic wave fields, has the form

$$\hat{\Psi} = x + iy = a(\cos(\omega t - kr) + i\sin(\omega t - kr)) = a\exp i(\omega t - kr). \qquad (4.6)$$

Time derivative of the potential displacement defines the potential-kinetic speed

$$\hat{V} = \frac{d\hat{\Psi}}{dt} = i\omega\hat{\Psi} = -\omega y + i\omega x = \upsilon_k + i\upsilon_p. \qquad (4.7)$$

The speed (4.6) defines the potential-kinetic momentum, *etc*. If the kinetic speed (and kinetic displacement) is the measure of intensity of motion, then the potential speed (and potential displacement) is the measure of intensity of rest. Kinetic and potential speeds define the corresponding energies, which, strictly speaking, have the opposite signs that point to their opposite character:

$$W_p = m(i\upsilon_p)^2/2 = -kx^2/2, \qquad W_k = m\upsilon_k^2/2 = -k(iy)^2/2. \qquad (4.8)$$

Their difference defines the modulus of total energy in a classical sense

$$W = W_k - W_p = ka^2 / 2 . \tag{4.9}$$

   Symmetrical potential-kinetic parameters give the complete description of potential-kinetic fields that is impossible in metaphysics and, hence, in classical, quantum and wave physics, which were created following Aristotle's logical rules of limited possibilities [14, 15]. The dialectical image of a judgment $\hat{\Psi}$ of the general binary structure

$$\hat{\Psi} = \Psi_p + i\Psi_k , \tag{4.10}$$

reproduces mathematically the real image and binary character of the original. The letter i in Eq. (4.10) designates (as was discussed in the previous section) the unit of negation, *i.e.*, points to the qualitatively opposite property Ψ_k (kinetic) with respect to Ψ_p (potential).

   Of course, if one chooses the potential displacement $x = a \sin \omega t$ then the kinetic one will be $y = a \cos \omega t$, *etc*. Due to this feature, ascribing to either of the two displacements the physical sense of "potential" or "kinetic" is a matter of taste (or convention).

   In physics, in those cases when the physical meaning of a complex function (4.10) is not understood (by a reason) and hence undefined, the imaginary term Ψ_k is regarded as unreal quantity not "susceptible of physical interpretation". In particular, a misunderstanding of "*just what does psi really mean*?" (the cited expression was taken from an epigram devoted to Schrödinger, which was spread among physicists at that time [8, page 130]) gave rise to a nothing-grounded interpretation of the wave Ψ-function, in quantum and wave mechanics, according to which the *real physical sense* has *only* its modulus squared [7, 16].

   In reality, as proved by all experience of physics and appears from the works [8, 10 - 15], "real" and "imaginary" parts of complex *wave* functions are both real. They represent two *qualitatively different* entities, in particular, the *potential* and *kinetic* features of the *wave* process described by the functions.

   Let us turn now to the physical sense of complex spherical harmonics, namely polar-azimuth components of the wave functions. But at the beginning we elucidate the sense of the wave function itself from our point of view. All details concerning the binary numerical field and the physical sense of *wave* functions are in the above cited works.

5. The physical meaning of the Ψ -function

Any physical parameter $\hat{P}$ of an arbitrary *wave field* is characterized by its particular measure or, in other words, by a period-quantum p_k; so that any $\hat{P}$ -parameter can be presented by the relative $\hat{\Psi}$ -measure:

$$\hat{\Psi} = \hat{P} / p_k . \qquad (5.1)$$

The relative $\hat{\Psi}$ -measure of the zero dimensionality of the $\hat{P}$ -parameter in the *wave* potential-kinetic field of matter-space-time of any nature is the wave function of the following general form

$$\hat{\Psi}(\omega t - \mathbf{kr}) = \hat{\Psi}(\omega t - k_x x - k_y y - k_z z) . \qquad (5.2)$$

$\hat{\Psi}$ -Function can be presented in the form of the product of its spatial and time components:

$$\hat{\Psi} = \hat{\psi}(\mathbf{kr})\hat{T}(\omega t) . \qquad (5.2a)$$

The spatial (amplitude) function $\hat{\psi}(\mathbf{kr})$ defines spatial waves, $\hat{T}(\omega t)$ defines time waves [15]. Thus, the $\hat{\Psi}$ -function is a variable wave real potential-kinetic binary number describing variations of a $\hat{P}$ -parameter in space and time. As a result the wave structure of any physical parameter $\hat{P}$ is presented by the following scalar measure:

$$\hat{P} = p_k \hat{\Psi}(\omega t - k_x x - k_y y - k_z z) . \qquad (5.3)$$

If p_k is the momentum of particles of the field, then the expression (5.3) describes the wave field of the momentum of particles.

