CONDENSED MATTER PHYSICS AND BIOPHYSICS -

APPLICATION OF EXCITON AND FERROELECTRICITY THEORIES ON BIOPHENOMENA

E.A.Hadžiselimović, Institute of Physics, University of Sarajevo
M.M.Marinković, Boris Kidrič Institute of Nuclear Sciences, Belgrade
B.S.Tošić, Institute of Physics, Faculty of Sciences, Novi Sad.

Introduction

Great effort are made last few decades in order to explain biological phenomena on the ground of physical laws and to introduce physical methods in biological researches as much as possible. Having in view the structural and dynamical characteristics of the biomatter it is obvious that condensed matter physics, compared with other parts of physics has a higher chance to render those efforts successful. The object of this paper is to estimate the possibilities and the field of application of the condensed matter physics in the frame of biological researches.

The first serious efforts to transcend the frame of a pure description in the analyses of processes taking place in the living matter led to the question whether the laws of physics are sufficient to explain the processes in the biomatter. So two extreme views were formulated: the vitalistic, that believed that the bases of life are not resting upon the physical laws and the opposite view according to which all biological phenomena are bound to obey the physical laws and that the life itself can be explained by those laws. The vitalistic view was at one time supported even by great embriologists, zoologists and others, such as G.Drish, L.S.Berg, A.G.Gurvich[1,2].

Bohr, Wigner, Elsaser and others attempted to make a compromise between those views[3-6]. Bohr was of the oppinion that physical laws may be used for the understanding of life processes but only if complemented by some nonphysical postulates (a generalization of the complementarity principle). Wigner made the next step and tried to describe the living, the feeding and the reproduction by a system of equations, the unknown quantities of which representing the degrees of freedom characteristic for the processes mentioned. Using the S-matrix formalism he demonstrated that his analysis leads to an inconsistent system of equations having a number of equations that exceeds the number of unknown quantities. He concluded that the analysis of biological processes can't be performed by

physical methods as the possibility of the existence of a set of variables satisfying simultaneously all those equations would be highly improbable. Eigen[7] pointed out that the mentioned Wigner's analysis is incomplete as it does not take into account the possibility of an influx of informations in the system under consideration. An additional information causes the selforganization of the system and is able to direct the processes such as the living, the feeding and the reproduction. So the number of independent equations is reduced and becomes equal to the number of unknown variables. That was for the first time that it become clear that the processes in the living matter are not to be treated as spontaneous but as directed. It was simultaneously pointed out that this directionality is not to be explained by nonphysical laws as it is explicitely due to processes taking place in a number of open and nonlinear thermodynamical systems. So the methods of nonlinear thermodynamics are able to explain the selforganization and the directionality of biological processes without to call for nonphysical arguments.

So Eigen offered a justification for the adherents, such as Schrödinger, Volkenstein, Apter, Raven and others[8-11] of the conception that the basis of life and of its origin are founded on physical laws. He also pointed out the way, one has to follow in applying physical laws in the analysis of the life phenomena. It consists in the efforts to find the basis of the life in those physical processes where the selfinstruction, due to the decrease of entropy is particularly present and perceptible.

Nonconservation and selforganization

The impression is that it is more difficult to explain the origin of life on the basis of physical laws than to explain the existing phenomena in an already constituted organism using those laws. The problem of the origin life was attacked by Oparin, Kalvin, Volkenstein, Monod and many others. It would be difficult to review all the ideas that appeared in connection with that problem. Here we confine ourselves to ideas of Prigogine and of his collaborators[12-13] as well as to those of Eigen.

Elaborating on the nonequilibrium thermodynamics Prigogine concluded that in open, nonlinear, thermodyna-

mical systems, conditions leading to a decrease of entropy i.e. an influx of information may take place. This he considers as a fundamental fact for the appearance of the autocatalysis and selforganization of the system leading finally to the transition from the inanimate to the living matter. According to Prigogine, the substantial element for the appearance of the autocatalysis is the entropy having a periodical time dependence characterized by a damping factor.

Starting from the fact that the autocatalysis may take place in chemical reactions and that those reactions are characterized by the fact that the number of molecules of the initial substances is not conserved we shall try, using an appropriate microscopic theoretical model, to estimate the character of the entropy due to the nonconservation effects. As a model we propose an exciton system. This model will be used in the following for the analysis of the particle system (the mixture of chemically reacting substances).

