On some algebraic problems arising in quantum mechanical description of biological systems

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Abstract

The biological hierarchy and the differences between living and non-living systems are considered from the standpoint of quantum mechanics. The hierarchical organization of biological systems requires hierarchical organization of quantum states. The construction of the hierarchical space of state vectors is presented. The application of similar structures to quantum information processing is considered.

1 Quantum Mechanics and Evolution

The most important discoveries in natural sciences are connected to quantum mechanics. There is also a bias that biological phenomena will be explained by quantum theory in future, since quantum theory contains all basic principles of particle interactions and these principles had success in molecular dynamics, the basis of life. Biology has however a number of concepts and facts not displayed explicitly in inanimate world. The following are of principle importance:

1. The properties of a living system are more than just a collection of its components properties. In other words, it is impossible to predict the whole set of properties of a complex biological system even having known all properties of its components.

2. The properties and functions of the components of a system depend on the state of the whole system. In other words, the same components being included in different systems may have different properties.

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3. There is an *Evolution* — a process of creating new entities, forms and functions on the base of the existing components.

For both biology and quantum physics the relation "the part - the whole" is extremely important, and not trivial: the factorization $\Psi(x) = \prod_i \psi_i(x_i)$ holds only for the systems of noninteracting particles.

The properties (2,3) listed above are implicitly based on the concept of scale: an entity to become a part of another entity should be in some metric smaller than it. If the metric is Euclidean, or at least Archimedian, the evolution of the Universe can be said to go from small scales to large scales. In this sense, the elementary particles and atoms had had their evolution: at early times of the Universe the nucleons had been built of quarks, the nuclei from nucleons and so long.

We do not have an answer to the question, why the evolution had taken the way it has been going through. However, *if the whole is more than the sum of parts and the properties of the parts depend on the state of the whole, there are some implications for quantum mechanics.*

To describe a state of an object $A_1$ (interacting with objects $A_2, \ldots, A_N$), which is a part of an object $B_1$ we have to write the wave function in the form $\{\Psi_{B_1}, \Psi_{B_1 A_1}\}$, where $\Psi_{B_1}$ is the wave function of the whole, and $\Psi_{B_1 A_1}$ is the wave function of a component $A_1$ belonging to the entity $B_1$. For instance, $A_1, A_2, A_3$ may be quarks, and $B_1$ may be proton. The objects $A_1, \ldots, A_N$ are inside $B_1$ and it is impossible to commute $[\Psi_{B_1}, \Psi_{B_1 A_1}]$ or to multiply them $\Psi_{B_1}, \Psi_{B_1 A_1}$, since the functions $\Psi_{B_1}(x)$ and $\Psi_{B_1 A_1}(x)$ live in different functional spaces.

We generally observe, that *each hierarchical level has its own symmetry.* This is $SU_3$ for quark level or isospin group for nuclei etc. So, each hierarchy level can be described by $(G_I, X^{G_I})$, where $I$ labels the scale, $G_I$ is the symmetry group at this scale, $X^{G_I}$ is a topology on $G_I$. The Euclidean space is a particular case of the translation group $G_I : x \to x + b$. The wave function of an object $B^{I_1}$ of the level $I_1$ consisting of $N$ objects $\{A_i^{I_2}\}_{i=1,N}$ can be written as

$$\Psi_B = \left\{ \psi_B^{I_1}(x^{G_I}), \psi_{B A_1}^{I_2}(x_1^{G_{I_2}}), \ldots, \psi_{B A_N}^{I_2}(x_N^{G_{I_2}}) \right\}. \quad (1)$$

In biology, as well as in physics, the symmetry breaking plays an important role. It is known, that the amount of information written in DNA, if calculated as one
nucleotide – one bit, is insufficient to describe the formation of adult organism. Thus, the information is likely to be written more effectively than just a technical plan of the organism. What is encoded, is probably a chain of bifurcation points to be undergone in growth process.

If the quantum mechanics is valid on the macroscopic scales, we can say that the hierarchy levels emerge as a result of a) evolution, b) self-organization, and formation of new entities from existing ones $\{\emptyset; \psi_{A_1} \otimes \psi_{A_2}\} \rightarrow \{\psi_B; \{\psi_{BA_1}, \psi_{BA_2}\}\}$, where the empty-set $\emptyset$ denotes the non-existing common “container” for two components $\psi_{A_1}$ and $\psi_{A_2}$; $\psi_B$ is a new entity formed by $\psi_{A_1}$ and $\psi_{A_2}$.

The hierarchy of biological system joins the hierarchy of non-living matter by means of the cell – unit of life, and its part, the genome, the sequence of macromolecules which prescribes the evolution of all living systems, from cell to organism.