Any $\hat{\Psi}$ -parameter satisfies the differential equation with the second partial derivatives with respect to spatial coordinates

$$\frac{\partial^2 \Psi}{\partial x^2} = -k_x^2 \Psi , \quad \frac{\partial^2 \Psi}{\partial x^2} = -k_x^2 \Psi , \quad \frac{\partial^2 \Psi}{\partial x^2} = -k_x^2 \Psi ,$$

or   (5.4)

$$\Delta \Psi = -k^2 \Psi ,$$

where $k^2 = k_x^2 + k_y^2 + k_z^2$ is the wave number squared of a fundamental frequency of the field. $\hat{\Psi}$ -Function satisfies also the equation with the second partial derivative with respect to time

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi \,. \tag{5.5}$$

Equations (5.4) and (5.5) form together the wave equation of the $\hat{\Psi}$-function

$$\Delta\Psi - \frac{1}{c^2}\frac{\partial^2 \Psi}{\partial t^2} = 0 \,, \tag{5.6}$$

where c is the definite base speed of wave processes at the corresponding (under consideration) level of matter-space-time.

   The sum of elementary solutions of Eq. (5.6) determines the structure of the wave field of an arbitrary parameter. Because in any point of a steady state wave motion the $\hat{\Psi}$-function is represented by the product of its spatial (called amplitude as well) $\hat{\psi}(\mathbf{kr})$ and time $\hat{T}(\omega t)$ factors, the wave equation (5.6) comes to the amplitude and time equations

$$\Delta\hat{\psi} + k^2\hat{\psi} = 0 \,, \tag{5.7}$$

$$\frac{\partial^2 \hat{T}}{\partial t^2} = -\omega^2\hat{T} \,, \tag{5.8}$$

where the *constant* parameters k and ω are defined from the boundary conditions.

   Equations (5.4) and (5.5) describe $\hat{\Psi}$-measures of arbitrary physical parameters; therefore, the distinction in their wave structures reduces to the difference of kinematic types of wave fields, at the equality of their discrete structure. Atomic wave fields-spaces are represented by the spherical-cylindrical fields.

   Thus, the $\hat{\Psi}$-function is the mathematical image of the wave process. $\hat{\Psi}$-Function defines not only the real picture, but also the possible picture of the field. Therefore, the $\hat{\Psi}$-function is simultaneously a prognostic probabilistic picture of the potential-kinetic field. In other words, the wave $\hat{\Psi}$-function is the natural measure of *physical probability of wave processes*, but by no means the probability of games of chance. By this reason the *wave equation* (5.7) is simultaneously the *equation of physical potential-kinetic probability* (prognosis) $\hat{\Psi}$ [17]. Let us elucidate now the solution of the wave equation (5.7) in outline using the notions stated above.

6. The symmetrical potential-kinetic structure of polar-azimuth functions

Complex polar-azimuthal functions (spherical harmonics)

$$Y_{l,m}(\theta,\varphi) = C_{l,m}\Phi_m\Theta_{l,m}(\theta)\exp[\pm i(m\varphi+\alpha)] \qquad (6.1)$$

are the particular solutions of polar and azimuthal equations,

$$\frac{d^2\Theta_{l,m}}{d\theta^2} + ctg\theta\frac{d\Theta_{l,m}}{d\theta} + \left(l(l+1) - \frac{m^2}{\sin^2\theta}\right)\Theta_{l,m} = 0 \qquad (6.2)$$

and
$$\frac{d^2\hat{\Phi}_m}{d\varphi^2} = -m^2\hat{\Phi}_m, \qquad (6.3)$$

to which comes the wave equation

$$\Delta\hat{\Psi} - \frac{1}{c^2}\frac{\partial^2\hat{\Psi}}{\partial t^2} = 0 \qquad or \qquad \Delta\hat{\Psi} + k^2\hat{\Psi} = 0, \qquad (6.4)$$

in spherical polar coordinates [8], where the wave number

$$k = \frac{2\pi}{\lambda} = \frac{\omega}{c} \qquad (6.4a)$$

is the *constant* quantity. In the last equality, ω is the fundamental frequency and c is the base speed of exchange of matter-space-time at a given level of matter-space-time; at the subatomic level $\omega = \omega_e = 1.869162\cdot10^{18}\ s^{-1}$ and c is equal to the speed of light [18].

