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E-ISSN : 2456-1045

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RESEARCH JOURNAL
VOLUME - 76 | ISSUE - 1

ADVANCE RESEARCH JOURNAL OF MULTIDISCIPLINARY DISCOVERIES

AUGUST 2022

INTERNATIONAL JOURNAL FOUNDATION
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Unity and Correlations of Entropic Components in physical and chemical regularities

ORIGINAL RESEARCH ARTICLE

ISSN : 2456-1045 (Online)
ICV Impact Value: 74.80
GIF- Impact Factor: 5.194
IPI Impact Factor: 3.56
Publishing Copyright @ International Journal Foundation
Article Code: PSSR-V76-I1-C1-AUG-2022
Category : PHYSICAL SCIENCE AND SPACE RESEARCH
Volume : 76.0 (AUGUST-2022 EDITION)
Issue: 1(One)
Chapter : 1 (One)
Page : 01-07
Journal URL: www.journalresearchijf.com
Paper Received: 28th SEPTEMBER 2022
Paper Accepted: 11th OCTOBER 2022
Date of Publication: 30th NOVEMBER 2022
DOI: 10.5281/zenodo.7379661

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ABSTRACT

All phenomena and processes in the nature and world proceed only in two energy directions: either along the force field gradient with minimum energy input (entropy) or against the gradient with maximum energy input (negentropy).

The graphs of S-curves and their nomograms characterize the dynamics of change in entropic components depending on the process main parameters. The condition of the system stationary state is the equality or constant of the correlation between its entropy and negentropy (equilibrium dynamics). Such regularities are found in many phenomena and conformational interactions in physical chemistry, nature, engineering and even economics. The examples of their functional contribution are given.

KEYWORDS: entropy, negentropy, conditions of systems stabilization, S-curves, their diversity, physical and chemical regularities, coronavirus, bioenergetics.

CITATION OF THE ARTICLE

Korablev G.A (2022) Unity and Correlations of Entropic Components in physical and chemical regularities”; *Advance Research Journal of Multidisciplinary Discoveries;* 76(1) pp.01- 07

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I. INTRODUCTION

The analysis of kinetics of various physical and chemical processes shows that in some cases the direct addition of velocities, kinetic or energy characteristics is performed, in others – their reciprocals are added.

In particular, such supposition is confirmed by the formula of electron transport possibility (W_∞) due to the overlapping of wave functions 1 and 2 (in steady state) during electron-conformation interactions [1]:

$$W_\infty = \frac{1}{2}\frac{W_1 W_2}{W_1 + W_2} \quad \text{......................(1)}$$

Equation (1) is used when evaluating the characteristics of diffusion processes followed by non-radiating transport of electrons in proteins [1].

And also: "From classical mechanics it is known that the relative motion of two particles with the interaction energy U(r) takes place as the motion of material point with the reduced mass μ:

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \quad \text{...................... (2)}$$

in the field of central force U(r), and general translational motion – as a free motion of material point with the mass:

$$m = m_1 + m_2 \quad \text{..........................(3)}$$

Such things take place in quantum mechanics as well" [2].

At the same time, the problem of quantum-wave dualism is not completely solved yet, although the application of de Broglie equation allows defining the borders of such phenomena. But the predominating property depends on the process conditions. And it is quite complicated to find out in advance which of them will operate in each particular case, although it is known that the wave pattern more often takes place at low energies, and corpuscular – at high ones.

The problem of diverse manifestation of the entropy concept is also of considerable interest. In thermophysical processes entropy (S) is the function of the system state whose differential in the elementary reversible process equals the ratio between the infinitely little quantity of heat transferred to the system and its absolute temperature:

$$dS = {}^{\delta Q}/_{T} \quad \text{.........................(4)}$$

In statistic thermodynamics the entropy of the isolated and equilibrious system equals the logarithm of the probability of its definite macrostate:

$$S = k \ln W, \quad \text{........................(5)}$$

where W – number of the system available states or degradation degree of microstates, k – Boltzmann's constant.

Therefore, the application and consideration of these laws has diverse manifestations, which are most fruitfully used in statistic thermodynamics. The concept of entropy stemming from the second law of thermodynamics is a criterion of process directedness and irregularity degree of systems.

Thus, these outstanding issues of physical chemistry require further investigation and discussion.

In this research an attempt is made to explain the foregoing problems from the point of the concepts on the directedness gradient of physical and chemical processes when their entropic components change.

