

GENERAL MECHANICS

G. B r a n k o v

Mechanics of Biomolecules and Bioelectronics

1. Mechanics of biomolecules

Last decades mark a notable progress, due to the fruitful integration of sciences like Physics, Chemistry and Biology. The methods of these sciences, applied in practice and helped by mighty microscopes, successfully reveal biological structures and processes on molecular and atomic level. With the application for decades now, of quantum mechanics in Physics and Chemistry a new stage has been reached. So in this aspect a considerable success has been achieved recently in biochemistry and biophysics as well. These methods should also be applied in Biomechanics and this is another problem to be discussed. The potentialities of the phenomenological approach are limited. It is known that phenomena and processes on a macro level are predetermined by the micro level. Atomic and molecular dynamics cause the processes in the living creatures. Investigating the movement within and among molecules is a mighty device when studying the essence of living cells and organs nature and function, as well as the nature of the genetic system.

Dulittle [5] thinks that DNA creates the project, but proteins, being both the bricks and the lime solution are those that carry it out.

The exploration of molecules, from a mechanical point of view, aims at studying their dynamic behaviour, i.e. determining of translations, velocities, acceleration, as well as establishing the role of electromagnetic interaction. The application of classical and quantum mechanical methods makes it possible for the scientists to plan correctly the experimental investigations, to interpret the observation results, to discover new relations, to predict new results, as well as to elaborate principally new technologies. Theoretical investigations have a practical importance in the development of protein and genetic engineering and in designing of new medical goods. New programmes have been worked out to read the heredity text stored in the human genotype, so as to correct any mistakes in it and to block out the faulty genes.

Three aspects of biomolecular dynamics are considered: vibration, rotation and movement [2].

Studying the biomolecular vibrations, scientists determine free and compulsory oscillation of molecules, their amplitudes and frequency. At the exploration of vibrations of complex globular protein molecules, it has been found out that the biggest are the vibrations near the surface, reaching 0.1 nm /1Å/, while in the interior they come to about 0.05 nm. The fluctuations of the side groups are greater than those in the framework. An anisotropy has been established, when studying the translation of atoms. This means that translations in definite directions prove greater than any others. In this way the surface of the a three axis ellipsoid has been established. The profound study of the dynamics of a single molecule of a complex configuration with many degrees of freedom is a difficult problem. For this reason the principle of substituting the complex molecule by a small one has been applied and thus the dynamic behaviour of the whole molecule has been approximately illustrated. We admit that the interaction of each atom within the molecule is reduced only to an interaction with it's neighbouring atoms. This means that at cyclic boundary conditions the three atom molecule could be interpreted as a small molecule. In case of nonlinear chains the dynamics of the molecule could be described by different laws and principles like Newton's law, the principle of d'Alembert, Hamiltons' variation principles, the equations of Lagrange. Investigations have been carried out for vibrations with small and big amplitudes. New, further more modern apparatus are needed for the successful development of the biomolecular vibration theory. They show the molecular dynamics process on the display and thus new theoretical generalizations could be made.

It is not only vibration of the separate segments but rotation round the covalent bonds that is carried out in the polipeptide chains. And together with the rotation of the atomic group, a motion of amino acid side group residues is performed too. During this rotation proteins can transport small molecules, electrons and protons over to the sectors, where needed. At this motion the atomic groups meet the resistance of the neighbouring molecules and it occasionally becomes the reason for the rotation seasure. It has been reported recently that eyesight molecules respond to light and a rotation of the "retinal" molecule is carried out in them due to the photon absorption.

Molecular movement is essential for all life processes. It is the core of hemodynamics, respiration and all fluctuation processes that take place within the organism. Molecular movement proves to be very important when studying the medical effect of the medicine molecules. Many scientists try to find out the mechanism of the medical effect of medicines, the way their molecules interact with the other molecules during that movement, the efficiency effect realization and so on. The aim is to establish a correlation between their electronic and confirmation structure, to find out the level and the distribution of their activity, to study the nature of the cellular "receptors" and to understand the "medicine-receptor" interaction. Thus, by means of the quantum pharmacology the profound research can be expanded in order to discover more specific and effective medicines, so that new ones can be designed.

