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Andrei Khrennikov (✉ Andrei.Khrennikov@lnu.se)

Linnaeus University

Irina Basieva

Linnaeus University

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“What is life?”: Open quantum systems approach

Irina Basieva¹ and Andrei Khrennikov¹

¹International Center for Mathematical Modeling in Physics and Cognitive Sciences, Linnaeus University, SE 351 95 Växjö, Sweden; correspondence to Andrei.Khrennikov@lnu.se

ABSTRACT

Recently the quantum formalism and methodology started to be applied to modeling of information processing in biosystems, mainly to the process of decision making and psychological behavior (but some applications to microbiology and genetics are considered as well). Since a living system is fundamentally open (an isolated biosystem is dead), the theory of open quantum systems is the most powerful tool for life-modeling. In this paper, we turn to the famous Schrödinger book “What is life?” and reformulate his speculations in terms of this theory. Schrödinger pointed to order preservation as one of the main distinguishing features of biosystems. Entropy is the basic quantitative measure of order. In physical systems, entropy has the tendency to increase (Second Law of Thermodynamics for isolated classical systems and dissipation in open classical and quantum systems). Schrödinger emphasized the ability of biosystems to beat this tendency. We demonstrate that systems processing information in the quantum-like way can preserve the order-structure expressed by the quantum (von Neumann or linear) entropy. We emphasize the role of the special class of quantum dynamics and initial states generating *the camel-like graphs for entropy-evolution* in the process of interaction with a new environment $\mathcal{E}$: 1) entropy (disorder) increasing in the process of adaptation to the specific features of $\mathcal{E}$; 2) entropy decreasing (order increasing) resulting from adaptation; 3) the restoration of order or even its increase for limiting steady state. In the latter case the steady state entropy can be even lower than the entropy of the initial state.

1 Introduction

This paper is an attempt to formalize the well-known Schrödinger’s speculations¹ on the special features of the information exchange between biosystems and their environments. We operate in the framework of quantum information and open systems^{2–6}.

We recall that in 1944 Schrödinger wrote the book that has big influence on the future interplay between physics and biology and development of biophysics¹. The book’s title poses one of the most fundamental questions of the modern science “*What is life?*”. We are still far from obtaining an answer to it, may be no closer than Schrödinger was in 1944. The main distinguishing feature of biosystems (from a physicist’s viewpoint) was presented by Schrödinger¹ as follows:

“What is the characteristic feature of life? When is a piece of matter said to be alive? When it goes on ‘doing something’, moving, exchanging material with its environment, and so forth, and that for a much longer period than we would expect of an inanimate piece of matter to ‘keep going’ under similar circumstances.”

See Appendix (Supplementary Information) for further discussion on Schrödinger’s views.)

1.1 Information biology

The main message of Schrödinger’s book¹ was that biosystems are subject not only to material or energy constraints imposed by the physical environment, but also to the information constraints imposed by the *information environment*. Biosystems are considered as *open systems* interacting with their physico-informational environments. Nowadays, this viewpoint is well accommodated in biology, see, e.g., Gatenby and Frieden⁷: “In a 1970 review⁸, Johnson characterized information theory (IT) as a “general calculus for biology. It is clear that life without matter and energy is impossible. Johnson’s manuscript emphasized that life without information is likewise impossible. Since the article, remarkable progress has been made toward understanding the informational basis for life...”

However, after a few years of successful applications of classical information theory to biology, the bio-community started to recognize its limitations⁷: “it seems clear that, in the 35 years since Johnson’s original article, IT using traditional Shannon methods has not become, as predicted, the “general calculus” of biology. Although the lack of wide spread application is probably the result of multiple limitations...” In⁷, Gatenby and Frieden stressed that in further applications of information theory in biology, “the focus will be on new methods...” In particular, researchers “address limitations of the IT methodology by applying new statistical and modeling approaches to information dynamics, including bio-informatics, dynamical systems, game theory, graph theory, and measurement theory.”

1.2 Information physics

We remark that the process of IT-reconsideration of biology was closely connected with the similar process in physics. Modern physics differs essentially from physics of the middle of the last century. Highlighting the role of information is one of the main outputs of development of physical theory, starting with Wheeler's "*It from bit*"⁹ to the recent *quantum information revolution* (known as the second quantum revolution in physics). (As it was declared at the second Vaxjö conference¹⁰ - "Quantum Theory: Reconsideration of Foundations: Quantum information is not just a new application of quantum theory, but its foundational basis; see also^{11-17, 4} for reconsideration of quantum foundations from the information perspective.)

In this paper, we present analysis of order-stability in biosystems based on the lessons from quantum physics, especially quantum information and open quantum systems⁵. In contrast to Schrödinger's attempt¹ to compare genuine quantum physical processes in the micro-world with biological processes, in this paper we compare not quantum physics and biology, but quantum and biological information processing¹⁸. This is a part of *quantum-like modeling*, applications of the formalism and methodology of quantum theory outside of physics, especially to cognition, psychology, decision making, but also microbiology and genetics; see pioneer works¹⁹⁻²¹, monographs²²⁻²⁶ and some papers²⁷⁻⁶² which are related to this work closer than other quantum-like studies (Nowadays, this topic is widespread; Google generates 286.000 results on "quantum-like").

1.3 Quantum-like modeling in biology: from cells to cognition and decision making

By the quantum-like paradigm⁵⁸, biosystems represent and process information by means of two coupled representations: a) physical (electrochemical) states, b) quantum information states. The latter states are "rough images" of the former (sections 4.2, 4.3). Such quantum-like, i.e., respecting the laws of quantum information theory, information processing has no direct connection with the genuine quantum physical processes in a biological organism. A biosystem is a black box performing quantum information processing. The ability to represent information in the quantum-like way was developed in the process of evolution of biosystems. It has no direct relation with system's spatial and temporal scales, temperature and other parameters of this sort (cf.⁶³⁻⁶⁷). In article⁴⁸, it was pointed out that the quantum representation of information is the distinguishing feature of all biosystems, from proteins, genomes, and cells to brains and ecological systems. One can speak about *quantum information biology*.