1. Initial data

The character of the change in the value of potential energy (ΔU) by its sign for different potential fields was analyzed [3] (the table is not given).

It was found out that the values of $-\Delta U$ and, consequently, $+\delta A$ (positive work) correspond to interactions proceeding along the potential gradient, and $+\Delta U$ and $-\delta A$ (negative work) take place during the interactions against the potential gradient.

After analyzing the first law of thermodynamics, we have the following [3]:

1) In the systems in which the interaction proceeds along the potential gradient (positive work), the resultant potential energy, as well as the reduced mass are found based on the principle of adding reciprocals of corresponding values of subsystems. This is the corpuscular process, in which entropy can serve as the theoretical concept.

2) In the systems in which the interactions proceed against the potential gradient (negative work) the algebraic addition of their masses, as well as the corresponding energies of subsystems is performed. This is the wave process, in which negentropy can serve as the theoretical concept.

3) The resonance stationary state of the systems is fulfilled under the condition of equality of degrees of their corpuscular and wave interactions. In thermodynamics of open systems the entropy products in stationary state are completely compensated by the negentropy flow.

4) All phenomena and processes in the nature and world, including a human, proceed only in two energy directions: either along the force field gradient

with minimum energy input (entropy) or against the gradient with maximum energy input (negentropy). The first direction corresponds to the notion of entropy and the second – to the notion of negentropy (negative entropy). In the dynamics of processes both phenomena are interrelated and complement each other.

2. Entropic nomograms

Coulomb interactions and their varieties are widely used in classical physics and quantum mechanics to evaluate structural interactions in simple and complex systems.

Thus in [1] Van der Waals, orientation and charge-dipole interactions are referred to electron-conformation interactions in bio-systems. And as a particular case – exchange-resonance transfer of energy. But biological and many cluster systems are electroneutral in structural basis. And non-Coulomb equilibrium-exchange energy interactions, i.e. non-charge electrostatic processes, are mainly important for them.

The structural interactions of summed electron densities of valence orbitals of corresponding conformation centers take place – processes of equilibrium flow of electron densities due to overlapping of their wave functions. The closer the values of their energy characteristics are, the easier the alignment of electron densities.

Heisenberg and Dirac [4] proposed the exchange Hamiltonian derived in the assumption on direct overlapping of wave functions of interacting centers:

$$\bar{H} = -I_0 S_1 S_2 \,,$$

where: $\bar{H}$ – spin operator of isotropic exchange interaction for a pair of atoms, I_0 – exchange constant, S_1 and S_2 – overlapping integrals of wave functions.

Initially, each free atomic structure has entropic equilibrium state of two opposite origins (orbital-nucleus) in the system of common reality (atom). Accordingly, in the binary system opposite entropic components from both atoms are interacting until the dynamics of entropic equilibrium stabilizes.

Such equilibrium-exchange conformation interactions regulate the stabilization of many organic systems (clusters, polypeptide chains, etc.). Therefore, in this approach the overlapping integrals of wave functions are modeled through the value of relative difference of energy parameters of interacting centers – coefficient α (in %) [5]-[6].

Such parameter is a direct characteristic of entropic equilibrium degree in the system. The initial values of energy and dimensional parameters for the majority of elements at different valence-active orbitals are given in [3] and other author's publications.

Applying the reliable experimental data we obtain the nomogram of structural interaction degree dependence (ρ) on coefficient α, the same for a wide range of structures (Fig. 1). Here, the values of α from 0 to 5 correspond to the conditions of entropic equilibrium, at which ρ=100%. This type of nomogram, as well as its dissymmetric variant (Fig. 2) give the possibility to evaluate the degree and direction of the structural interactions of phase formation, isomorphism and solubility processes in multiple systems, including molecular ones [5]-[6].

The less is α, the higher is the interaction wave component degree according to Fig. 2 (negentropic curve). And in Fig. 1 the increase of α characterizes the increase in corpuscular and electrostatic properties in microsystems (entropic curve). Thus, the notion of entropy is numerically modeled via coefficient α and negentropy – via 1/ α.