The equations of Newton, Lagrange and others could be used when studying

the movement of the molecule at the corresponding initial conditions and in accordance with the medicine application, orally or by an injection.

The successful elaboration of the problem of vibration, rotation and movement requires corresponding experimental investigations as regards to the mechanics of the system of "biomolecules-biofilms".

The folding and unfolding of the globular molecules presents a characteristic motion, which probably is of great functional importance. One could get an idea of this motion mechanism out of the specific movement of the sulphur molecule, studied by Paul Flory and collaborators [7]. When sulphur is heated, its atoms arrange in long linear chain sets of macro molecules. After cooling the long chains rearrange in cyclic molecules of different sizes. Most characteristic is the eight-angle cyclic molecule. These cyclic S_8 molecules

form a crystalline solid. A principle question has to be put up not only in this case but as regards to the organic globular molecules as well, because these molecules are the factors, causing this strict, geometric structure. What kind of movement the atoms accomplish from the linear chain toward the eight-angle molecule. Most probably the distribution of the valent electrons which cause the strictly determined valent angles alters automatically in case of a thermodynamic change. An attempt has been made to develop a mechano-mathematical model.

All atoms and molecules emit and absorb light. Each atom acts as a transmitter and an absorber of specific electromagnetic radiation in a gaseous medium. The atom can effectively emit and absorb radiation only at definite frequencies. The frequency range comprises the spectrum characteristic of each atom. Leitsiancky and Lurie consider the problem of determining the trajectory of an electrically charged particle with mass m and electrical charge e in a magnetic field of tension H . They use the basic movement equation

$$m \frac{dv}{dt} = e \left[\mathbf{v} \times \mathbf{H} \right] .$$

The equation gives the tangent and the normal of the trajectory:

$$m \frac{dv}{dt} = e \left[\mathbf{v} \times \mathbf{H} \right] \tau ,$$

$$m \frac{v^2}{\rho} = e \left[\mathbf{v} \times \mathbf{H} \right] \mathbf{n} .$$

Out of the second equation we achieve:

$$\frac{mv_0^2}{\rho} = ev_0 H \sin \varphi ,$$

where φ is the angle between the velocity vector v and the tension vector H , this angle being a constant.

The latter equation gives the curvature expression

$$\rho = \frac{mv_0}{eH \sin \varphi_0},$$

which is a constant. Out of this one can draw the conclusion that the trajectory is a screw line.

The second group of molecules, basic for the living processes in the organism, are the molecules of the DNA and RNA nucleic acids which carry the genetic information.

The primary and most essential question regarding the DNA structure, its double spiral form discovered by Watson and Crick in 1953 is being precised and improved still now. This structure includes four types of different "basic couples" as synonyms of "genetic letters", which connect both spirals. These four letters comprise the alphabet of genetic heredity.

According to W. Arber [1], a Nobel prize winner, the genes are arranged in great DNA fibre molecules. He reports that the *Escherichia coli* genes are set in one single molecule of DNA, which consists of about four millions of basic couples. The information carried by this genotype bluntly repeats Bible's information. Human genotype stores information, corresponding to that preserved in a library, containing about 1000 volumes of the Bible. The DNA spirals consist of neucleotides, which are monomerial units. In fact they are phosphate groups and desocsyribo saccharose residues (pentagonals). Each residue of the saccharose is connected to one of the four types of bases: guanine (G), cytosine (C), timine (T) and adenine (A). Both DNA chains are bound together by means of two couples of basic bonds. (A-T and C-G). Hydrogen bonds are formed between the bases [4].

In the recent years biologists and biochemists have began manipulating DNA by cutting, modifying and reconstructing them again in a unit. This potentiality could be used to change utterly the outlook of biology, which has of course its positive and negative sides.