The hierarchy levels of living and non-living matter

| Living matter | Non-living matter |
|---------------|------------------|
| ...           |                  |
| ecosystem     |                  |
| population    |                  |
| organism      |                  |
| organ         |                  |
| cell          |                  |
| organell      |                  |
| genome        |                  |
|               |                  |
| molecule      |                  |
| atom          |                  |
| nucleus       |                  |
| nucleon       |                  |
| ...           |                  |

The place on an entity in the hierarchy tree and its distance from the position of the organism it belongs to determines the dynamical repertoire of the entity.

The evolutionary distance between maximal and minimal parts of the organism determines its ability of self-recovering. For instance, if one end of *Hydra oligactis* (a simplest animal living in water) is cutted off, the remaining cells react to the absence of this part by rearranging themselves and giving growth to new cells and form a complete animal. This process involves at least three levels:

\[ \text{Organism} \rightarrow \text{Cell} \rightarrow \text{Cell component}. \]

Let $T(G_A)$ be an irreducible representation of the symmetry group $G_A$ which corresponds to the wave function of the intact organism. The self-repairation process
can be then described by following 3 level diagram:

\[
\{\psi_A; \{\psi_{AC_1}, \ldots, \psi_{AC_N}\}\} + \Gamma \rightarrow \{\psi_A; \{\psi_{AC_1}, \ldots, \psi_{AC_K}\}\} + \{\psi_{C_{K+1}}, \ldots, \psi_{C_N}\}
\]
\[
\rightarrow \{\psi_A; \{\psi_{AC_1c_1}, \psi_{AC_1c_2}, \ldots, \psi_{AC_Kc_L}\}\}
\]
\[
\rightarrow \{\psi_A; \{\psi_{AC_1}, \ldots, \psi_{AC_N}\}\}
\]  \hspace{2cm} (2)

On the first stage, affected by destructive action \(\Gamma\), the part of the system, a block of \((N - K)\) cells is cutted of. The remainder

\[
\{\psi_A; \{\psi_{AC_1}, \ldots, \psi_{AC_K}\}\}
\]  \hspace{2cm} (3)

does not form a complete organism any longer; the product of representations \(\bigotimes_{i=1}^{K} T(G_{C_i})\) does not contain \(T(G_A)\). So, the wave function of the remainder \(\text{[3]}\) breaks down to the third level hierarchy wave function \(\{\psi_A; \{\psi_{AC_1c_1}, \psi_{AC_1c_2}, \ldots, \psi_{AC_Kc_L}\}\}\), providing a possibility of building a representation tensor product, which contains \(T(G_A)\). On the third level the wave functions are being rearranged according to this tensor product and the missed second level blocks are being rebuilt.

The observations at all levels of the evolutional hierarchy, from simple organnels to complex ecosystems suggest that basically, only neighboring levels interact. The quantum nature of the interactions in this hierarchy may be used to understand, why a cutted skin recovers, but the arm cutted of is not being recovered. If the lost part of the organism has \(M \gg 1\) hierarchical levels a \(M\)-level cascade process should run in the remainder to rebuild the lost part. A process of this type will require significant flux of energy, and at the same time a tremendous flux of negative entropy, to restore the symmetry of the wave function of the whole organism by rearranging the wave functions of its components.

\section{Pauli principle}

Pauli principle: \textit{Two fermions of the same system can not be in the same quantum state.} This is a consequence of the fact that the wave function of a fermion system should be antisymmetric with respect to particle transposition.

If we disregard the interaction of neighboring levels only, we can say that, \textbf{two fermions belonging to the same system of the next hierarchical level can not be in the same state}. Therefore, it is impossible for two electrons in atom to have the same quantum numbers \((n, l, m)\), but is it possible for two electrons of the same \textit{molecule} to be in the same state? It seems evident that two electrons of different macroscopic objects can be in the same state. \textit{But is it really possible for two electrons of the same molecule?}
So, the real question is: what should we really mean by “the hierarchy level next to atom”? There is no common sense answer to this question, but if the generalization of Pauli principle formulated above, is valid, and the only question is what is the next hierarchical level, the matter can be experimentally investigated, at least in principle. To some extent, the idea of possible experiment of this type have been suggested by D. Home and R. Chattopadhyaya [4]. If biological macromolecules, the DNA, can be used as a device for quantum measurement, it means that if a photon absorbed by a DNA molecule, the wave function of the whole molecule flops from one quantum state into another. But the DNA molecule itself consists of smaller molecules. So, there are two alternatives: either the absorption of a photon changes the wave function of the DNA only by changing the wave function of one of its components, or it changes the wave function of the whole DNA. In the latter case, due to the interaction between the whole and its parts, the absorption of the photon at one edge of DNA can can be immediately detected at the opposite edge, at least in principle.

