

The Information Modeling of Optical Objects in the Nanoscience

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Abstract:

This paper presents the basic ideas and concepts for the development of information models of optical objects in the nanoscience. Quantitative ratios among regularities in trigonometric spectral analysis as a possible connection between the projection of natural (point-source) radiator and absorbing atomic section are shown. This approach has been applied to the correlation between these patterns and atomic spectroscopy (specifically, terms and ionization potentials of neutral atoms with s and p shells. This has made it possible to build information models of radiation and atomic absorption on certain principles of field continuum quantization. The paper analyzes the possibilities and limitations of the information method of calculating the singlet odd electronic states of the diatomic homonuclear molecule from their dependence on the quasi-adiabatic ionization potential and on the quantum numbers of the atoms forming the molecule.

Keywords:

Information Models of Radiation and Absorption, Optical Octaves, Trigonometric Projections, Continuum Quantization, Atomic and Molecular Terms

1. Introduction

It is commonly considered that, on the one hand, quantized energy of optical radiation in photons has no reliable underpinning in theoretical physics [1, pp. 1189 and 1213]; on the other hand, there is a system of harmonic octaves that correlates with the optics of radiation sources [2, p. 109] by characteristics of their trigonometric functions (TFs) [3].

The goal of this paper is to study optical and trigonometric regularities to find the physical essence of the first provision of correlations between the empirical data of both approaches by building an information model (IM) of radiation (IMR), of atomic absorption (IMAA), of additivity of terms (IMAT).

With its semantics that has historically included essential meanings (Arab, *tangens*; a shadow that is inalienable from an object, a satellite, tangent; cognate of Lat. *tangibilis*: felt by touch, from *tangere*: to touch, border, take possession of), the tangent seemed to be the relevant value for studying optical correlations. However,

experience has shown that the suitable quantity is not tg is but tg^2 is, which not only eliminates negative radiation energy values but helps to identify characteristic features of the junctures on the tangent curve.

Extreme points (junctures) of octaves must correlate with the radiation source trigonometry because the projection (cross section) of the natural source could be correlated with $x\pi$ -fold measured radiation angles, where $x < 1$. If the magnetic/light field energy propagates at a phase velocity, then the photon energy correlates with the wave frequency in vacuum and/or relevant wavelength like the self-congruent codes of data and data-processing method.

That is the reason that neither energy nor wavelength taken separately can be the target quantity that carries streams of information from the radiation source to the receiver; the target quantity is the combined dependence of their variation, i.e., exactly $\Delta E(\Delta\lambda)$ as some hypothetical *instrument function* of source energy variation ΔE via the *slit width* variation $\Delta\lambda$. Then, this quantity could be further considered as the relevant argument for defining information characteristics in the IMR or IMAA.

Any domain of science essentially deals solely with information. Ontologically, information is ideal relative to data but material relative to the interpreting subject. The information model reflects only an object's essential properties and is, therefore, its characteristic description that helps one to understand reality. In information science the information model is a representation of objects, relations, limitations, rules, and operations that is meant to identify the essential semantics of data for a chosen domain (problem area).

Thus, the information model as understood hereafter is the totality of information on the state and functioning of an analyzed system, arranged according to certain rules; for example, chromatic (information) models are models created in the natural language of the semantics of color concepts and their ontological predicates, i.e., in the language of essences and meanings of the color canons commonly reproduced in world culture. Some cases of chromatic models include the atomic model of intelligence (AMI), inter-faith immanence of religions (IFIR), and model of axiological social semantics (MASS), etc., which are all based on the theory and methodology of chromatic [4].

Generally, any system perceives only information that it can absorb. Since the resonant characteristics of this part of information will be common to the components of the absorbing system, this information as information absorbed (perceived) may be the very internal ontologically ideal information that we link with the characteristic components of the modeled object.

Thus, only such information is classified as *bound* that correlates with functions, not with the structures and composition (system components and their interactions) of the system that ontologically belong to the material level. At this approximation the information related to this level can be classified as free. It is therefore easy to give the semantic definition of information: information is an agreed distribution of the source's codes across relevant codes of the bound and free states of the receiver.

Since the information model as a totality of information characterizes the essential properties and typical features of objects, information model development is not confined to trivial simplifications according to the normal criterion of retaining only the characteristic information about a complex system. An optimal case of an

information model is the dimension of a physical quantity with all of the minor parameters eliminated, which makes it easy for the researcher to validate the formalization of his reasoning's.

2. Experimental Data Analysis

To solve the problem, we made a detailed analysis of TFs in the following sequence: $\pi/4$ constituted the angle $\varphi_1 = 0.78539$ radians. This is the first octave point for a step of 45° . The next points of that octave ($\varphi_2 = 1.57077$, $\varphi_3 = 2.35615$, etc.) appeared to match accurate to five characters with the known energy scale in electron-volts ($E_1 = 0.78539$, $E_2 = 1.57077$, $E_3 = 2.35615$, etc.). Therefore, the formula $\lambda = ch/E$ was used to find wavelengths λ and definite numbers q and Z that corresponded to the running numbers of indexes of φ and E .