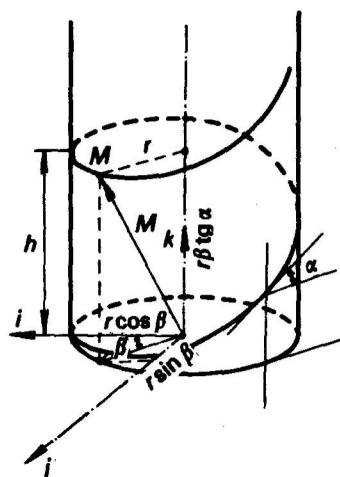


Fig 1

The spiral is 22 Å in diameter and the space between the residues along the spiral is 2.55 Å or 3.46 Å. The angle of the spiral varies from 70° to 90°. It is accepted that molecular dynamics is characteristic of the sub nanosecond area. The most important movements are supposed to be the lowest vibration frequencies (4 GHz).

In some cases they could reach hundreds of GHz.

The position of a random point M from the spiral [Fig.1] could be defined by the radius vector expression.

$$M(\beta) = re(\beta) + \lambda\beta k,$$

where $e(\beta) = \cos \beta i + \sin \beta j$

By each coil, the spiral lifts with $2\pi\lambda$.

The tangent vector is:

$$M\beta = \frac{dM}{d\beta} = re\left(\beta + \frac{\pi}{2}\right) + \lambda k$$

or

$$t = \frac{dM}{ds} = \frac{r}{\sqrt{r^2 + \lambda^2}} e\left(\beta + \frac{\pi}{2}\right) + \frac{\lambda}{\sqrt{r^2 + \lambda^2}} k$$

Then

$$\cos(t, k) = \frac{\lambda}{\sqrt{r^2 + \lambda^2}},$$

which means that the angle between the tangent and the axis z is a constant.

Curvature and torsion expressions can be determined by the formulae:

$$k = \frac{r}{r^2 + \lambda^2}, \quad \kappa = \frac{\lambda}{r^2 + \lambda^2},$$

i. e. k and κ are constants.

The angular instant velocity is defined by the expression

$$\omega = \frac{1}{\sqrt{r^2 + \lambda^2}} k,$$

and is a constant too.

The screw spiral is a system of atoms with many degrees of freedom.

In the general case each atom has two degrees of freedom vibration u_t in the direction of the tangent and vibration u_r in the direction of the radius

(the normal). Vibrations are considered to be free and small i.e. they deviate a little from the equilibrium state.

The movement equation of a random atom i from the mono spiral is:

$$m_i \sqrt{r^2 + \lambda^2} \ddot{\beta}_i = \sum_1^n F_i = \sum_1^n k_{ij} \beta_j ,$$

where β_i are generalized angle coordinates; $\sqrt{r^2 + \lambda^2}$, $\ddot{\beta}_i$ — the acceleration in the direction of the tangents; F_i — restoring forces; k_{ij} — elasticity coefficients.

A condition has been put for an interaction accomplished mainly among the neighbouring atoms. So a group of three atoms will be considered here, their masses being m_1 , m_2 and m_3 , equally spaced at an a distance.

The kinetic and potential energy expressions are:

$$T = \frac{1}{2} m_1 r_c^2 (\dot{\beta}_1^2 + \dot{\beta}_3^2) + \frac{1}{2} m_2 r_c^2 \dot{\beta}_2^2 ,$$

$$V = \frac{1}{2} k (\beta_2 - \beta_1)^2 + \frac{1}{2} k (\beta_3 - \beta_2)^2 ,$$

where

$$r_c = \sqrt{r^2 + \lambda^2} = r \sqrt{1 + \frac{\lambda^2}{r^2}} .$$

The movement equations are:

$$m_1 r_c^2 \ddot{\beta}_1 = k (\beta_2 - \beta_1) ,$$

$$m_2 r_c^2 \ddot{\beta}_2 = k (\beta_1 - 2\beta_2 + \beta_3) ,$$

$$m_3 r_c^2 \ddot{\beta}_3 = -k (\beta_3 - \beta_2) .$$

The spiral vibration at the action of outer forces is:

$$m_i r_i \ddot{\beta}_i + \sum_1^n k_{ij} \beta_j = F_i \sin(\omega, t) .$$

Lagrangean equation at forced vibrations is:

$$\frac{d}{dt} \left[\frac{\partial T}{\partial \dot{\beta}_i} \right] - \frac{\partial T}{\partial \beta_i} + \frac{\partial V}{\partial \beta_i} = Q(t) , \quad (i = 1, \dots, n)$$