3 Wave functions of living and non-living systems

The living and non-living systems are different in the complexity, in the Kolmogorov sense. The Hamiltonian for a non-living system can be constructed using the representations of the symmetry groups of its components and their interactions. This description is shorter than a time series of its matrix elements $E_{mn}(t)$ taken at each moment of time. For a living system the shortest description of the evolution operator may be the time seria $E_{mn}(t)$ itself, or its subseria.

Let us formulate the difference in the language of group theory:

1. We can assert, that for nonliving systems the knowledge of irreducible representations of the component wave function and a symmetry group which accounts for their interaction completely determines the wave function of the whole.

2. The wave function of a living system is constrained, but not completely determined by the representations of symmetry group of its components. This means, that even if we know the wave functions of all components of a living system we still can not predict the behavior of the system without a separate knowledge of the next level wave function, i. e. the wave function of the whole.

To conclude with, we should mention that possible distinction between living and non-living systems, itemized above in this paper, makes a new point in the Schrödinger cat problem

$$\frac{1}{\sqrt{2}}|\text{cat dead}\rangle + \frac{1}{\sqrt{2}}|\text{cat alive}\rangle = ?$$
In hierarchical formalism, the wave function of a *dead cat* is constructed from the direct products of the irreducible representations of its parts. The wave function of the *alive cat* comprise the wave function of the whole cat as well. So these two wave function live in different functional spaces.

### 4 Density matrix

The standard approach to introduce the density matrix is to consider the quantum states of the “system+environment”: \( |\psi\rangle = \sum_{ij} C_{ij} |\phi_i\rangle |\theta_j\rangle \), where \( \{ |\phi_i\rangle \}_i \) are the state vectors of the system, with \( \{ |\theta_i\rangle \}_i \) are those of the environment, *i.e.* the rest of the Universe. In coordinate representation

\[
\psi(x, y) = \langle y | \langle x | \psi \rangle = \sum_{ij} C_{ij} \phi_i(x) \theta_j(y) \equiv \sum_i c_i(y) \phi_i(x). \tag{4}
\]

In any measurement performed on quantum system the wave function can be considered as a superposition of the different states of the system taken with weights \( c_i(y) \) dependent on the state of the environment. This means the operators of physical observables related to the system act only on \( |\phi_i\rangle \) vectors: \( A|\phi_i\rangle |\theta_j\rangle = (|\phi_i\rangle)|\theta_j\rangle \) and the average value of the observable \( A \) is given by

\[
\langle A \rangle \equiv \langle \psi | A | \psi \rangle = \sum_{ii'} \rho_{ii'} \langle \phi_i | A | \phi_{i'} \rangle \equiv Sp(\rho A) \tag{5}
\]

where \( \rho_{ii'} = \sum_j C_{ij}^* C_{i'j} \) is the density matrix. (The orthonormality of the state vectors of the environment is assumed \( \langle \theta_i | \theta_j \rangle = \delta_{ij} \))

The density matrix \( \rho_{ii'} \) being hermitian is usually represented in the diagonal form

\[
\rho_{ii'} = \langle \phi_{i'} | \hat{\rho} | \phi_i \rangle, \quad \text{where} \quad \hat{\rho} = \sum_i |i \rangle \omega_i \langle i |, \quad Sp \rho = \sum_i \omega_i = 1,
\]

where the eigenvalue \( \omega_i \) is the probability of finding the system in the \( i \)-th eigenstate.

In context of biological systems, we can expect the probability of quantum states of the subsystem (A) to be dependent basically on the state of the system (B) it is embraced in. For instance, the state of the nuclei is basically dependent on the state of the cell, and much less on the states of other systems; the state of the cell in its turn depends on the state of the organ etc. There is a temptation to identify \( |\theta_j\rangle \) with the states of the system and \( |\phi_i\rangle \) with the states of the subsystem. This is not the same as in standard quantum mechanics, because \( A \cap B = A, A \cap E = \emptyset, A \cup B = B, A \cup E = U \), where \( A \) is subsystem of \( B \), \( E \) is the environment of \( A \) and \( U \) is the Universe.
If the system $B$ consists of $k$ parts $A_1, \ldots, A_k$, then we can write the wave function of the form

$$\ket{\psi} = \sum_{i_1, \ldots, i_k} C^j_{i_1, \ldots, i_k} \ket{\phi_{i_1}} \otimes \cdots \otimes \ket{\phi_{i_k}} \ket{\theta_j}$$  \hspace{1cm} (6)$$

The equation (6) is an approximation accounting all effects of the environment on the subsystem $A_k$ only by means of the effect of the system $B$ to its subsystem $A_k$. We shall call $\phi$ the microlevel and $\theta$ the macrolevel wave functions.