As a matter of fact, whereas the dependence of all the TFs on $\Delta E = const$ and $\Delta\lambda \rightarrow const$ produced harmonics and progression, respectively, the TFs from $\Delta E(\Delta\lambda)$ showed the characteristic properties of the radiation spectrum in the information model of radiation. This is obviously determined by the fact that, according to the definition of *information*, the codes of the information source and receiver appeared to be concordant because of the natural type of the point-source radiator and receiver projection.

If the continuum quantization begins from $\lambda = 1578.63$ nm, then it is necessary to approach the possibility of developing the information model of quantization (IMQ) that could be based at a zero approximation on the above-found trigonometric function ratios between the IMR and the IMAA.

The criterion of manifestation of extreme radiation points in octaves were values of amplitudes of $A \tan^2 E/\Delta E(\Delta\lambda)$ at $\pi/4$ -fold values with a period of 2π , i.e., according to formula $\Delta E_n = (E_n - E_{n-8}) = 2\pi$. This allowed us to identify for each octave certain junctures linked with the wavelength, energy, and amplitude of radiation.

The numerical correspondence between the values of energy and radiation angles made it possible to establish correlations with the basic provisions of physical optics as well. As an example, the TF behavior at $\lambda \rightarrow \infty$ came to notice. The point of 1578.6 nm (the first term of the new octave) was the crossing point of the curves $\sin^2 E/\Delta E(\Delta\lambda)$ and $\cos^2 E/\Delta E(\Delta\lambda)$, whereas the functions $\tan^2 E/\Delta E(\Delta\lambda)$ and $\sin^2 E/\Delta E(\Delta\lambda)$ asymptotically tended to the value of $ch\Delta E$.

While the first octave began in the IR region (1578.6 nm - $\pi/4$), it reached its peak at 789.3 nm ($\pi/2$), which almost matched the known upper conditional limit of 780-790 nm for visible light.

The bottom limit of the visible region at 395.7 nm (π) also fitted within its commonly accepted range of 390-400 nm. Is it accidental that the point at 526.2 nm ($3/4 \pi$) also appeared to be at the interface between the *warm* and the *cold* colors of visible light, while it had earlier been relevant for an *average standard observer* [5].

The next points of the first octave corresponded to the UV limit with the peak reached at 263.1 nm ($3/2 \pi$) and the limit of the vacuum UV region (197.3 nm - 2π). Could we consider all these *coincidences* accidental, while they were arrived at by researchers from different areas of *light, color, and human* studies long before we had found these TF points? Table 1 shows different junctures of the derived function $\tan^2 E/\Delta E(\Delta\lambda)$ for the first triad of octaves.

The data from Table 1 were used to find the following ratios for all octave terms: octave order numbers were found using the equation $n = Z_{2ji} / q_{2ji}$; the order number q (with values from 1 to 8) for each octave was found using relation

$$E q = \varphi Z \quad (1)$$

where q is the correlation factor; Z is the integer number that corresponds to the order number of characteristic TF lines/bands in all of the optical region that begins from the crossing point of the functions $\sin^2 E / \Delta E(\Delta\lambda)$ and $\cos^2 E / \Delta E(\Delta\lambda)$. The same formula was used to find the order number values in each q period (from 1 to 8) in octaves II and III. How can this be interpreted?

Table 1. The correlation of the first octave quantities with the quantum numbers of TF*

$q, \varphi \setminus n$		I			II			III		
q	$\varphi, \text{rad.}$	Z	λ, nm	E, eV	Z	λ, nm	E, eV	Z	λ, nm	E, eV
1	0.78539	1	1578.63	0.79	9	175.40	7.07	17	92.86	13.35
2	1.57077	2	789.31	1.57	10	157.86	7.85	18	87.70	14.14
3	2.35615	3	526.21	2.36	11	143.51	8.64	19	83.09	14.92
4	3.14159	4	394.65	3.14	12	131.55	9.42	20	78.93	15.71
5	3.92692	5	315.73	3.93	13	121.43	10.21	21	75.17	16.49
6	4.71231	6	263.10	4.71	14	112.76	11.00	22	71.76	17.28
7	5.49769	7	225.52	5.50	15	105.24	11.78	23	68.63	18.07
8	6.28308	8	197.33	6.28	16	98.67	12.57	24	65.78	18.85

* For the compared semantics of numbers n, q, φ, z , see Table 2.

The above-proposed assumption that the sought quantity that carries streams of information from the radiation source to the receiver is neither energy nor wavelength but the dependence of their variation, i.e., precisely $\Delta E(\Delta\lambda)$ as some hypothetical *instrument function* of the limits of the source energy variation ΔE via the *slit width* change $\Delta\lambda$, has obviously turned out to be true. This quantity could then be further considered as a relevant argument for identifying the information characteristics of radiation in the IMR and/or IMAA. We shall make a correct comparison of the results with the known single-electron buildup of atoms with many electrons by giving a short overview of the known situation.

