



## About unitary quantum theory and catalytic process theory

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### ABSTRACT

In article is considered approximately unitary quantum equation with oscillating charge for single particle. The Laws of the conservation are got after averaging on ensemble of the particles. Using of this equation allows with united position to explain many mysterious phenomenas of the catalytic processes and nature.

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### Introduction

In the standard quantum theory, a micro-particle is described with the help of a wave function with a probabilistic interpretation. This does not follow from the strict mathematical formalism of the nonrelativistic quantum theory, but is simply postulated. A particle is represented as a point that is the source of a field, but can not be reduced to the field itself and nothing can be said about its "structure" except with these vague words. Modern quantum field theory can not even formulate the problem of finding a mass spectrum.

This dualism is absolutely not satisfactory as the two substances have been introduced, that is, both the points and the fields. Presence of both points and fields at the same time is not satisfactory from general philosophical positions – "razors of Ockama". Besides that, the presence of the points leads to non-convergences, which are eliminated by various methods, including the introduction of a re-normalization group that is declined by many mathematicians and physicists, for example, P.A.M. Dirac.

The original idea of Schroedinger was to represent a particle as a wave packet of de Broglie waves. As he wrote in one of his letters, he "was happy for three months" before British mathematician Darwin showed that such packet quickly and steadily dissipates and disappears. So, it turned out that this beautiful and unique idea to represent a particle as a portion of a field is not realizable in the context of wave packets of de Broglie waves. Later, de Broglie tried to save this idea by introducing nonlinearity for the rest of his life, but wasn't able to obtain significant results. It was proved by V.E. Lyamov and L.G. Sapogin [1] that every wave packet constructed from de Broglie waves with the spectrum  $a(k)$  satisfying the condition of Viner-Pely (the condition for the existence of localized wave packets)

$$\int_{-\infty}^{\infty} \frac{|\ln(a(k))|}{1+k^2} \geq 0$$

becomes blurred in every case.

There is a school in physics, going back to William Clifford, Albert Einstein, Erwin Schrödinger and Louis de Broglie, where a particle is represented as a cluster or packet of waves in a certain unified field.

According to M. Jemer's classification, this is a 'unitary' approach. The essence of this paradigm is clearly expressed by Albert Einstein's own words: «We could regard substance as those areas of space where a field is immense.

From this point of view, a thrown stone is an area of immense field intensity moving at the stone's speed. In such new physics there would be no place for substance and field, since field would be the only reality . . . and the laws of movement would automatically ensue from the laws of field.»

However, its realization appeared to be possible only in the context of the Unitary Quantum Theory (UQT) within last two decades. It is impressive, that the problem of mass spectrum has been reduced to exact analytical solution of a nonlinear integro-differential equation. In UQT the quantization of particles on masses appears as a subtle consequence of a balance between dispersion and nonlinearity, and the particle represents something like a very little water-ball, the contour of which is the density of energy.

Following, in essence, this general idea, the UQT represents a particle as a bunched field (cluster) or a packet of partial waves with linear dispersion, and the particle is identified with some field.

Dispersion is chosen in such a way that the wave packet would periodically disappear and appear in movement, and the envelope of the process would coincide with de Broglie wave. Based on this idea, the relativistic-invariant model of such unitary quantum field theory was built.

The relativistic invariant equation for our wave packet is following [2-12]:

$$i\lambda^\mu \frac{\partial \Phi}{\partial x^\mu} - \frac{c\Phi}{\eta} \int \left( \bar{\Phi} \lambda_\mu u^\mu \frac{\partial \Phi}{\partial x^\mu} - u^\mu \frac{\partial \bar{\Phi}}{\partial x^\mu} \lambda_\mu \Phi \right) \frac{dV}{\gamma} = 0 \quad (1)$$

where  $\Phi$  is the function of coordinates  $x_\mu = (ct, \mathbf{x})$ ,  $\mu = 0, 1, 2, 3$ , describing different characteristics of our wave packet,  $u_\mu = \left(\frac{1}{\gamma}, \frac{\mathbf{v}}{\gamma}\right)$  is the four-velocity of the particle,  $\lambda_\mu$  is some number matrix and matrices  $\lambda_\mu (32 \times 32)$  satisfy the commutation relations

$$\lambda^\mu \lambda^\nu + \lambda^\nu \lambda^\mu = 2g^{\mu\nu} I, \quad \mu, \nu = 0, 1, 2, 3,$$

where  $g^{\mu\nu}$  is the metrical tensor. This fundamental equation of UQT describes, in our opinion, all properties of elementary particles. It is possible to derive from (1) the Dirac equation and also the relativistic invariant Hamilton – Jacoby equation [3,4]. We have succeeded in solving only the simplified scalar variant of eq. (1). However, the solution obtained has allowed to determine theoretically [7,8] the elementary electrical charge and the fine-structure constant  $\alpha$  with high precision (our theoretical value  $\alpha = 1/137.962$ ), the known experimental value  $\alpha = 1/137.3552$ . Our efforts to find more complete solution of eq.(1) were unsuccessful. Note, our approach based on UQT has nothing in common with Standard Model of Elementary Particles.

It is important to note that Sir Isaac Newton did not apply the conception of material point at all, although it is ridiculous to imagine that such a natural and trivial idea could not come into his mind. We do not know the way of the thinking of that great man. But we know about his marvellous insight, and it may be quite probable that Newton felt and foresaw intuitively all difficulties which the physics science should meet when using the conception of a material point, and he wanted to warn the physicists of future generations: Be careful! The notion of a material point is dangerous!

Really, we see today- after more than two and a half century - that the most troubles of the quantum theory arise if a particle is considered as a material point. A rich bouquet of divergences is the result of this approach. Nevertheless, such an approach is very convenient if it should be used correctly. Let us remember that in accordance with the Newton corpuscular theory, beams of light should be considered as a flow of certain particles. They are emitted in all directions by a luminous body and move in empty space or homogeneous medium uniformly and linearly. In other words, in the same way as usual ordinary material particles do in the absence of any external forces. Newton explained the phenomena of reflection and refraction of light beams on the interface between two homogeneous mediums as a result of the certain forces action directed orthogonally to this interface. These forces, according to Newton, change the normal velocity component, but do not touch the tangential one, and the analysis of this effect has allowed to derive the laws of reflection and refraction. However, the inability of his theory to explain the effects of partial reflection and passage phenomena as well as Newton rings (his own discovery) brought him to almost forgotten but quite modern today theory of bouts (fits). Newton thought that to make complete explanation of all the processes it is necessary to assume that particles of light may experience bouts of reflection and bouts of passage as well. Assume the light falling on to a flat surface. Some part of beams passes and other is reflected. Following quantum description of that effect

the particle connected with the incident wave at the moment of impact has a certain probability to pass or to be reflected. In this situation Newton just used the word “bouts” instead of “probability”.

It is absolutely clear that ideas set forth below will be crude approximation, because no one equation of particle’s motion is able to describe even the most simple interference process in the case of translucent mirror. During that process material particle is divided into two parts, that later shall destroy each other in destructive interference. If we would like to make correct description of single particle, then situation from viewpoint standard quantum mechanics becomes dismal and purely probabilistic. At any moment of time a particle may be in only one non-coherent state: no one particle can move in two different directions simultaneously. Nevertheless, it seems there is a whole class of processes where such description has certain sense. Moreover, UQT have allowed calculating the spectrum of the masses of the elementary particles [9,13,14].

### Materials and Methods

The equation with oscillating charge has been derived soon after the thin structure constant value estimation was obtained. For the first time this equation was just postulated [15,16] and used for description of cold nuclear fusion process due to mutual deuteron interaction.

This equation has the following form

$$m \frac{d^2 \mathbf{r}}{dt^2} = -2Q \text{grad } U(\mathbf{r}) \cos^2 \left( \frac{mt}{2\eta} \left( \frac{d\mathbf{r}}{dt} \right)^2 - \frac{m\mathbf{r}}{\eta} \frac{d\mathbf{r}}{dt} + \varphi_0 \right) \quad (2)$$

where  $m$  is the mass,  $r$  the radius vector,  $U(r)$  the external potential,  $\varphi_0$  the initial phase and  $Q$  the constant part of particle’s charge. The multiplier 2 in eq.(2) is needed for correct transition to equation of classical mechanics because the averaged charge will be two times smaller.

Great dissatisfaction still remains because equation (2) has only been postulated. More over, the fact that not every particle is charged strictly restricted equation’s use. A little bit later [17-20] that equation was “derived” from Schroedinger equation and it was understood that it had been specific charge oscillated. However, for more simplicity we are going to use “oscillating charge” term. It was H. Poincare who noticed for the first time that if the charge or mass of the particle were equally decreased it would not influence equations of motion and could not be experimentally detected.