Let $A$ be an observable acting on the microlevel of a system containing $k$ subparts. Then, as a result of the summation over all macrolevel states, the average value of the observable $A$ is

$$\langle A \rangle = \sum_{i_1, i_2, \ldots, i_k} C^j_{i_1, i_2, \ldots, i_k} \langle \theta_j | \langle \phi_{i_1} | \ldots \langle \phi_{i_k} | A | \phi_{i_1} \rangle \ldots \rangle | \phi_{i_k} \rangle = \rho_{i_1} \langle i | A | i' \rangle,$$  \hspace{1cm} (7)$$

where $i \equiv (i_1, \ldots, i_k)$, $|i\rangle \equiv |\phi_{i_1}\rangle \ldots |\phi_{i_k}\rangle$ is the multiindex of the microlevel state. If the operator $A = A_1$ acts only on the first ($i_1$) subsystem of the microlevel, the density matrix for this subsystem is obtained by the averaging over all other ($i_2, \ldots, i_k$) subsystem and the macrosystem state

$$\rho^{(1)}_{i_1 i_2 \ldots i_k, k} = \sum_{i_1, i_2, \ldots, i_k} C^j_{i_1, i_2, \ldots, i_k} C^j_{i_1', i_2', \ldots, i_k}.$$

In analogy with quantum computing algorithms [6], we can introduce operators which acts on the microlevel depending on the state of the macrolevel

$$\hat{B} = \ket{\theta_m} B_{ik}^m \langle \theta_m | i \rangle \langle k |$$  \hspace{1cm} (8)$$

The mean value of the corresponding observable in a two level hierarchical system is

$$\langle B \rangle = \langle \psi | \hat{B} | \psi \rangle = \sum_{i, i'} C^j_{i i'} B_{ii'}^j C^j_{i j}.$$  

5 Recording information in hierarchical quantum systems

The tree-like hierarchical structures can work similar to wavelet based data compression. For example, let us consider a set of $l = 2^{N-1}$ quantum bits. If these qubits are embraced in $N = 3$ level hierarchical system, shown in Fig. 2, then, instead of 4 original qubits $\phi^2_{11}, \phi^2_{12}, \phi^2_{21}, \phi^2_{22}$, on each level of the hierarchy we construct a Haar wavelet [7] like basis:

$$\begin{align*}
|\phi^1_1\rangle &= \frac{|\phi^2_{11}\rangle + |\phi^2_{12}\rangle}{\sqrt{2}}, \\
|\phi^1_2\rangle &= \frac{|\phi^2_{11}\rangle + |\phi^2_{22}\rangle}{\sqrt{2}}, \\
|\phi^0\rangle &= \frac{|\phi^1_1\rangle + |\phi^1_2\rangle}{\sqrt{2}} \hspace{1cm} |\psi^1_1\rangle &= \frac{|\phi^2_{11}\rangle - |\phi^2_{12}\rangle}{\sqrt{2}}, \\
|\psi^1_2\rangle &= \frac{|\phi^2_{11}\rangle - |\phi^2_{22}\rangle}{\sqrt{2}}, \\
|\psi^0\rangle &= \frac{|\phi^1_1\rangle - |\phi^1_2\rangle}{\sqrt{2}}.
\end{align*}$$  \hspace{1cm} (9)$$
Figure 2: Hierarchical quantum system used for information recording. The state vector of the whole system is $|\Phi\rangle = \{|\phi^0\rangle, \{|\phi^1\rangle, |\phi^2\rangle\}, \{|\phi^0_{11}\rangle, |\phi^0_{12}\rangle, |\phi^0_{21}\rangle, |\phi^0_{22}\rangle, |\phi^1_{11}\rangle, |\phi^1_{12}\rangle, |\phi^1_{21}\rangle, |\phi^1_{22}\rangle\}\}$. Since the $\phi$ states are linear combinations of $\phi$ and $\psi$ states of the previous level, finally the whole information is stored in 4 independent states of the 2 top levels:

$$\Psi = \{|\phi^0\rangle, |\psi^0\rangle, \{|\psi^1_1\rangle, |\psi^1_2\rangle\}\}.$$  

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References

[1] Nicolis G., Prigogine I. *Self-Organization in Non-Equilibrium Systems*, Wiley, New York, 1977.

[2] Lima-de-Faria A. *Evolution without selection*. Elsevier, 1988.

[3] Alberts B., Bray D., Lewis J., Raff M., Roberts K. and Watson J.D. *The molecular biology of the cell*, Garlance Publishing Inc., New York, 1994.

[4] Home D. and Chattopadhyaya, R. DNA molecular cousin of Schrödinger’s cat: A curious example of quantum measurement. *Phys. Rev. Lett.* 76(1996)2837-2839.

[5] Feynman, R.P. Statistical mechanics, W.A. Benjamin Inc. Massachusetts, 1972.

[6] Nielsen M.A. and Chuang I.L., *Phys. Rev. Lett.* 79 (1997)321-324.

[7] Daubechies, I., *Comm. Pure. Apl. Math.* 41(1988) 909-996.