What is the main distinguishing feature of the quantum-like representation and processing? It is a possibility of processing unresolved uncertainties. Mathematically, they are encoded in states' *superpositions*. What is the main advantage of such information processing (operating with superpositions)? It saves computational resources: biosystems working in the quantum-like regime need not resolve all uncertainties and determine probability distributions at each step of state's processing. Here the state is interpreted not as a physical or chemical state, but as an information state of the biosystem *S* (sections 4.2, 4.3). In paper⁵⁸, we apply this idea to modeling quantum representation of information processing by the brain. Quantum information states are connected to the standard neural codes, for example, "excited-quiet" code (section 4.3), see Fig. 1. Cognitive superposition does not mean simultaneous coexistence of excited and quiet neural states realized by some sort of quantum magic; rather, it accounts for a potential of transferring to new cognitive eigenstates in case of some particular change of the cognitive basis.

In our quantum-like model, order-stability in biosystems is a consequence of such superposition based information processing. This is an unusual *explanation of stability as arising from processing of ambiguities without attempting to resolve them*. From evolutionary stand point such behavior is advantageous for systems that are particularly *context sensitive*. In a complex environment, living-context of an *S* is highly variable and, for *S*, it is resource consuming to determine the probability distribution of all variables involved in its functioning. So, we explore *contextuality* as one of the distinguishing features of the quantum theory⁶⁸⁻⁷².

We also stress that the quantum(-like) representation of information is *linear* (see section 4.2) and *S* processes its state very rapidly (see section 4.1). Linearity is heavily explored in the use of the vector representation of correlations, by the so-called *entangled states*. (cf. with quantum computing, e.g.,²). Evolution of highly correlated information states is described by simple linear equations, quantum master equations.

Quantum-like modeling extends the domain of applications of the quantum formalism and methodology outside of physics. It is a fruit of the quantum information revolution and it generally establishes the information interpretation of quantum physics^{11,17, 4}. Another supporting stream of research is quantum logic where the main role is played by the structure of the logic operations and rather than by their physical carriers (e.g.,⁷²).

1.4 Stability of order in biosystems from the viewpoint of open quantum systems

We present a quantum information reformulation of Schrödinger's discussion on bio-stability as based on entropy-exchange with biosystem's environment. Our suggestion is to treat entropy on the basis of quantum information theory (as the von Neumann entropy⁷³ or linear entropy). By using this theory, we follow the aforementioned recommendation of Gatenby and Frieden to focus on new methods in the information approach in biology. The quantum entropy represents uncertainty in

Figure 1. Illustration for quantum-like representation of uncertainty generated by neuron's action potential (originally published in⁵⁸).

distribution of quantum information states. This kind of entropy is crucially different from classical entropy. In particular, the Second law of thermodynamics can be violated and, for an isolated system, the quantum entropy is preserved. For open quantum systems, the problem of escaping transition to disorder can be formalized with quantum Markov dynamics. Within this theory, it is demonstrated (with concrete quantum master equations) that a biosystem S with quantum-like information processing can preserve and even decrease its entropy in the process of information exchange with its environment $\mathcal{E}$ and, in this way, preserve or even improve its order structure.

We highlight the role of *the camel-like behavior of the quantum entropy* (section 2.3) in the process of interaction of the system with the surrounding environment and propose a bio-information interpretation of such behavior: 1) entropy (disorder) increasing in the process of adaptation to the specific features of a new environment; 2) entropy decreasing (order increasing) resulting from adaptation to the environment; 3) the restoration of order or even its increase for limiting steady state. In the framework of quantum Markov dynamics, we present an illustrative example of such behavior, see (9), (10) and Figures 2 and 5.

We describe (section 2.5) the class of quantum Markov dynamics for which the camel-like behavior is impossible; they are well known in physics - the unital dynamics.

Apart from the basic quantum entropy, the von Neumann entropy⁷³, we analyze behavior of the linear entropy reflecting decoherence of the system's quantum state (section 2.6). As we see (Fig. 5), quantum Markov dynamics can prevent decoherence and even increase the state's coherence. This feature of quantum state dynamics is very important for modeling information processes in (open) biosystems.

We conclude by highlighting the problem of the description of the possible states of a living system S and speculate that such states should generate the camel-like dynamics of the quantum entropies for all possible surrounding (physico-informational) environments (section 3).

Since the authors hope that the paper can attract attention of biologists who are not acquainted with quantum theory, the paper contains the compact description of the quantum formalism and open systems' dynamics (section 2.1, 4.1).

2 Results

2.1 A few words about quantum (von Neumann) entropy

Denote by $\mathcal{H}$ a complex Hilbert space endowed with the scalar product $\langle \cdot | \cdot \rangle$. For simplicity, we assume that *it is finite dimensional*. The space of density operators is denoted by $D(\mathcal{H})$. The space of all linear operators in $\mathcal{H}$ is denoted by the symbol $\mathcal{L}(\mathcal{H})$. In turn, this is a linear space. Moreover, $\mathcal{L}(\mathcal{H})$ is a complex Hilbert space with the scalar product, $\langle A | B \rangle = \text{Tr} A^* B$. We shall also consider linear operators acting in $\mathcal{L}(\mathcal{H})$. They are called *superoperators*.

Quantum entropy was invented by von Neumann⁷³ and, for a density operator ρ , it is defined as

$$\mathcal{S}(\rho) = -\text{Tr} \rho \ln \rho, \quad (1)$$

This is a natural generalization of the classical Shannon entropy. Since any density operator is Hermitian, there exists an orthonormal basis (e_j) consisting of eigenvectors of ρ , i.e., $\rho e_j = p_j e_j$ (where $p_j \geq 0$ and $\sum_j p_j = 1$). In this basis the matrix of ρ is diagonal and the matrix of the operator $\rho \ln \rho$ has the form $\text{diag}(p_j \ln p_j;)$ hence $\mathcal{S}(\rho) = -\sum_j p_j \ln p_j$. However, the von Neumann entropy has the Shannon form only w.r.t. the special basis. We present three basic properties of the von Neumann entropy: 1) $\mathcal{S}(\rho) = 0$ if and only if ρ is a pure quantum state, i.e., $\rho = |\psi\rangle\langle\psi|$; 2) for a unitary operator U , $\mathcal{S}(U\rho U^*) = \mathcal{S}(\rho)$; 3) the maximum value of entropy is approached on the state $\rho_{\text{disorder}} = I/N$ and $\mathcal{S}(\rho_{\text{disorder}}) = \ln N$, where N is the dimension of the state space. It is natural to call $\rho_{\text{disorder}} = I/N$ *the state of maximal disorder*.