Let us notice at the same moment that quantum mechanics is the more fundamental science than classical mechanics. As it approaches the limit quantum mechanics results in classical mechanics. However, that fact had not prevented Schroedinger to “deriving” his “famous” equation from relations obtained within Newton mechanics. Schroedinger himself (and many other researchers) considered it not as rigorous deduction but a peculiar illustration because it is impossible to derive this equation strictly from classical mechanics, and this equation was, in fact, postulated. Quite similarly, the equation with oscillating charge is not contained in Schroedinger equation, and further we propose some illustration of correspondence between these two equations.

We will “derive” equation (2) from Schroedinger equation in the following way. Let us do it for one-dimensional case, since 3-dimensional generalization is too complicated. Complete Schroedinger equation with potential  $U(x)$  is following:

$$\frac{\eta^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) + i\eta \frac{\partial}{\partial t} \Psi(x,t) = U(x)\Psi(x,t) \tag{3}$$

We will seek the solution of this equation in non-traditional form:

$$\Psi(x,t) = \cos(kx) \int \exp(itg(\varphi)) dt, \tag{4}$$

where

$$\varphi = \frac{mt}{2\eta} \left( \frac{dx(t)}{dt} \right)^2 - \frac{mx(t)}{\eta} \frac{dx(t)}{dt} + \varphi_0 \tag{5}$$

The  $x(t)$  function is some function of time and is not connected in any way with independent variable  $x$ . By substituting (4) in equation (3) we get:

$$i\eta^2 k^2 \int \exp(itg(\varphi)) dt + 2imU(x) \int \exp(itg(\varphi)) dt + 2\eta m \exp(itg(\varphi)) = 0 \tag{6}$$

For the very small kinetic energies the following relation always holds true:

$$\eta^2 k^2 \ll 2mU(x).$$

Then we may neglect the first integral in (6). Differentiating the remnant part in time and reducing general exponential factor we obtain:

$$2U(x)\cos^2(\varphi) + 2mt \frac{dx(t)}{dt} \frac{d^2x(t)}{dt^2} - m \left( \frac{dx(t)}{dt} \right)^2 - 2mx(t) \frac{d^2x(t)}{dt^2} = 0 \tag{7}$$

If we use the relation

$$x(t) \approx t \frac{dx(t)}{dt},$$

that may be considered true for short time-intervals, then in equation (7) items 2 and 4 are canceled and we obtain:

$$U(x)\cos^2(\varphi) = \frac{m}{2} \left( \frac{dx(t)}{dt} \right)^2 \tag{8}$$

In the equation (8) left side is oscillating potential energy, right is kinetic energy. Unfortunately, we do not observe mutual transformation of kinetic energy into potential one and back (as it is in classical mechanics of different conservative systems). It seems that potential energy oscillate because the whole packet appears and disappears together with the charge. At the other side, kinetic energy apparently is connected with Fourier harmonic components of moving packet that results in appearance and disappearance of mass due to dispersion in the process of moving. Then we shall assume that independent variable  $x$  should be replaced by  $x(t)$  in the potential; we have no other simple ideas. In that case we get the following equation:

$$U(x(t))\cos^2(\varphi) = \frac{m}{2} \left( \frac{dx(t)}{dt} \right)^2, \tag{9}$$

which may be considered as typical Lagrangian like:

$$L = \frac{m}{2} (\dot{x}')^2 - U \cos^2(\varphi) \tag{10}$$

where  $x$  depends on time and following shorter symbols are used:

$$x = x(t), \dot{x}' = \frac{dx(t)}{dt}, \ddot{x}'' = \frac{d^2x(t)}{dt^2}, U(x) = U$$

If we integrate that Lagrangian, then we obtain the expression for the action. Further, we can find Euler-Lagrange equation; that will be the equation of motion. For this purpose we integrate Lagrangian (9) in respect to time and obtain the action functional, and compile the variation of this functional. We get the equation:

$$\begin{aligned} & -U' \cos^2(\varphi) + \frac{2}{\eta} U m \dot{x}' \cos(\varphi) \sin(\varphi) - m \ddot{x}'' - 2U' \dot{x}' \cos(\varphi) \sin(\varphi) \left( \frac{m \dot{x}' t - m x}{\eta} \right) \\ & + 2U \sin^2(\varphi) \left( \frac{m \dot{x}' t \ddot{x}'' - m \ddot{x}'' x - m \dot{x}'^2}{\eta} \right) \left( \frac{m \dot{x}' t - m x}{\eta} \right) \\ & - 2U \cos^2(\varphi) \left( \frac{m \dot{x}' t \ddot{x}'' - m \ddot{x}'' x - m \dot{x}'^2}{\eta} \right) \left( \frac{m \dot{x}' t - m x}{\eta} \right) \\ & - \frac{2}{\eta} U m \ddot{x}'' \cos(\varphi) \sin(\varphi) = 0 \end{aligned} \tag{11}$$

If we agreed that within infinitesimal time interval the velocity and acceleration of particle are nearly constant, i.e.

$$x \approx \dot{x}' t, \dot{x}' \approx \ddot{x}'' t,$$

Then only the first and the third items remain. Thus, we can rewrite (11) in habitual form:

$$\frac{dU(x)}{dx} \cos^2(\varphi) = m \frac{d^2x(t)}{dt^2} \tag{12}$$

In 3-dimensional case we obtain the same result. Notice, equation (12) is non-autonomous according to expression (4) for  $\varphi$ .

It is possible to “derive” from Schroedinger equation also our autonomous equation in form (12). For this purpose we will seek the solution of equation (3) also in form (4), but with another phase:

$$\phi = \frac{mc^2 t}{\eta} + \frac{mt}{2\eta} \left( \frac{dx(t)}{dt} \right)^2 - \frac{mx(t)}{\eta} \frac{dx(t)}{dt} + \varphi_0 \tag{13}$$

Then after substitution at Shroedinger equation and after the same transformations as previously we will get new first-order equation considered as a Lagrangian:

$$U(x(t))\cos^2(\phi) - \frac{m}{2} \left( \frac{dx(t)}{dt} \right)^2 + mc^2 = 0 \tag{14}$$

After integrating (14) in respect to time and compiling the variation we get equation in form (12), but with the phase in form (13). In expression (13) there are terms with slow and fast oscillation that satisfy following inequality:

$$\frac{mc^2}{\eta} \gg \frac{m}{2\eta} \left( \frac{dx(t)}{dt} \right)^2$$

Now we may first of all neglect the smaller term in comparing to the bigger one, and then reject fast oscillating term, in so far as it will not influence final result at. Thus we have the autonomous equation that may be written as follows:

$$m \frac{d^2 \mathbf{r}}{dt^2} = -Q \text{grad } U(\mathbf{r}) \cos^2 \left( -\frac{m \mathbf{r}}{\eta} \frac{d\mathbf{r}}{dt} + \varphi_0 \right) \tag{15}$$

Of course, this method will not delight anybody, but it differs a little from generally accepted cancellation of divergences in quantum field theory, when infinities being subtracted one from the other are canceled.

It may be noticed that autonomous equation (15) might be obtained at once after substituting relations (11) into (5). It should be especially noticed that resulted first-order equations like (9) and (12) won't be primary integrals of the second-order equations (2) and (15) and last equations are crude approximations. More over the entire "derivation" may be a subjected to criticism. Our main task, however, was to illustrate that the above-mentioned equations have certain relation with Schroedinger equation. By the way, in "hidden parameters" theorem it was logically proven that within rigorous Schroedinger equation there is no place for such hidden parameter as initial phase. That is why the rigorous deduction of our equations from Schroedinger equation is absolutely impossible. Hereafter we will try to explain how it should be understood at all.

We deal in quantum theory with pure probabilities and such approach is based not upon our inability to control or exactly measure different parameters of the existing processes, but upon accidental character of many parameters by its nature. In other words, the chance that observed probability reflects the influence of uncontrolled hidden parameters may be excluded from consideration, if these parameters are not clearly detected or are not included into theory. According to that quantum mechanics assume that alternative events have equal probabilities and consider it as a physical fact. More generally, it is considered as a basic thesis limited reproduction of the atomic events to be made in thoroughly controlled similar experimental conditions.

The main aim of the Science is the understanding of outward things and description of all going processes by means of Mathematics. One of the ways – is gaining experimental information and putting it in good order in our mind. That process requires considering as fundamental or initial some minimal quantity of facts, and the other facts as their logical corollaries. Such division into fundamental facts and their logical corollaries depends on analytical abilities as well as on existing in Science of an overarching paradigm and some times on our preferences as well. For example, it is unnecessary to consider mathematical beauty of a theory as truth criterion (P.A.M.Dirac). As alternative example we can use Lorentz fundamental transformations (at our point of view they are quite not good-looking) or Maxwell equations, which beauty till introduction of mono-field (P.A.M.Dirac again) was rather doubtful.

