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A Conceptual View onto the Physical Foundations of Astrobiology
Provisional Outline of a Research Program

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> De natura rationis non est res, ut contingentes;
> sed, ut necessarias, contemplari.
> Spinoza: Ethica 2p44[1]

1 Introduction

At the same time, when talking about the *origin of life* one is also talking about the *definition of life* in the first place. And when defining *life on the planet Earth* one is also defining *life in the Universe* altogether. In other words: There is a close relationship between an arbitrary planet in an arbitrary solar system and cosmology (thus local and global aspects of the Universe) on the one hand, and between physics and biology on the other. Hence, astrobiology has not only its methodological as well as systematic foundations in biology, but also in physics proper. And it moreover possesses a metaphysical horizon, because, if there is a choice among classes of Universes in the beginning (defined in cosmological terms), there is a discrepancy between the actual and the possible – and hence, there is not only energy, but information, too.

The problems raised here are rather ancient problems indeed: Their scientific discussion can be traced back as far as to Aristotle who connects topics like the origin of life with cosmology itself. For him, the Universe has a specific purpose. This is mainly because Aristotle cannot actually imagine that the Universe could spontaneously assemble itself generating the high degree of complexity that can be observed. What he did not know at the time was that despite the results of a first inspection, the underlying selection mechanism is well able to create order out of disorder, given enough time.[2] For him, it is the *soul* (psyche) instead that is the organizing principle of living forms. It is thus steering dynamical processes within organisms by being functionally related to other organs, being responsible then for growth, preservation, aging, motions and so forth. Hence, the soul can be visualized as the propulsion, the driving mechanism, for the organic metabolism that gains the properties of a cybernetic system as can be seen in terms of the heart-lung-cycle given by Aristotle comprising of feedback loops whose deeper meaning nevertheless remained hidden for quite a while.[3]

Almost 2300 years later, after a long historical development in the achievements of the sciences (and the advent of Darwinian theory), it is Schrödinger who in his well-known book on the nature of life comes back to the point that physics underlies what can be observed in phenomenological terms.[4] With his concept of what he calls "aperiodic crystals" he lays the ground for the later results by Watson,

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[1] „It is in the nature of reason to visualize the things not as accidental (contingent), but as necessary." Baruch de Spinoza: Ethica Ordine Geometrico Demonstrata (Ethics demonstrated according to the geometrical method), part 2, proposition 44. Quoted here from ed. Konrad Blumenstock, Wissenschaftliche Buchgesellschaft Darmstadt, 1980, vol. 2, 232/233.

[2] See in detail: Armand Marie Leroi: Die Lagune oder Wie Aristoteles die Naturwissenschaften erfand. Theiss (Wissenschaftliche Buchgesellschaft Darmstadt), 2017, 94, 97. (par.)

[3] Ibid., 177–195, Appendix B4: 431 sq. (par.)

[4] Erwin Schrödinger: What is Life? The Physical Aspects of the Living Cell. (Trinity College Dublin, 1943), Cambridge University Press, 1967.

Crick and others on the structure of DNA. He notes that entropy and order are deeply connected to each other, and he defines an organism as one that can be maintained by extracting order from the environment.[5] So he can discuss the two aspects of producing order from disorder as well as producing order from order, respectively. Within this framework, the generation of order, asking for a decrease of the total entropy of a system (as we know today) does not actually contradict the second law of thermodynamics, because the entropy balance of the complex organization within a living organism is well-compensated by the production of heat which is released into the environment.

The problem of energy and entropy balance was however not really topical in the essentially biological discussion of Darwinian principles ongoing since their introduction by Darwin himself in 1859. But a recent re-conceptualization of Darwinism presented by Stephen Jay Gould in 2002 refers explicitly to the physical foundations of this theory. Practically all modern protagonists dealing with the formation of structure and the models of self-organization, mainly put forward in the seventies and eighties of the last century, are named in this book, obviously inspired by the results of the Santa Fe school.[6]

However, Darwin's theory (in the nowadays perspective) starts from RNA and DNA molecules. And today, we would prefer a picture of the origin of life that is *primordial* in the sense that it does not presume the existence of complex chain molecules of this type. Hence, it is not so much the material that is important for the onset of living forms, but instead, it is the *co-operative dynamics* (co-evolution) among system-like structures that initializes life in the strict sense. Probably, we could couple the beginning of life to the effects of selection for which complex structures such as RNA or DNA would be necessary, while within the stage of onset selection is nothing but a process of taking mutually into account what the essential conservation laws do actually prescribe. If the Universe is filled with entities that extract work by measuring displacements from equilibrium in the environment which are sources of energy (and information), as Stuart Kauffman claims[7], then life as we know it differs only in terms of the specified interaction between the micro-level and macro-level of organisms, joining the evolution of genotype to that of phenotype. We will come back to this.

But it was not before 1997 that all these first rudiments of insight were put together in the shape of a cosmological theory drawing heavily on the interdisciplinary context. This was when Lee Smolin published his book on the life of the Universe.[8] From the beginning on he notes that "Physics must underlie and explain biology because living creatures, like all things in the universe, are made out of atoms which obey the same laws as do every other atom in the world. An approach to physics that does not make the existence of life comprehensible must eventually give way to one that does."[9] On the other hand, what is certainly invariant in the physical description of nature is *thermodynamics*. From this field of physics we learn something else: "Nothing can live in an environment in thermal equilibrium. If life is to exist there must then be regions of the universe that are kept far from thermodynamic equilibrium for the billions of years it takes for life to evolve. We then want to ask, What is required of the universe so that it contains such regions? The answer to / this question is easy. There

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[5] Ibid., 60 sqq., 68–73. (par.)

[6] Stephen Jay Gould: The Structure of Evolutionary Theory. Belknap of HUP, Cambridge (Mass.), London, 2002. Gould mentions not only the line of thinking originally introduced by D'Arcy Wentworth Thompson: On Growth and Form. CUP 1917, including Conrad H. Waddington who published together with Erich Jantsch: Evolution and Consciousness. Human Systems in Transition. Addison-Wesley, Reading (Mass.), 1976, assembling a large number of other protagonists following the same line of thinking in self-organization and chaos theory such as René Thom: Structural Stability and Morphogenesis, Benjamin, Reading (Mass.), 1975, Ilya Prigogine who published together with Grégoire Nicolis: Self-Organization in Non-Equilibrium Systems, Wiley-Interscience, New York etc., 1977, and Brian Goodwin who published together with Richard Sole: Signs of Life. How Complexity Pervades Biology. Basic Books, New York, 2002, but also protagonists of the Santa Fe school such as Stuart Kauffman: The Origins of Order, OUP 1993, and Per Bak: How Nature Works: The Science of Self-organized Criticality. Copernicus, Göttingen, 1996.

[7] Stuart Kauffman: Investigations. OUP 2000, 82.

[8] Lee Smolin: The Life of the Cosmos. OUP 1997.