Multi-electron atom description is currently based on the single-electron atom classification because this is the only method of spectroscopic calculations of excited states; for example, if we accept that the zero energy E_o corresponds to the basic atomic state and

$$E_n = h\nu \quad (2)$$

corresponds to the excited atomic state, then we can find for each atom a sequence of numbers that are referred to as the spectral terms of this atom, i.e.,

$$T_n = E_n - E_o = E_n \quad (3)$$

In the simplest Bohr atomic model electrons are placed on certain (allowed) orbits along the atomic nucleus. When it moves to a lower orbit, an electron loses a quantum of energy and emits a quantum of light. In contrast, the transfer to a higher orbit requires additional energy; usually, it is absorbed by electrons in the form of photons with a definite wavelength.

The current state of the theory of atomic spectra permits quite strict consideration only for single-electron atoms, i.e., the atom of hydrogen and hydrogen-like ions He^+ , Li^{2+} , Be^{3+} , etc. The theory of multi-electron atomic spectra is based on the approximation of a central self-congruent field, where the state of the atom as a whole is determined by the sum of states of all its electrons, taking account of their interaction [2, pp. 36-39]. The detailed analysis of the single-electron application to the multi-electron atom is broadly represented in contemporary papers [2; 6], and we shall not dwell on this.

According to D.N. Klyshko, the metaphysical language is based on the notion that the concept of a *photon* is expressed not only in the mathematical symbols of quantum mechanics but is a *real* physical entity with some a priori properties (*elements of physical reality* as formulated by A. Einstein) and that any electromagnetic radiation field consists of a set of these autonomous entities (disregarding very weak vacuum environment nonlinearity) like an ideal gas that consists of non-interacting atoms. *"The state of affairs in quantum physics is paradoxical: its basic concept of photon as an elementary particle of light field has no clearly defined position in the formal quantum theory. ...in my opinion, "a photon as an elementary particle of the light field" is the basic concept of optical metaphysics...To judge by currently published works, a photon is something that objectively exists in space and time..."* Klyshko analyzed this issue in detail and concluded that *"a photon as an elementary particle of the optical field has no clear rational definition. Thus, according to the suggested definition, it is a category of metaphysics."*[1, pp. 1191-1192].

On the other hand, the concepts of a photon and a quantum of light have thus far been used as synonyms: *a photon as an elementary particle is a quantum of electromagnetic radiation (light)*. However, it has been added that radiated light is usually continuous and becomes quantized only when absorbed by matter, which agrees with the basic provisions of quantum mechanics and the generally accepted definition of the photon in the International lighting vocabulary that *a PHOTON is an elementary particle of radiation, the energy of which (QUANTUM) is the product of the Planck constant and the electromagnetic radiation frequency* [5, p. 19].

What will then appear if we take into account the above-obtained results of the TFs as interpreted in the IMR and the IMAA? Can we consider that a photon is the radiation unit Z and, at the same time, a quantum is number of photons Z_n ? Should we distinguish between the concepts of a photon and a quantum of energy and introduce their relevant formalization as verified by Popper's methods, taking account of the given properties of photon? Shall we not still adhere to the metaphysical idea of photon a ardently discussed by D.N. Klyshko?

Let us assume that the electromagnetic field radiation consists of photons Z . Their energy can therefore be expressed in a discrete sequence of values that is divisible by the indivisible portion, i.e., one quantum of Z . On the other hand, if a photon is a unit of light (an optical region of the electromagnetic field) and a quantum refers to the number of photons, we shall come to the following conclusion from the standpoint of the information approach.

A *photon* as an elementary particle of electromagnetic field has a certain energy in the IMR; thus, a *quantum* must be understood as the photon energy converted in the IMAA according to the IMQ and (1):

$$E = ch/\lambda = \phi Z/q \quad (4)$$

where q and Z are the above-identified order numbers in the octave (period) and in the entire optical region, respectively, λ is the wavelength, ϕ is the angle of the IMR projected to the IMAA, and c is the speed of light.

On the assumption that a photon is source radiation with an energy $h\nu$ measured in eV and a quantum is the *angle* of its incidence to the projection/atom measured in radians, equation (4) holds, which logically includes both, the number of photons Z and their quality q relevant to the respective parameters of electrons as self-congruent codes of information processing. Since $1 \text{ eV} = 1 \text{ rad}$ and other relevant values according to (4) in the first and subsequent octaves, respectively, the elementary principles of radiation quantization $Z = qE/\phi$, with the relevantly developed IMQ as the function of IMR (TF) and IMAA (TF), have been confirmed from the standpoint of the dimension theory as well.

In the strict sense photons and quanta interpreted from these standpoints have been differentiated in physical terms not only by quantity but by quality as well. If we consider that h in (1) is merely the factor of proportionality between the energy and the frequency continuum, what will then be the physical sense of their quantization? Does it consist only in discretization $\hbar = h/2\pi$ or could there have been some other natural ways to identify discontinuities in the energy and frequency continuums?

3. Classification of Atomic Spectra

Since photon energy quantities can be expressed via ratios of q , Z , ϕ according to the following equation (1), then $ch = \lambda\phi Z/q$, therefore, $h = Z\phi/qv$.