Newton mechanics, uniquely, allows the prediction (in a determined way) the future of a system if the initial data are known. Statistic mechanics arises from the necessity of complicated mechanical systems' analysis, when small and even uncontrollable inexactitude of initial data results in almost unforeseen consequences and so makes concessions to very complicated computational processes. Nevertheless, the base of statistical mechanics remains determined process.

Within standard quantum mechanics the situation absolutely differs. According to it, dynamics and statistics are indivisible, and not even the most genius mathematician with the most powerful super computer principally can not avoid a statistical description. And here an atavistic thought appears that in reality quantum description is incomplete, and in future, when new

"hidden" parameters yet unknown for quantum mechanics will be introduced, the descriptions of predicted determined dynamic regularity may arise. For the first time that challenge was strictly issued and solved by mathematician John von Neumann for the Schroedinger equation: there are no such "hidden" parameters in standard quantum theory with Schroedinger equation.

The equation with oscillating charge has such "hidden" parameter – the initial phase. Naturally, the question arise, how to reconcile it with von Neumann proof. Here we can notice that equation with oscillating charge is a crude approximation at very small energies and therefore, formally, it is not strict quantum-mechanical equation and results of von Neuman theorem can not be applied.

It is quite understandable that equation with oscillating charge can not strictly describe interference processes since according to it moving particle should have bifurcation's states (particle should physically divide). This is absolutely impossible in the case of motion equations in classical mechanics. That is why using of our equation is apparently limited to cases of small energies and to cases when there is evidently no interference, or strong diffraction. In other words, in the case, when the wave packet is being reflected or dispersed as a whole only, then the use of equation with oscillating charge is possible.

Moreover, according to such approach the question about particle' photon emission when particle starts moving with acceleration remains unclear. Generally speaking, intimate mechanism of photon emission remains a big mystery. We assume the picture of such a process in images and movements exists and we hope will be discovered in future.

There is very interesting parallel between Schroedinger equation and equation with oscillating charges. It is known that in the case of charged particle movement in plane condenser with the constant tension to be applied classical uniformly accelerated motion  $x = at^2$  appears. For the equation with oscillating charge such analytical solution exists. Let show that Schroedinger equation has physically similar solution also. Viz., let potential in Schroedinger equation be equal  $U(x) = rx$ . Then complete Schroedinger equation is as follows:

$$\frac{\eta^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} - rx\Psi + i\eta \frac{\partial \Psi(x,t)}{\partial t} = 0 \quad (16)$$

We will seek the solution in rather unusual form:

$$\Psi(x,t) = b \exp\left(i \frac{ma^2 t^3}{2\eta} - i \frac{matx}{\eta}\right) \quad (17)$$

By substituting (17) in (16) we get (after reducing):

$$-2ma^2 t^2 + (ma - r)x = 0.$$

This relation will be fulfilled if

$$x = \frac{2ma^2}{ma - r} t^2. \quad (18)$$

This result confuse untrained reader, because in equation (16)  $x$  and  $t$  are independent from each other variables. Such idealization is inherent and convenient in mathematics, but the real situation is slightly others: during motion the truly independent variable is time only. Generally speaking, coordinate is dependent variable and at given velocity is connected with time by means of the relation (18).

If in (18) impose the requirement  $r \rightarrow 0$  (potential vanishes), then absolutely strange particular solution appears

where the particle is able to move with constant acceleration and to generate energy no of an unknowns where origin (!!!) Of course, it is out of understanding how such initial conditions could be created. That effect remains valid even if we put  $r \rightarrow 0$  directly in equation (15).

From the standard physics point of view the motion of quantum particle within the field of constant potential never differs from the motion in empty space free from any field, because, as a rule, potential is determined up to arbitrary constant (well known calibration) and that constant may be always selected so as potential would be equal zero. Such a solution of the equation (15) for wave function with increasing frequency (energy) has been discovered independent from us by Dr. Bill Page - USA (particular report) in the form of combinations of Airy functions. The same solutions can be obtained for Dirac equation.

Curious, but we have similar situation in classical electrodynamics. If during acceleration of a charge one takes into account force acting on a charge itself, then the braking due to radiation arises. In different works this effect is called in different way: bremsstrahlung, Lorenz frictional force or Plank's radiant friction. That force is proportional to third derivative of coordinate  $x$  relative to time and was experimentally proved many years ago. If we write the equations of motion for the charge moving in space free from external fields impact and if the only force acting on the charge is the "Plank radiant friction", then we would obtain following equation:

$$m \frac{d^2 x}{dt^2} = \frac{2e^2}{3c^3} \frac{d^3 x}{dt^3}$$

It is evident that equation in addition to trivial and natural particular solution

$$v = \frac{dx}{dt} = \text{Const}$$

has general solution where particle acceleration is equal

$$a = \frac{d^2 x}{dt^2} = C_1 \exp\left(\frac{3mc^3 t}{2e^2}\right),$$

i.e. is not only unequal to zero, but more over it unrestrictedly exponentially increases in time for no reason whatever!!! For example, L.Landau and E.Lifshits in their classical work "Theory of the field" wrote apropos of this: "A question may arise how electrodynamics satisfying energy conservation law is able to give rise to such an absurd result in accordance to which a particle was able to unrestrictedly increase its energy."

The background of that trouble is, actually, in infinite electromagnetic "eigen mass" of elementary particles. If we write in equations of motion finite charge mass, then we, in essence, arrogate to it formally an infinite, formally, negative "eigen mass" of not electro-magnetic origin, that together with electro-magnetic mass should result in finite mass of particle. But as far as subtraction of one infinity from another is not mathematically correct, that leads to troubles as described above".

We are going to tell about such astonishing solutions, where excess energy appears in nature. We think that processes of energy generation being in nature have left their signs both in quantum theory and electrodynamics. We should note that such traces are fully absent in classical mechanics. Mathematical characteristic of these equations and their decisions were in detail analysed in [9-11].

## Results and Discussion

### The equation with charge oscillating

Using the equation with charge oscillating has allowed much simply physically explain: the tunnel effect, resonance scattering on short potential and practically all rest quantum effects. But, the main, behaviour of the particles in potential wells can be accompanied both generation, and absorption to energy, but laws of the conservation appear only when averaging on ensemble. For single processes there is only probability that or other events and in this case, under small energy, laws of the conservation are absent, otherwise was determinism.

The eq.2 with charge oscillating has only two analytical decisions:  $r \sim t^2$  when moving in constant field of the flat capacitor and  $r \sim \sqrt{t}$  when moving in dipole field. For it in general is absent the integrals of the motion. The autonomous equation has an integrals of the motion, but analytical decisions for it is not found. The numerical decisions of both equations have a qualitative alike natures of the motion. Let consider the behaviour of the particles in potential wells.

### Particles in Potential Wells

In this section we will consider only one-dimensional problems. In classical mechanics the problem of rolling a particle into a finite-depth well is very simple from the physical point of view. Classical solutions of motion equations in the case of a potential well with symmetrical sides correspond to situation when a particle always rolls into the well and then leaves it at the same initial velocity. Moreover, in classical mechanics it is impossible to roll a particle into a well with symmetric sides in such a way that it remains there. If not for friction this would be true.

For the mechanics of a particle with an oscillating charge there are three possible modes of behavior, which, as it was found out, do not depend on the type of the potential well; it must only be finite and have equal sides:

1. A particle at small initial velocity and having certain initial phase can roll into the well and start oscillating there for a long time with damping, its charge will be constantly reduced, and finally this particle turns into "a phantom". From point of view of our theory, the wave packet representing this particle is spread all over the Universe. Moreover, there appears to be a certain threshold for the energy. If the energy is below this threshold, the particle will not roll out of the well at all. The value of the energy threshold depends on the type of potential. Oscillations without loss of energy and charge are also possible.
2. A particle can roll into the well and roll out at a speed higher, equal or lower than the initial speed. In other words, a particle passing the well can either increase or reduce its energy. The energy conservation law for a single particle is not always valid.
3. A particle rolls into the well and starts oscillating there, and its energy will increase until it rolls out of the well with a much higher energy. It can even roll out in the direction opposite to the initial movement (reflection). Such processes seem to explain multiple experiments made by J.Griggs, Yu.Potapov, T.Misuno, A.Samgin, N.Tesla, R.Tandberg, P.Correa, etc. [9-11]. In books [9-11] this processes have a name "Mathernity Home".

The autonomous movement equation in the case of a potential well in the shape of hyperbolic secant

$$U(x) = -U_0 \operatorname{sech}(x^2)$$

will look as follows:

$$m \frac{d^2x}{dt^2} + \frac{4U_0 Q x \cos^2\left(mx \frac{dx}{dt} + \varphi_0\right) \sinh(x^2)}{\cosh^2(x^2)} = 0 \tag{19}$$

where  $m, Q, \varphi_0$  are mass, charge and initial phase of a particle respectively.