A double spiral fragment is being discussed /Fig.2/. In case of equal

vibrations in both spirals, the cross bonds /bases/ exhibit no deformations or strains. But when there is a difference in the amplitudes or in the vibration phases, and in case of certain structural changes in one of the spirals, local deformations and vibrations in the cross bonds appear.

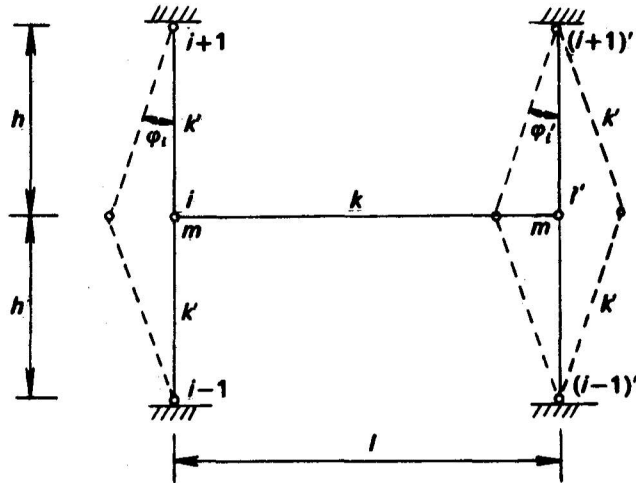


Fig. 2

We admit that atoms $(i + 1)$, $(i - 1)$, $(i + 1)'$, $(i - 1)'$ are immovable. Vertical and horizontal vibrations may be accomplished only by atoms i and i' . Normal /normal modes/ vibrations of the system $i - i'$ are being considered. A normal mode is achieved at a synchronized vibration or at the first main vibration.

The second normal mode could appear when atoms i and i' vibrate at equal angles but in opposite phases, i.e. $\varphi_i = -\varphi_{i'}$ - second basic vibration. At this vibration the spring stretches out and then shortens again. It tries to restore it's initial position. Every movement of the system $(i - i')$ could be presented as a combination of these normal modes. The first atom receiving a translation u_i different from $u_{i'}$, the free vibrations of the system can be described by the following equation:

$$m \ddot{u}_i = k \left[u_i - u_{i'} \right] - 2k' u_i.$$

The extension of the springs $\overline{i-i+1}$ and $\overline{i-i-1}$ and their symmetrical ones could be defined respectively by the expressions $u_i \varphi_i = h \varphi_i^2$ and $h \varphi_{i'}^2$.

The kinetic energy of the system being,

$$mh^2 \left[\dot{\varphi}_i^2 + \dot{\varphi}_i'^2 \right] .$$

The potential energy expression is :

$$\begin{aligned} V &= \frac{1}{2} kh^2 \left[\varphi_i' - \varphi_i \right]^2 + 2k'h^2 \left[\varphi_i' - \varphi_i \right]^2 \\ &= \frac{1}{2} h^2 \left[\varphi_i' - \varphi_i \right] \left[k + 4k' \right] . \end{aligned}$$

By means of these expressions there could be written the corresponding equations. The fragment discussed is in an extended form along a plane.

A triple spiral fragment is considered.