We note that, for an isolated quantum system, the dynamics is represented by unitary evolution operator $U(t)$ (for the Schrödinger and von Neumann equations). Thus, in contrast to the classical case, the entropy of an isolated quantum system. is not changed and its order structure is preserved; the disorder inside the system does not increase with time.

2.2 Quantum Markov dynamics

Basics of the theory of open quantum systems are presented in section 4.1; the general evolution equation (23) for the state $\rho(t)$ of a system S interacting with the surrounding environment $\mathcal{E}$ is very complicated. In physics, various approximations are normally considered. One of the most useful approximations is derived under the assumption of *weak coupling* between S and $\mathcal{E}$. This is *the quantum Markov dynamics* given by the *Gorini-Kossakowski-Sudarshan-Lindblad* (GKSL) equation^{5,6} (in physics, it is commonly called simply the Lindblad equation; this is the simplest quantum master equation):

$$\frac{d\rho}{dt}(t) = -i[H, \rho(t)] + L[\rho(t)], \quad \rho(0) = \rho_0, \quad (2)$$

where Hermitian operator (Hamiltonian) H describes the internal dynamics of S and the superoperator L , acting in the space of density operators, describes an interaction with environment $\mathcal{E}$. This superoperator is often called *Lindbladian* and it can be expressed in the form:

$$L\rho = \sum_j \gamma_j \left(C_j \rho C_j^* - \frac{1}{2} \{ C_j^* C_j, \rho \} \right), \quad (3)$$

where operators $C_j \in \mathcal{L}(\mathcal{H})$ and, for a pair of operators F_1, F_2 , $\{F_1, F_2\} = F_1 F_2 + F_2 F_1$, is their anticommutator. The C_j are called “collapse operators” or “quantum jump operators”. Note that the solution $\rho(t)$ remains a positive density matrix with trace 1 if it starts with such ρ_0 (so this general form of dynamics preserves the trace in the same way as Schrödinger dynamics does). The coupling constants $\gamma_j \geq 0$ describe the strength of interaction between the system S and its environment $\mathcal{E}$. They can be interpreted as inverse relaxation time (the higher the value of this constant, the faster the meltdown of oscillatory behaviour). Generally each jump operator C_j describes the special type of interaction of the system S with the environment $\mathcal{E}$ and it is characterized by its own relaxation time τ_j and interaction constant $\gamma_j = 1/\tau_j$.

The key aspect of the GKSL-equation is that, whereas the standard Schrödinger equation produces incessant periodic oscillations in all probability amplitudes for all observables (unless the state is an eigenvector of the Hamiltonian H), the GKSL-equation eventually produces stabilization of its solution to a steady state⁶:

$$\lim_{t \rightarrow \infty} \hat{\rho}(t) = \hat{\rho}_{\text{steady}}. \quad (4)$$

This state represents the approach of the stationary regime of reaction to the environment influence.

The GKSL-equation is a quantum master equation for Markovian dynamics. To formulate the Markov property, consider the evolution superoperator $\mathcal{T}_t : \mathcal{L}(\mathcal{H}) \rightarrow \mathcal{L}(\mathcal{H})$,

$$\rho(t) = \mathcal{T}_t \rho_0. \quad (5)$$

It has the form

$$\mathcal{T}_t = e^{t\Gamma}, \text{ where } \Gamma\rho = -i[H, \rho] + L[\rho]. \quad (6)$$

This representation implies that the map $t \rightarrow \mathcal{T}_t$ is the superoperator semigroup, i.e., $\mathcal{T}_0 = I$, and

$$\mathcal{T}_{t_1+t_2} = \mathcal{T}_{t_2} \circ \mathcal{T}_{t_1}, t_1, t_2 \geq 0. \quad (7)$$

The latter equality represents Markov property:

$$\rho(t+s) = \mathcal{T}_{t+s} \rho_0 = \mathcal{T}_s \rho_t, \text{ for any } s \geq 0, \quad (8)$$

to determine system's state at any instant of time $t' \geq t$, it is sufficient to know its state at time t .

2.3 Modeling order-stability in biosystems: Camel-like dynamics of quantum entropy

We stress that the GKSL-equation has been widely applied outside of quantum physics to a variety of problems in cognition, psychology, decision making, and economics^{2,18,32,34,35,48} (cf. also with⁷⁴).

As the basic model example for quantum entropy dynamics, we consider the following simple GKSL-equation:

$$\rho'(t) = -i[H, \rho(t)] + \gamma(C\rho(t)C^* - \frac{1}{2}\{C^*C, \rho(t)\}). \quad (9)$$

Here γ is the coupling constant representing the strength of interaction between S and its environment $\mathcal{E}$. We want to present the model example of the order-stable dynamics that matches the biological order preserving behavior. We select the Hamiltonian of S and the interaction operator C as follows:

$$H = \sigma_x = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, C = \begin{vmatrix} 0 & 1 \\ 0 & 0 \end{vmatrix}, \quad (10)$$

(In section 2.5, one can find a hint why we selected the operators in this way.)

System's Hamiltonian is the Pauli matrix σ_x . We select the initial state as the density matrix

$$\rho(0) = \frac{1}{2} \begin{vmatrix} 0.1 & -0.1i \\ 0.1i & 0.9 \end{vmatrix}. \quad (11)$$

The curves in Fig. 2 correspond to the values of the coupling constant $\gamma = 0, 1, 2, 3, 4, 5$. For $\gamma = 0$, the system is isolated and it preserves its entropy (straight line). The environment $\mathcal{E}$ that is described by the interaction operator (Lindbladian L determined by one operator C) has the strong ordering effect on the system. The increase of the coupling constant γ implies quicker stabilization and lower entropy of the steady state.