[9] Ibid., 25.

must be things in the universe that are much hotter than the rest of it, and are able to maintain themselves as constant sources of light and heat for enormous periods of time. […] The existence of stars is thus the key to the problem of why the cosmos is hospitable to life."[10]

This line of argument is purely physical and very economical indeed, because it summarizes sober "general" results and their conclusion without referring to any heuristic or non-physical foundation. Now, if we make existence topical, then there must have been something that caused this existence in the first place. Existence demands emergence and development of what has emerged. We can call this "evolution". In other words: *The Universe becomes historical*. But note also that "[h]istory arises when the space of possibilities is too large by far for the actual to exhaust the possible."[11] Hence, contrary to what would have been the opinion for a large number of centuries, in our nowadays perspective, the Universe is not ergodic at all, but it is intrinsically *non-ergodic*.[12] From this Smolin concludes: "What then surely is most new about our modern understanding of life is the idea of evolution, for it enables us to see life not as an eternally repeating cycle, but as a process that continually generates and discovers novelty. And, by the same token, what is most new about modern cosmology is the discovery that the universe is also evolving."[13]

At a fundamental level, the known laws of physics will produce the conceptual framework in order to discuss this cosmological evolution. But there is the possibility that additional laws might be found which are characteristic for more complex forms in the Universe. One hint can be found within the *systemic perspective*. "The basic understanding that life on this planet constitutes an interconnected system must be considered to be one of the great discoveries of science."[14] And Smolin comes back to thermodynamics with a view to practical applications of the systemic framework: "Thermodynamics provides the simplest way to distinguish clearly between a planet with life, such as Earth, and dead planets such as Mars and Venus. The reason is that the atmosphere of the Earth is permanently in an enormously improbable state, very far from thermodynamic equilibrium. […] We may conclude from this that there must be some outside agents that are maintaining the earth's atmosphere permanently in such an unstable state far from equilibrium. There are such agents, they are the living things of the biosphere. For the great cycles that continually replenish the oxygen, carbon, and other elements of the biosphere are driven by the metabolic processes of living things. / If a planet has life, one can see it easily by determining whether its atmosphere is in thermal equilibrium. […] If we can get a spectrum of the light from a planet, we can see immediately if it has life or not by analyzing it to find the composition of the atmosphere. […] The basic mechanisms of natural selection thus imply that any planet with only a little life must be in a transient stage: any stable occupation of a planet by life must involve the whole planet. / As in similar cases such as the disks of spiral galaxies, the only possible explanation for the stability of such a non-equilibrium system is the existence of feedback mechanisms that control the rates of the various cycles involved."[15]

It is here where Smolin refers to ongoing work of the Santa Fe school: "What is new [in Per Bak and Stuart Kauffman] is the idea that when one has many species that evolve together in an ecosystem, new collective effects emerge which determine things like the rates at which old species become extinct and new ones appear. / What Bak, Kauffman, and others have accomplished by taking a global view of evolution is the beginnings of a theory in which the Gaia hypothesis is only the rare and extreme case of a completely general phenomenon, which is that the evolution of the different species are coupled to each other. […] It can happen, for example, that several species can evolve together to reach stable symbiotic relationships. Lynn Margulis has proposed that such events may account for the origins of both eukaryotic cells and multi-celled creatures."[16]

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[10] Ibid., 28 sq.

[11] Stuart Kauffman: At Home in the Universe. The Search for the Laws of Self-Organization. OUP 1995, 186.

[12] Stuart Kauffman: Investigations, op. cit., 144.

[13] Smolin, op. cit., 143.

[14] Ibid., 146.

[15] Ibid., 147–149.

[16] Ibid., 150–151.

As to the authors mentioned this looks like an exclusively American perspective. And indeed, it would be necessary to also quote the European contributions of the Paris school (Thom) and Brussels school (Prigogine) as to that, including the relevant colleagues involved at the time. Note the difference: While the Santa Fe approach discusses *self-organized criticality* for phenomena which are observable in the common configuration space (Euclidean space-time), Prigogine (and Thom) putting forward models of *structure formation*, together with the advocates of *chaos theory* (Mandelbrot, Feigenbaum et al.) speak about self-organization in phase spaces. The interaction and possibly joint origin of these approaches are not yet sufficiently clarified (and in fact, rarely discussed). As to the underlying astrophysics however, the idea is obvious: "There are hot stars radiating into cold space. The biosphere can organize itself because it finds itself in the middle, and is able to harness the flow of energy to drive the processes that continually form the complex molecules that are necessary for life. […] This line of thought suggests that *there should be a general theory of self-organization, which is based on the thermodynamics of systems* that are far from equilibrium because they are infused by a steady flow of energy. Such a theory might tell us that in these situations the level of organization, rather than of entropy, increases steadily in time. [Moreover] [a] system must have a potential for organization. […] What a flow of energy does is to change the game, so that improbably structured configurations become probable."[17]

For the thermodynamic non-eqilibrium the systemic perspective will offer the possibility to introduce network-shaped interactions among a multitude of active agents that "play the game of evolution".[18] The necessary ingredient for this is the notion of "cycle" processes (or loops). Smolin refers here to the work of Harold Morowitz to whom we will come back in more detail later. Cyclic interactions turn out to be the most fundamental form of interactions at the roots of evolution: "Such cycles underlie the basic processes of the biosphere, and they involve all of the basic elements of life. Morowitz proposes that these cycles are more fundamental than life; and will arise in any chemical system that has a steady flow of energy through it. According to him, the formation of these cycles may have been the first step in the self-organization of the biosphere, occurring perhaps even before the evolution of the proteins and nucleic acids."[19] And Smolin continues: "Life perhaps might be seen to have evolved a way to ride these flows and / cycles the way a surfer rides the flow of energy in water waves. […] To get to life, then, we need to add several more elements to the basic picture of how open systems may organize themselves. The first is that living organisms always have clear boundaries between themselves and the outside world. […] at the level of the biosphere as a whole, the material that makes up the biosphere is kept isolated from the rest of the universe by the action of the Earth's gravitational field, while the atmosphere and ozone layer serve partly to control its exchange of radiation with the outside universe.

A second point is that if a system is to reach a steady state then there must be some stability […] So we expect feedback to be a ubiquitous element of far-from-equilibrium, open systems, in which a stable configuration has been reached."[20]

Although in Smolin's approach the systemic perspective is not being discussed in detail, but certainly implicit all the time, the idea showing up is that in the end, *the Universe is the maximal system* which is structured into a large set of sub-systems (in other words: is *a system of systems*).[21] What is

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[17] Ibid., 153. (my emphasis)

[18] Rainer E. Zimmermann: Metaphysics of Emergence. Part 1: On the Foundations of Systems. xenomoi, Berlin, 2015.

[19] Smolin, op. cit., 154.

[20] Ibid., 154 sq.

[21] For a proposal concerning an appropriate definition of systems while referring to Stuart Kauffman see Zimmermann, op. cit., 27 sq. – There is one caveat however with respect to Kauffman's definition of agents which is implicit in the definition of systems, cf. ibid., 37. This will be discussed elsewhere at a later occasion. Note also that the concept of "a system of systems" implies possible applications of category theory.

also implicit only in this approach is the concept of information.[22] Nevertheless, all important aspects of a global approach to cosmological evolution of which biological evolution turns out to be a specialized complex case, can be obtained from the book: "I would like to call a *self-organized, non-equilibrium system* one which is: a distinguishable collection of matter, with recognizable boundaries, which has a flow of energy and possibly matter, passing through it, while maintaining, for time scales long compared to the dynamical time scales of its internal processes, a stable configuration far from thermodynamic equilibrium. This configuration is maintained by the action of [autocatalytic] cycles involving the transport of matter and energy within the system and between the system and its exterior. Further, the system is stabilized against small perturbations by the existence of feedback loops which regulate the rates of flow of the cycles."[23]

As to the specific difference of living and non-living systems (in order to avoid vitalism) Smolin continues: "[A] galaxy is a self-organized structure, but it is not alive. For something to be alive it is certainly necessary that it be part of a self-organized, non-equilibrium system. But no definition of life could suffice that ignored the role that information and control play in the workings of a living cell. […] The first is that in a living cell the rates at which its chemical processes take place are controlled by enzymes which are proteins. The second is that the synthesis of the enzymes is made and controlled by information that is coded symbolically in the structures of certain nucleic acids. The third is that the cell can reproduce itself, and that, when it does so, the nucleic acids coding it also reproduce themselves. /

We may then make the following definition: A *living system* is

A a self-organized non-equilibrium system *such that*
B its processes are governed by a program which is stored symbolically *and*
C it can reproduce itself, including the program.