The resulting octave is verified by the following criterion: an atomic/molecular charge and/or term must be divisible by an elementary charge and/or term. In its respect, this indicates the possible multiplicity of the TF parameters with a multiplicity of radiation exposure angles. If the original energy in the IMR was $E_1 = 0.78539$, which corresponded to angle $\phi = 0.25 \pi$, then, according to (1) $E_1 = 0.25 \pi Z/q$.

It follows that, according to Tables 1-2, Z is both a quantity that expresses energy and the original quantum number that gradually increases at a quantization step of 0.25π .

To put it in another way, whereas the previous quantization step was 2π

$$\hbar = h/2 \pi = 0.159 E/v \quad (5)$$

the quantization value in the IMR according to (1) and (5) is

$$\hbar = 0.125 Z/v$$

Firstly, it distributes the integer values of Z number of photons absent in (5)

$$Z = 1.272E;$$

Secondly, it is the dependence on quantum numbers that is mediated in (1).

It its respect, q found reveals qualitative differences of photons in each octave; according to the value of the angle ϕ ,

$$q = 4\phi/\pi \quad (6)$$

or, according to Table 1,

$$q = \phi_n/\phi_1 \quad (7)$$

Thus, first, q is not only the order number of TF junctures in each octave but also the qualitative index of the quantization principle according to (6)-(7). According to (4) and (6), however, Z includes this quality of q and still retains the properties of the numerical index in (1), which allows us to suppose that, taking account of the semantics of q , the factor of the conversion of the photon energy $\varphi_1 Z$ into electron energy $E = eU$ is an integer angle factor according to (5) and (7).

Secondly, the correlations between the TF quantities and the LS scheme given in Table 1 for a single-electron atom have made it possible to compare (1) with (2). It follows that dimensions $[E]$ and $[Z]$ are identical but Z can point to the number of photons that are numerically comparable in the IMAA with the basic quantum number n at the approximation of the LS single-electron scheme.

Thirdly, formula (4) is notable, where the angle value is replaced with the frequency ν and the quantum energy value (the number of photons, Z), which directly confirms the previous conclusion upon substitution to the Planck formula:

$$E = h\nu = \varphi_1 Z \quad (8)$$

It is possible to explain from these standpoints the dimension correspondences between the radiation energy and the radiation incidence angle ($1 \text{ eV} = 1 \text{ rad}$) because all of the TF formulas included not absolute energy values but relative ones, i.e., their variations relative to variations in wavelength. The issue is that, according to the above-given test data, the criterion of the radiation maximums/minimums was variation in the radiation energy ΔE and/or radiation absorption by the atom at values that are divisible by Δn and $\Delta \lambda$.

Thus, these data indicate that it is exactly the message content together with an adequate method of its processing that should be considered as the characteristic property of information. As shown above, this is exactly the property that is found in the recurrent TFs with the semantics of the self-congruent codes of a radiation (information) source and receiver. These properties show that the discretization of the light continuum as the self-congruence of codes of an interpreter, i.e., a discretization method (n, q, Z, φ) and continuum data ($E = h\nu$), made it possible to quantize light and matter.

Since these theses are also verifiable in a test with photons polarized at 0, 45, 90, and 135 degrees, Popper's principle will be compatible with the requirement by Klyshko, who is sure that *quantum physics* as characterized by a continuously efficient relationship between experiments and mathematical models must be separated from the unproductive and mostly verbal *quantum metaphysics* that is not controlled by experiments but lays claim to a profound description of quantum phenomena.

"Obviously, physics as an experimental science cannot do without such criteria as Popper's refutability principle or Bridgman's operationalism (at least for some key concepts)" [1, p. 1189].

If these concepts appear to be the above-derived operational definitions for quantum numbers of TFs, this can also be relevant for the description of multi-electron atoms; they must then undoubtedly be subject to the refutability principle.

Usually, the concept of spectroscopy includes the analytical method based on separating electromagnetic radiation by the wavelength λ , i.e., by the radiation/absorption energy $E = ch/\lambda$. If the product is $\lambda E = ch = \lambda \varphi_1 Z = \text{const}$, then,

considering the semantic diversification of the photon energy $E_\varphi(Z)$ and a quantum as a number of photons Z_n , the product $\lambda_{at}(Z) E_\varphi(Z)$ must show a linear dependence on Z_n as the characteristic TF quantity:

$$\lambda_{at}(n) = (aZ_n + b) / E_\varphi(n) \quad (9)$$

where Z_n is the order number of the term in the Lyman series that includes the number of photons, i.e., is observable in absorption and λ_{at}^n is the transfer wavelength that corresponds to Z_n to the relevant TF energy; a and b are empirical factors. In the current variant of the Bohr model they correlate with the screening constants σ in the LS scheme [6, p. 197] because they also increase proportionately with the increase in Z in each PT group.