The plots below represent the results of a numerical solution of equation (19) by the Runge-Kutta-Merson method under following starting conditions:

$$U_0 = 1, m = 1, Q = 1, x_0 = -1, v_0 = 1/20$$

The resulting modes of the particle's behavior under equal starting conditions greatly depend on the initial phase, and its variations result in a very rich behavior. Let us demonstrate this fact. A particle with  $\varphi_0 = 0.1$  rolled into the well and rolled back (was reflected) with a higher energy (Fig. 1). Under the same starting conditions and with an initial phase value of  $\varphi_0 = 0.2$  passage of the particle through the well was observed with nearly the same energy (Fig. 2.) and at  $\varphi_0 = 3.2$  increasing oscillations inside the well were observed (Fig.3), where a particle could accumulate energy (a "maternity home" solution).

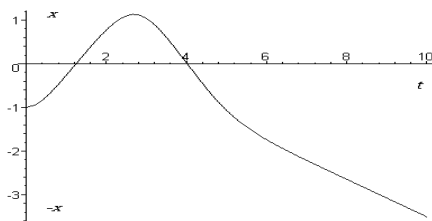


Fig.1. Reflection from potential well with a certain speed increase.

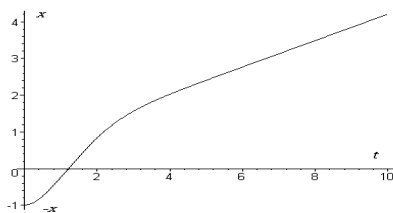


Fig.2. Passage of the well without reflection with a small energy change.

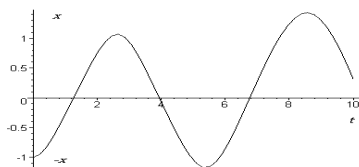


Fig.3. Oscillation in well with energy growth ("maternity home" solution).

Certainly, such a process is not characteristic only for the case of the hyperbolic secant potential. A numerical research of our problem with other potentials was made, yielding similar results. (Remark: It was recently found out that hyperbolic secant potential plays a special role in quantum mechanics, and it turned out that barriers of this type are in general non-reflective, but for solutions of equation with an oscillating

charge all this is not valid.) Let us take as an example a potential of the Gauss bell-curve:

$$U(x) = U_0 \exp\left(-\frac{x^2}{\sigma^2}\right) \tag{20}$$

The movement equation is following:

$$\frac{d^2x}{dt^2} + \frac{2Qx \exp\left(-\frac{x^2}{\sigma^2}\right) \cos^2\left(mx \frac{dx}{dt} + \varphi_0\right)}{m\sigma^2} = 0$$

where  $m, Q, \varphi_0$  are mass, charge and initial phase respectively. This equation was solved under starting conditions  $Q = 8, \sigma = 1, m = 1, x_0 = 0.1, v_0 = 0.5$  and under different initial phases. When initial phase  $\varphi_0 = 0.1$  the particle oscillates, increase its energy and overcomes the potential barrier, as can be see in Figure.4.

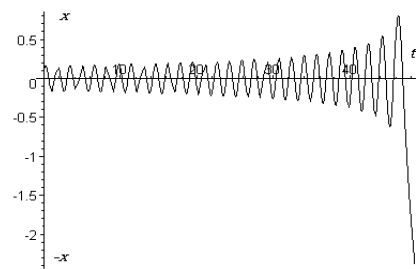


Fig.4. Passage of well with oscillations and energy growth ("Mathernity Home" solution).

For other starting conditions  $x_0 = -4, v_0 = 0.01, \varphi_0 = 2$  we get a process where the particle is spread all over the Universe, and not only its energy, but also its charge is reduced, and it turns into a "phantom". Fig.5 serves as an illustration.

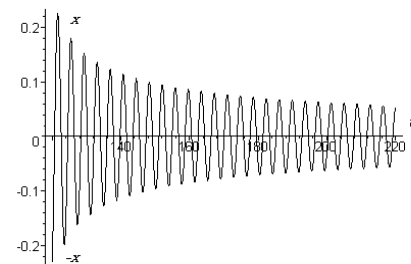


Fig.5. Particle oscillation in well and its gradual disappearance ("crematorim" solution).

There are the conditions under which the particle in the well does not disappear, but loses almost all its kinetic energy when leaving the well. Thus, under the following starting conditions and parameters of the particle:  $m = 5, Q = 10, \sigma = 1, \varphi_0 = 1.57, x_0 = -5, v_0 = 0.1$  our simulation yields the result illustrated in Fig.6.

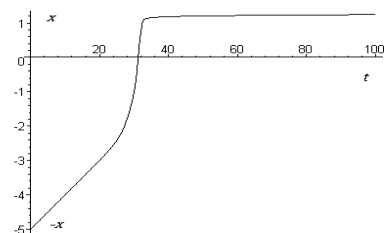
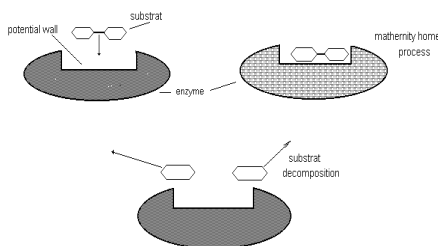


Fig.6. Passage of well with nearly full loss of energy.

Such processes, however, are observed only in finite-depth wells, i.e. those having a bottom. In wells of the coulomb type or H.Yukawa type these processes do not take place, and no oscillations are observed (this does not mean, however, that they are totally absent there). The particle simply falls to the bottom of the well. In the Coulomb potential the fall happens approximately in accordance with the law  $x = at^{2/3}$ . Of course, the relativistic effect of mass accumulation will lead to the following relation in the limit  $x=ct$ .

If non-autonomous equations are used for modeling, the qualitative behavior results will look the same, so we omitted them.

The well known problem of “shortage” of energy in many biochemical reactions with the ferments (enzymes) participation looks even more mysterious. For example, in the deeply studied reaction of polysaccharides disintegration in presence of lysozyme the following take place: a molecule of polysaccharide appears in a special cavern in a big molecule of lysozyme, sole time later its debris is thrown out (Fig.7.)



**Fig.7. Disintegration of polysaccharides molecule in presence of lysozyme**

The energy of broken bound in polysaccharides is about 3 eV, and the energy of thermal motion is 0.025 eV only. So it is absolutely incomprehensible where does the lysozyme take energy necessary to break polysaccharide from. There is no any satisfactory mechanism to explain this type of reaction (although they are a lot of the explanation). As physics say, “the problem was pigeonholed”.

The most astonishing is the fact that in all excess energy liberation can not be explained by chemical reactions or changes of phase. If sometimes nuclear reactions take place (in accordance with modern science that could not be at all) they are able to explain a hundredth or a thousandth part of the heat energy liberated. There is no doubt that all these facts belong to the new physical theory, because there are no any reasonable explanations for these facts in the network of the old theory at all.

#### Possible Uniform Approach to the Theory of Catalytic Processes

Consider for the sake of simplicity only two types of chemical reactions: decomposition and synthesis, when a complex molecule decomposes under certain conditions into two or more component atoms or molecules, or two atoms or molecules unite and create a new chemical compound. In order for this to happen, in a synthesis reaction two particles should be united. The complicated interaction potential, which is today unknown even for the simplest chemical reactions, plays a complicated role, most often that of a barrier.

According to Arrhenius' theory (today accepted by everybody), only those collisions are chemically effective, when the participating molecules have an excess of the energy over the average value. The difference between the minimal energy

of a molecule, necessary for the reaction to take place, and reaction resultant from the bump to happen, is called activation energy  $E_a$ . It depends on the temperature of the system.

When the number of active molecules  $N_a$  represents a small share of the total number of molecules  $N$ , their number can be expressed through the Boltzmann-Gibbs activation energy as follows:

$$N_a = N \exp\left(-\frac{E_a}{RT}\right) \quad (21)$$

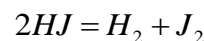
It is known that a temperature increase usually considerably increases the reaction rate. Van't Hoff discovered that the reaction rate increases by 2-4 times, when the temperature raises by 10 degrees, and if the temperature raises by 100 degrees, the reaction speed grows approximately by 1000 times.