Azimuthal spiral molecular vibrations could be established out of the experimental investigations. A group of atoms, presenting a symmetrical particle with an inertial moment J and an attached side group is being considered. The former group can be studied schematically as an attached pendulum. These pendulums prove to be different because of the different side groups. But the acceptance of this peculiarity leads to a very complex problem. Because it is small vibrations that are explored, there could be accepted a constant inertial moment. The azimuthal vibrations of the first three particles, equally spaced at an a interval /Fig. 3./ are taken into account. We admit that the fourth particle is attached immovably. It is accepted that the three particles have equal interval moments and that the spiral spring has a k stiffness. The azimuthal turns are denoted by φ_1 , φ_2 and φ_3 . An admittance has been made that the molecule moves freely in the biological fluid and that the movement of the particles is harmonious due to the recreative torsion forces.

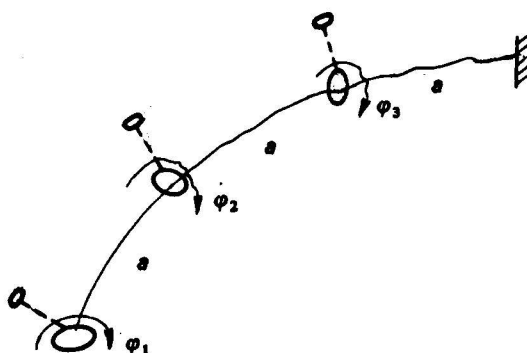


Fig.3

Kinetic and potential energy equations could be written as follows:

$$T = \frac{1}{2} \sum_i J \dot{\varphi}_i^2 = \frac{1}{2} J \left[\dot{\varphi}_1^2 + \dot{\varphi}_2^2 + \dot{\varphi}_3^2 \right];$$

$$V = \frac{1}{2} \frac{k}{a} \left[\varphi_3^2 + \left(\varphi_2 - \varphi_3 \right)^2 + \left(\varphi_1 - \varphi_2 \right)^2 \right].$$

By means of the Laplace equations we have:

$$-J\ddot{\varphi}_1 = \frac{k}{a} \left[-\varphi_2 + \varphi_1 \right];$$

$$-J\ddot{\varphi}_2 = \frac{k}{a} \left[-\varphi_3 + 2\varphi_2 - \varphi_1 \right];$$

$$-J\ddot{\varphi}_3 = \frac{k}{a} \left[-2\varphi_3 - \varphi_2 \right];$$

The frequency equation, as well as the cubic equation for root determination, the three algebraic equations and so on can be composed in the familiar way.

The fragment considered is assumed stretched out on a plane, while actually it lies on a cylindrical surface.

2 Bioelectronics

Bioelectronics or molecular electronics is an integrity of microelectronics and biological systems, possessing a natural ability to transport electrons on a molecular level. This is a new field of activity, still in its earliest phase of development. Great future innovations are lying ahead for this new branch of science, and they will surely mark a new stage in technical and science evolution.

The basic task of bioelectronics is to synthesize molecules, working as single electric chain elements, such as conductor, resistance capacity and so on, and then to combine these elements in amplifiers, memory devices and so on. These devices are being used in the modern electric apparatus and could be made smaller in size but greater in capacity and quicker in reaction. The aim is to use proteins for electron transport. Such proteins, for example are cytochrome and ferredoxine proteins. Our task is to understand how these proteins carry out that transport of electrons and to develop electron conductors on a molecular level.

The main impulse for the development of bioelectronics comes from the requirements of military and cosmic agencies to produce complex electron systems of minimal dimensions, weight and energy. Incredible results have been achieved in the early sixties in this aspect due to the silicone chips. But the further

improvement meets certain difficulties of a technical character. This was the reason for the micro electronic industry to search for new methods. So different possibilities for solving of this problem have been excavated. In this aspect great attention is paid to Bioelectronics nowadays. The final task of each bioelectronic investigation is to repeat the electron transfer in nature on an electron level.