The spherical harmonics (6.1) are also the solutions of Schrödinger's equation of quantum mechanics

$$\Delta\hat{\Psi} + \frac{2m}{\hbar^2}(W + \frac{Ze^2}{4\pi\varepsilon_0 r})\hat{\Psi} = 0, \qquad or \qquad \Delta\hat{\Psi} + k^2\hat{\Psi} = 0. \qquad (6.5)$$

In the latter case, k is the *variable* quantity dependent on the distance from the origin of coordinates, r:

$$k = \pm\sqrt{\frac{2m}{\hbar^2}(W + \frac{Ze^2}{4\pi\varepsilon_0 r})}. \qquad (6.5a)$$

Schrödinger's equation is usually presented in the following forms

$$-\frac{\hbar^2}{2m}\Delta\Psi + U\Psi = i\hbar\frac{\partial\Psi}{\partial t} \qquad \text{or} \quad \hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}, \qquad (6.6)$$

where

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + U \qquad (6.6a)$$

is Hamilton's operator (Hamiltonian), W and

$$U(r) = -Ze^2 / 4\pi\varepsilon_0 r \qquad (6.6b)$$

are, respectively, total and potential energies of an electron in the field of a nucleus of hydrogen-like atoms. A critical analysis of an introduction of the *variable* wave number k (6.5a) in the wave equation by Schrödinger and peculiarities of his radial solutions had been carried out in the works [7, 16].

A formal introduction of the potential function $U(r) = -Ze^2 / 4\pi\varepsilon_0 r$ in the wave number k by Schrödinger (while $k = 2\pi/\lambda$ and λ cannot continuously vary in space in dependence on distance [7]) does not quite mean that the polar-azimuth distribution (6.1) has a relation to electrons. As a pure mathematical function, (6.1) is not related to the electron potential function (6.6b) (or to any other one either).

The potential-kinetic polar-azimuth function (6.1) consists of two elementary polar-azimuth functions, potential and kinetic, which have the following form

$$Y_{l,m}(\theta,\varphi)_p = C_{l,m}\Phi_m\Theta_{l,m}(\theta)\cos(m\varphi + \alpha), \qquad (6.7)$$

$$Y_{l,m}(\theta,\varphi)_k = C_{l,m}\Phi_m\Theta_{l,m}(\theta)\sin(m\varphi + \alpha). \qquad (6.8)$$

If the normalizing factor of polar-azimuth functions (6.1) is assumed to be equal to the numerical unit, these functions are called the reduced functions and designated as $\tilde{Y}_{l,m}(\theta,\varphi)$.

The reduced *potential* polar-azimuth functions $\tilde{Y}_{l,m}(\theta,\varphi)_p = \tilde{\Theta}_{l,m}(\theta)\cos m\varphi$ (for $\alpha = 0$) are presented in Table 6.1. Graphs of the *potential* polar-azimuth functions $Y_{l,m}(\theta,\varphi)_p$ (or $\tilde{Y}_{l,m}(\theta,\varphi)_p$) are drawn in Fig. 6.1 (with circumferences, defining the cones of extremal values of polar angles).

Recall that the wave function $\hat{\Psi}$ of both solutions, ordinary (6.4) and Schrödinger's (6.5) wave equations,

$$\hat{\Psi} = \hat{R}_l(kr)\hat{Y}_{l,m}(\theta,\varphi)\hat{T}(\omega t) = \Psi_p + i\Psi_k \qquad (6.9)$$

contains the same spherical harmonics

$$\hat{Y}_{l,m}(\theta,\varphi) = \Theta_{l,m}(\theta)\hat{\Phi}_m(\varphi) = C_{l.m}P_{l.m}(\cos\theta)C_m \exp[\pm i(m\varphi+\alpha)], \qquad (6.9a)$$

where $C_{l,m}$ and C_m are coefficients depending on the normalizing conditions, $P_{l,m}(\cos\theta)$ are Legendre adjoined functions, $\Phi_m(\varphi)$ are azimuthal functions, α is an initial phase of the azimuthal state.

Table 6.1. The reduced potential polar-azimuth functions $\tilde{Y}_{l,m}(\theta,\varphi)$