As we can see from Fig. 2, entropy's dynamics has four stages:

- 1. Increasing and approaching the maximum value: the interaction with a new environment $\mathcal{E}$ and learning its features increases disorder in the system S .
- 2. Decreasing and approaching the minimum value: by using the results of learning during the first stage, S recovers order.
- 3. Slight increasing: the process of further interaction with $\mathcal{E}$ can bring a new portion of disorder into S .
- 4. Stabilizing: S approaches the steady state ρ_{steady} .

We call graphs of such shape, Fig. 2, *camel-like graphs*. For small interaction constant γ (long relaxation time $\tau = 1/\gamma$) there are two humps, with the second hump essentially dumped; increase of γ leads to stronger dumping of the second hump and then to its disappearance; for say $\gamma = 5$, the "camel" becomes one humped. The presence of the second hump and its

Figure 2. Order-stable (camel-like) dynamics of the quantum (von Neumann) entropy.

dependence on γ is a finer characteristics of dynamics and we shall concentrate on the presence of the first (relatively big) hump. The entropic camel is characterized by the inequality:

$$\max_t \mathcal{S}(\rho(t)) \gg \mathcal{S}(\rho_{\text{steady}}). \quad (12)$$

For large γ , we have even the inequality:

$$\mathcal{S}(\rho_0) > \mathcal{S}(\rho_{\text{steady}}). \quad (13)$$

The main distinguishing feature of such dynamics is that its steady state is not characterized by entropy's maximum value corresponding to the first hump of the *camel-like graph* (cf., with the typical behavior of a physical system, section 2.5). *The entropy of the steady state can be essentially lower than the entropy approached at the first stage of dynamics - adaptation to the features of the environment $\mathcal{E}$ and search for adequate reaction to it.* After this stage, S begins to improve its functioning and to increase the degree of internal order, consequently the entropy decreases. In Schrödinger's terms¹, after the stage of adaptation to the environment's features the system S starts to "absorb order" from $\mathcal{E}$ (to absorb negative entropy, in Schrödinger's words). Illustrative biological examples are presented in section 3.3.

Of course, not any environment would deliver order. A typical quantum physical environment delivers disorder and generates the *dissipation process* leading to entropy's increase. In such situation, the steady state is characterized by the maximum of entropy (section 2.5, Fig. 4). To be more precise, we have to speak not about order-stable or disorder-generating environments, but about interactions which generate order or disorder.

We emphasize that, for the camel-like dynamics, *the entropy of the steady state ρ_{steady} can be essentially lower than the entropy of the initial state ρ_0 .* For very strong coupling with the environment (graph for $\gamma = 5$), the final entropy is practically zero. Hence, adaptation via interaction with $\mathcal{E}$ can improve the level of order in S . The system absorbs from the environment the information useful for internal ordering. Thus, a special class of open quantum systems exemplified by dynamics (9), (10) is a very good candidate for mathematical modeling of order-stability in biosystems.

Schrödinger by himself tried to explain the aforementioned situation by using the notion of "negative entropy"¹:

"Every process, event, happening -call it what you will; in a word, everything that is going on in Nature means an increase of the entropy of the part of the world where it is going on. Thus a living organism continually increases its entropy - or, as you

may say, produces positive entropy -and thus tends to approach the dangerous state of maximum entropy, which is of death. It can only keep aloof from it, i.e. alive, by continually drawing from its environment negative entropy - which is something very positive as we shall immediately see. What an organism feeds upon is negative entropy. Or, to put it less paradoxically, the essential thing in metabolism is that the organism succeeds in freeing itself from all the entropy it cannot help producing while alive.”

2.4 Applicability of quantum Markov dynamics to modeling of interaction of biosystems with environments

Finally, we discuss briefly the applicability of the Markov approximation given by the GKSL-equation to modeling of interaction of a biosystem S with its environment $\mathcal{E}$. The basic condition for derivation of the GKSL-equation from the general dynamics, see (23), is *weak coupling* of S with $\mathcal{E}$ (see, e.g.,^{5,6}). This condition is very natural in the biological framework. While any biosystem S is fundamentally open, its coupling to the surrounding environment should be weak; otherwise functioning of S can be destroyed by $\mathcal{E}$. For example, strong interaction with electro-magnetic radiation may cause immediate death. In the same way, intensive absorption of information coming, e.g., from mass-media and other sources can lead to information overload, to a state of stress, and even to death. Schrödinger pointed out¹ that isolation mechanisms play the crucial role in survivability of a biosystem¹). Hence, from this viewpoint the GKSL-equation is a natural approximation of (23).

2.5 Entropy's dynamics for disorder-generating open quantum system

In this section we describe a typical behavior of quantum physical systems. The results presented here illustrate how biosystems should not behave, to stay alive. The unitality of quantum dynamics is discussed as a condition for non-camel graphic behavior. In what follows, it is useful to use the terminology of quantum information theory^{2,3}.

A quantum channel is any trace-preserving completely positive map (superoperator) $\mathcal{T} : \mathcal{L}(\mathcal{H}) \rightarrow \mathcal{L}(\mathcal{H})$.

A quantum channel is called *unital* if $\mathcal{T}(I) = I$, where I denotes the unit operator. The dynamics of a typical physical system is characterized by unitality.

We formulate the following simple (but very important for our reasoning) result:

Theorem 1. *For a quantum channel $\mathcal{T}$,*

$$\mathcal{S}(\mathcal{T}\rho) \geq \mathcal{S}(\rho). \quad (14)$$

for all quantum states if and only if $\mathcal{T}$ is unital.

This result is a part of open quantum system theory folklore; for reader's convenience, we presented it in section 5.