What I think most recommends a definition such as this one is that it grounds the existence of life in physics […] far from equilibrium thermodynamics. At the same time, it makes clear to what extent living things have properties which […] cannot be understood purely in terms of the general theory of non-equilibrium systems.[24]

But if the cell satisfies the above definition, why do galaxies not? Or the Universe altogether as to that? The problem is how far the parts A through C of the definition can be carried over to large regions of the Universe that consist of matter (energy-mass) and information (entropy-structure). Smolin argues: "As to the first part of the definition, it may very well be reasonable to regard the whole universe as a self-organized system. But to push the analogy to the point that the universe fits the definition of a living system, we would have to regard the laws of nature themselves as a program. I don't think that this could be sustained. For one thing there is, as far as we know, no sense in which the laws of nature could be represented symbolically, as something analogous to a computer program. […] It may turn out in the end that the laws of nature are representable by an algorithmic system, but I do not know any reason why this must be so. Furthermore, there are very interesting arguments, such as those raised by Roger Penrose in his recent books, that this should be impossible.[25]

Referring to Penrose here means that what is being disputed is the existence of a strict formal algorithm which organizes the world similar to a computer program. However, some possible solutions (such as a straightforward generalization of algorithmic programs derived from quantum information, or a symbolic storage in terms of gravitational signatures, perhaps hidden in black holes – what by the way, would also support Smolin's cosmological selection conjecture[26]) might be able to circumvent

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[22] This appears to be the rule in general as far as the prevalent literature is being concerned. One exception may be the important book by Marcello Barbieri: The Organic Codes. CUP 2003, dealing with the concept of reconstruction from incomplete information. Here he even introduces the concept of meaning, though mostly (but not exclusively) with a focus to fully developed cell structures.

[23] Smolin, op. cit., 155.

[24] Ibid., 156.

[25] Ibid., 157.

[26] Rainer E. Zimmermann: Cosmological Natural Selection Revisited. Some Remarks on the Conceptual Conundrum and Possible Alleys. http://www.arXiv.org/pdf/physics/0304053 (2003) See also id.: The Modeling of Nature as a Glass Bead Game. In: Eeva Martikainen (ed.), Human Approaches to the Universe. An Interdisciplinary Perspective. Agricola Society, Helsinki, 2005, 43–65.

this. As to the concept of information with a view to physics, José M. Díaz Nafría and myself have collected some results from fields that are rarely combined until now.[27]

Finally, Smolin concludes: "It is thus fascinating to note that a universe that has the capacity for efficient star formation is already going to have the basic ingredients necessary to turn self-organized non-equilibrium systems into living systems. […] the universe as a whole must itself be a self-organized, non-equilibrium system. The reason for this is that it is impossible to have a self-organized, non-equilibrium system which exists permanently inside a larger system which is itself in thermal equilibrium. [open systems need an environment that is also not in equilibrium] / It then seems that our life is situated inside a nested hierarchy of self-organized systems that begin with our local ecologies and extend upwards at least to the galaxy. Each of these levels are non-equilibrium systems that owe their existence to processes of self-organization that are in turn driven by cycles of energy and materials in the level above them."[28]

2 Emergent Complex Systems

Once, we decide to approach the problem of initial emergence in terms of systems, we have the following two-fold situation: *On the one hand*, we have to look for a plausible mechanism of emergence for those networks that define the nucleus of systems in the first place. *On the other hand*, even for fundamental systems of this kind, thermodynamics must be valid after all. Hence, we have also to look for a plausible mechanism of emergence for thermodynamics itself. The basic idea is the following: If we share the viewpoint that concepts like "system" (and emergence, matter, information, space, time as to that) are simply conceptualizations of observable entities that are ill-determined in ontological terms, but that are practical notions suitable for the building and communicating of theories (always given that theories are sets of consistently defined propositions), then theories of nature are to nature what the picture is to the object of which it is a picture. In other words: We always deal with the mapping of mappings rather than with a concrete type of reality. This nested hierarchy of mappings is what we call "actuality" (which is the world as it is conceptualized according to what we can observe). Alternatively, we can talk of "modality" (a concept introduced originally by Spinoza for visualizing the world in terms of the two attributes of substance that are accessible to human beings: matter and mind, respectively). This is significantly different from what we call "reality" in the strict sense, when meaning the world as it is independent of human observations. Hence, the most we can do is to describe the world's actuality according to the principles of the sciences (providing the appropriate mapping techniques) – this is included in the field of sceptical philosophy – and then to heuristically extend our research to the foundation of actuality which is reality proper. This is included in the field of speculative philosophy. We can say that we understand the emergence of an entity in nature, if we can derive it from its foundations. The problem is that we can only derive something that is consistently conceptualized before. But as we can clearly realize, the concepts we use in order to formulate our theories are constrained to the domain of actuality. In a sense, the corresponding entities could be included in the domain of reality to a certain extent, but the latter domain will be incredibly larger than the former domain. Hence, our scientific language is not adequate for describing the foundations. This is why we have to find a suitable interface between the two which is at the same time the starting point for theories concerning actuality.

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[27] Rainer E. Zimmermann, José M. Díaz Nafría: Emergence and Evolution of Meaning: The GDI Revisiting Program. Part 1: The Progressive Perspective: Top-Down. Information, 2012, 3, 472–503. (doi: 10.3390/info3030472) and also José M. Díaz Nafría, Rainer E. Zimmermann: Emergence and Evolution of Meaning: The GDI Revisiting Program. Part 2: The Regressive Perspective: Bottom-Up. Information 2013, 4, 240–261. (doi: 10.3390/info4020240) as well as Rainer E. Zimmermann, José M. Díaz Nafría: The Systemic Perspective as a Paradigm for Unified Approaches in the Sciences. (Panel I of the wcsa2012 conference, Vienna) In: Giulia Mancini, Mariarosalba Angrisani (eds.), Mapping Systemic Knowledge, Lambert Academic, Saarbrücken, 2014, 14–34.

[28] Smolin, op. cit., 158 sq.

As we notice now that in the beginning it is necessary to assume the validity of the system paradigm as well as of thermodynamics in the first place, we have to ask for the position of this required interface.[29] Because the line of argument is somewhat involved here, we shortly refer to a former passage of my book on systems quoted above[30] in order to clarify the general idea without going too much into detail. (Some of the issues utilized are not yet sufficiently clarified in theory.)