l	m	$\tilde{Y}_{l,m}(\theta,\varphi) = \tilde{\Theta}_{l,m}(\theta)\cos m\varphi$			
0	0	1			
1	0	$\cos\theta$	5	0	$\cos\theta\,(\cos^4\theta - 10/9\,\cos^2\theta + 5/21)$
	± 1	$\sin\theta\,\cos\varphi$		± 1	$\sin\theta\,(\cos^4\theta - 2/3\,\cos^2\theta + 1/21)\,\cos\varphi$
2	0	$\cos^2\theta - 1/3$		± 2	$\sin^2\theta\,\cos\theta\,(\cos^2\theta - 1/3)\,\cos2\varphi$
	± 1	$\sin\theta\,\cos\theta\,\cos\varphi$		± 3	$\sin^3\theta\,(\cos^2\theta - 1/9)\,\cos3\varphi$
	± 2	$\sin^2\theta\,\cos2\varphi$		± 4	$\sin^4\theta\,\cos\theta\,\cos4\varphi$
3	0	$\cos\theta\,(\cos^2\theta - 3/5)$		± 5	$\sin^5\theta\,\cos5\varphi$
	± 1	$\sin\theta\,(\cos^2\theta - 1/5)\,\cos\varphi$			
	± 2	$\sin^2\theta\,\cos\theta\,\cos2\varphi$	6	0	$\cos^6\theta - 15/11\,\cos^4\theta + 5/11\,\cos^2\theta - 5/231$
	± 3	$\sin^3\theta\,\cos3\varphi$		± 1	$\sin\theta\,\cos\theta\,(\cos^4\theta - 10/11\,\cos^2\theta + 5/33)\,\cos\varphi$
4	0	$\cos^4\theta - 6/7\,\cos^2\theta + 3/35$		± 2	$\sin^2\theta\,(\cos^4\theta - 6/11\,\cos^2\theta + 1/33)\,\cos2\varphi$
	± 1	$\sin\theta\,\cos\theta\,(\cos^2\theta - 3/7)\,\cos\varphi$		± 3	$\sin^3\theta\,\cos\theta\,(\cos^2\theta - 3/11)\,\cos3\varphi$
	± 2	$\sin^2\theta\,(\cos^2\theta - 1/7)\,\cos2\varphi$		± 4	$\sin^4\theta\,(\cos^2\theta - 1/11)\,\cos4\varphi$
	± 3	$\sin^3\theta\,\cos\theta\,\cos3\varphi$		± 5	$\sin^5\theta\,\cos\theta\,\cos5\varphi$
	± 4	$\sin^4\theta\,\cos4\varphi$		± 6	$\sin^6\theta\,\cos6\varphi$

The difference between the general solutions of ordinary (6.4) and Schrödinger's (6.5) wave equations is caused by the difference of their radial equations (because of the different wave numbers k, see (6.4a) and (6.5a)), which leads to the different radial solutions $\hat{R}_l(kr)$. We will not show here Schrödinger's radial equation and its solutions, they are analysed in detail in [7, 16].
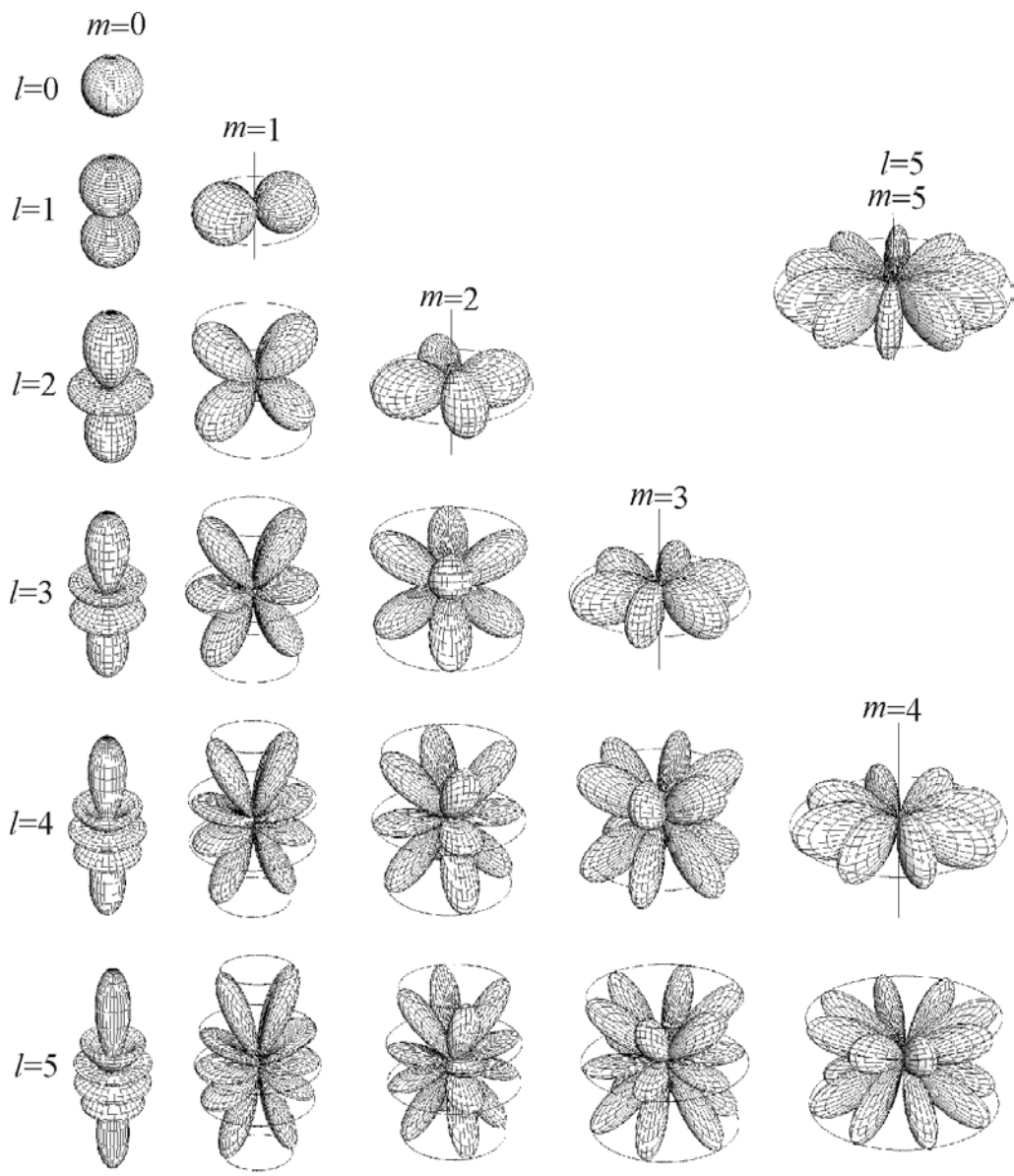
Fig. 6.1. Graphs of the potential polar-azimuthal functions $\left|\Theta_{l,m}(\theta)\cos m\varphi\right|$