If the temperature raises by 10 degrees, and it is assumed that the activation energy remains constant (which is possible under small temperature intervals), the temperature effect on the number of active molecules can be estimated. Let us assume that the activation energy for a certain reaction under  $300^0 K$  is 24000 cal. In this case:

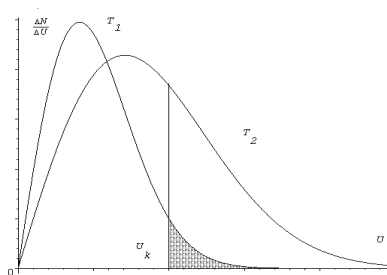
$$\frac{N_a}{N} = \exp\left(-\frac{24000}{2 \cdot 300}\right) \approx 4.1 \cdot 10^{-18}$$

and such a reaction with 4 active molecules at  $10^{18}$  will certainly be very slow. Under  $T = 310^0 K$  the same exponent will equal  $16 \cdot 10^{-18}$ , i.e. the number of active molecules will quadruple. There will be 16 of them per each  $10^{18}$  molecules. The average molecular energy reserve will increase only by 3-4%.

It should not be assumed that everything is so nice and the reaction speed increase is due only to the higher number of collisions between molecules and to the increased number of active molecules. For example, the increase in the number of gas molecule collisions under the growing temperature  $T$  will be proportionate to  $\sqrt{T}$ . But the change of speed in a homogeneous reaction



cannot always be accounted for only by the Van't Hoff rule. If we calculate the number of molecular collisions  $HJ$  using the molecular-kinetic theory equations in 1 cubic cm per second at the pressure of 1 atm., it will be of the order of  $10^{28}$ , and the speed of this reaction with a 100% efficiency of each bump must be gigantic, and everything should be over in  $10^{-10}$  seconds, which never happens in reality.



**Fig.8. Distribution of molecules by kinetic energy ( $T_1 < T_2$ ).**

This happens, because not every bump ends with interaction. Thus, a molecular bump for biomolecular reactions is a necessary condition, but not a sufficient one.

By Arrhenius, the reaction speed constant  $k$  can be expressed by the following equation:

$$k = A \exp\left(-\frac{E_a}{RT}\right)$$

where  $A$  is the pre-exponential multiplier, constant for this case. In accordance with Maxwell-Boltzmann ideas, Fig. 8 contains a sketch of two curves of gas molecule distribution by kinetic energies under two different temperatures  $T_1 < T_2$ . Along the axis of ordinates the ratio between the number of gas molecules  $\Delta N$ , the energy of which is between  $U$  and  $U + \Delta U$ , to the energy value interval  $\Delta U$ , is shown, and along the abscissa axis the energy  $U$ . Only such molecules are capable of entering into the reaction, whose kinetic energy is not less than a certain value of  $U_k$ , meeting the activation energy. The number of hot molecules capable of entering a reaction under  $T_1$  is graphically shown by the crosshatched region. It is seen that this number is greatly increased if  $T_2 > T_1$ , which happens in accordance with equation (21), and the average kinetic energy grows much slower, because it is simply proportionate to the absolute temperature. The source of molecular activation may lie not only in heat, but also in radiant or electric energy, the energy of radioactive particles, and... a catalyst. For a reversible reaction, the heat effect equals the difference between the activation energies of the direct and reverse reactions.

Not all chemical processes happen spontaneously. There are reactions that go only in one direction with full consumption of the initial substances (explosive processes). Such reactions, as a rule, cannot spontaneously go in the reverse direction.

The situation is much more interesting with reversible reactions. If we mix, for example, hydrogen and iodine warmed up to  $800^{\circ}K$ , they will react and hydroiodine will be formed. If  $HJ$  is not removed from the reaction space, the iodine and hydrogen will never be totally consumed. Under these conditions, the state of dynamic chemical equilibrium will be achieved, which could otherwise be achieved by warming  $HJ$  to  $800^{\circ}K$ , because we are dealing with a reversible reaction (only under these conditions).

Real equilibrium is characterized by the fact that it can be approached from two sides. In a state of equilibrium the concentrations of all the substances in the system remain unchanged under these conditions, since the speed of the direct and reverse reactions is the same.

Real equilibrium in case of a thermodynamically reversible process is shifted under very slight changes in the external conditions, strictly following these changes. It is believed that any transfer to a less stable state is always connected with some work expense from outside. The farther the system is from the balanced state, the more capable it is principally of entering into reactions. But this capacity is not at all always manifest under the said conditions. For example, a mixture of  $H_2$  and  $O_2$  is very reactive, but under room temperature no changes in the concentration of the substances taken are observed in it. Such examples are numerous. These systems are in a state of an

unstable false equilibrium, and changes are not observed in them simply because the process speeds are infinitely small. There are lots and lots of such false equilibrium systems, and we can even say that we are living in a world of false equilibriums. However, if the process is accelerated by heating or by a catalyst, the false equilibrium will be broken and a reaction will take place. In other words, false equilibrium is almost always caused by kinetic problems (difficulty) during a reaction.

According to the Sadi Carnot theorem, the efficiency equals

$$\eta = \frac{A}{Q} = \frac{T_2 - T_1}{T_2}$$

where  $T_2$  and  $T_1$  are the temperatures of the heater and the cooler. Be it quickly or slowly (equilibrium thermodynamics does not deal with this at all), every chemical reaction goes in such a way as to tend to a state of real equilibrium. If the reaction takes place in a system under constant pressure and temperature, the change of enthalpy  $\Delta H$  (heat content) can be presented as a sum of two terms: the change of the Gibbs free energy  $\Delta G$  and the change of the bound energy  $\Delta L$ :

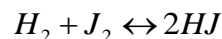
$$\Delta H = \Delta G + \Delta L.$$

The Gibbs free energy  $G$  is sometimes called the isobaric-isothermal potential, and it is not the free energy under constant volume and temperature, which in theoretical thermodynamics is usually denoted by the letter  $F$ . The bound energy  $\Delta L$  is expressed by the product of absolute temperature  $T$  multiplied by the change of the state function (change of entropy)  $\Delta S$ . In this case:

$$\Delta G = \Delta H - T\Delta S \quad (22)$$

Fig.9 shows the dependence of the free energy on the relative content of  $HJ$  in the mixture

( $H_2 + J_2$ ). If, for instance, in the system



being in a state of equilibrium free energy has the value designated by the ordinate at point  $C$  (Fig.9), any deviation of the composition of the mixture of initial and end substances from the equilibrium to the right or to the left from point  $C$  requires certain work, so the free energy must increase both with an increase in the partial pressure of  $HJ$  and with an increase of partial pressures (concentrations) of  $H_2$  and  $J_2$ . It follows that under the chemical equilibrium a gas system of  $H_2, J_2$  and  $HJ$  has the minimum value  $G_{min}$ . On the way from the mixture of  $H_2$  and  $J_2$  (point  $A$ ) to the equilibrium mixture composition, loss of free energy must be observed -  $\Delta G < 0$ . The same  $\Delta G < 0$  on the way of the mixture composition change from  $B$  to  $C$ . With equilibrium mixture composition at point  $C$

$$\Delta G = 0$$

the condition of chemical equilibrium is  $\Delta G = 0$ , and the criterion of reactivity is the requirement  $\Delta G < 0$  under constant pressure and temperature. In other words, the reaction is possible, if  $G$  decreases, and once it begins, it will go on spontaneously. The moving force of the whole process is the value of  $\Delta G$ . Loss of this free energy in a reaction going on under a constant pressure and temperature does not depend on the route of the process and equals the maximum reaction work, i.e.  $-\Delta G = A$ .



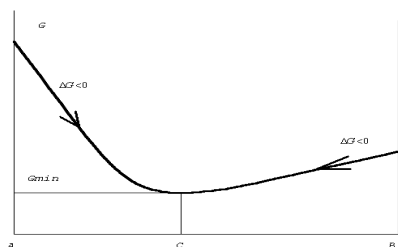


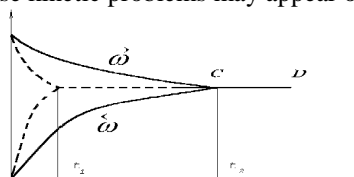
Fig. 9.

Of course, if for a certain process  $\Delta G > 0$ , then, from the point of view of the existing science, there is no point in trying to hold it under the said conditions. Let us note that earlier the criterion of chemical affinity was considered to be the value of the positive heat effect  $Q$ . Under low temperatures this is almost true, because the product  $T\Delta S$  in equation (22) becomes very small and  $\Delta G$  nearly coincides with  $\Delta H$ . Much later it was discovered that there were many reactions with heat absorption, which usually go on under very high temperatures. If  $T\Delta S > 0$ , the second term of equation (9) can be more than  $\Delta H$ , and then  $\Delta G$  will have a negative value, which makes such reactions possible. Here is an example. Reaction



which under normal conditions goes on from right to left, can, nevertheless, go on from left to right. For it  $\Delta H_{1000} = 62 \text{ kcal}$ ,  $\Delta G_{1000} = -26.1 \text{ kcal}$ , i.e. below zero. *The Unitary Quantum Theory gives us hope that for reactions of the left-right type the effect of high temperature may be replaced by a relevant catalyst.*

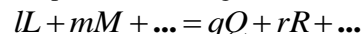
Equilibrium chemical thermodynamics only establishes a principal possibility of a reaction and solves the problem of achieving the equilibrium, but it does not answer the question of how quickly this equilibrium can be achieved, because the time is altogether absent from this theory. In no case it can be assumed that the lower the negative value of  $\Delta G$ , the quicker the process, because kinetic problems may appear on the way.