The Hamiltonian of the exciton system is[14]

$$H=\sum_{\vec{k}}\left\{Z(\vec{k})B^{+}_{\vec{k}}B_{\vec{k}}+\frac{1}{2}\gamma(\vec{k})\left[B^{+}_{\vec{k}}B^{+}_{-\vec{k}}+B_{-\vec{k}}B_{\vec{k}}\right]\right\}, \qquad (1)$$

$$Z(\vec{k})=\Delta+\chi(\vec{k});\quad \Delta\approx 5eV;\quad \chi,\gamma\approx 0.05-0.5\,eV.$$

Owing to the term proportional to Y, the exciton number is not conserved. Starting from the equations of motion for the operators $B^{+}B$, BB and $B^{+}B^{+}$ one finds the following time dependences:

$$\begin{aligned}
B^{+}_{\vec{k}}(t)B_{\vec{k}}(t)&=\alpha_1+\alpha_2 B^{+}_{\vec{k}}(0)B_{\vec{k}}(0)+\alpha_3 B_{-\vec{k}}(0)B_{\vec{k}}(0)+\alpha_3^{*}B^{+}_{\vec{k}}(0)B^{+}_{-\vec{k}}(0),\\
B_{-\vec{k}}(t)B_{\vec{k}}(t)&=\beta_1+\beta_2 B^{+}_{\vec{k}}(0)B_{\vec{k}}(0)+\beta_3 B_{-\vec{k}}(0)B_{\vec{k}}(0)+\beta_4 B^{+}_{\vec{k}}(0)B^{+}_{-\vec{k}}(0), \qquad (2)\\
B^{+}_{\vec{k}}(t)B^{+}_{-\vec{k}}(t)&=\beta_1^{*}+\beta_2^{*}B^{+}_{\vec{k}}(0)B_{\vec{k}}(0)+\beta_3^{*}B^{+}_{\vec{k}}(0)B^{+}_{-\vec{k}}(0)+\beta_4^{*}B_{-\vec{k}}(0)B_{\vec{k}}(0),
\end{aligned}$$

where

$$\beta_1\equiv\beta_1(\vec{k},t)=-\alpha_3;\quad \beta_2\equiv\beta_2(\vec{k},t)=2\beta_1;\quad \alpha_1\equiv\alpha_1(\vec{k},t)=\frac{\Omega_y^2}{2\Omega^2}(1-\cos 2\Omega t);$$

$$\beta_3\equiv\beta_3(\vec{k},t)=-\frac{\Omega_y^2}{2\Omega^2}+\frac{\Omega^2+\Omega_z^2}{2\Omega^2}\cos 2\Omega t-i\frac{\Omega_z}{\Omega}\sin 2\Omega t;\quad \beta_4\equiv\beta_4(\vec{k},t)=-\alpha_1;$$

$$\alpha_2\equiv\alpha_2(\vec{k},t)=1+\frac{\Omega_y^2}{\Omega^2}(1-\cos 2\Omega t);\quad \Omega^2=\Omega_z^2-\Omega_y^2;\quad \Omega\equiv\Omega(\vec{k});\quad \Omega_z\equiv\hbar^{-1}Z(\vec{k});$$

$$\alpha_3\equiv\alpha_3(\vec{k},t)=\frac{\Omega_y\Omega_z}{2\Omega}(1-\cos 2\Omega t)+i\frac{\Omega_y}{2\Omega}\sin 2\Omega t;\quad \Omega_y\equiv\Omega_y(\vec{k})=\hbar^{-1}\gamma(\vec{k}).$$

It has to be pointed out that the substitution of (2) in (1) leads to a Hamiltonian that remains time independent. Nevertheless, the specific time-dependence of operators as given in (2) leads to some biophysically important phenomena such as the irreversible absorption of light energy, high dissipation and an entropy having a periodic time-dependence characterized by a damping factor (see e.g.[15-17]). Our concern here is primarily the entropy. It is possible to find a basic set leading to exciton energy eigenvalues[17] equal to those that would result after a u-v transformation of the Hamiltonian (1)[18]. The eigenvalues belonging to the particle number operator are time-dependent for this basic set. The quantum mechanical mean values for the energy and the particle number are:

$$\langle x|H_k|x\rangle = \tfrac{1}{2}(E_K - Z_k) + E_k \tilde{N}(\vec{k},0);\ \langle x|\tilde{N}(\vec{k},t)|x\rangle = \tilde{N}(\vec{k},t) = \tfrac{1}{2} f + (1+f)\tilde{N}(\vec{k},t) \quad (3)$$

$$E_K = \sqrt{Z_K^2 - \gamma_K^2};\ f = f(\vec{k},t) = [\gamma_K^2 - Z_K(Z_K - E_K)]E_K^{-2}(1-\cos 2\Omega_K t);\ \Omega_K = \hbar^{-1}E_K$$