Obviously, the important starting point of systems is their underlying network of interacting agents.[31] Following an idea of Stuart Kauffman's, we think of *agents* in this generalized sense as self-reproducing, auto-catalytic systems which achieve a new kind of closure in a given space of catalytic and work tasks propagating work out of non-equilibrium states and playing natural games according to the constraints of their environment.[32] In particular, (physical) space is visualized then, as being comprised of autocatalytic autonomous Planck scale agents co-evolving with each other serving at the same time as some sort of crystallization of seeds of classicity (in the physical sense). This co-evolution is taking place according to what Kauffman calls *4th law of thermodynamics*: The maximum growth of the adjacent possible in the flow of a non-ergodic Universe maximizes the rate of de-coherence and thus the emergence of classicity. There is also a hierarchy of such agents depending on the explicit complexity of those in question ("higher-order agents"). Games of various types of agents are nicely illustrated by Szabó and Fáth.[33] But on the fundamental level of physics, Kauffman mentions the possibility to visualize *spin networks* as knots acting on knots to create other knots in rich coupled cycles not unlike a metabolism. Hence, they (or their constituents) show up as a sort of "fundamental agents".[34]

If we take up the viewpoint of Kauffman's seriously, then it appears to be straightforward to find the fundamental agents in the loops of *loop quantum gravity* (and the associated *quantum information theory*) in the first place: This is because it is the loops which combine in order to form spin networks. In fact, six of them co-operate in order to produce one hexagon of the network. The conceptual reason for this is that the associated entropy satisfies the criterion for a thermodynamic cycle process such that

$$\tfrac{1}{4}\, l_p^2 \int da \leq 0,$$

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[29] In earlier discussions I have spoken of the „injection of structure“ into the vicinity of the cosmological Big Bang, at a time, when it was fashionable to apply Prigogine's approach to relativity theory. See e.g. Rainer E. Zimmermann: The Lepton Brusselator. Creation of Structure in the Early Universe. J. Gen. Rel. Grav. 14 (11), 1982, 1051–1060. Also: id.: Homogeneous Cosmologies and their Stability Behaviour. New Physics (Korean Physical Society), 22 (3), 1982, 291–315. And finally id.: Non-Equilibrium Thermodynamics of Cosmological Event Horizons. In: Proc. Annual GAMM Meeting, Hamburg, ZAMM 64 (4/5), 1984, T402–T404.

[30] Taken here from Metaphysics of Emergence, op. cit., 37–46.

[31] We shortly recall the above-mentioned definition from my book: "We call *system* a network of interacting agents producing a space with a well-defined boundary that is open in the sense of thermodynamics."

[32] This is referring to an earlier manuscript version of Kauffman's book „Investigations“, cf. the address www.santafe.edu/sfi/People/ kauffman/Investigations.html. In the actual book version, autonomous agents are defined as self-reproducing systems which can at least perform one thermodynamic work cycle.

[33] György Szabó, Gábor Fáth: Evolutionary Games on Graphs. www.arxiv.org/pdf/cond-mat/0607344 (2006)

[34] Obviously, this remark has not become part of the book version. (Stuart Kauffman: Investigations. Oxford University Press, 2000) But without doubt, the idea has been to visualize fundamental systems as fundamental agents on the Planck level. Cf. Investigations, op. cit., 253–265. The quotation goes back to the original paper from which the book manuscript eventually derived: Santa Fe institute, working papers, 96–08–072, 162 sq. In his earlier books, Kauffman does not mention this explicitly, probably because their publication preceded Kauffman's co-operation with Lee Smolin. (Stuart Kauffman: The Origin of Order. Oxford University Press, 1993. And also id.: At Home in the Universe. Oxford University Press, 1995.) See also more recently Stuart Kauffman, Lee Smolin: A possible solution to the problem of time in quantum cosmology, www.arxiv.org/pdf/gr-qc/9703026 and id. & id.: Combinatorial dynamics in quantum gravity, www.arxiv.org/pdf/hep-th/9809161 . I have summarized some of the aspects in Rainer E. Zimmermann: Classicity from Entangled Ensemble States of Knotted Spin Networks. A Conceptual Approach. www.arxiv.org/pdf/gr-qc/0007024

where the integral is a closed path integral (loop integral) and *a* is the surface area generated with respect to one hexagonal fragment of the spin network. (It is l_P the Planck length.) By the definition of loops above we clearly recognize that this procedure is not referring to some physically "vacuous" geometrical meaning, but that instead, this geometrical picture is physically loaded due to the parallel propagator with its gravitational or curvature connotation, respectively, and the explicit group action involved: Hence, with a *loop* we mean here a closed curve α such that $T[\alpha] = - \mathrm{tr}\, [U_\alpha]$, where

$$U_\alpha (s_1, s_2) \sim P \exp \{ \int^{s2}_{s1} A_\alpha (\alpha(s))\, ds \}$$

is the parallel propagator of the vector field A_α along α defined by (the s_i being points of α)

$$d/ds\, U_\alpha (1, s) = da_i(s)/ds\, A_i(i(s))\, U_\alpha (1, s).$$

The SO(3)-field A is here essentially the difference of the SU(2)-spin connection and the extrinsic 3-curvature called *real Ashtekar connection*:

$$A_i^j (x) = \Gamma_i^j (x) - k_i^j (x).$$

The important result (Rovelli) is that *each spin network state can be decomposed into a finite linear combination of products of loop states.*

Obviously, this bears a strong resemblance to the classical Wilson loop representation (hence, we think here of a kind of *loop transport* according to Stuart Kauffman's idea of agents), and is also essentially a Feynman-type integral which gives the probability for a (physical) system to go from one state to another state:

$$< x2, t2 \mid x1, t1 > = \int^{XN}_{X1} D(x(t)) \exp i/\hbar\, S,$$

where S is he action of the form

$$S := \int^{t2}_{t1} dt\, L(x, x').$$

Here, L is the Lagrangian. (The probability is the above expression squared. This is equivalent to the Schrödinger picture of quantum physics on the one hand and a model for quantum computation on the other.) As Freidel and Krasnov (as early as 1999) as well as Reisenberger and Rovelli (in 2000) have shown, spin networks and spin foams, respectively, can be visualized as Feynman integrals of that sort such that the formal Feynman perturbation series of the partition function

$$Z = \int D \phi \exp (- S[\phi])$$

is given by

$$Z = \Sigma_J\, N(J)\, \Sigma_e\, \Pi_{f \in J} \dim a_f\, \Pi_v\, A_v(e),$$

where J is a 2-complex, and the vertices, edges, and faces are labelled accordingly. It is N(J) the number of vertices of J divided by the number of symmetries of J.

There is a number of important cross-relationships which connect the notion of loops with the notion of knots: Louis Kauffman's bracket algebra (the boundary algebra of containers and extainers) turns out to be the precursor of the Temperley-Lieb algebra important in order to construct representations of the Artin braid group related to the Jones polynomial in the theory of knot invariants.[35] As

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[35] For more details concerning Kauffman see Rainer E. Zimmermann: Matter and Information as Attributes of Substance. Eur. Phys. J. Special Topics 226, 2017, 177–180. Also id.: Topoi of Systems. On the Onto-Epistemic

the elementary bracket algebra is to *biologic* what Boolean logic is to classical logic, this has important epistemological consequences. On the other hand, the Jones polynomial can itself be visualized in terms of quantum computers, because a similar partition function of type $Z_K = < \text{cup} \mid M \mid \text{cap} >$ with creation and annihilation operations, respectively,

$$\text{cup} := \mid a > : C \to V \otimes V,$$

$$\text{cap} := < b \mid : V \otimes V \to C,$$

M being the braiding, and $< K > := \Sigma_\sigma < K \mid \sigma > d^{||\sigma||}$, can be related to the process of quantum computation (as can, by the way, the spin network formalism itself.) As spin networks are nothing but graphs, the *agency* in question here is motion on graphs or *percolation of energy and information in networks* such that phase transitions can be represented in terms of an appropriate cluster formation of connected components. This is what points to a close relationship to *cellular automata* utilized for the simulation of evolutionary processes (cf. Conway's game of life or Wolfram's approach). Stuart Kauffman has associated this with the emergence of collectively autocatalytic sets of polymers, and in fact with the onset of forming classicity with regards to physics.