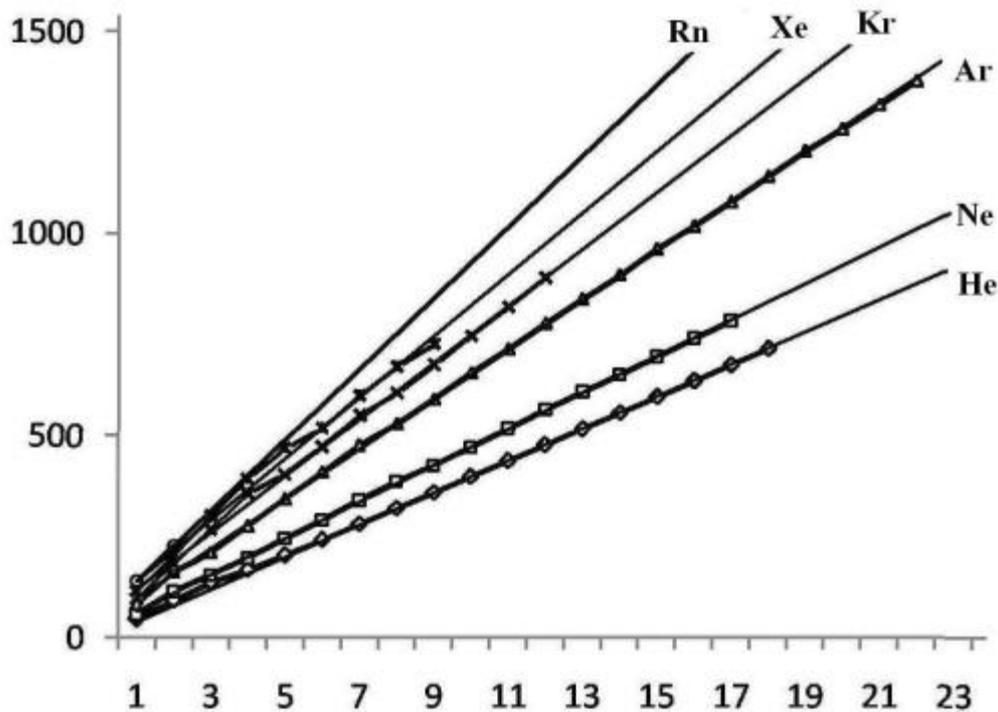


Figure 1. Regressions of $\lambda_{at}(n) E_\varphi(n)$ IIIVa group : the values of (Z_n) are given along the x axis, the values $\lambda_{at}(n) \cdot E_\varphi(n)$ nm eV are given along the y-axis.

In its respect, this has made it possible to substantiate the correlation between the properties of TFs and atomic terms, which has been confirmed by the test data given in Figure 1 for known terms of the neutral atoms of IIIVa PT group [8; 9].

First of all, since ionic potential were essentially the limit for T_n , where the electron traveled beyond the limits of the Coulomb nucleus field, this regression made it possible to approximate the values of higher terms up to the atomic ionization potentials; secondly, it made it possible to divide the terms by the full moments $J = L + S$ of the electron shells as "quantum optics often deals with linear problems, which makes it simpler to compare it with classic models" [1, p. 1189].

It follows from this comparison that the IMAA fully corresponds with the known atom description but, importantly, made it eight times more detailed by φ and still adequately retained the properties of atomic systems. In particular, the ratio between the atomic term wavelength $\lambda_{at}(Z)$ and Z -relevant IMQ energy $E_\varphi(Z)$ reveals the previously unknown linear regression $\lambda_{at}(Z) E_\varphi(Z)$ as a function of quantum numbers Z_n , and J , which is given in Figure 1.

4. Molecular Spectra

The purpose of the present part was to establish the dependence of the odd singlet electronic terms of H_2 , $T_e = \min W_a(R) - \min W_X^I \sum_g^+(R)$ [where $W_a(R)$ is the adiabatic potential of the a state], on the terms T_n of the atoms forming the molecule. This approach is based on the correlation between T_e (e - the equilibrium distance) and the sums of T_n of atoms a and b with equality or the minimum difference in their quantum numbers n and l :

$$T_e^{a,b} = K_i \sum_{a,b} T_{n,l}^{a,b} \quad | \quad \Delta T_{n,l}^{a,b} \rightarrow \min (\Delta n=0;1; \Delta l=0;1) \quad (10)$$

which was pointed out in [7] as the property of relative additivity of atomic terms (AT). Hereinafter, Eq (10) will be called the IMAT equation, and K_i will be assumed experimentally determined by the coupling coefficient.

To compare the atomic and molecular spectra, it would be convenient to measure the values of the terms from the ground state, in accordance with Fig. 2, by equating the energy of the ground state to zero. In the case of a molecule, consideration of additional terms (in comparison with the atom) due to vibrational and rotational motion leads to the necessity of neglecting the zero energy ω_e'' of the vibrations of nuclei in the ground state and averaging the anharmonicity effects and zero energies ω_e' of excited states.

On the basis of known conditions for H_2 ($\omega_e''/2 \approx \omega_e'$) we can approximately express these corrections in terms of the shift of the energy scale of the molecule by $\omega_e''/2$. Hence the quasi-adiabatic ionization potential

$$I_m(e) = I_m - \omega_e''/2$$

makes it possible to equate to zero the ground state of the hydrogen molecule, so that the principal quantum numbers of the atoms forming the molecule will be equal to the quantum numbers of the individual atoms in this state. We thus found the first single-valued point of the desired correlation ($n_a = n_b = 1$).