Since it is the question about a bose gas, the entropy can be deduced in the standard way, i.e. counting the microstates and it has the form:

$$S(\vec{k},t) = \frac{\mathcal{E}(\vec{k},t)}{\theta}\left[e^{\frac{\mathcal{E}(\vec{k},t)}{\theta}} - 1\right]^{-1} - \ln\left[1 - e^{-\frac{\mathcal{E}(\vec{k},t)}{\theta}}\right];\ \mathcal{E}(\vec{k},t) = \frac{E(\vec{k})}{1+f(\vec{k},t)};\ \theta = k_B T \quad (4)$$

Taking into account the expression (3) for the function f it is obvious that the entropy has a periodic time-dependence.

The analysis derived here may be applied in a straightforward way on a chemically reacting particle system. The Hamiltonian of the particle mixture can be written as:

$$\hat{H} = \sum_{\nu,\vec{k}} \left\{ \chi_\nu(\vec{k}) a_\nu^+(\vec{k}) a_\nu(\vec{k}) + \tfrac{1}{2}\gamma_\nu(\vec{k})\left[a_\nu(-\vec{k})a_\nu(\vec{k}) + a_\nu^+(\vec{k})a_\nu^+(-\vec{k})\right]\right\} \quad (5)$$

Operators $a_\nu^+(\vec{k})$ create a molecule of the substance ν in the state $\vec{k}$. The Hamiltonian (5) being constructed in analogy to the multilevel exciton Hamiltonian, the cross terms (i.e. the terms $\chi_{\mu\nu} = \gamma_{\mu\nu} = 0$ for $\mu \neq \nu$) are deleted. It is obvious that this model represents a model of the mixture of noninteracting gases. The coefficients χ_ν are taken as $\chi_\nu(\vec{k}) = A_\nu + \hbar^2 k^2 (2M)^{-1}$ where the first term A_ν is the Pauling energy of hybridization that induces the molecules to unify, the second term being the kinetic energy of the molecule. For $\gamma(\vec{k})$ it is

assumed that it is proportional to the kinetic energy, i.e. $\omega_\nu(k) = G_\nu \hbar^2 k^2 (2M_\nu)^{-1}$ where $G_\nu \leq 1$. Taking into account the molecular masses and the usual values of the hybridization energies, the coefficients χ and γ are of the order of 10 k_B so that for room temperatures one has $\chi, \gamma \ll \theta$. This inequality will be used in the following for the calculation of the entropy. This calculation, starting from the Hamiltonian (5) will not be quoted here as it is too clumsy but it finally leads to the following conclusions:

a) After a sufficiently large increase of time the entropy becomes an oscillatory function of time having a damping characterized by the factor $t^{-\frac{3}{2}}$. This result is just in accordance with Prigogine's and Eigen's criteria for the appearance of the autocatalysis.

b) After a sufficiently large increase of time the pressure becomes periodically equal to zero which means the singularity in the entropy flux. It is out of doubt that sudden jumps, i.e. drops of the entropy flux meaning the increase of information, can play a fundamental role in the autocatalytic process. It is precisely in those moments that the substantial information, able to direct the reaction, is transmitted.

Concluding this paragraph it should be pointed out that the mixture of substances itself can be a seat of excitons and ferroelectric excitations which on their part may also have an oscillatory entropy with damping. It can be shown that in the system particles + antiparticles, the entropy of the particle system may decrease at the expense of the increase of the entropy of the quasiparticle system so that the quasiparticle system may play the role of a source of information for the particle system.

Proton currents in the O - H - O bonds

In the preceeding paragraph it was pointed out that a system of ferroelectric excitations in a mixture of biological substances (such as proteins and nucleic acids) can serve as a source of information for the particle mixture. Here we shall analyse the possibility of protonic currents in O-H-O bonds and their properties. According to Crick's and Watson's ideas[19-21], the proton currents cause the

instabilities in the O-H-O bonds, those bonds constituting the binding elements of the DNA. Those instabilities and the recombination processes open the possibility for the crossingover.