**Fig. 10. Establishment of chemical equilibrium. Along axis x- time, along axis y- reaction speed. Firm line – without catalyst, dotted line – with catalyst. CD – chemical equilibrium line;  $t_1 \ll t_2$ .**

The questions of chemical reaction speed, the effect of different factors on speed, and the reaction mechanism are the subjects of chemical kinetics. Using different methods: changes of temperature, pressure, concentration, introduction of catalysts, radiation with light, it studies the speeds of achieving an equilibrium. If the definition of the “energy capacity” of  $\Delta H$  and the “work capacity” of  $\Delta G$  in the process requires only the knowledge of enthalpy and the free energy of the formation of the initial and the end substances under given conditions, the process speed depends not only on what substances there are in the right and left parts of the equation; it also always depends on intermediary products and, mainly, on catalytic processes.

Chemical reaction speed  $\omega$  in straight direction:



where  $l$  molecules of substance  $L$  react with  $m$  molecules of substance  $M$ , etc., is expressed by the following equation:

$$\omega = k C_L^l C_M^m \dots \quad (24)$$

where  $C_L, C_M$  are the concentrations of the substances  $L$  and  $M$ , i.e. the number of molecules in a volume unit or a proportionate value, and  $k$  is the reaction speed constant. The reaction speed in the reverse direction is totally similar:

$$\omega = k C_Q^q C_R^r$$

At the equilibrium  $\omega = \omega$ , and, consequently,

$$\frac{C_Q^q C_R^r \dots}{C_L^l C_M^m \dots} = \frac{k}{k} = K$$

This is the equation of the active mass law for chemical equilibrium in ideal systems, and  $K$  is the equilibrium constant.

The active mass law is intuitively clear: for a reaction to happen, the molecules of the initial substances should bump, i.e. the molecules should as a result of chaotic heat movement approach each other to a distance of the atomic dimension order. The probability of finding in a certain small volume at a given moment of time  $l$  molecules of substance  $L$ ,  $m$  molecules of substance  $M$ , etc. will be proportionate to the probability of compound event  $C_L^l C_M^m$ . Hence, the number of bumps within a unit of time in a unit of volume is proportionate to this value, which leads to equation (24).

This law can have a different interpretation: the reaction speed is proportionate to the derivative of the concentration of the reacting substances in time.

It is clear that the observed speed of a reversible reaction will be as follows:

$$\omega = \omega - \omega$$

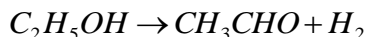
But the seeming simplicity of chemical kinetics is broken by catalytic processes. Catalytic reactions are such reactions, the speed of which is changed by other substances (catalysts) introduced into the system, the composition and quantity of such catalysts remaining unchanged by the end of the reaction. However, catalysts take part in the process. In biochemical processes a huge role belongs to organic catalysts – ferments (enzymes). In case of homogeneous catalysis, the catalyst is in the same phase with the reacting substances. In case of heterogeneous catalysis, reactions go on the surface of the catalyst, which forms an independent phase.

Today it is believed that all catalytic reactions from the thermodynamic point of view are spontaneous processes, i.e. they are accompanied by reduction of free energy, and the catalysts do not shift the state of chemical equilibrium, but accelerate its achievement. One and the same catalyst accelerates, as a rule, both the direct and the reverse reactions. All catalysts have a selective effect, accelerating not any reaction at all, but one that is thermodynamically possible. Dehydration of ethyl alcohol on different catalysts is a vivid example:

Under 350 degrees C on  $Al_2O_3$  reaction is

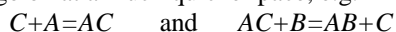


Under 350 degrees C on Cu reaction is



On other catalysts and under different temperatures butadiene  $CH_2CHCHCH_2$ , butylalcohol  $C_4H_9OH$ , diethyl ether  $(C_2H_5)_2O$ , and other substances are received from ethyl alcohol. It is clear that the type of ethyl-alcohol dehydration is defined exclusively by the catalytic substance.

Acceleration of reaction in homogeneous catalysis is a more or less understandable process and is explained by formation of intermediary compounds (sometimes of a whole chain of them). If a reaction  $A+B=AB$  requires a greater activation energy  $E_a$  and goes on slowly, introduction of catalyst  $C$  allows for holding the process in two stages through an intermediary compound, which process will require smaller activation energies and go on at a much quicker pace, e.g.



The catalyst  $C$  remains unchanged in quantity. D.Mendeleyev thought, however, that even in homogeneous catalysis there may exist another mechanism: the catalyst may sometimes simply reduce the value of  $E_a$  in the reacting molecules.

But if the processes in homogeneous catalysis seem fairly clear, in heterogeneous catalysis, which is much more selective than homogeneous and is very widely used, all is in the dark, and the number of heterogeneous catalysis theories is probably only slightly less than the number of heterogeneous catalytic processes themselves. This statement is in no way original. It is enough to read an article by G.Bond [21] with a characteristic title: «Catalysis: Art or Science?». Of course, it is only the opinion of a single researcher, but... here is what wrote in [22] the well-known German specialist in chemical catalysis A. Mittasch:

*«When a question was raised of the practical use of the ammonia direct synthesis process discovered by F.Gaber, K.Bosch, to whom the matter was entrusted, set a task before his team – to replace expensive and rare substances like platinum, osmium and uranium, with more affordable ones, or to improve the known but rarely used catalysts in such a way that they could be used in the industry... We paid principal attention to mixtures of iron with other metals, but in laboratory experiments we, besides iron, mixed every element A from the periodic table with any element B as such, or in the form of compounds with different ratios and by different methods» (!!!).*

A.Mittasch and all his multiple employees from the Baden plants of IG Farbenindustrie solved the problem: the required catalyst was found. They also received patents for hundreds of other catalysts discovered in the process of solving the problem.

Modern chemists say that the method of primitive and nearly meaningless sorting out remains the main one in the search of the necessary catalyst.

Thus, the results of practical work have advanced greatly, but no general catalysis theory has been created for a very long period of the existence of catalytic processes and reactions.

The chemists first faced the catalysis phenomena in 1800's, and today they have a right to expect an understanding of the essence of them. It did not happen, however, and very serious reasons appeared for being discontent with those theories and

hypotheses, which reflected only separate, and not always principal, aspects of the phenomenon.

The theories satisfied only their authors, but were not understandable and acceptable for others, and, most importantly, were totally useless as a help to experts in the selection of this or that catalyst.

Let us shortly list the main research results received in heterogeneous catalysis experiments.

1. All solid bodies with all kinds of chemical compositions possess a certain surface activity and can be conducive to initiating and accelerating chemical reactions. But the surface activity of some bodies is so small that these bodies are practically unfit for catalyzing reactions that need even a minimum activation energy. The surface activity of some other bodies is sufficient, and they can be widely used as catalysts for a big number of reactions. Such was the conclusion made, for example, by D.Mendeleyev [23], although there are many other researchers who came to the same conclusion independently.

2. Since the catalytic activity, in particular, the orienting actions of catalysts, mainly depends on the chemical composition, the latter is the key factor defining the catalytic qualities of solid bodies. This conclusion was made by D.Mendeleyev, I.Langmuir, A.Mittasch, G.Konovalov, and many others.

3. Together with the chemical composition, the physical state of a body is another factor defining the catalytic qualities of solid bodies, first of all, the excess saturation of the body's surface due to an excess of free energy. Such are the conclusions of D.Mendeleyev, G.Konovalov and P.Roginsky, and others.

4. Out of more concrete physical reasons defining the qualities of solid catalysts, porosity and crystallographic state were identified. Nearly all researches came to this conclusion.

5. The catalytic surface of solid bodies represents, as a rule, a largely heterogeneous surface, i.e. the sum of sections differing in their adsorption and catalytic qualities.

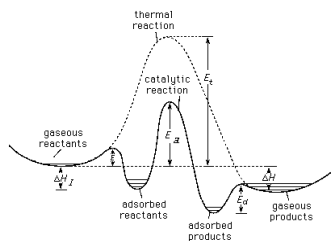
The best results are produced by catalytic surfaces of the "spongy" type. It is interesting to note that it was observed by M.Faraday, who devoted much of his time to catalytic processes.

Moreover, D.Mendeleyev defines the essence of catalysis through such a form of chemical interaction between catalysts and reagents as provides for continuous chemical interaction and excludes stoichiometric relationships.