At integer values of the wave number m, the particular solution of the wave equation (6.4) has the standard form. If we present the number m in the form $m = \frac{1}{2} 2s$, where $s \in N$, we arrive at

$$\hat{\psi} = A_l \hat{R}_l(\rho)\Theta_{l,s}(\theta)e^{\pm is\varphi} = A_l\sqrt{\pi/2\rho}H^{\pm}_{l+\frac{1}{2}}(\rho)\Theta_{l,s}(\theta)e^{\pm is\varphi} \quad (6.10)$$

or

$$\hat{\psi} = A_l\sqrt{\pi/2\rho}(J_{l+\frac{1}{2}}(\rho)\pm iY_{l+\frac{1}{2}}(\rho))\Theta_{l,s}(\theta)e^{\pm is\varphi}, \quad (6.11)$$

where A_l is the constant factor; $\rho = kr$; $H^{\pm}_{l+\frac{1}{2}}(\rho)$, $J_{l+\frac{1}{2}}(\rho)$ and $Y_{l+\frac{1}{2}}(\rho)$ (or $N_{l+\frac{1}{2}}(\rho)$) are the Hankel, Bessel and Neumann functions, correspondingly.

The form of the function (6.10) uniquely shows that it describes the kinematic structure of *standing spherical waves* in wave physical space. Thus the solution (6.11) yields the spatial geometry of disposition of specific points (nodes and antinodes) in which the wave $\hat{\Psi}$ function takes the zero and extremal values. With this, polar-azimuthal functions, potential and kinetic, define the *angular spatial coordinates*, respectively, of nodes and antinodes of the standing spherical waves, and nothing more.

Two terms in (6.11) are the potential and kinetic *spatial* constituents of the $\hat{\Psi}$-function; they have the following form

$$\hat{\psi}_p = Ac_l(\rho)/\rho = A\sqrt{\pi/2\rho}J_{l+\frac{1}{2}}(\rho)\Theta_{l,m}(\theta)e^{\pm im\varphi}, \quad (6.12)$$

$$\hat{\psi}_k = \pm As_l(\rho)/\rho = \pm A\sqrt{\pi/2\rho}Y_{l+\frac{1}{2}}(\rho)\Theta_{l,m}(\theta)e^{\pm im\varphi}. \quad (6.13)$$

The half-integer solutions of (6.4), at $l = m = (1/2)s$, have the form

$$\hat{\psi} = A\hat{R}_s(\rho)\Theta_s(\theta)e^{\pm i\frac{s}{2}\varphi}, \quad (6.14)$$

where

$$\hat{R}_s(\rho) = \sqrt{\pi/2\rho}H^{\pm}_{\frac{s}{2}+\frac{1}{2}}(\rho), \quad (6.15)$$

$$\Theta_s(\theta)e^{\pm i\frac{s}{2}\varphi} = C_s\sin^{\frac{s}{2}}\theta(\cos\frac{s}{2}\varphi\pm i\sin\frac{s}{2}\varphi). \quad (6.16)$$

We see that the polar extremes of half-integer solutions lie in the equatorial plane.

All spatial components are determined with the accuracy of a constant factor *A*, imposed by boundary conditions, which have no influence on the peculiarity of distribution of the *nodes* on radial spheres. The superposition of even and odd solutions defines the *even-odd solutions*. Odd solutions describe the nodes, lying in the equatorial plane of atomic space. In this plane there are also solutions in the form of *rings* in space (graphically shown further) separated by radial unstable shells.

$\hat{\Psi}$ -Function represents any parameter of the *wave* field [8] such as, for example, potential-kinetic displacement, potential-kinetic speed, physical potential-kinetic probability, *etc*.