Assuming further that the ionization potentials of the atoms $I^{a,b}$ and molecule $I_m(e)$ also conform to the property of IMAT, we can write the relation

$$K_i = I_m(e)/(I_A^a + I_A^b) \quad (11)$$

which correlates uniquely in quantum numbers $n \rightarrow \infty$ and thus gives the second extreme point of the desired correlation. Since we are proceeding from the linear character of the empirically demonstrated relationship (10) between all the terms of the atoms and molecule, evaluating the coupling coefficient K_i , one can assume that all the remaining electronic terms of H_2 will fall on the straight line $T_e(\sum_{ab} T_n^{a,b})$, connecting these two uniquely found points ($n = 1$ and $n = \infty$).

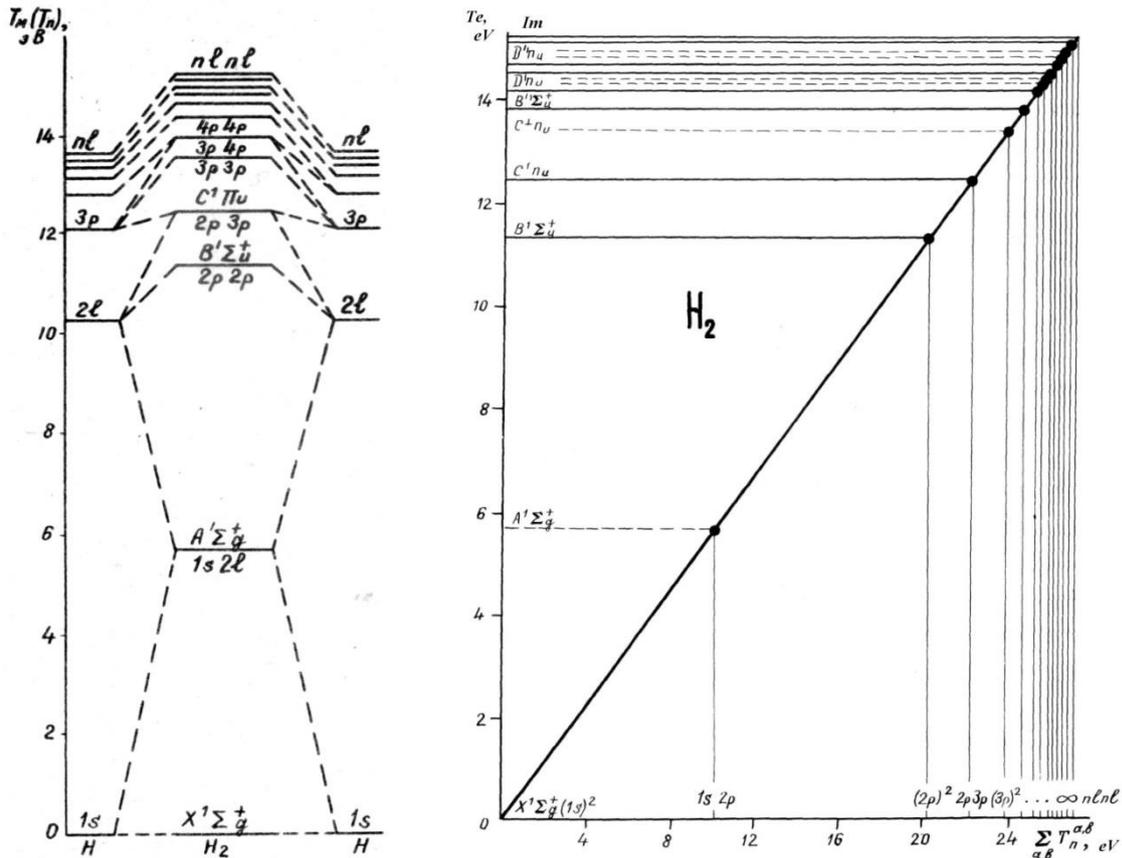


Figure 2. Terms T_n of the hydrogen atom and quasi-adiabatic terms T_e of the hydrogen molecule [8].

The analytical dependence (10) describes with sufficient accuracy ($\sigma=0.0025$) the electronic terms of the molecule in terms of the adiabatic ionization potential or the shift of the scale in the approximation (11) and the quantum numbers of the atoms forming the molecule.

It is well known that the predominant realization of single-electron transitions, i.e., excitation of one optical electron, corresponds to the greatest probability of electric-dipole transitions. In correspondence with this, and also with the principles of delocalization and indistinguishability of electrons, one can assume that the contribution to the electron charge density connected with allowed single-electron transitions is formed by two equal parts of the electron charge density of the two atoms of a diatomic homonuclear molecule. Then the ratio of the number of optical electrons (i.e., unity) to the number of valence electrons s_e can indicate the degree of participation

$$K_i = 1/s \quad (12)$$

of the valence electrons in forming the chemical bond.