Consider open quantum systems dynamics and master equation (2) for the density operator of the system S , $\rho_0 \rightarrow \rho(t) = \mathcal{T}_t \rho_0$. Suppose that, for any $t \geq 0$, the dynamical quantum channel $\mathcal{T}_t$ is unital, i.e.,

$$\mathcal{T}_t I = I, \quad t \geq 0. \quad (15)$$

Inequality (14) implies that, for any t ,

$$\mathcal{S}(\mathcal{T}_t \rho_0) \geq \mathcal{S}(\rho_0). \quad (16)$$

Markov property implies that, for any $t > 0$,

$$\mathcal{S}(\mathcal{T}_s \rho(t)) \geq \mathcal{S}(\rho(t)), \quad \text{for any } s \geq 0. \quad (17)$$

Thus, entropy does not decrease at any instant of time t (for the unital dynamics). (We recall that we consider finite dimensional state spaces; in the infinite-dimensional case, the situation is essentially more complicated^{75,76}.) We obtained a kind of the Second Law of Thermodynamics, but for open (quantum) systems (see paper⁷⁶ for more precise formulation of this law):

If the system's evolution can be described by unital dynamics, then the von Neumann entropy gain during evolution is nonnegative.

If a quantum dynamics is non-unital, then quantum entropy can decrease and fluctuate (section 2.3, Fig. 2).

Theorem 2. *Dynamical channel $\mathcal{T}_t$ is unital, for some time-interval $[0, \delta]$, $\delta > 0$, if and only if the unit operator satisfies the equation:*

$$LI = 0 \quad (18)$$

Proof 1). Since $\mathcal{T}_t(I) = I$, we have $\frac{d}{dt} \mathcal{T}_t(I) = 0$, and, hence, $\mathcal{T}_t(I)\Gamma I = 0$. The dynamical channel is invertible, since $\mathcal{T}_t = e^{t\Gamma}$, where $\Gamma : \mathcal{L}(\mathcal{H}) \rightarrow \mathcal{L}(\mathcal{H})$ is a bounded linear (super)operator (we consider a finite dimensional case). Hence, $\Gamma I = i[H, I] + LI = 0$ and (18) holds. 2). Now, let (18) hold, then $\Gamma I = 0$ and $\mathcal{T}_t I = e^{t\Gamma} I = I$.

Figure 3. Order-generating dynamics of the quantum (von Neumann) entropy for maximally disordered state.

In fact, we found that unitality on any (in principle, an arbitrary small time-interval) implies global unitality, on $[0, +\infty)$, because condition (18) implies the global unitality.

Proposition 1. *If, for each state, the entropy gain is nonnegative on an arbitrary small time-interval, then the dynamical channel $\mathcal{T}_t$ is unital for all $t \in [0, +\infty)$, and, hence, the entropy gain is nonnegative on $[0, +\infty)$.*

Of course, here the condition “for each state” is crucial. Consider dynamics (9) with H and C given by (10), but select the initial condition $\rho_0 = I/2$. (This state has the maximal entropy $\ln 2$). The entropy dynamics is represented at Fig. 3, in contrast to Fig. 2, there is no any interval with entropy increasing.

Theorem 2 and Proposition 1 imply the following form of the the Second Law of Thermodynamics for open quantum systems:

Theorem 3. *For GKSL-dynamics, the von Neumann entropy gain during evolution is nonnegative, iff (equivalent) conditions (15), (18) hold.*

Now we rewrite equation (18) in terms of the operator representation of the Lindbladian L .

$$0 = LI = \sum_j \gamma_j (C_j C_j^* - C_j^* C_j) = \sum_j \gamma_j [C_j, C_j^*]$$

We recall that in functional analysis a linear operator is called normal, if it commutes with its adjoint operator:

$$[C, C^*] = 0. \quad (19)$$

Thus normality of all operators C_j is sufficient for unitality of dynamics and, hence, the entropy gain is nonnegative (globally). In the simplest case (see equation (9)), the sum is reduced to one term, and the condition (19) is necessary and sufficient for unitality and entropy increase. (One can easily check that the operator C in (9)) given by (10) is not normal.) For example, consider equation (9) with some Hermitain interaction operator C , say $C = \sigma_z$ (Pauli z -matrix) with the same Hamiltonian and initial condition as before (see (10), (11)); see Fig. 4 for graphs (for the same value of $\gamma = 0, 1, \dots, 5$). We see that entropy monotonically increases and approaches its maximal value $\ln 2$.

Figure 4. Disorder-generating dynamics of the von Neumann entropy.

2.6 Dynamics of linear entropy

As we know, the von Neumann entropy approaches its minimal value, $\mathcal{S} = 0$, for pure states. This points to a connection between the degrees of purity and order in a system. How can one define purity of a quantum state? Pure states are represented by density operators of the form $\rho = |\psi\rangle\langle\psi|$. As any projector, such a state is an idempotent operator, i.e., $\rho^2 = \rho$. Since this projector is one dimensional, $\text{Tr } \rho = 1$. Hence, if a quantum state is pure, then $\mathcal{P}(\rho) \equiv \text{Tr } \rho^2 = 1$, and vice versa. The quantity $\mathcal{P}(\rho)$ is called purity of ρ . Purity equals one iff the state is pure.

On the basis of purity, one introduces a new sort of entropy, linear entropy (see, e.g.,³) given by

$$\mathcal{S}_L = 1 - \mathcal{P}(\rho). \quad (20)$$

This entropy behaves similarly to the von Neumann entropy:

- 1. $\mathcal{S}_L(\rho) = 0$ if and only if ρ is a pure quantum state.
- 2. For a unitary operator U , $\mathcal{S}_L(U\rho U^*) = \mathcal{S}_L(\rho)$.
- 3. The maximum of entropy is approached on the state $\rho_{\text{disorder}} = I/N$ and $\mathcal{S}_L(\rho_{\text{disorder}}) = 1 - 1/N$, where N is the dimension of the state space.

In particular, the linear entropy of an isolated quantum system is constant. Open quantum system dynamics can generate camel-like shapes of the linear entropy, cf. Figures 5 and 2 (a camel-like shape) as well Figures 6 and 3 (monotonic increase).