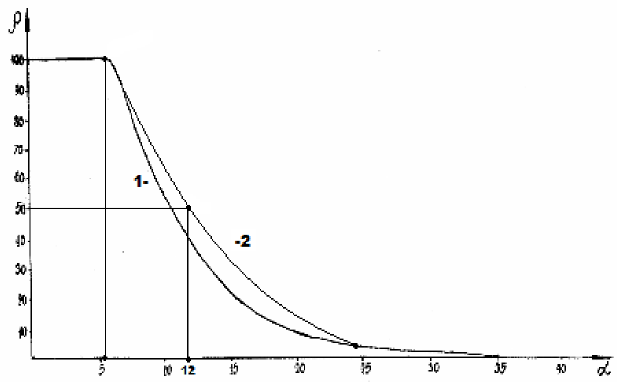


Fig. 1. Nomogram of the dependence of structural interaction degree (ρ) on coefficient α

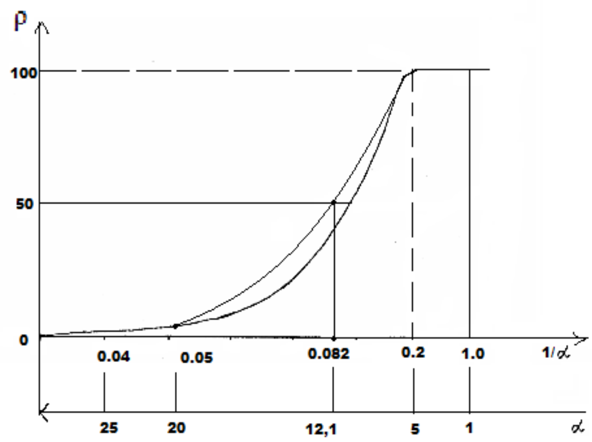


Fig. 2. Nomogram of the dependence of structural interaction degree (ρ) on coefficient 1/α

Many phenomena and processes in nature, engineering and even economics are described by the same graphs called S-curves. Such S-curves and initial nomograms are graphical characteristics of non-equilibrium dynamics of changes in entropic components.

3. Conditions of equilibrium and correlations of entropic parameters

The execution of par. 3 of Initial Data is classified depending on the peculiarities of process dynamics. Thus, in electromagnetic wave the difference in the path of vector components is 90°. In general case, during the rotational motion of the system of two similar vectors ($\vec{R}$) with the phase difference of 90° their resultant is as follows:

$\vec{C} = 2^{1/2}\vec{R}$, where for the given angle tg45°=1…..(6)

If such process is complemented by the movement in spiral dynamics, vector ($\vec{C}$) becomes the tangent vector and forms the spiral rotation angle, for which:

$tg\varphi = C/R = 2^{1/2}$, where geodesic angle φ equals 54.733°……………………. (7)

At this angle a silk worm winds the silk thread onto a base.

Thus, during a purely rotational motion the condition of equilibrium of vector components of entropic characteristics is fulfilled, and during the spiral one their ratio equals $2^{1/2}$. During a translational motion the conditions of either equilibrium or constant ratio of values of their components are fulfilled. At the same time, exponential dependencies are revealed in statistic processes. Such approach defines general principles of many physical regularities.

1) Characteristic of spin-orbital interaction – fine structure constant $\alpha = \frac{r}{\lambda}$, where r – electron classical radius, λ – its Compton wavelength.

2) In [7]; [8] the concepts of breaking point during the extension of thread plastics by its winding pitch are used, where: σ_α – axial, σ_β – circumferential stresses, which are replaced by value N_α – axial "strain" and N_β – circumferential "strain" by the following equation:

$$\frac{\sigma_\beta}{\sigma_\alpha} = \frac{N_\beta}{N_\alpha} = tg^2\varphi \quad = 2 \quad ……………. (8)$$

"This condition allows obtaining the stress-ration system of threads with the minimum weight of the item" [8].

In harmonic oscillations of the body the potential energy ratio conditioned by quasi-elastic force to kinetic energy equals $tg^2\delta$, i.e.:

$$E_п/E_к = tg^2\delta \; ……………………… \quad (8a),$$

where δ – angular characteristic of oscillations.

If δ=φ, the system gets the entropic equilibrium state.

3) In quantum mechanics the ratio of magnetic moment of the particle to its mechanical moment is called the gyromagnetic ratio g. Here $g_s = 2$, if the electron magnetic moment is conditioned only by the spine component and $g = 1$, if it is formed by the orbital motion of electrons. Such g values and their ratios characterize the corresponding entropic dependencies.

4) Planck's equation (quantum transition):

$h = E/\nu$, where E – orbital energy, constant in stationary state, the process proceeds along the field gradient (entropy), ν – electromagnetic wave frequency (negentropy), h – Planck's constant.

