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LETTER TO THE EDITOR

STRUCTURAL ORDER AND PARTIAL DISORDER IN BIOLOGICAL SYSTEMS

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An attempt to define a general, theoretical framework for the investigation of relationships between structure and function in biological systems was made ten years ago (Baianu and Marinescu, 1968; Comorosan and Baianu, 1969). It was then proposed that as a consequence of relational principles, biological variability, dynamics and conditions of experimental observation (and/or other "hidden" causes which are internal, or external to biological systems), one is often concerned with biological functions which are neither fully nor uniquely specified in terms of the underlying molecular structures. This rather general uncertainty, or limitation, was called "fuzziness"† of structures with respect to the associated biological function, and many examples of its occurrence were given by Nicolas Rashevsky (1971) in relational biology and the theory of organismic sets.

A simple example of the kind of relation which we had in mind was given in *loc. cit.* The relation "three points A, B and C form a triangle" is preserved as long as A, B and C are not co-linear and therefore there are an infinite number of different structures satisfying this relation. The relation fails to be satisfied only for those positions of C for which A, B and C are co-linear.

Similarly, in biology, one encounters many situations in which a certain relation, or biological function is maintained over a whole range of structures, or processes (which are not necessarily all well-defined, or specified) and therefore the definition of biological functions in terms of "the performing structures" is limited by a certain "fuzziness". Problems

†In the fields of automata and systems theory this concept takes on a stochastic meaning (Zadeh and Desoer, 1963; Arbib, 1966, 1969), without reference to a relational framework.

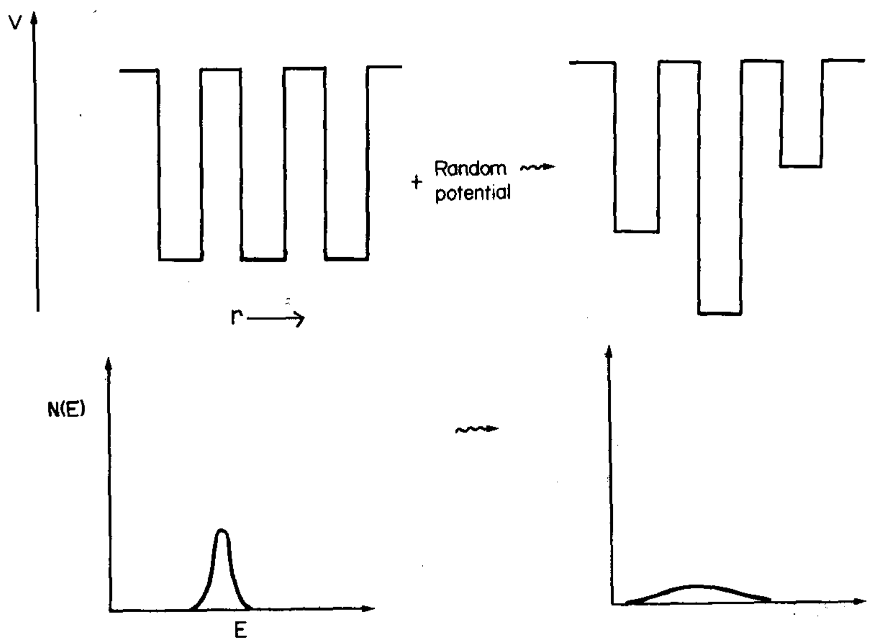

Figure 1. Model of the potential energy of an electron according to Anderson (1958). The densities of states are also shown in the lower half of the figure.

associated with biological multistability (Baianu, 1970), structural stability, qualitative biodynamics (Baianu, 1971a) and catastrophe theory also involve this property.

Mathematically, if the molecular configurations capable of performing a certain biological function form a topological space J, then the mapping, f, from J to the topological space F of biological functions is an *epimorphism*, or a many-to-one continuous map. This has the important, but mathematically trivial, consequence that given a biological function, such as "reproduction" or protein biosynthesis, one cannot find a reverse, well-defined mapping f^{-1} which would uniquely assign to each biological function exactly one, well-defined molecular configuration. It is interesting that the topological equivalence of geometrical shapes, for example, involves itself a "fuzziness" at the geometrical level and suggests that definitions of "biological functions" rely implicitly on the existence of certain topological equivalences between the associated molecular structures. Hence, at all times, there is a "fuzziness" in the relationship between structures and biological function.

Since all biological systems have partially disordered structures, which are continuously changing in a certain range, it would be interesting to consider the "fuzziness" associated with the presence of partial disorder. As a first step in this direction, let us recall the effects of disorder in certain physical, solid systems.