The application of biomolecules in Electronics has been subjected to scientific investigations for more than about 25 years. One of the first products in this field is the biosensor, which has great abilities for control and measurement not only of biological but of other processes as well. According to Richard Taylor, a specialist in applied technology, the biosensors are some of the most exiting technologies for measurement, which are to be presented in the near future. The biosensor is a combination of biomolecules and metal. It will help creating entirely new technologies in many unthought of fields of science. Biosensors contain an organic molecule, which responds selectively and quickly to the smallest and insignificant changes in the surrounding environment. The first biosensors usually contain an enzyme that acts indirectly, exciting a reaction between two chemical substances and then measuring this reaction. The second generation of biosensors, already coming forward, consists of biologically created molecules, which can directly sense and measure the presence of a specific substance.

Most progressive biosensors belonging to the third and the fourth generations are the biochips – silicone chips, combined with a living material. These devices might possess a density, millions of times greater than that of the standard silicone chips [8]. Their work resembles the human brain activity and is known as analogous signalization.

Possibilities have been studied to produce biochips as the first step for the creation of a biocomputer.

Various really existing arranged biological systems like furrowed muscle fibers have been investigated. Biological systems of this kind have a three-dimensional lattice structure, and present a possibility to create a biochip.

One of the outstanding micro electronic achievements is the development of sensor devices. They consist of a biologically sensitive element, closely connected or integrated with a transducer. So as to use the specific character and the sensitivity of biological systems in a combination with the computing ability of microprocessors, two opposite uncharacteristic science branches in the biosensor. Modern biosensor's conception belongs mainly to the ideas of L e l l a n d C l a r k [8] and collaborators /1962/. They admit that enzymes can combine with electrochemical detectors so as to form "enzyme electrodes" that could make a basic sensor. Organic molecules, nucleic acids, enzymes, membranes, cells, tissues and others can act as biological elements. Potentiometers, ammeters and calorimeters could play the role of transducers. Biosensors' fundamental abilities should be studied generally in both destinations of their components in order to optimize not only each one of their characteristics separately but their complex behaviour, as regards to response, selectivity and stableness.

Some investigators aim at studying the problem of how genes of different origin could be transferred and transplanted in different organisms and in what way this technology could be used in the development of sensors. P. Warner [8] states the opinion that genetic manipulation will play a certain role in biosensorelaboration, the way it is with many other fields in biotechnologies.

Protein engineering has appeared as a result of the exploration of different possibilities for the development of biosensors. In protein engineering the covalent protein structures are being modified by adding, substituting or abolishing of groups in such a way that the chemical characteristics of the molecules prove different from the ones displayed at the initial state. The lack of knowledge about the succession of amino acids, and about the crystalline structure are the reason for the empirical approach to be applied. Here again it is not sufficient to discuss the specific protein structure in a static condition. It is necessary to know protein dynamics.

Biosensors have various fields of application. They are used for a continuous and automatic control of metabolites, medical drugs and glucose in blood.

An apparatus has been elaborated for detecting of low concentrations of biological particles as viruses, bacteria and other cells in a solution. It is required that the observations are carried out "in vivo" so as to control the disease in a completely automatic way.

Biosensors can keep under control the surrounding environment and detect toxic substances in the air and in the water as well.

3. Conclusions

Biophysics and Biochemistry are sciences closely related to Biomechanics. They have gained great advance during the recent decades, due to the application of the quantum mechanics' methods. Biomechanics has great achievements because of the complex combining of the corresponding biological sciences with the classical mechanical methods. Investigations on a phenomenological level of approach have proved out to possess limited prospects. It is known that phenomena and processes on a macro level are predetermined by the micro level. This is what imposes dynamics of atoms to be studied, because there lie the causes for the processes observed in all living organisms. Dynamics of big molecules, (protein and nucleic acid molecules) play a fundamental role in the living processes.

The theory of biomolecules has been successfully applied in "Bioelectronics", which means "molecular electronics". Many research workers have decided to use biomolecules and especially electron transport in most modern fields of science.

They aim at studying and applying the living nature methods in building of apparatus, in various industrial processes, in medicine, as well as in the surrounding environment control, military installations, Space. Biosensors, biochips, are successfully developed and they have caused a real technical and science revolution. With the elaboration of the biocomputer new perspectives

have been found out in protein and gene engineering, as well as in computer apparatus installations.

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