One of its advantages is that it is easier to calculate than the von Neumann entropy (To calculate the von Neumann entropy, one has to find the eigenbasis of ρ and this can be computationally difficult.) The main distinguishing feature of the linear entropy is straightforward coupling with purity of the quantum state. This sort of entropy is also used as a measure of *decoherence* (see, e.g.,^{77,78} for applications for analysis of experimental data). The latter can be treated as the loss of purity.

For a quantum physical system, typically open system dynamics leads to decoherence, loss of purity; linear entropy approaches one. The basic feature of biosystems is their ability to beat decoherence and increase states' purity - the camel-like behavior of the linear entropy.

For linear entropy we can formulate the analog of Theorem 3:

Decoherence

Figure 5. Order-stable (camel-like) behavior of the linear entropy (decoherence).

Theorem 3a. For GKSL-dynamics, the linear entropy gain during evolution is nonnegative, iff (equivalent) conditions (15), (18) hold.

For example, consider curves of unital dynamics in Fig. 4. Its evolution of the linear entropy is presented in Fig. 6.

3 Discussion

3.1 What type of open system dynamics has to be associated with biosystems?

It is useful to try to assign some biological meaning to unitality, $\mathcal{T}_t I = I$. In the N -dimensional case, we can consider the state $\rho_{\text{disorder}} = I/N$. This is the state of maximal disorder (with respect to the von Neumann and linear entropies), $\mathcal{S}(\rho_{\text{disorder}}) = \ln N$ and $\mathcal{S}_L(\rho_{\text{disorder}}) = 1 - 1/N$. The unital dynamics is characterized by transformation of the maximal disorder state into itself, i.e., $\mathcal{T}_t$ cannot decrease disorder and generate order of some degree. However, it is not clear whether a biosystem can be alive in the state of total disorder, ρ_{disorder} . Generally, we consider the unitality as a condition excluding the possibility of the camel-like dynamics for all possible states.

The camel-like dynamics of a quantum system represented by the curves in Fig. 2, 5 is a good candidate for modeling of living systems. The main problem is the absence of mathematical formalization of the camel-like behavior. Violation of the unitality condition implies only that, for some states, entropy has the camel-like form. But, generally non-unitality does not imply the camel-like dynamics for all states, as one would like to have for biological systems.

3.2 States of live systems

This interplay between the form of dynamics and states' features is a complex issue, since not only the description of possible interactions with environments (encoded in the coefficients of the Lindbladian), but even the description of the class of possible states $D_S(\mathcal{H})$ of a bio-system S is a difficult problem. It is natural to assume that $D_S(\mathcal{H})$ is a proper subspace of the space of all density operators $D(\mathcal{H})$. A similar problem is well known even in quantum physics. Textbooks may claim that all density operators correspond to physically realizable states, but experts know that only special quantum states can be prepared experimentally.

The states of our interest are limited to those compatible with life. Denote the space of such states by the symbol $D_{\text{life}}(\mathcal{H})$. Subclasses of the states correspond to the health (including aging) conditions of the life. The description of the mathematical

Decoherence

Figure 6. Disorder-generating dynamics of the linear entropy (decoherence).

structure of the space D_{life} is a complex problem. We mention one concrete question: Is $D_{\text{life}}(\mathcal{H})$ a convex set? We recall that the set $D(\mathcal{H})$ is convex and this fact has very important consequence for the basic probabilistic features of the quantum information processing^{79,80}. The environmental states describe the conditions of system's environment, but they are manifested only in the L -operator.

In view of the above consideration, maybe attempting to describe a class of dynamics that generate, for all states belonging to $D(\mathcal{H})$, the camel-like behavior of the von Neumann entropy is not at all a fruitful research strategy. Instead, we can define for each GKSL-dynamics the class of states $D(\mathcal{H}|\mathcal{E})$ generating the camel-like behavior; so $D(\mathcal{H}|\mathcal{E})$ is the union of the all such trajectories of the entropy of S for the environment $\mathcal{E}$. Then it is natural to suppose that

$$D_{\text{life}}(\mathcal{H}) \subset \bigcup_{\mathcal{E}} D(\mathcal{H}|\mathcal{E}),$$

with union w.r.t. all possible environments supporting alive-states. We remark that for the unital dynamical systems the set of states $D_{\text{life}}(\mathcal{H})$ is empty.

We have the following picture of the life-state evolution. Let ρ_0 be the initial state at the moment when S meets new environment $\mathcal{E}$ and let $\rho_0 \in D(\mathcal{H}|\mathcal{E})$. Then a camel-like trajectory of the system's entropy is generated and the steady state ρ_{stead} is approached. If $\mathcal{E}$ stable, then S is comfortable in it and the entropy is constant (with small fluctuations). Let now S meet a new environment $\mathcal{E}'$ (that can be generated, e.g., by change of some parameters describing the state of $\mathcal{E}$). Then if $\rho_{\text{stead}} \in D(\mathcal{H}|\mathcal{E}')$, then a new camel-like trajectory is generated and so on.

In principle, we can consider a life-evolution trajectory, starting with $\rho_0 = \rho_{\text{birth}} \in D(\mathcal{H}|\mathcal{E}_{\text{birth}})$. A life-trajectory consists of camel-like blocks, and the last block violates the camel-like structure of entropy: here entropy behaves in accordance with behavior of physical dissipating systems and entropy grows to the maximal value.

3.3 Adaptation to the environment: illustrative examples

3.3.1 A human adaptation to surrounding environment³²

Suppose that somebody, say, Ivan suddenly finds himself in an unknown forest; he shall find a possibility to feed himself, adapt to weather conditions, secure his life from animals and so on. At the first stage, he investigates features of the forest-environment and adapts his behavior to these features: disorder in his information representation of this context increases. Then he starts to explore the results of adaptation and his life becomes more ordered, up to stabilization to a steady state corresponding to this forest-environment.

This is an example for discussion of the meaning of the second hump of our entropy camel. From the curves in Fig. 2, we see that with the increase of the coupling constant the second hump disappears. It seems that it corresponds to the following situation: a biosystem S has adapted to the environment $\mathcal{E}$ and started to explore the features of $\mathcal{E}$. However, if γ is relatively small, S was not able to adapt to all basic features of the environment and in the process of exploration, S meets some new features of $\mathcal{E}$. So, the process of adaptation continues, but on a smaller scale. This generates the second hump and only then the state's stabilization. Of course, there can be many humps with decreasing amplitude.