Let us examine the O-H-O bond of the length 2L assuming the following model potential in the region of the bond:

$$V(x) = V_1 \delta(x) + \frac{1}{2} V_2 [\delta(x-L) + \delta(x+L)] \qquad (6)$$

This potential simulates the double well potential which is assumed for the O-H-O bond. The advantage of this potential is that it admits the exact solution of the eigenvalue problem as well as the penetration from bond to bond since the transmission coefficient is different from zero.

The differential equation of the problem is:

$$\frac{d^2\phi}{dx^2} - \lambda^2 \phi = W_1 \delta(x)\phi + \frac{1}{2} W_2 [\delta(x-L)+\delta(x+L)]\phi, \quad \lambda^2 = \frac{2mE}{\hbar^2} \qquad (7)$$
$$W_i = \frac{2mV_i}{\hbar^2}; \; i = 1,2$$

The problem can be solved using the Fourier expansion, since the solution has to be periodical, the period being 2L. For $E<0$ the following secular equation is obtained:

$$\operatorname{cth}\xi = \frac{2}{M(1+\beta^2)}\xi + \frac{\beta^2 M}{2(1+\beta^2)}\frac{1}{\xi}; \qquad \begin{matrix} M = L|W|; & W_1 = -|W| \\ \xi = \lambda L; & W_2 = -\beta^2|W| \end{matrix} \qquad (8)$$

with the corresponding solution in the form:

$$\phi_i(x) = C \tilde{\tilde{\operatorname{sh}}} \lambda_i x; \quad i = 1,2; \quad \tilde{\tilde{\operatorname{sh}}} \lambda x = \tilde{\tilde{\operatorname{sh}}} \lambda (x \pm 2L). \qquad (9)$$

The equation (8) is solved for the case of KH_2PO_4, i.e. it is assumed that L=3.5 nm and $2\Omega = |E_1 - E_2| = 200\text{-}400\ cm^{-1}$.

It may be demonstrated that the functions ϕ_i are not orthogonal so that one takes the following combinations:

$$\psi_1 = \tilde{\tilde{\operatorname{sh}}} \lambda_1 x - A e^{i\varphi} \tilde{\tilde{\operatorname{sh}}} \lambda_2 x; \quad \psi_2 = \tilde{\tilde{\operatorname{sh}}} \lambda_1 x + i A \xi e^{i\varphi} \tilde{\tilde{\operatorname{sh}}} \lambda_2 x \qquad (10)$$

the parameters A, φ, ξ and the constants C_i are determined from the orthonormality conditions. In the result of the numerical analysis one has:

$$\langle \psi_1 | H | \psi_1 \rangle = -340\,cm^{-1} - i\,152\,cm^{-1}; \quad \langle \psi_2 | H | \psi_2 \rangle = -3682\,cm^{-1} + i\,152\,cm^{-1}$$
$$2\Omega = \operatorname{Re} E_1 - \operatorname{Re} E_2 = 281\,cm^{-1} \qquad (11)$$

For ψ_i given in (10) the probability current reigning in

the bond is different from zero and in the same way is the proton current. The expression is:

$$j_1 = -\frac{\hbar C_1^2 e}{m}(\lambda_1 \widetilde{ch}\lambda_1 x \widetilde{sh}\lambda_2 x - \lambda_2 \widetilde{ch}\lambda_2 x \widetilde{sh}\lambda_1 x)A \sin\varphi; \quad j_2 = -\frac{C_2^2}{C_1^2}\xi j_1 \operatorname{ctg}\varphi. \quad (12)$$

The proton currents are odd functions with respect to , both are approximately of the same value and are confined in the interval from 0 for x=0 to $\pm 5\mu A$ for $x = \pm L$.

Concluding this paragraph it should be noticed that:
a) Proton currents exist in O-H-O bonds.
b) They have the maximal value on the boundary of the bond which makes the penetration in the neighbouring bond possible.
c) The system of individual bonds analysed here may be used to construct a linear structure endowed with ferroelectric excitations. Taking (11) into account it is seen that the excitations taking place in the linear structure are expected to be instable with a lifetime of the order of 10^{-14}s.