The radial component $\hat{R}_l(kr)$ of the wave function $\hat{\Psi}$ (6.9) describes the radial field of displacements of the wave parameter, which the $\hat{\Psi}$ -function represents in the wave equation (the density of potential-kinetic phase probability in the work [8], in the case of Eq. (6.4)), the polar component $\Theta_{l,m}(\theta)$ describes the polar displacements, and $\hat{\Phi}_m(\varphi)$ describes the azimuth displacements.

Potential and kinetic solutions (6.7) and (6.8) are mutually conjugate because the conjugate functions

$$\hat{\Psi} = \Psi_p + i\Psi_k \quad \text{and} \quad \hat{\Psi} = i(\Psi_p + i\Psi_k) = (-\Psi_k)_p + i(\Psi_p)_k \quad (6.17)$$

satisfy the wave equation.

The potential solutions define the coordinates of rest, whereas the conjugate kinetic solutions define the coordinates of maxima of motion. Thus, the potential solutions give us the spatial coordinates of equilibrium domains (nodes of standing spherical waves) in the wave atomic space.

From the above it is clear why we should distinguish between the two solutions, potential and kinetic, do not mixing them. Rest and motion (nodes and antinodes) are the two *qualitatively different* states of wave processes.

Now it is obvious as well that the so-called p_y-orbital of quantum mechanics, presented in Fig. 1.1, relates to the *kinetic* solutions (just like d_{yz}- and d_{xy}-orbitals in (1.7)), so that we have no rights to consider the kinetic p_y-orbital together with the potential p_x-orbital, responding to $l = 1$ and $m = 1$ (see Fig. 6.1).

Kinetic harmonics are the same, in form, as potential harmonics, but they are displaced (turned) in space in the azimuthal direction, around the z-axis,

with respect to potential harmonics (just like $\cos m\varphi$ with respect to $\sin m\varphi$ in (6.7) and (6.8)) so that the kinetic extrema are between the corresponding potential extrema (as alternated nodes and antinodes in standing waves).

Basing on the clarification of the nature of the polar-azimuthal functions, let us answer now to the following question: what information is actually contained in spherical harmonics presented in Fig. 6.1?

7. Nodal structure of spherical standing waves in atomic spaces

The form of the radial equation and its solutions $\hat{R}_l(kr)$ depend on the concrete problem, which imposes the definite requirements on the wave number k (see (6.4a), (6.5a) and (6.10)).

However, for any model of an object of study, the radial solutions define the characteristic spheres of extrema and zeros of the radial function. For a variety of problems, it is sufficient to know at most that such characteristic spheres exist. This is why we do not analyze here Schrödinger's radial equation and its solutions: it is not the matter in question of this paper.

Evidently, the polar and azimuth equations (6.2) and (6.3) are common (universal) for all models of objects of study if they are described by the general wave equation (6.4). As was mentioned above, Schrödinger's equation (6.5) comes to the same polar and azimuth equations as well.

Radial solutions $\hat{R}_l(kr)$ (6.10) are defined by roots of Bessel functions [19, 20] only in the case of the constant wave number k (6.4a) that distinguishes them from Schrödinger's solutions based on the variable wave number k (6.5a). They give the equilibrium spherical shells of standing spherical waves in the wave field of potential and kinetic displacements.

Polar-azimuthal functions (6.1) define polar-azimuthal coordinates of *nodes and antinodes of standing spherical waves*, located on these shells [8].

Polar components $\Theta_{l,m}(\theta)$ of the $\hat{\Psi}$-function (6.9) define characteristic parallels of extrema (principal and collateral) and zeros on radial spheres (shells).