5) Movement velocity equation

V = S/t, where S – way during the mechanical motion with energy consumption (negentropy), t – time, it always increases and is directed along the gradient (entropy). Lorentz curve (the figure is not given) also indicates the availability of space-time dependence. In these cases, the constant motion rate is the condition of stationary state, which is found both in the microcosm of atoms and molecules and in the macrocosm during the movement of planets.

6) During the rotational motion of the charged particle in gravitation field [9]:

$$\ln(\frac{G}{\varepsilon_0}) = tg^2(a_0\varphi) \; ………………….. \quad (9)$$

Where: ε_0 – electric constant, G – gravitational constant, $a_0 = 1.00233$ – quantum correction to electron gyromagnetic ratio in an atom, which may, in this case, characterize the influence of particles motion precession.

7) From the thermodynamic definition of entropy:

T = dw/ds, where dw – thermal energy, therefore, the average temperature (T) is constant both in biological systems and for planets.

8) In chemical kinetics Le Chatelier principle is fulfilled: "At the external action upon the equilibrium system the equilibrium will shift in the direction of the process, which resists this action".

9) Initial conditions are in accordance with the complementarity principle by N. Bohr: for complete description of quantum-mechanical phenomena it is necessary to apply two conflicting (complementary) sets of classical notions, the summation of which provides the exhaustive information about these phenomena as integral ones. For example, the description of an object as a particle and as a wave.

In such examples:

1. If the processes proceed along the gradient (entropy), the parameters are as follows: t, α, E, σ_α, r, ε_0, $E_п$.

2. If the processes proceed against the gradient (negentropy), the parameters are as follows: S, ρ, ν, σ_β, λ , μ, G, $E_к$, l.

4. S–curves in economics

S-curves are often used in economic investigations, for instance, GDP dynamics, amount and volume of products, forecast of innovation potential, etc. Thus, the graphs of demand line (entropy analogy) and supply line (negentropy analogy) are used to evaluate the rational market price (Fig. 3) [10].

From the graph it is seen that the rational market price is fixed if the demand and supply lines are in equilibrium.

The diagram of GDP world dynamics is demonstrative, which almost corresponds to the negentropy graph (Fig. 4) [11]. The main decrease in GDP growth has started since 2018 and it becomes very significant during the coronavirus pandemic.

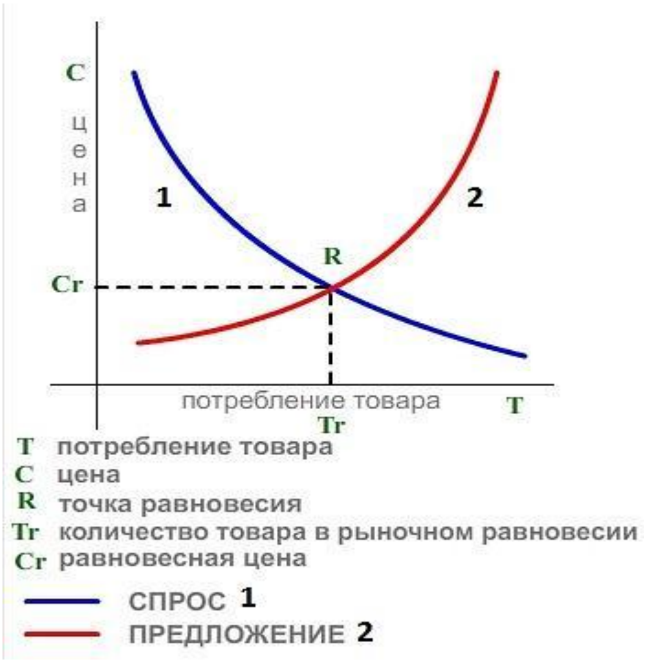
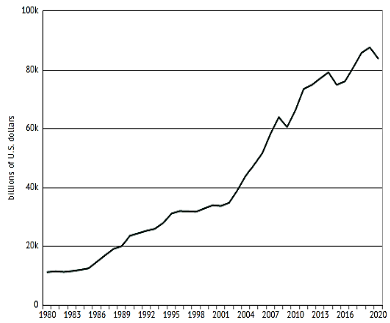


Fig. 3. Graph of demand and supply

At the same time, GDP of China has been constantly increasing, though with delay, even in 2020. In order to avoid GDP stagnation, some negentropic economies should probably get some complement of entropic component. The Chinese experience and coronavirus busting experience already exist in the world. Thus, the countries with rather small percentage of state companies took in the situation faster and are better managing this problem.