But there is still another point to that: In the approach of Barrett and Crane (1997[36]), the idea is to generalize topological state sum models in passing from three to four dimensions by replacing the characteristic SO(3) group with SO(4), or its appropriate spin covering, SU(2) x SU(2), respectively. The concept of spin networks is also generalized then, by introducing graphs with edges labelled by non-negative real numbers (called „relativistic spin networks"). Applying this kind of „spin foam" model to Lorentzian state sums demonstrates their finiteness in turn implying a number of choices made from physical and/or geometrical arguments. The really interesting aspect of this is its relation to the group SL(2,C): because this is the double cover of SO(3,1) and the complexification of SU(2) which in turn is the double cover of SO(3). On the other hand, SL(2,C) is the group of linear transformations of C^2 that preserve the volume form. Thanks to an e-mail crash course on these matters referring to the Barrett-Crane model and made available online by John Baez and Dan Christensen (2000), where they use the terminology of the former's quantum gravity seminar[37], it is easy to understand that constructions in the sense of Barrett-Crane turn out to be invariant under SL(2,C). In other words, we essentially deal with states in C^2 which are *spinors*. And it is from quantum theory and special relativity, especially by the important work of Roger Penrose already in the sixties and seventies of the last century, that we know about their relevance. On the other hand, as Baez notes, a state in C^2 can also be called a *qubit*. So „[w]hat we [a]re really doing, from the latter viewpoint, is writing down ‚quantum logic gates' which manipulate *qubits* in an SU(2)-invariant [in fact, SL(2,C)-invariant] way. We [a]re seeing how to build little Lorentz-invariant quantum computers. From this viewpoint, what the Barrett-Crane model does is to build a theory of quantum gravity out of these little Planck-scale quantum computers." (Baez, Christensen, e-mail discussion, 2000, 42) This is obviously very much on line with the arguments of Zizzi, Lloyd and others. Moreover, it is referring to the explicit level of spin networks: That is, the aforementioned „boundary layer" between the physical world and its foundation (otherwise called a *subject* or *natura naturans*) shows up as a „shift of quantum computing" processing the fundamental information necessary for performing the transition from foundation to world (or in other words: for actually *producing a world* out of its foundation).

Foundations of Matter and Information. (= Chapter 6) In: Mark Burgin, Wolfgang Hofkirchner (eds.), Information Studies and the Quest for Transdisciplinarity. Unity through Diversity. World Scientific, Singapore etc., 2017, 191–214.

[36] John W. Barrett, Louis Crane: Relativistic Spin Networks and Quantum Gravity. https://arxiv.org/abs/gr-qc/9709028

[37] Unfortunately I am unable to retrieve this file from the web page of John Baez now, possibly due to his more recent shift of interest, but the reader may find the following instructive: John C. Baez, J. Daniel Christensen, Thomas R. Halford, David C. Tsang: Spin Foam Models of Riemannian Quantum Gravity, www.arxiv.org/pdf/gr-qc/0202017 .

Utilizing the “skeleton-of-the-universe view” (Zimmermann, 2004), the idea would be to insert various steps of a hierarchy of complexity in the overall functor diagram from topological quantum field theory (cf. John Baez):

$$\begin{tikzcd}
\mathrm{nCob} \arrow[r] & \mathrm{Hilb} \\
\mathrm{SpinF} \arrow[u, "em"] \arrow[r] & \mathrm{Hilb} \arrow[u, shift right] \arrow[u, <-, shift left, "id"']
\end{tikzcd}$$

This diagram is commutative, if an adequate emergence (*em*) mapping is being defined. Here, SpinF is the category of spin foams, and nCob is the category of n-dimensional cobordisms. (For the time being, we can safely set n = 4.) Hence, there remain three things to do:

(a) to show that loops are fundamental agents in that their loop motion (their self-assembly and combination into spin networks) corresponds to Stuart Kauffman’s definition of agents.
(b) to actually describe what the mapping *em* looks like in detail.
(c) to introduce intermediate stages of hierarchy into that mapping.

In the meantime, as for task (a), we can at least offer an *outline of proof*: From recent work of Donnelly’s (2008[38]) we know that the appropriate entropy we have to deal with is the von Neumann entropy of the form $S(\rho) = \mathrm{tr}\,(\rho \ln \rho)$, where ρ is a suitable density matrix. In Kitaev and Preskill (2006[39]) as well as Rovelli and Vidotto (2010[40]) we find that for spin networks in loop quantum gravity, it is especially the Braunstein-Ghosh-Severini (BGS) entropy which is relevant here: This refers essentially to a quantum field theory on a space $\Omega \subseteq \Sigma$ with $H_\Sigma = H_\Omega \otimes H_\Omega^C$ as adequate tensor product of the associated Hilbert spaces such that $\rho_\Omega = \mathrm{tr}_{H(\Omega,\,C)} |\psi\rangle\langle\psi|$. In particular, for the loops of this theory, the appropriate Hilbert spaces are defined by the cyclic functions of an SU(2) connection A. Hence: $\{\psi;\ \psi(A) = f(U(A, \gamma_1)\ [\ldots]\ U(A, \gamma_L))\}$, where $|\psi\rangle$ is a spin network state. The density matrix of the underlying graph Γ turns out to be the Laplacian matrix $L(\Gamma)$ (essentially the difference between degree matrix and adjacency matrix) divided by the degree-sum of such a graph. Then, the loop integral over γ: $\int_\gamma dS(\Omega) \geq 0$ fufils Stuart Kauffman’s condition for an autonomous agent.

In a sense, the “skeleton-of-the-universe view” can be thus visualized as a generalized kind of an algorithmic approach such that the physical phenomena of the universe (i.e. of the observable physical world) emerge as a result of algorithmic procedures that are coded into a *procedural space* that is logically prior to the action of fundamental quantum computation. Note however that it is left open whether this algorithm is strictly defined or subject to (fuzzy) hermeneutic interpretation instead.

And, while talking about all of that, we notice that this is the outcome of the modeling procedure. In other words, the systematic approach outlined above is itself a model, i. e. a mapping of the world, not the world itself. We utilize the concepts of *space*, *network*, and *system* according to our epistemological principles: As such networks serve as a formal skeleton (or circulation) for a space and for a system, respectively, while they are graphical representations of both of them. The concept of space serves also the graphical representation of what we call a system. The system is the concept we have of what we are able to observe in concrete terms. But what we observe is only part of the world. (Our ontological directive is: The world is not as we observe it.) But we are products of that world ourselves. Hence, there is the necessity of a *cognitive meta-theory* for our other theories which tells us something about the basic limitations of our possible knowledge. *This entails the necessity of a self-loop: Humans model the world by inventing theories according to the cognitive constraints this same world is imposing upon humans.* Theories thus constitute categories of meaning. If humans show up then as communities of communities of fundamental (natural) agents, they are, with respect to the latter, *emergent structures* in nature. And so are all of their reflexive concepts. Hence, the concept of (human) meaning

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[38] William Donnelly: Entanglement Entropy in Loop Quantum Gravity. www.arxiv.org/pdf/0802.0880

[39] Alexei Kitaev, John Preskill: Topological Entanglement Entropy. www.arxiv.org/pdf/hep-th/0510092

[40] Carlo Rovelli, Francesca Vidotto: Single Particle in Quantum Gravity and Braunstein-Ghosh-Severini Entropy of a Spin Network. www.arxiv.org/pdf/0905.2983

itself is emergent with respect to fundamental *proto-meaning* defined in terms of the directed behaviour of fundamental agents.[41] This may be utilized as a grounding of the concepts of *pre-reflexive* and *reflexive meaning*, respectively. Hence, the Universe is meaningful from the outset, but it is only humans who develop reflexive meaning such that they actually know that there *is* meaning.