Azimuthal components $\hat{\Phi}_m(\varphi)$ define characteristic meridians of extrema and zeros. Potential and kinetic polar-azimuthal functions $\hat{Y}_{l,m}(\theta,\varphi)$ select together the distinctive coordinates of extrema and zeros on the radial shells.
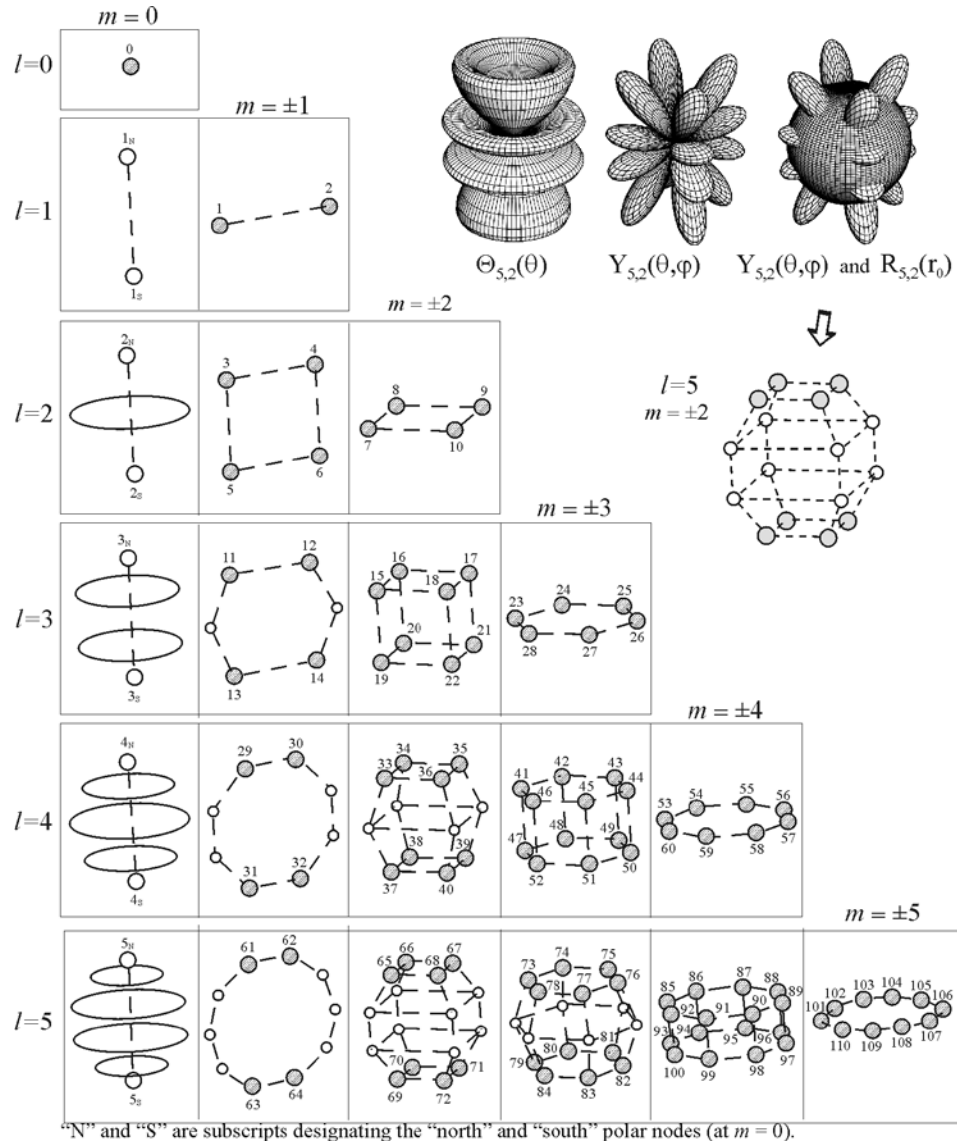
"N" and "S" are subscripts designating the "north" and "south" polar nodes (at $m = 0$).

Fig. 7.1. Spatial solutions $\psi_{l,m}(\rho,\theta,\varphi)_p = C_\Psi R_l(\rho)\Theta_{l,m}(\theta)Cosm\varphi$ (for $r = const$) of the wave equation (6.4) for *spherical standing waves* presented in the form indicating the space distribution of *potential* extrema-nodes (discrete elements of the shell-nodal structure of atoms); numbers 1, 2, 3, …, 110 are the ordinal numbers of the principal potential polar-azimuth nodes coinciding with atomic numbers of the elements Z [8].

The geometry of characteristic states on radial shells is expressed by extrema and zeros of the polar-azimuthal components of the $\hat{\Psi}$-function.

The *potential* solutions of the $\hat{\Psi}$-function (for $l = 0, 1, 2, 3, 4, 5$) are depicted graphically in Fig. 7.1 for a constant value of the radial coordinate r. In this figure, with an example for $l = 5$ and $m = \pm 2$, it is also shown how the presented discrete (nodal) structure of the three dimensional wave space is obtained from the aforementioned solutions for the different wave numbers l and m.

The graphs of the solutions indicate that there are *principle* (designated in Fig. 7.1 by shaded points) and *collateral* (designated by the smaller unnumbered hollow points) extrema, which determine, correspondingly, stable and metastable states of probabilistic events.

Principal *potential* polar-azimuthal nodes are numbered in Fig. 7.1 by ordinal numbers. The principal polar-azimuth extrema (potential and kinetic, $m \neq 0$) mainly define the geometry of radial shells of atomic space, whereas collateral extrema ($m \neq 0$) play the secondary role. Both principal and collateral extrema are points-nodes of the steady-state discrete geometry of the wave field of matter-space-time of atoms.

As it turned out, the shell-nodal structure, presented in Fig. 7.1, is reminiscent of *spherical resonant cavities* [21] (described by Bessel functions as well) having internal oscillating electric and magnetic mode fields.

And what is more, as appears from the comprehensive analysis [8, 13], all types of *elementary crystal lattices represent*, in essence, elementary *nodal structure of standing waves* in a limited three-dimensional wave physical space.