3.3.2 A cell adaptation to lactose-glucose environment³⁴

Another example is the lactose-glucose metabolism in a cell. If the proportion of glucose-lactose in cell's environment is changed, e.g., the concentration of glucose goes down and the concentration of lactose goes up, a cell S should change the regime of glucose-lactose consumption: at this stage entropy increases, since S cannot immediately update the information on the concentrations. Then when S "becomes sure" that the glucose concentration became low, it starts to consume lactose and entropy goes to its minimum value. Then S approaches the steady state corresponding to lactose consumption.

3.3.3 Epimutations³⁵

In contrast to the previous examples, epimutation changes not only bio-information processing (change in gene expression), but even the physical structure of the cell as, e.g., promoter methylation and histone modifications. At the stage of, e.g., promoter methylation (as the reaction to a new environment) entropy increases, then it goes down and finally stabilizes.

3.3.4 Neuron interacting with electrochemical environment⁵⁸

Quantum information representation of a single neuron's state is briefly presented in section 4.3 (see⁵⁸ for details). However, a neuron s is not an isolated biosystem; it interacts with other neurons via electric signals as well as with the surrounding chemical environment, including a variety of hormones; denote this environment by $\mathcal{E}$. Thus we are again in the framework of the theory of open quantum systems. In our model, by being involved in some cognitive task the neuron s receives signals from $\mathcal{E}$. The entropy of the quantum information state increases. The neuron is "in doubts" and it tries to adapt its state to the signals coming from other neurons as well as to the chemical context. After this period of adaptation, s starts to fire synchronically with other neurons involved in the same cognitive task. The quantum entropy decreases to its minimum. The electric state of synchronic firing corresponds to the steady state in the quantum information representation.

In reality, a cognitive task is performed not by a single neuron, but by a neural network. In particular, synchronicity is achieved inside this network. Hence, a biosystem S is a neural network, its quantum information states are (generally entangled) states of neurons inside S . Synchronic firing corresponds to a steady state of S .

The second hump of the entropy curves can be generated according to the general scheme. If S is too weakly connected with other neural networks that are relevant to performance of the cognitive task, then, after the first stage of interaction and adaptation with $\mathcal{E}$, S can get signals which do not match the previous adaptation. They generate a new state update and a new hump that is essentially lower than the first one.

3.4 Concluding remarks

Stimulated by the famous book of Schrödinger¹ and further studies on applications of IT to biology (e.g.,^{7,8}), we consider a biosystem S as an information processor operating in the physico-informational environment $\mathcal{E}$. Since any alive biosystem cannot be treated as an isolated system, we proceed with the theory of open systems. Quantum theory of open systems is the most general formalism describing interaction of S and $\mathcal{E}$ containing classical theory as a special case. This is a methodological reason for employing the quantum information framework. The use of this framework is strongly supported by intensive quantum-like modeling outside of physics, in cognition, psychology, decision making, microbiology (see introduction of this paper). In paper⁵⁸, quantum-like representation of information by the brain was constructed as the superposition representation of uncertainty generated by neurons' action potentials. By using quantum information representation, a biosystem transforms complex nonlinear dynamics of electrochemical states into linear dynamics of quantum-like states (section 4.2). In contrast to dynamics generated by typical physical environments, this quantum-like dynamics does not lead a biosystem to the state of the maximal entropy.

We emphasize the role of the quantum master equations and specific quantum states resulting in the camel-like shape of the graph of quantum entropy (von Neumann and linear). We point to the condition of unitality of dynamics as the condition excluding the camel-like behavior of entropy and, hence, the possibility to use such systems for modeling interactions of biosystems and surrounding (information) environments. In this paper, dynamics was represented by completely positive maps (as is commonly used in quantum physics). However, biological application may involve more general dynamics, cf. with Diosi⁸¹ who "considered all positive dynamics, not restricted for the Lindblad-Gorini-Kossakowski-Sudarshan complete-positive subclass."

Returning to Schrödinger's book¹, we can say that the theory of open quantum systems provides the possibility to embed his speculations into the formal mathematical framework (at least to some degree).

4 Materials and Method

4.1 Dynamics of the state of a system interacting with its environment

As was already emphasized, any biosystem S is fundamentally open. Hence, dynamics of its state has to be modeled via an interaction with surrounding environment $\mathcal{E}$. The states of S and $\mathcal{E}$ are represented in the Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$. The compound system $S + \mathcal{E}$ is represented in the tensor product Hilbert spaces $\mathcal{H} \otimes \mathcal{K}$ ^{5,6}. This system is treated as an isolated system and in accordance with quantum theory, dynamics of its pure state can be described by the Schrödinger equation:

$$i \frac{d}{dt} |\Psi\rangle(t) = \mathbf{H} |\Psi\rangle(t), \quad |\Psi\rangle(0) = |\Psi\rangle_0, \quad (21)$$

where $\Psi(t)$ is the pure state of the system $S + \mathcal{E}$ and $\mathbf{H}$ is its Hamiltonian. This equation implies that the pure state $|\Psi\rangle(t)$ evolves unitarily: $|\Psi\rangle(t) = U(t) |\Psi\rangle_0$. Here $U(t) = e^{-it\mathbf{H}}$. Hamiltonian (evolution-generator) describing information interactions has the form

$$\mathbf{H} = H_S \otimes I + I \otimes H_{\mathcal{E}} + H_{S,\mathcal{E}},$$

where $H_S \in \mathcal{L}(\mathcal{H})$, $H_{\mathcal{E}} \in \mathcal{L}(\mathcal{K})$ are Hamiltonians of S and $\mathcal{E}$, and $H_{S,\mathcal{E}} \in \mathcal{L}(\mathcal{H} \otimes \mathcal{K})$ is the interaction Hamiltonian. This equation implies that evolution of the density operator $R(t)$ of the system $S + \mathcal{E}$ is described by the von Neumann equation:

$$\frac{dR}{dt}(t) = -i[\mathbf{H}, R(t)], \quad R(0) = R_0. \quad (22)$$

However, the state $R(t)$ is too complex to be handled consistently: the environment includes too many degrees of freedom (both physical and informational). Researchers are interested only the state of S ; its dynamics is obtained via tracing of the state of $S + \mathcal{E}$ w.r.t. the degrees of freedom of $\mathcal{E}$ (see^{5,6}):

$$\rho(t) = \text{Tr}_{\mathcal{K}} R(t). \quad (23)$$

Generally, this dynamics is mathematically very complicated. A variety of approximations is used in applications. As was stressed in section 2.2, one of the most useful approximations is given by the Gorini-Kossakowski-Sudarshan-Lindblad equation.