This confirms that the singularities of the latter are actually determined by the characteristic parameters of the electronic transitions (in particular, T_e), which can be obtained for simple molecules from an analysis of the rovibronic band systems in electronic absorption spectra.

From here it follows that, first, one can estimate the order (multiplicity) of the chemical bond $P_{ab} = s_e/2$ between atoms a and b in the molecule ab from the value of K_i (IMAT). For convenience we will call a compound with a definite bond order a molecule integer further on and will denote the bond multiplicity by the left lower index of the element symbol.

Second, the value of T_e must be proportional to the sum of two identical terms $T_n^a = T_n^b$ of the two atoms: $T_e^{ab} \sim (T_n^a + T_n^b)$, which is connected with the correspondence of the atomic and molecular terms to definite changes of their charge states. Since these changes correspond directly to redistribution of the electron density upon a single-electron transition, we can write $\Delta n^{ab}=0$ for the symmetric (relative to the plane separating the nuclei) charge redistribution of the two atoms in the molecule and $\Delta n^{ab}=1$ for the asymmetric charge redistribution of the two atoms due to the arising of polarization forces upon an electronic transition.

Thus, from the data IMAA - IMAT and values of K_i , which actually determines proximity to the characteristic value $1/s_e$, one can determine the unknown electronic terms of definite molecule intemers.

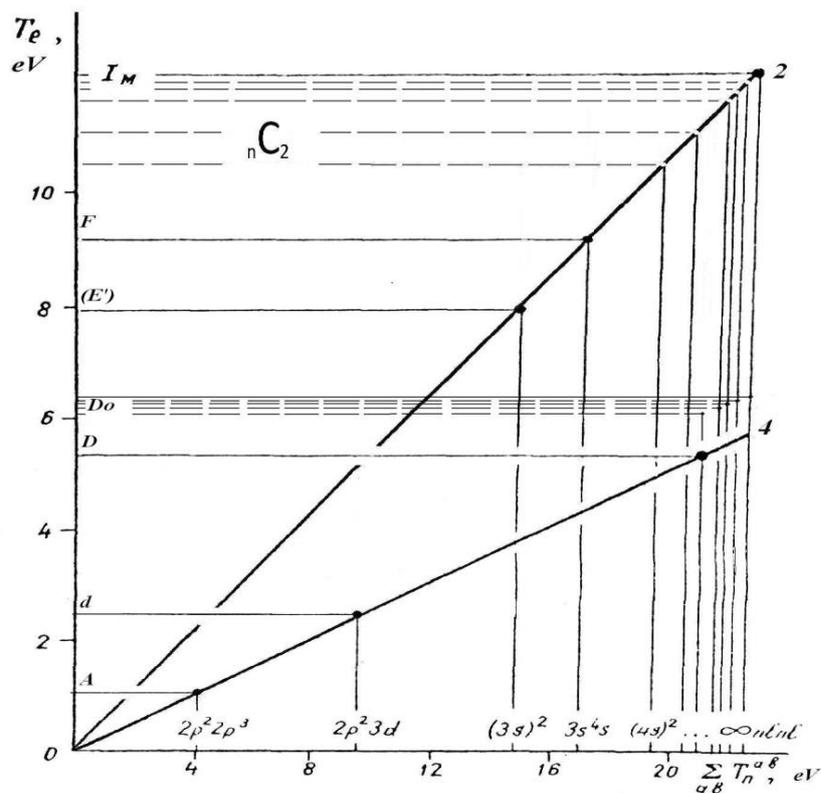


Fig.3. Correlation between electronic terms of the molecule ${}_n\text{C}_2$ and sums of terms of the atoms forming it [8;9].

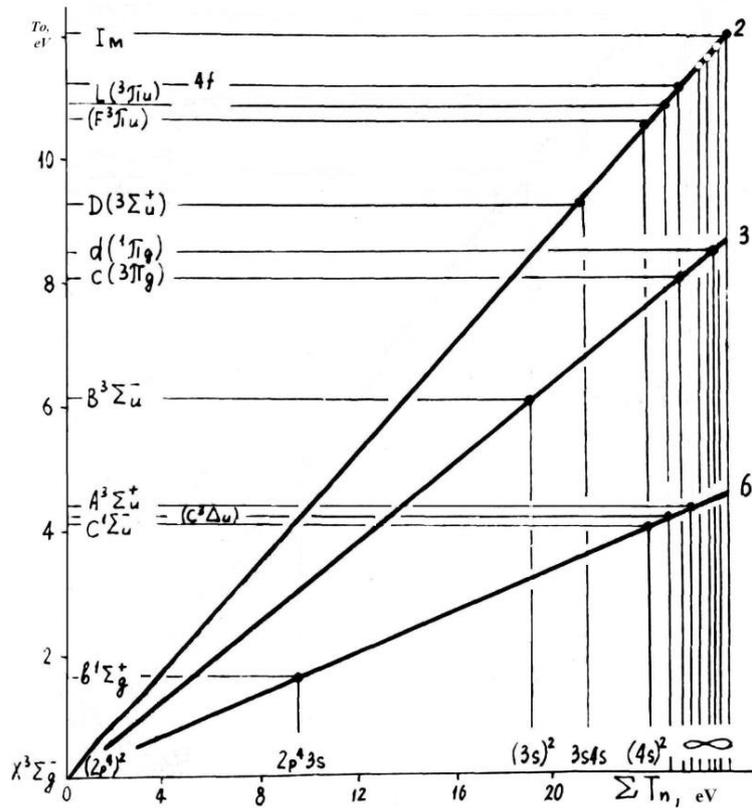


Fig.4. Correlation between electronic terms of the molecule nO_2 and sums of terms of the atoms forming it [8;9].