Starting from the effects of partial disorder superimposed onto a regular structure, or lattice, P. W. Anderson proposed in 1958 a simple theoretical model for certain quantum transport processes in solids. This has provided a source of inspiration for further developments in the electronic theory of partially disordered crystals and non-crystalline systems (recent reviews were recently presented by Sir Nevill Mott *et al.* (1975) and by Mott and Davis (1979)).

In this model, the potential energy of an electron at regular sites is perturbed by a random potential, as shown in Figure 1. In such situations, transport was shown to occur not by motion of free carriers (or spin waves) but by "some quantum-mechanical jumps of the mobile entities from site to site" (Anderson, 1958). The solutions of the Schrödinger equation for any energy in the band, in this case, are no longer the extended Bloch states (as in perfect, metallic crystals), but are *localized in space.* The electrical properties expected on the basis of Anderson localization in a disordered solid, or fluid, are significantly different from those derived for perfect crystals. Furthermore, the functioning of semiconductor devices such as metal-oxide-silicon (MOS) field effect transistors can be correctly explained only by this model, which includes a significant amount of disorder.

Since the Anderson localization occurs in most systems which are partially, or almost totally, disordered, we can reasonably expect that it would also occur in most biological structures which, as it will be shown, are partially disordered.

For many years, biological structures, such as nucleic acids, proteins and membranes, have been considered exclusively as "crystalline" and the problems raised by disorder were circumvented rather than solved (Hosemann and Bagchi, 1962). Undoubtedly, this approximation was a necessary first step and had produced well-known results in molecular biology. We can reasonably expect that the disorder present in these systems should be reflected in a "fuzziness" of structures associated with the currently defined biological functions. The number of attempts made to consider the effects of structural disorder on the interpretation of experimental results for biological structures has recently increased (Burge and Draper, 1967; Baianu, 1974, 1978; Moody, 1975; Nelander and Blaurock, 1978; Baianu and Burge, 1979).

The simplest, partially disordered, lattice is "one-dimensional", such as the system formed by stacking erythrocyte membranes (Baianu, 1974, 1978). The molecular arrangement in the plane of the membrane is highly disordered, while the long-range structure formed by the membrane lamellae has only about 2–5% stacking disorder. It is now certain that disorder has important repercussions for the structural data analysis and interpretation.

Nerve myelin, which was considered for many years as crystalline, is now recognised to be paracrystalline (Hybl, 1977), that is, partially disordered, and the disorder is at least in two dimensions (Nelander and Blaurock, 1978). This must have important consequences for its function (Baianu, 1972). Since the membrane matrix is, generally, semi-conducting one would expect localized states to exist in this system and mobility edge phenomena (see for example, Mott *et al.*, 1975) to be observed. Similarly, extracted, powdered DNA is a semi-conductor in the solid state (Baianu and Vicol, 1970), and through the observation of its electrical properties, as well as their change in the presence of magnetic fields, one should be able to derive conclusions concerning its electronic structure, in a manner analogous to the experiments on MOS devices (Nicholas *et al.*, 1977; Stradling, 1978). (The experiment would, however, involve changes of the magnetic field in steps of the order of 0.05 G.)

The effects of disorder on the observation processes are not yet investigated but the presence of localized states brings about the possibility of observing new quantum observables (Rosen, 1977 and references therein), through the interaction with measuring apparatuses of adequate design. These new observables need not be biological and certainly they are not less physical than those measured with a traditional apparatus. One class of measuring instruments which are likely to produce this kind of result should include a *coherent* source (such as a laser) and should detect *transient* signals (for example, pulsed lasers and pulsed NMR spectrometers). Thus, transient methods have recently allowed the observation of local structure in electrolyte glasses (Baianu *et al.*, 1978). The extension of the applicability of these techniques to biological structures is one of the experimental problems now being investigated.

The relational variability of biological systems therefore requires adequately developed concepts and mathematical instruments. Attempts in this direction were mostly carried out in connection with: the theory of organismic sets (Baianu, 1970, 1971a, 1977; Baianu and Scripcariu, 1973), (M, R)-systems (Baianu, 1973, Baianu and Marinescu, 1974) and automata (Baianu, 1971b). This has led to new mathematical structures and general theorems concerning their realizability in biology. The above discussion also suggests that it has become necessary to bridge the gap between the functional (relational biology) approach and the structurally-based approaches in molecular biology. In this process, "fuzziness" and structural disorder should play an important role.