Two more remarks are in order here: First of all, most of what we have said so far is compatible with more recent work of Stuart Kauffman's. He lists as conditions for emergent life: auto-catalytic reproduction, work cycles, boundaries, self-propagating work and constraint construction, choice.[42] Although he discusses life in particular, these conditions can be generalized in a straightforward manner, as he says: "[...] the laws that govern the whole are not to be found in any specific physical realization of such a system, but rather in the mathematics of this broad class of dynamical systems, whatever their material realization."[43]

The second point is the following: There is actually a conceptual problem with the concept of causality here. This is mainly because causality is made very strong within the framework of quantum gravity. As far as I can see, this goes back to the original idea of Fotini Markopoulou's that emerged when discussing the causal past of events in terms of Heyting algebras.[44] Central to this is the construction of the functor *Past*: $C \rightarrow$ Set from the causal set to the events in the past of each $p \in C$. As can be seen from earlier expositions, this functor relies on the equally fundamental construction of past light cones in the sense of relativity theory. But it is not clear yet how far this conception can be applied with respect to the foundations of space and time, because it is essentially a result of classical physics only.[45]

3 Further Consequences of Thermodynamics

Hence, what we recognize is that it is the initial structure of the Universe itself that determines the dynamical unfolding of the original potential. This is mainly achieved by applying thermodynamic principles to networks and thus systems. The starting point for looking at the initial conditions however is the additional field of *phase transitions*, in particular with a view to their universal properties in nature. In fact, these have been introduced in a completely different field of theoretical physics: It is the *Kibble-Zurek mechanism* that describes the non-equilibrium dynamics and formation of topological defects in a system subject to a phase transition. Originally developed for the primordial quantum states of the Universe, it turns out that the first principles of the mechanism exhibit a wide range of universality in physics. In a sense, this idea triggered somehow the efforts taken as to the inflationary model of the Universe. And this work was also involved in the discovery of the Higgs boson in elementary particle physics.[46]

The general idea goes back to the original assumption in cosmology that at high temperature (characteristic for the early state of the Universe) a simple gauge symmetry principle would be relevant such that there would be only one type of "force" available. At lower temperatures however the initial symmetry would be spontaneously broken creating the variety of forces and particles we can actually observe today. The expansion of the Universe would thus produce correlations among physical fields on

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[41] Although one could as well argue that the evolutionary continuity of forms of consciousness actually prevents the application of proto-concepts.

[42] Stuart Kauffman, Philip Clayton: On emergence, agency, and organization. Biology and Philosophy 21 (2006), 501–521.

[43] Ibd., 518.

[44] Fotini Markopoulou: The internal description of a causal set: What the universe looks like from the inside. www.arxiv.org/pdf/gr-qc/9811053

[45] Fotini Markopoulou, Lee Smolin: Causal Evolution of Spin Networks. www.arxiv.org/pdf/gr-qc/9702025

[46] For a recent review of the essential theory including experimental test devices see Adolfo del Campo, Wojciech H. Zurek: Universality of Phase Transition Dynamics: Topological Defects from Symmetry Breaking. www.arxiv.org/pdf/1310.1600 Also in Jerome Gauntlett (ed.), Symmetry and Fundamental Physics (Tom Kibble at 80), World Scientific, Singapore etc., 31–87. For even more recent results see also Logan W. Clark, Lei Feng, Cheng Chin: Universal Space-Time Scaling Symmetry in the Dynamics of Bosons across a Quantum Phase Transition. Science 354 (6312), 2016, 606–610.

larger and larger scales by progressive cooling down. By what is referred to as a "rapid quench" a random pattern of disorder becomes gradually ordered. The limit of correlation scales is defined by the velocity of light determining the Universe's causal horizon.[47]

This can be combined with the inflationary model according to Alan Guth and others, especially with a view to reservations this model has not been able to overcome in the long run. But it appears that if the Big Bang was a bounce (for which there is some theoretical evidence after all due to recent results of the Pittsburgh school), preceded by another large, smooth Universe like the one we actually observe, then many problems can be solved which inflation was invented to solve, but this time without utilizing inflation at all. Mechanisms can be described that could be responsible for growing quantum fluctuations into nearly scale-free, Gaussian density fluctuations to seed cosmic structure formation.[48] Based on the ekpyrotic Universe he himself helped to be introduced (in 2001), Turok refers to a version of the Friedmann equation of the form

$$H^2 = (\mathring{a}/a)^2 = (8\pi/3)\ G\ (\Delta V + \rho_m/a^3 + \rho_r/a^4 + \rho_{aniso}/a^6) - k/a^2 + (8\pi/3)\ G\ \rho_{ek}/a^{3(1+w)}.$$

Here ΔV is the potential energy density in the false vacuum that behaves like a large cosmological constant, k is spatial curvature and the densities are those of matter, radiation, and anisotropy, respectively. It is *a* the usual cosmological scale factor (the expression on the left-hand side indicating the Hubble parameter squared), and G the gravitational constant. The additional term on the far-right-hand side describes the ekpyrotic energy density, and w is very large as compared to 1. In the classical Friedmann equation of this type, the cosmological constant is usually eliminated by replacing $\rho \to \rho - \Lambda/8\pi G$.

Despite some reservations left (e.g. that the false vacuum is not only highly speculative so far, but also part of a particle picture that might be inadequate for gravitation as derived from the classical Einstein equations), this approach looks much better than the inflationary case with its drawbacks. And there is another interesting point to this which will become relevant for our research tasks here: Turok stresses the point "that energy is *not* a conserved quantity in an expanding universe. The relevant conserved quantity is the volume of phase space (or its logarithm, the entropy), and it is this quantity, *not the energy*, which should be used to estimate the probability of finding a given initial state."[49]

Hence, the Kibble-Zurek mechanism as it is presented concisely in the paper of del Campo and Zurek himself[50] gives an alternative for inflation by capturing the essence of the non-equilibrium dynamics involved in the crossing of the phase transition at a finite rate.[51] However, as it turns out, appropriate observations have been made for a large class of physical phenomena pointing after all towards some kind of universality of the proposed mechanism. But not for the early cosmology of the Universe.

The general intention however is straightforward: To find the dynamics for spontaneous emergence of structure derived from thermodynamic foundations. In other words: This spontaneous formation of structure is visualized as a necessary, not as a contingent process taking place in Nature.

We come back now to the work of Morowitz[52]: We know from our remarks on entropy that the formation of structure is closely coupled to the stochasticity of the events involved. This is the statistical side of the phase transitions mentioned above. After discussing terrestric conditions of life and the associated processes in detail for 400 pages, the authors introduce phase transitions in chapter 7 as an instrument to generate a reasonably universal method of research – in other words: in order to follow the line of argument we have explicated already before. The intention of the authors is stated clearly: "One of our main thesis in this monograph is that the origin of life cannot be understood as a

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[47] I am paraphrasing here Neil Turok: Tom Kibble and the Early Universe as the Ultimate High Energy Experiment. In: Jerome Gauntlett (ed.), op. cit., 1–29, here: 2.