Despite the electronic-microscopic research, it is still unclear what are the active centers of heterogeneous catalysis on a "spongy" surface.

The questions of whether they are peaks or wells have long been debated. Are they angles, ribs, or planes? No experimental answers have been found so far.

The accelerating action of a catalyst can be formally explained by the S.Arrhenius equation, if we assume that the molecule activation energy  $E_a$  in catalytic reactions is normally less than in non-catalytic ones. It has proven to be true. For example, in case of non-catalytic decomposition of ammonia  $NH_3$ , the value  $E_a$  is of the order of 80 kcal/mole, and in case of catalytic decomposition  $E_a \sim 40$  kcal/mole, i.e. twice less! Due to reduction of  $E_a$ , acceleration of catalytic reactions is achieved as compared with non-catalytic reactions.



**Figure 11: Energy profiles for catalytic and thermal (noncatalytic) reactions in the gaseous phase.  $E_a$  is activation energy for catalytic reaction;  $E_t$  is activation energy for thermal reaction;  $E$  is activation energy of absorption of gaseous reactants;  $E_d$  is activation energy of desorption of gaseous products;  $\Delta H_1$  is heat of chemisorption of reactants;  $\Delta H$  is heat of overall reaction. (Encyclopedia Britannica).**

At first this conclusion was made by S. Arrhenius himself, but he did not suggest any concrete ideas concerning the mechanism of reducing  $E_a$ . D. Mendeleev went farther and compared the effect of a catalyst with heat energy! Understanding that heat energy could appear from nowhere, he, nevertheless, reduced the value of  $E_a$  with the help of molecule deformation. Today it is absolutely clear that such deformation still needs energy, and it would be naïve to think that D. Mendeleev did not understand it. Of course, it could only be a local energy directed specifically to reducing the value of a certain connection, and not heat energy distributed uniformly over the interaction volume, but even such energy in today's science has nowhere to appear from. This is illustrated by Fig. 11. From this figure it is clear that the reacting particles and particles appearing after the reaction are sort of divided by a potential barrier with the height  $E_t$ . An analogy with the tunnel effect suggests itself, but it is very superficial, because the usual quantum tunnel effects do not exist here, and these phenomena are similar only in results.

A natural question arises. If the reaction goes on from left to right, can there be a catalyst that would conduct the reaction from right to left without consumption of energy  $\Delta H$ ? Both states are divided by a high barrier, and there are lots of reactions, which do not go from left to right without a catalyst at all. The unitary quantum theory gives hope for realization of such phenomena, although within the existing science it is impossible without consumption of energy  $\Delta H$ . Next we will give a short statement of the main ideas of Mendeleev [23] concerning chemical catalysis.

Chemical interaction of two reagents always takes place when they touch each other, i.e. in contact. The reason of chemical modification  $E_a$  of two different substances lies in the emergence of conditions "changing the movement peculiar to masses of solitary homogeneous bodies». In a heterogeneous system, "at the meeting place of two bodies, in the touching point... real perturbations and deviations of movement will take place, of a different type as compared with a free surface. The difference of movement on the surface is defined by the influence of particles and atoms of one type with the surface ones, and in case of a meeting between two bodies, changes on their surfaces will be defined by the influence of their own and alien atoms and particles».

In a homogeneous system, when "a chemical phenomenon takes place in a homogeneous gas mixture, or in a solution of

two bodies, it cannot be regarded as alien to the change taking place on the contact surface, because a particle surrounded by other particles, different from it, must more or less change its state as compared to the one it has when surrounded by similar particles".

Thus, according to D. Mendeleev, [23], a contact of two different substances  $A$  and  $B$  facilitates modification of their valent state and may lead to redistribution of their "component elements", i.e. the composition and structure, or otherwise, may cause chemical interaction between them. In this sense, a contact is similar to the effect of temperature; "internal movement changes brought about by a contact with an alien body can quantitatively and qualitatively correspond to such internal movement changes as may happen due to the said physical conditions, e.g. from temperature changes. This brings catalytic or contact phenomena closer to dissociation ones, although does not allow for intermixing thereof".

It is clear from the above-cited statements that D. Mendeleev was very brief on the concrete matters of the catalysis mechanism. In his ideas of "perturbations" and "deviations in movement" happening in contact some chemists (A. Balandin, multiple theory [24]) saw signs of an explanation of the catalysis mechanism through molecule deformation, others – through the chemical orientation of reactions. Since every complex molecule has a certain chemical state, any "perturbation" or "deviation in movement" (oscillations) of its atoms can be regarded as a modification of its form and as a more significant modification of its structure, up to a free radical formation. Of course, there is much room for interpretation. D. Mendeleev only put the question of the catalysis mechanism and slightly raised the curtain, but he did not solve the problem, and was not even going to do it. He finished his main article on catalysis [23] with only a hint of "finding a method for research, which must... lead to clarification not only of the position of contact reactions in connection with other types of chemical transformations, but of the very mechanism of chemical modifications".

We have already noted that for molecule deformation in the existing science there is a need for energy, and the main stumbling block lies in the unclear character of the mechanism of reducing the value  $E_a$ , because without the Unitary Quantum Theory it is incomprehensible where such energy can come at all. It is this very circumstance that is the main reason of catalysis being so far an art, and not a science!

#### **General approach to catalysis phenomena connected with energy generation**

As a rule atoms but not molecules participate in primitive reactions. In the case of gas mixtures, for example, the latter should be in atomic state. If examined for example the reaction between nitrogen and either the oxygen or the hydrogen, these gases do not react in general conditions, and moreover the nitrogen, due to its chemically passive behavior, resembles rare gases, because it either does not react at all, or reacts at extremely high temperatures. The Nitrogen reacts with the Oxygen and forms the Nitric oxide only at the temperature of  $4000^{\circ}C$  and with the Hydrogen it forms Ammonia not only at high temperature and pressures but in the obligatory presence of a catalyst. That happens due to the extremely high energy of the Nitrogen dissociation, about  $\sim 170.22$  kcal/mole that is essentially more than energy of the thermal motion at usual

temperatures. At  $3000^0 K$  and normal pressure Nitrogen is dissociated at 0.001 portion, in the same conditions Hydrogen and even Oxygen are dissociated more than at one tenth. However so huge temperatures are not used in the large-scale production of Ammonia and Nitric Acid, but a special catalyst is required (as a rule it is a heterogeneous one).

It is known that both plants and animals assimilate Nitrogen, of course first having transferred it into the atomic state. The mechanism of atomic Nitrogen assimilation by animals is connected with the activity of the nitrogenase ferment. The attempts to reproduce that reaction in artificial conditions without ferment or catalyst failed.

During the last years it was shown for the first time that the molecular Nitrogen is able to form complexes with some transition metals, and then conditions were found for the reduction of Nitrogen molecule combined within the complex to hydrazine. Such binuclear complexes correspond to the idea of model catalytic system with two active centers that work simultaneously.

The conventional today point of view is that this process consists of the following ones: for the Nitrogen molecules activation it is necessary to spend some energy for the first  $\pi$ -bond, at the further stage of Nitrogen regeneration it requires essentially less energy. It was possible to overcome the high activation barrier at the first stage due to the electron redistribution within the complex. At this stage, electrons populate the antibonding  $\pi$ -orbitals of Nitrogen molecules and reduction of electron density at bracing  $\sigma$  and  $\pi$ -orbitals takes place. Electron re-distribution on the Nitrogen molecule's orbitals happens due to the participation in that act of some  $d$ -electrons of transition metals that promote the  $N-N$  connection slackening.

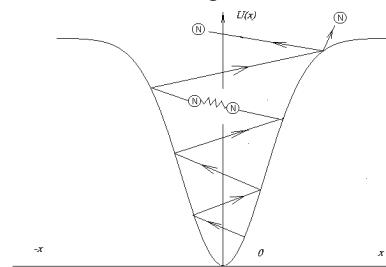
To realize the described electron transmission within the complex transition metal – Nitrogen molecule a correspondence definite geometrical and energetic factors is required.

In fact, the scheme presented is a quantum-chemical picture of cooperative action model, typical for ferments. We should note that influence of ligands' and protonic solvents on the Nitrogen molecule activation and further reduction has not been shown in that scheme. Meanwhile such an influence on the catalysis exists, that has been confirmed by experiments, and that fact brings the model even closer to enzymatic reactions. Quantum-chemical models of the process of activation and molecular Nitrogen reduction in living organisms with the participation of ferruginous albumen ferredoxin – electron supplier for the purpose of  $N-N$  bond loosening have been developed.

But the above mentioned explanation of the Nitrogen splitting into the atomic state (recall that it requires an enormous energy and it remains unknown where to take it from) is not free of criticism above because any bond's loosening should be paid off by a tremendous quantity of energy.