LITERATURE

Anderson, P. W. 1958. "Absence of Diffusion in Certain Random Lattices." *Phys. Rev.*, **109**, 1492–1505.

Arbib, M. "Automata Theory and Control Theory. A Rapprochement: *Automation.* **3**, 161–189.

———. 1969. "Stochastic Automata." In *Theories of Abstract Automata.* New Jersey: Prentice-Hall.

Baianu, I. 1970. "Organismic Supercategories—II. On Multistable Systems." *Ibid.*, **32**, 539–561.

———. 1971a. "Organismic Supercategories and Qualitative Dynamics of Systems." *Ibid.*, **33**, 339–354.

———. 1971b. "Categories, Functors and Automata Theory." *Abstr. 4th Congress LM.P.S.*, p. 82.

———. 1972. "Energetical considerations in E.E.G. interpretations." *Ann. Univ. Bucuresti*, **21**, 61–67.

———. I. 1973. "Some Algebraic Properties of (M, R)-Systems." *Bull. Math. Biol.*, **35**, 213–217.

———. 1974. "Structural Studies of Erythrocyte and Bacterial Membranes by X-ray Diffraction and Electron Microscopy." Ph.D. Thesis. London University.

———. 1977. "A Logical Model of Genetic Activities in Lukasiewicz Algebras: The Non-Linear Theory." *Bull. Math. Biol.*, **39**, 249–258.

———. 1978. "X-ray Scattering by Partially Disordered Membrane Systems." *Acta Crystall.*, **A34**, 751–753.

———, N. Boden, M. Mortimer and D. Lightowers. 1978. "A New Approach to the Structure of Concentrated Aqueous Electrolyte Solutions by Pulsed N.M.R." *Chem. Phys. Lett.*, **54**, 169–175.

——— and R. E. Burge. 1979. "X-ray Diffraction Studies of Bacterial Cytoplasmic Membranes." *Biochim. Biophys. Acta* (in press).

——— and M. Marinescu. 1968. "Organismic Supercategories: I. Proposals for a General Unitary Theory of Systems." *Bull. Math. Biophys.*, **30**, 625–635.

——— and M. Marinescu. 1974. "On a Functorial Construction of (M, R)--Systems." *Rev. Roum. Math. Pure and Appl.*, **19**, 389–391.

——— and L. Vicol. 1970. "Semiconductibility of DNA at low temperatures." *Disc. Conf. Macromol. and Biopolymers*, Prague.

Burge, R. E. and J. C. Draper. 1967. "Structure of the Cell Wall of the Gram-negative Bacterium *Proteus vulgaris.*" *J. Mol. Biol.*, **28**, 189–204.

Comorosan, S. and I. Baianu. 1969. "Abstract Representations of Biological Systems in Supercategories." *Bull. Math. Biophys.*, **31**, 59–71.

Hosemann, R. and S. N. Bagchi. 1962. *Direct Analysis of Diffraction by Matter.* Amsterdam: North Holland.

Hybl, A. 1977. "Paracrystalline Nature of Myelin." *J. appl. Crystall.*, **10**, 141–146.

Moody, M. F. 1975. "Diffraction by Dispersions of Spherical Membrane Vesicles—I. The Basic Equations." *Acta Crystall.*, **A31**, 8–16.

Mott, N. F. *et al.* 1975. "The Anderson Transition." *Proc R. Soc. Lond. A.*, **345**, 169–205.

Mott, N. F. and E. A. Davis. 1979. *Electronic Processes in Non-crystalline Materials.* Oxford: Clarendon Press.

Nelander, J. C. and A. E. Blaurock. 1978. "Disorder in Nerve Myelin: Phasing of the Higher Order Reflections by Means of the Diffuse Scatter." *J. Mol. Biol.*, **118**, 497–532.

Nicholas, R. J., R. A. Stradling and R. J. Taylor. 1977. "Evidence for Anderson Localization in Landau-level tails." *Solid State Commun.*, **23**, 341–345.

Rashevsky, N. 1971. "Relational Forces and Structures Produced by Them." *Bull. Math. Biophys.*, **33**, 321–338.

Rosen, R. 1977. "Observation and Biological System." *Bull. Math. Biol.*, **39**, 663–678.

Stradling, R. A. 1978. "Quantum Transport." *Phys. Bull.*, **29**, 559–562.

Zadeh, L. A. and C. A. Desoer. 1963. *Linear Systems Theory.* New York: McGraw-Hill.

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