[48] Ibid., 16 sq. (par.)

[49] Ibid., 11.

[50] Adolfo del Campo, Wojciech H. Zurek, op. cit., 32–35.

[51] Ibid., 33.

[52] Eric Smith, Harold J. Morowitz: The Origin and Nature of Life on Earth. CUP 2016.

compounding of rare or arbitrary events, but must be understood as a cascade of *system rearrangements* that were in certain essential ways robust, and at least locally, necessary."[53] This is very much the same tenor we have recognized in the aforementioned approaches in terms of a purely physical perspective.

The authors continue: "Two lines of argument lead to this conclusion, one empirical and the other from the theoretical perspective […] From the empirical side, we have exhibited a number of specific subsystems in which patterns appear to proceed upward from low-level organic chemistry or geo-energetics and not downward from controlling macromolecules or structures. These suggest that constraint and stability flowed from what was generic and necessary rather than from what was particular and perhaps accidental. From the theoretical side, independent of the particular cases in which we happen to have functional or historical reconstructions of living subsystems, we know that living matter obeys certain mathematical laws governing fluctuation and stability, which include the familiar laws of thermal physics but extend also to higher-level structures. The most important problem these address is that many small-scale degrees of freedom have been entrained in states of order that are robust on the timescales we observe directly, and these ordered states have persisted for billions of years. Whatever chemicals and contexts conducted the biosphere on its path of emergence, a theory of biogenesis can only make sense within the larger framework of physical and mathematical law if almost all intermediate stages were robust, and at least most transitions were likely."[54] And the authors identify as the key concept of system rearrangement in the mentioned sense that of phase transition.[55]

It is here where Smith and Morowitz link their argument to what the physicists have done before with the global perspective of cosmology in mind. However, in systematic as well as methodological terms, to demonstrate the smooth transition from a top-down approach starting with cosmological concepts to a bottom-up approach selecting an individual planet as to execute research concerning the emergence of living structures, remains still a not yet completely conceptualized objective.

Nevertheless, with stressing the importance of what they call "Phase Transition Paradigm for Emergence" we have a generic starting point for approaching this goal. The idea is essentially the following: In systems that show large-deviations scaling, probability distributions for fluctuations simplify to the following form:

$$P_{\text{fluct}} \sim e^{-Ns}$$

with N defining scale and s defining structure also called rate function. The limit is such that for $N \to \infty$, $1/N \ln (P_{\text{fluct}}) + s \to 0$. The rate function in a large-deviations limit is also called the *entropy*.

As example the authors take a canonical one: the *Central Limit Theorem*. Let us take a random variable X with a probability density of the form

$$P(x \leq X \leq x + dx) = p(x)\, dx$$

with mean $E(X) = \mu$ and finite variance $E(X - \mu)^2 = \sigma^2$. In the case of aggregation define the sum $X^{(N)} = X_1 + \ldots + X_N$. Re-scale in the form of $Y^{(N)} = X^{(N)}/N$. Then the distribution of $Y^{(N)}$ converges for large N to the distribution

$$P(x \leq Y^{(N)} \leq x + dx) \to (2\pi\sigma^2/N)^{-1/2} \exp\,(-\,N(x - \mu)^2/\sigma^2)\, dx$$

with the appropriate terminology. Hence, N here is simply the number of samples in the aggregate (i.e. the scale factor) while the rate function $s = (x - \mu)^2/\sigma^2$ depends on x which characterizes the structure of fluctuations about an invariant mean. The universality in the statistics can be visualized in terms

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[53] Ibid., 425.

[54] Ibid.

[55] Ibid., 426.

of a generalization of the way the central limit theorem collapses an infinite diversity of higher-order moments in the microscopic density p(x) into the two-dimensional family of Gaussian limit densities.[56]

If joint fluctuations are constrained because some quantity $X = X_1 + X_2$ takes a fixed value in the aggregated system, then the jointly most probable configuration is the maximizer $\delta S = 0$ along the surface of constraint $\delta X_1 = - \delta X_2$. As $\delta X_1 \to 0$, then

$$\partial S_1/\partial X_1 = \partial S_2/\partial X_2 = \partial s_1/\partial(X_1/N_1) = \partial s_2/\partial(X_2/N_2). \ (*)$$

Intensive and extensive state variables provide dual characterizations of a system as long as the entropy function is convex. Introduce the notation $\lambda = \partial S/\partial X$. The Legendre transform of entropy S with respect to an extensive state variable X, F say, is then constructed by

$$F = X\, \partial S/\partial X - S = X\lambda - S.$$

Again, the derivative of F with respect to λ recovers X. Hence, given an entropy function from a large-deviations scaling limit, we may describe a system either by the quantity X it contains, or the gradient λ of S at which the quantity X is maintained. The argument for maximum probability that leads to equation (*) may then be expressed as the classical thermodynamic equilibrium condition that coupled systems take on their most likely macroscopic configuration when the intensive state variables dual to any exchangeable quantities are equal.[57]

The concept of an optimally informative quantity in a problem of statistical inference is captured in the notion of a *sufficient statistic*: The state variables in particular, are sufficient statistics for maximum-entropy distributions in which they are arguments of the entropy. Call a system S_X such that its state is a joint state of n random (microscopic state) variables x_i. The number of possible configurations for S_X is given by

$$\prod_{i=1 \dots n} | X_i |,$$

where $| X_i |$ is the cardinality of number of elements in X_i when the latter is the set from which the x_i take their values. Any function $\sigma_x\{x_i\}$ that is many-to-one such that it takes its values from a set of cardinality much smaller than the expression for X_i above is called *summary statistic*. This is also called *sufficient for y*, if $P(y| \{x_i\})$ has the property that

$$P(y| \{x_i\}) = P(y| \sigma_x\{x_i\}).$$

Here, y is a new random variable that shall be estimated and whose distribution of values is generated from the value of the state $\{x_i\}$. Then the above indicates that we can know no more about the values of y given knowledge of the whole state $\{x_i\}$ than we know given the value that $\sigma_x\{x_i\}$ takes. Hence, the number of possible distinct forms for $P(y| \sigma_x\{x_i\})$ is limited to the smaller cardinality rather than the much larger one.[58]

The entropy-maximizing distribution over micro-states is the least constrained distribution consistent with the values of the state variables. For this reason, any reduction in entropy required, as the boundary conditions on a system change, is eligible as a measure of information gained about the system's micro-states as a result of the change of the macro-state. Therefore the entropy of a macro-state has the interpretation of the amount of information *missing* in the corresponding distribution about sampled micro-states.

Smith and Morowitz take the underlying conceptions for their viewpoints onto statistics from the works of Edwin T. Jaynes that start with two seminal papers from 1957. Although they differ from his

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[56] Ibid., 437–439. (par.)

[57] Ibid., 440–442. (par.)