That process seems more natural in accordance with the UQT. The bottom of nearly any potential well may be fully approximated by a parabola. Then the use of results obtained in Fig.3 is possible. Let a Nitrogen molecule get into a cavern or some cavity on the catalyst surface during the adsorption. Then the natural oscillation of that molecule starts. During the oscillation, its energy starts growing and becomes more than the energy of the Nitrogen dissociation, in the result two Nitrogen atoms will fly out of the cavity and they will have enough time

to react without any energy problem (with an Oxygen atom, for example). That is sketched on Fig. 12.



**Fig.12. Oscillation of Nitrogen molecule in potential well of catalyst.**

After that the cavern is ready for next “free of charge” repetitions. Of course a satisfactory initial phase of Nitrogen molecule getting inside is required to realize exactly the “maternity home” solution, because at other phases the molecule flying in starts to deliver to the vacuum its kinetic energy thus realizing the “crematorium” solution. Probability of that or other solution strongly depends on the catalyst geometry and material by potential equation and on the value of the most probable material molecule velocity and structure. The cavern itself can be compared with the catalyst active center. If such a well were changing its form for whatever reason or an alien object were sticking in then the divergent oscillations would stop, that amounts to the active center “poisoning”.

The material of well' walls should fulfill the only task – to reflect in a proper way the object getting into it. That is the general requirement for all ferments and catalysts. And of course the type of the wall potential plays a very significant role, but the most important are its dimensions and form, that from the most general considerations should be about nanometers (an upper estimate). Exactly that explains the widest universality of some catalysts like the platinum black, clays, and aluminosilicates. As it is known these catalysts work perfectly in different reactions.

In the case of enzymes the form of cavities have dimensions and potential specific for each type of ferment (molecule architectonics, key-lock system) and sometimes the molecules of definite form only may take places and oscillate. That apparently explains the high specificity of enzymes reactivity. The case of molecule decomposition mentioned above looks quite simple in idea. But ferments and heterogeneous catalysts are able to synthesize in spite of repulsive forces that associating atoms have to overcome. We shall assume the existence of simultaneous orthogonal oscillations of atoms-respondents within one general well or in few next one to another wells. Then the energy of these oscillations at “maternity home” solution implementation will be spent for overcoming of repulsive forces hampering reaction.

*We should specially note that the energy during that process is liberated locally within the area of some concrete molecular or atomic bond and meanwhile the energy destroys that bond but does not disperse over the surrounding medium, so the process hardly can be detected by temperature increase.* In that simple variant of heterogeneous catalysis the constant of chemical equilibrium will not shift.

In the framework of the mechanism proposed the positive influence of effect of aggravation: becomes more clear: the catalyst activity is considerably increasing due to the assembling of big molecular masses, that is probably necessary because the solution “maternity hospital” is more likely for big masses.

Coenzymes may play a similar role. In addition, the influence of *pH* at enzymic processes is explained, because a Hydrogen free atom or bare proton can easily “connect” to nearly any chemical object and so it may radically change the character of oscillations within the well. Temperature also strongly influences these processes because enzyme form is strongly connected with it (as a rule an enzyme is a protein).

To shift equilibrium constant of a chemical reaction requires changes of the system entropy, that cannot be excluded for enzymatic processes, because ferments can deliver negative entropy, as we have mentioned above. Today it is considered impossible, but who is able to foresee the future?

We can not exclude that idea of energy generation within a potential well is just waiting for the creation of general theory of catalysis. Here we should recall brilliant words of a famous Russian specialist on physical chemistry Professor A.N. Kharin (Taganrog, 1955) who always said at his lectures: “*The problem of chemical catalysis is the most incomprehensible in the modern physical chemistry and it won't be solved until physicist discover some new mechanism able to explain the liberation of the energy that lowers the reaction barrier.*”

Our UQT allows, as we hope, to make the first shy steps in right direction.

### Conclusions

It is known that the human society nowadays faces the problem of a new steady energy source, as far as the reserves of *burned* (in the literal sense of a word) natural fuel – oil, gas, coal and so on rapidly run out.

Over the last decade it became evident that further intensive development of modern power engineering and transport leads the humanity into a large-scale ecological crisis. Rash decrease of fossil fuel resources against the background of the natural annual growth of power consumption forces industrially developed countries to expand their net of nuclear energy installation. That in more and more increases the risk of their exploitation. The problem of nuclear wastes utilization becomes more actual. Taking that alarming tendency into account a lot of scientists and experts definitely express their opinion in favor of speeding up the search for new alternative energy sources and new energy carriers application in power engineering and transport. In particular they fix their eyes on Hydrogen, as its sources in the World Ocean waters are inexhaustible. Additional irrefutable advantages of that fuel are the relative environmental safety of its use, eligibility for heat-engines without any noticeable changes of their construction, high-calorie capacity, possibility of permanent storing, transportability by existing transport network, nontoxic character and etc. However an essential problem, that has not been overcome till nowadays, is the diseconomy of its industrial production. More than 600 companies, concerns, university laboratories and social scientific and technical societies in Western Europe, USA, Australia, Canada and Japan toil at reduction of prices of the process of Hydrogen generation (see magazine “Motor transport”, № 4, 1992, page 38). Successful solution of that important problem will revolutionary change World economy and will be able to sanitize the environment by reducing carbon-dioxide wastes.

There is a whole range of well-known water decomposition techniques: chemical, thermo-chemical, electrolysis and others, but all of them have the same imperfection, the using of expensive high-grade energy in engineering process of hydrogen generation. More over this high-grade energy liberation requires the scarce fossil fuel (coal, natural gas, oil products) or power

energy produced at electric power stations. It suffices to say that the conventional industrial electrolysis requires for one cubic meter of Hydrogen generation of 18-21,6 mega-watt-seconds, and taking into consideration the generation of electric power itself general power consumption exceeds 50 mega-watt-seconds, that makes the Hydrogen extremely expensive (about US \$2 per cubic meter).

At the same time our Earth is literally bathing in the heat energy flow, received from the Sun. And the task comes “to insert” that inexhaustible source of free-of-charge low-potential heat into the industrial procedure of Hydrogen generation. Hydrogen exceeds natural gas by its calorific value in 2,6 times, oil in 3,3 times. It addition, the cleanness of the process of Hydrogen burning, transportability, possibility of direct transformation of the chemical energy into the electric one should be added. Moreover, the sources of Hydrogen are practically inexhaustible. But we will have to develop inexpensive, technologically applicable, large-scale method of Hydrogen generation requiring low energy consumption. Due to that reason the electrolysis can not be used for this purpose.

From that point of view the water bio-photolysis with the use of non-organic catalysts or enzymes and solar energy attracts out attention. Of the most interest was the hydrogenase application. The process of water bio-photolysis consists of two stages. At the first stage the flow of solar energy acts upon the mediator-carrier. As carriers compounds with strong electron-seeking characteristics, for example, viologenic dye (*Y, Y*-dipyridine derivative) or nicotineamideadeninedinucleotide (NAD<sup>+</sup>) are used. Mediator with a high oxidative-reduction potential being excited by radiation takes electrons away from the water molecule and passes into the reset state. Molecular Oxygen is liberated, it does not oxidize the mediator in the reset stage.

At the second stage there is the electron transfer with the help of bacterial ferment of hydrogenase from the mediator in the reset form to protons with combining of molecular Hydrogen. Till now the efficiency of the process of water bio-photolysis under this scheme is too low, and the system itself is not stable enough, but researches in that field are successfully continuing. That classical direction appeared not far ago and promised to be interesting being quite close to equilibrium with environment.

However some times ago there was a report on practically spontaneous water decomposition by Oxygen and Hydrogen under the influence of catalyst. That partially confirms the accuracy of ideas described above. For example there was a private communication about a Japanese Kamuro Dozi, who used for this purpose catalyst of cupric oxide. The other two groups (one in Philippines, and the other in USA) are already testing a vehicle powered by mixture of Oxygen and Hydrogen to be generated by catalytic decomposition (with low energy consumption) of common water. The authors have even attached a plate with the inscription: “They said it couldn't be done!” to the reactor where water decomposition take place. The vehicle itself is provided with a label: “Powered by ordinary water”. The Mixture of the oxygen and hydrogen in usual condition is very stabile object. The Products of the decomposition of water and water itself are divided by high potential barrier, catalysis helps to realize tunnel transition. There is a widely known opinion of most chemists: “*If any reaction does not proceed that means that an appropriate catalyst has not been developed yet*”.

Of course if it were created a source of electric power similar to working in Switzerland device of Paul Baumann of "perpetuum mobile" type, there would not be necessity in using of water electrolysis or even it catalytic decomposition for the purposes of motor transport because that would decide all existing principal energy questions. But never the less solar energy should be used as utter as possible because that approach will not move general heat equilibrium of the Earth.

There is no necessity to add anything about further perspectives for professional researcher and advanced thinking reader.

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