Conclusion

We have demonstrated the possibility to apply the methods belonging to the condensed matter physics to the realm of phenomena taking place in the prebiological phase. More specifically: owing to those methods, the microscopic theoretical schemes and models for the basic concepts actually used in the analysis of the prebiologic phase, are derived from the first principles. Those concepts are: the irreversible light-energy absorption, the high dissipativity, the periodical entropy characterized by a damping and the appearance of proton currents in the system of O-H-O bonds.

Concluding this analysis one should remind that the prebiological phase presents a more difficult problem for the research as compared to the phase concerning the processes in the already constituted biomatter. The researches belonging to the latter phase are highly developed and divers. Theoretically as well as experimentally rheology and other blood phenomena are examined. A lot is already done to shed some light on the transfer of mass, energy and information moving within the living organisms. Great efforts are made to clarify the nature of the cancer and of its origins. The biophysics of membranes is also a field

of intense research, Frölich, Davydov and many others taking part in it. The eye and the vision are also the object of physical researches, attempts being made to develop microscopic theories of the eye and of the vision by the application of methods from crystalooptics. Methods taken from physics are successfully applied in the realm of neurobiology. Nerves and processes in nerve networks are examined experimentally as well as theoretically, the analogy with electric networks being successfully applied. The details concerning the mentioned researches may be found in appropriate references[22-27].

References

1)L.S.Berg,Nomogenez ili evolucija na osnove zakonomernosti,1922.
2)A.G.Gurvič, Teorija biologičeskogo polja, M.Medgiz, 1944.
3)N.Bohr, Atomnaja fizika i čelovečeskoe poznanie,M.,I.L. 1961.
4)N.Bohr, Uspehi fizičeskih nauk, 76, 21, 1962.
5)E.Wigner, Etjudi o simmetrii, M., Mir, 1971.
6)W.Elsaser, The Physical Foundation of Biology, Oxford, Pergamon Press, 1958.
7)M.Eigen, Molekularnaja samoorganizacija i rannie stadii evolucii, UFN 109, 545, 1973.
8)E.Schrödinger, What is Life, Cambridge U Press, 1951.
9)M.V.Volkenstein, Molekuli i žiznj, M., Nauka, 1965.
10)M.Apter, Kibernetika i razvitak, M., Mir, 1970.
11)H.Raven, Ontogenez, M., Mir, 1964.
12)I.Prigogine, Structure, Dissipation and Life in Theoretical Physics and Biology, North Holland, Amsterdam, 1964.
13)I.Prigogine,C.Nicolis, Biological Order, Structure and Instabilities, Quart.Rev.Biophysics 4, 2/3, 107, 1971.
14)V.Agranovič, Zh.Eksp.Teor.Fiz. 37,430,1959.
15)E.Hadžiselimović,M.Marinković,B.Tošić, Non-Conservation of Excitons as a Mechanism of Light Energy Capturing to appear in Int.J.Quantum Chem.
16)E.Hadžiselimović,M.Marinković,B.Tošić, Phys.Stat.Sol. (b) 100, 1980.
17)E.Hadžiselimović,M.Marinković,B.Tošić, On Possible Microphysical Foundations of Chemical Reaction's Autocatalysis, submitted to Int.J.ofQuantum Chem.
18)N.Bogoliubov,J.of Phys.9, 23,1947.

19)J.D.Watson, F.H.C.Crick, Nature 177, 964, 1953.
20)F.H.C.Crick, On Molecules and Man, London, Seattle U Press 1968.
21)J.D.Watson, Molecular Biology of Gene, BenjaminInc. 1977.
22)B.Katz, Nerve, Muscle and Synapse, McGraw Hill, 1966.
23)L.Dintenfass, Blood Micro-rheology, Appleton-Century-Crofts, 1971.
24)E.N.Lightfoot, Transport Phenomena and Living Systems, J.Wiley and Sons, New York, 1974.
25)J.Tooze, The Molecular Biology of Tumor Viruses, Cold Spring Harbor Laboratory, 1973.
26)J.D.Goddard,J.S.Schultz,R.J.Bassett, On Membrane Diffusion with near Equilibrium Reaction, Chem.Eng.Sci. 25, 665-683, 1970.
27)S.W.Kuffler,J.G.Nichols, From Neuron to Brain, Sinauer, Sunderland, Mass. 1976.