Thus, the spatial shell-nodal structure presented in Fig. 7.1 uniquely determines the structure of matter at the atomic and molecular levels, in particular, the intra-atomic structure and the structure of crystals [22].

The quasi-similarity of the geometry of external shells, for the same quantum number m and different quantum numbers l, clearly seen from Fig. 7.1, reveals the nature of Mendeleev' Periodic Law [8, 22 - 24] and specifies the role of electrons in chemical bonds formation [25]. A great body of other important consequences, originated from the above solutions, relates to the new data concerning the atomic structure, periodicity, symmetries, the nature and structure of isotopes [26], *etc*. These and other relevant data are not the matter in question of this paper, they can be found in the reference works of the author.

8. Conclusion

A series of different notions, touched in this paper, is that minimal ground which was necessary for elucidation of the groundlessness of one of the key concepts of modern physics, namely hybridization. In this connection, the physical nature of the wave $\hat{\Psi}$-function and spherical harmonics has been elucidated. It was shown that polar-azimuthal factors of the wave function $\hat{\Psi}$, potential and kinetic, being the solutions of the ordinary wave equation in spherical polar coordinates and of Schrödinger's wave equation, define the *angular spatial coordinates*, respectively, of nodes and antinodes of standing spherical waves.

Dialectical binary numerical field, introduced in the approach presented, coinciding in form with the field of complex numbers (lying in the *complex plane*), is the basis for this study. In dialectical numerical field (lying in *real* three-dimensional *space*), both "real" and "imaginary" terms of complex wave functions and, hence, of their constituents, spherical harmonics (polar-azimuthal functions), are real. They reflect polar opposite, potential and kinetic, properties of an object (or a process) of study, which the given complex wave function represents and describes.

Important consequences follow from the analysis brought concisely to light in this paper. The erroneousness of the concept of *hybridization* because of the natural unquestionable inadmissibility of abstract mixing of physically immiscible is the first of these consequences. The mixing objects are actually the *qualitatively opposite real features*, potential and kinetic (like, for example, material and ideal, quantity and quality, form and contents, motion and rest, cause and effect, past and future, absolute and relative, wave and quantum, *etc*). Since the hybridization is in the base of the quantum mechanical atomic model and quantum chemistry, the above fact naturally calls in question, whether do they correctly describe reality? We have the base to doubt in it that confirms the similar conclusions obtained in other works on this subject [7, 16].

Obviously, a denial of the legality of "hybridization" amounts to a denial of the superposition principle, *i.e.*, the basis of quantum mechanics. Hence, the validity of the QM atomic model calls sound doubts.

Actually, the comprehensive analysis, carried out in the work [8], showed that mono-center (mono-nuclear) atomic model rather does not correspond to reality. As it turned out, an atom is substantially more complicated that it appears from the quantum mechanical atomic model. Atoms are similar to

"star" associations of the nucleon world, represented by elementary structural units, namely H-atoms (we refer to them protons, neutrons and hydrogen atoms) in the composition of complex atoms.

Although, within the framework of quantum electrodynamics (which was developed on the basis of QM by correcting its shortcomings and broadening possibilities), most of the experimental facts in atomic physics (after incredible efforts undertaken by mathematical physics in the past century) are *calculated* now relatively correctly. However, the last circumstance cannot justify the fully developed current *status quo* in atomic physics and related fields because physics must not only to "*calculate all the results*" [27], but also to *comprehend* nature.

Any theory initiates an experiment originated from this theory; therefore the experiment very often "confirms" such a theory, to a certain degree, although this theory maybe does not reflect reality completely (see, for example, the work devoted to electron spin [28]). This is why theorists must not ignore the fact (noted in his time by Bohr [29]) that the correspondence of any theory with the experiment does not quite mean that the given theory is true and uniquely possible. And what is more, the possibilities of modern mathematics are so impressive that it can present any abstract figment of an imagination as a profound theory and fit it to the experiment. Therefore, we have the firm ground to state that QM incorrectly *describes* the atomic structure.

It make sense to say in addition (for the readers interested in this matter) that a new atomic theory, some elements of which were concisely touched in this paper in connection with the notion of hybridization, is also based on *dynamic model of elementary particles* [18]. The word "*dynamic*" means that the discrete elements of inter- and intra-atomic spaces (just like of elementary particles and their constituents) are not static, being in continuous dynamic exchange of matter-space-time with all interrelated embedded wave fields-spaces of the Universe [11]. The new atomic model originated from the new atomic theory, called the *shell-nodal* or *multi-center* (or *molecule like*) atomic model [30], entirely elucidates a large body of experimental facts of physics (including Rutherford's experiment on scattering of α- and β-particles in substance [31]). This model allows also putting and solving the questions impossible in the framework of modern atomic theory.

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