5. Conclusion

Thus, a new approach to developing information models of radiation (IMRs), quantization (IMQs), and atomic/molecular absorption (IMAA)/(IMAT) linked the projection of natural sources of light with light-absorbing atoms via relationships between light functions and trigonometric functions (TFs).

This provision has been confirmed by the resulting correlation between trigonometric functions and ionization potentials of neutral atoms with the filling of the s & ndp shells, as well as by the verified information connection between atomic terms and TF junctures by linear regressions that make it possible to provide reliable predictions of unknown terms and/or their classification. The discovered correlation between the optical region continuum and its octaves in the IMR has allowed us to assume the possibility of elaborating new quantization principles because the photon and the quantum turned out to have a numerical *angle-energy* correlation in the IMQ and IMAA; as a result, we have provided a potential alternative to the single-electron classification of multi-electron atoms in the nanoscience.

The approximate correlation of definite attributes of atomic terms according to the Russell—Saunders scheme (LS connection) with TF parameters is presented in Table 2.

Table 2. The correlation between the LS scheme and TF parameters

	LS*	IMQ	PT	IMAA	IMAT
n	Principal quantum number ($n=1, 2, 3, \dots, \infty$)	Octave no. $n=q_{2\pi}Z_{2\pi}$	Period no. 1(K), 2(L), 3(M)...	Atomic term no.** $n = Z_n + 1$	Min difference $\Delta n = 0; 1$
l	Orbital quantum number ($l= 0, 1, 2, 3, \dots$)	no. (.) in all region $l=n-1=Z_n$	No. group (no. of valence electrons)	Number of valence electrons in atomic terms	Min difference $\Delta l = 0; 1$
Z	Element no. (total number of electrons)	TF no. (.) in all region $Z_\gamma = q \cdot E / \varphi N_o$. of photons)	Element no. (total number of electrons)	Total number of electrons $Z_e = E_\varphi / \varphi_1$	Electronic shell $s_e = I / K_i$
q	<i>L, S, J</i> quantum numbers of shells 0(S), 1(P), 2(D)...	TF (.) no. in each octave $q = 4\varphi / \pi$	TF (.) no. in each period $q = \varphi_n / \varphi_1$	Term value in atom $q = \lambda_n \cdot \varphi \cdot Z / ch$	<i>nlnl</i> – quantum number (on Rydberg)
φ	$\hbar = h/2\pi$ (360°)***	$\varphi_1 = \varphi / q$ (45°)	$\varphi_1 = \pi / 4$ (45°)	$h = \pi \cdot \lambda_n \cdot Z / 4c$ (45°)	$\varphi_m = \arctg K_i$
E	$E = hv$	$E = Z \cdot \varphi / q$	$E_\varphi = \varphi_1 \cdot Z$	$E_n = ch / \lambda_n$	$E_m = K_i \sum E_n$

*The Russell—Saunders scheme works in the Coulomb field of the nucleus of a single-electron atom, i.e., with rules of sampling for dipole radiation $\Delta J=0, \pm 1$ and $\Delta m = 0, \pm 1$ [6, p. 117]. ***n* has a polysemantic meaning, i.e., it characterizes the Bohr atom orbit, order number of the term, and the PT in both the IMAA and LS ($2n^2$). ***Projections of vectors *L, S, J* in the LS scheme are quantized \hbar -fold to 360° angles [2, pp. 38 and 212].

As spectroscopic information models deal only with functions and/or bound data, the issue is neither structure nor mechanical particles and/or their interaction according to this principle: there are no probabilities (statistics factor) in the IMR, IMQ, and IMAA/IMAT but strict reproducibility (scientific criterion).

However, the developed information models require verification in order not to fall to the metaphysical part of quantum mechanics, in the words of D.N. Klyshko. The issue is that "the possibility to predict new effects, capacity for integration, classification, and systemization of phenomena, universality, compactedness, simplicity, and clarity are obviously the basic criteria to compare the advantages of alternative languages" [1, p. 1212].

It can be assumed that continued studies of the IMR, IMQ, and IMAA/IMAT will create powerful tools and means for other optical correlations and/or information models that can produce new optical theories. Together with our results, this can be a definite contribution to prospective developments in the information-based interpretation of the concept of a photon in terms of quantum optics.

Careful analysis of the correlation results obtained from Eq. (10) for all 360 well-known electronic terms of 50 diatomic homonuclear molecules shows the reality of a reliable and correct interpretation of electronic absorption spectra of a simple molecule independently of the presence in the absorbing volume of the mixture of its intermers.

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