ДАТА	ЗНАЧЕНИЕ	ИЗМЕНЕНИЕ, %
2020	83 844,99	-4,23%
2019	87 552,44	2,17%
2018	85 689,96	6,16%
2017	80 716,20	6,17%
2016	76 022,14	1,59%
2015	74 829,37	-5,35%
2014	79 059,95	2,69%
2013	76 989,92	2,92%
2012	74 805,34	1,90%
2011	73 413,65	11,00%

Fig. 4. Graph of world GDP

5. S-curves and COVID-19

Non-equilibrium dynamics can be also demonstrated in virus etiology, which can be interpreted as smooth transition from atomic-molecular interactions on the microlevel to a formally similar process in macrosystems. This analogy is confirmed by the graph (Fig. 5) for the Russian coronavirus scenario [12] in its most complicated period before the omicron virus emergence. Using the comparative methods with reference nomograms, we can make some assumptions about further progress of the coronavirus scenario [13].

Fig. 5. Number of diseases in the given time period

6. Entropic principles of bioenergetics

Bioenergetics of live systems defines a wide range of their functional capabilities. And first of all – life span. Longevity problems have always been Date ed and investigated in the world and their results have been considered and applied at different times, though with various degrees of success. The life span has been most rapidly increasing after 1920-s mainly due to more developed medicine (but not only this). Gene-protectors, normalizing the dysfunction of organs, are currently applied to prolong a human's life. Treatment methodologies with the application of statins to decrease low-density cholesterol level are developed and used [14]. The resources of gene engineering, which, changing human genome, could contribute to the treatment of hereditary diseases, are investigated. In this paper such problematic issues are considered from the point of the principles of entropic correlations.

The heart works this way: work phase (systole) is always accompanied by functionally equal rest phase (diastole). It was determined long ago that in heat processes in an open thermodynamic system the entropy is completely compensated by the negentropy flow. Therefore, the equality or parity correlation of these entropic parameters is the condition of static stability of any system. In non-equilibrium dynamics such entropic correlations are vividly presented in the form of graphs called S-curves. For example, the curves of functional dependencies of parameters in epidemiologic scenarios.

Two simple common rules should be fulfilled for live systems in view of their longevity and entropic correlations:

1. The amount of calories absorbed should equal the amount of calories spent.
2. The time spent for rest of a live organism should equal the time spent for work.

The type of nutrition is very important but its composition is not always essential.

It is important and necessary to understand and correctly use such principles in our biophysical philosophy when making the energy exchange in our own lives, whatever difficult such approach would seem.

II. CONCLUSION

This approach is not brand new and the given examples are not single. Already in 1943 E. Schrodinger in his book "What is life?" explained that the negative entropy produced by an organism in a live system balances the positive entropy flow. Thus, thousands of years ago Chinese medicine found out that all phenomena of the world and nature can be considered as the interaction of two opposite geneses of one reality. And the principle of unity and struggle of opposites is fulfilled in dialectics.

From the point of these ideas, physiotherapy and reflexotherapy can be considered as the methodology of equalizing the potentials of two manifestations of energy geneses, which are the entropy and negentropy in modern concepts. And the nature today, as before, fulfills its principles. For example, it struggles against viruses by collective immunity. The twentieth century, the century of wars, epidemics and revolutions, brought a lot of human losses. But the population increase rate was the highest in all of the human history. At present, in the time of ecological problems, there is an important principle: all carbon dioxide produced must be absorbed.

The established entropic principles are in many ways demonstrated both in nature and engineering, and can be effectively used.

Thus, for hundreds of years a silkworm has been winding the silk thread onto the base at the angle of 54.733 degrees (geodesic angle). In engineering, a special high-strength thread has been wound on the spaceship body at the same angle for quite a while. There are other less known examples: linen winding onto the base or operation of some devices in agricultural engineering, etc.

Since these regularities are unknown for broad scientific community, their application in practice is evidently insufficient. But it is necessary to take these principles into account in the technology of preparing hybrid products consisting of two or more components (or fractions), for example, when producing milk-containing compositions. The products obtained this way will have better quality than the ordinary ones.

This methodology has a special meaning in material science, for example, in steel alloying. In such cases, the problematic issues of phase-formation and extension of solid solutions arise. This approach allows finding the optimum solutions to evaluate the interaction degree of atomic-molecular structures (ρ).

Using this entropic methodology and its nomogram, it is possible to evaluate the processes of isomorphism and formation of solid solutions in simple and complex systems.

These are the practical opportunities for applying this methodology in scientific research and technological innovations.

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