4.2 Emphasizing linearity of the quantum model

Quantum-like modeling is not an attempt to reduce the biological functions to quantum physics. Here classical biophysical processes, in genes, proteins, cells, bodies, brains are represented within quantum information theory.

One of the advantages of this representation is its linearity. The quantum state space is a complex Hilbert space and dynamical equations are linear differential equations. The classical biophysical dynamics beyond quantum information representation is typically nonlinear and very complicated. The use of the linear space representation simplifies the processing structure. The use of the quantum information representation means that generally large clusters of classical biophysical states are encoded by a few quantum states: the quantum structure arises as the result of coarse graining. It leads to essential information compressing. It also implies increase of stability in state-processing.

This is a rather unusual viewpoint on the use of quantum information representation as lowering complexity and instability of information encoding and processing.

4.3 Quantum information representation for the electrochemical processes in brain's neural networks

Quantum-like models are formal operational models that can be used for the description of information processing in biosystems (in contrast to studies in quantum biology - the science about the genuine quantum physical processes in biosystems). At the same time, it is important to discuss possible connection of quantum information processing in a biosystem with the electrochemical processes in it. This is an interesting and very complicated problem. An attempt to proceed in this direction was presented in paper⁵⁸ for brain's neural networks. The quantum information formalization of states of neural networks is connected with electrochemical processes in the brain. The key-point is representation of uncertainty generated by the action potential of a neuron as quantum(-like) superposition of the basic mental states corresponding to a neural code, see Fig. 1 for illustration.

Consider a single neuron S . Its quantum information state corresponding to the “classical neural code” *quiescent and firing*, 0/1, can be represented in the two dimensional complex Hilbert space $\mathcal{H}_{\text{neuron}}$ (qubit space). At a concrete instant of time neuron's state can be mathematically described by superposition of two states, labeled by $|0\rangle, |1\rangle$:

$$|\psi_{\text{neuron}}\rangle = c_0|0\rangle + c_1|1\rangle. \quad (24)$$

where $\langle 0|1\rangle = 0$ and $\langle \alpha|\alpha\rangle = 1, \alpha = 0, 1$. The coefficients c_0 and c_1 are complex amplitudes for potentialities that S is quiescent or firing. Superposition represents uncertainty in action potential, “to fire” or “not to fire”. This superposition is the quantum information representation of physical, electrochemical uncertainty.

The states of a group of neurons S , say a neural network in the brain, is described by the tensor product of single neuron states; generally these are entangled states. (Entangled states are basic states for quantum computing² that explores state’s inseparability. Thus, in our quantum-like model the brain also explores this computational resource. However, brain’s functioning is not based on the algorithmic information processing (see, e.g., Penrose⁶³ for a discussion)):

$$|\Psi\rangle = \sum_{\alpha_j=0,1} C_{\alpha_1 \dots \alpha_n} |\alpha_1 \dots \alpha_n\rangle, \quad (25)$$

where the complex amplitudes $C_{\alpha_1 \dots \alpha_n}$ are normalized by 1.

5 Proof of theorem on quantum entropy increasing

Proof. We recall that in this paper we proceed with finite dimensional state spaces. Consider the space of dimension d . By the monotonicity of quantum Kullback–Leibler information (relative entropy), $S(\mathcal{T}\rho || \mathcal{T}\rho') \leq S(\rho || \rho')$, where $S(\rho || \rho') = \text{Tr}[\rho \log \rho] - \text{Tr}[\rho \log \rho']$. Then,

$$\begin{aligned} S(\rho || I/d) &= \text{Tr}[\rho \log \rho] - \text{Tr}[\rho (-\log d)] \\ &= \log d - (-\text{Tr}[\rho \log \rho]) = \log d - S(\rho). \end{aligned}$$

If $\mathcal{T}$ is unital, i.e., $\mathcal{T}I = I$, we have

$$\begin{aligned} S(\mathcal{T}\rho) - S(\rho) &= [\log d - S(\mathcal{T}\rho || I/d)] - [\log d - S(\rho || I/d)] \\ &= S(\rho || I/d) - S(\mathcal{T}\rho || \mathcal{T}(I/d)) \geq 0. \end{aligned}$$

Thus, we conclude that

$$S(\mathcal{T}\rho) \geq S(\rho),$$

if $\mathcal{T}$ is unital. Conversely, if

$$S(\mathcal{T}\rho) \geq S(\rho)$$

for all states ρ , we have $S(\mathcal{T}(I/d)) \geq S(I/d) = \log d$ so that $\mathcal{T}(I/d) = I/d$. Thus, we have proven that $S(\mathcal{T}\rho) \geq S(\rho)$ for all states ρ if and only if $\mathcal{T}$ is unital.

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Figures

Figure 1

Illustration for quantum-like representation of uncertainty generated by neuron's action potential (originally published in58).

Figure 2

Order-stable (camel-like) dynamics of the quantum (von Neumann) entropy.

Figure 3

Order-generating dynamics of the quantum (von Neumann) entropy for maximally disordered state.

Figure 4

Disorder-generating dynamics of the von Neumann entropy.

Figure 5

Order-stable (camel-like) behavior of the linear entropy (decoherence).

Figure 6

Disorder-generating dynamics of the linear entropy (decoherence).

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