[58] Ibid., 446–447. (par.)

views in the interpretation of a number of mathematical details[59], they nevertheless utilize his approach within the context of Bayesian inference. Jaynes refers heavily on the earlier works of Josiah W. Gibbs and Harold Jeffreys, respectively.[60] Beside the issue of state function, controversy has possibly arisen at the time due to the unusual discussion of the difference between Boltzmann and Gibbs entropies which can be found in the same volume of collected essays.[61] The state (or partition) function has the following relevance for our topic here:

Traditionally, the sum over all configurations of the exponential function that maximizes entropy is called *partition function* for the ensemble. Its equilibrium form is given by

$$Z = \exp(-\beta F) = \prod_{i=1\ldots N} \sum_{si\in(-1,1)} \exp(-\beta H)$$

with $\beta = 1/kT$ (and T in units of k). This function can be visualized as *a count of the number of likely states of the system, each weighted by the exponential term in the probability distribution*. This term reflects a count of states in the environment's heat reservoir after the spin system has accounted for energy βH. Hence, the partition function can also be understood in terms of a count of the number of states available in the system/environment pair constrained by the total energy of which most is held in the environment. If there is no constraint so that the distribution is uniform, the partition function is normalized so that it simply counts the total number of microscopic system states. The temperature is the boundary condition imposed by the environment that will determine how strongly the system's internal energy skews the distribution of states. Here, F is the *Helmholtz free energy*.

The essential idea is based as an example on a version of the Curie-Weiss model describing magnets with spins "up" and "down", respectively. The s_i then give the dynamical variable for spin i. The microscopic energy function is of the form

$$H = -\tfrac{1}{2}\,\varepsilon - \varepsilon/N \sum_{(i,\,j)} s_i\, s_j - h \sum_{i=1\ldots N} s_i.$$

On the other hand, H is a function of the magnetization μ only, because in that case internal and external interactions are symmetric. Thus

$$H = -\,\varepsilon\mu^2/2\,N - h\,\mu$$

with the magnetization $\mu = 2n - N$, if n spins point upwards. The number of otherwise equivalent microscopic configurations that all have this same value of magnetization is given by

$$\binom{N}{n}$$

which is nothing else than $N!/(n!\,(N-n)!)$. As N becomes large, the concentration of vertices near the equator of a suitably chosen hypercube (for N = 4, say) increases. If co-operative effects can restrict possible micro-states to be distributed in certain regions, they can drastically reduce the number of such micro-states available (they can thus reduce entropy) and increase the information about the micro-state in the thermal distribution.[62]

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[59] Cf. ibid., 448.

[60] Cf. E. T. Jaynes: Information Theory and Statistical Mechanics, I, II (1957), in: R. D. Rosenkrantz (ed.), E.T.Jaynes: Papers on Probability, Statistics, and Statistical Physics. Kluwer, Dordrecht, Boston, London, 1989 (1983), 6–16, 19–38. The important issue is the differently introduced concept of entropy and the subsequent discussion essentially based on general state functions that are equally well applicable to classical as well as quantum mechanics.

[61] Cf.: The 1962 Brandeis Lectures, Gibbs vs. Boltzmann entropies, in: R.D.Rosenkrantz (ed.), op. cit., 40–76, 79–86.

[62] Smith, Morowitz, op. cit., 455–457. (par.)

Jaynes then clarified somewhat the role of the constraining of state variables and the structure of the inference problem implied by them, making clear how the thermodynamic entropy can be understood as an application of information entropy to systems whose internal states are incompletely determined by their boundary conditions.[63] This gives the combinatorial basis after all of the Gibbs-Shannon entropy in the following way: Take a system with N distinguishable objects which may take any one of K states. If every assignment of objects to states is equally probable, the frequency of samples that have n_i objects in state i, for i = 1…K and $\sum_{i=1…K} n_i = N$, is

$$P(n_1 … n_K) = (1/K^N)\, N!/(n_1! … n_K!).$$

Here, the laws of large numbers cause *scale* to separate from *structure* (as we have seen in the beginning), because the multinomial coefficient (due to Stirling's formula for the logarithm) converges on the approximation

$$\ln N!/(n_1! … n_K!) \approx - N \sum_{i=1…K} n_i/N \ln n_i/N = N\, h(n_1/N … n_K/N),$$

where h is now the Gibbs-Shannon entropy function of the frequencies displayed in brackets which sum to unity. When we pass now from equilibrium to non-equilibrium, then we have to note that the biosphere is not just an open system, because it is not created by reversible processes and not an equilibrium ensemble (and thus does not furnish a contradiction between being highly ordered on the one hand and the principle of maximum equilibrium entropy on the other – already a result in Boltzmann and Schrödinger). Smith and Morowitz formulate: "The macroscopic entropy that is thermodynamically meaningful must be an information measure for the distribution from which it is computed. [This is the content of the large-deviations definition of entropy function shown here.] The state variables which are its arguments must also be appropriate sufficient statistics for that ensemble […] The function of these variables […] which is a macroscopic entropy function for an equilibrium ensemble will not generally be the actual entropy function for a non-equilibrium ensemble.[64] […] The equilibrium entropy does, however, provide a bound on the degree of stably sustained order […]"[65] It is here where the properties of *driven systems* (i.e. systems that are driven away from equilibrium by means of their constraints) becomes important. In driven systems, states are occupied only if they can be reached by energy or materials between the time these enter the system and the time they exit: "In some systems, including many popular reaction-diffusion models, the approximate equilibrium entropy at successive times contains enough information to determine dynamics with the aid of a set of transport coefficients. More generally, factors that can affect transition rates and which are not captured in the equilibrium entropy alone can range from the response of reaction rates to catalysts, to the construction – within a system – of far from equilibrium structures such as compartments, surfaces, scaffolds, or turnstyles which may partition reactants into separate near-equilibrium, but decoupled, subsystems. The rate structure away from equilibrium, and the history dependence it induces in the system's response to its boundary conditions, can be considerably more complex than the probability structure at equilibrium."[66] Nevertheless, the theory of stability for driven systems remains one of counting which is a consequence of the state function picture: Those macro-trajectories are stable that have the largest number of stochastic ways to be entered or maintained, and the fewest ways to be exited.[67]

The decisive link between this approach by Smith and Morowitz and the physical preparations of theory starting from cosmology remains to be defined in minute detail. However, the most important aspect of this approach – namely not to centre the discussion around the biological individual, but around the global biosphere altogether (quite in line with the Gaia hypothesis of Margulis and Lovelock,

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[63] Ibid., 487. – He thus arrives at insight to a reliable error correction, if discussing the case of equilibrium systems.

[64] The whole sentence in emphasis in the original text.

[65] Smith, Morowitz, op. cit., 505.

[66] Ibid., 506.

[67] Ibid., 507. (par.)

in fact) – sketches the general tendency implied: “Darwinian evolution is not a defining pre-condition for life, but rather a consequence of the nature of individual-based organization within a living state specified at other levels. The biosphere as a whole rather than any particular kind of individuality or ecological community-structure within it is the locus at which life is identified as a distinctive planetary phenomenon.”[68] All the systems in question are selected on the basis of functions they have executed: “Whether the selection occurs by means of thermal relaxation at or away from equilibrium, or later through a Darwinian dynamic, the mechanics of aggregation has only data from the past to draw upon. This is a statement that the processes of the assembly and maintenance are *causal* in the physical sense of the term. It can be refined to say that they are *Markovian* – that all information from the past relevant to dynamics is represented in features of the current state […]”[69]

4 The Quantum Picture

The advantage of the phase transition paradigm is its universality with respect to both macro-processes as well as micro-processes, respectively. Hence, it can be applied equally well to both the classical and the quantum domain of physics. Note that some time ago, John Baez and Jacob Biamonte have dealt in detail with the linking of classical stochastic dynamics to quantum physics.[70] What they find is that stochastic mechanics within the framework of a large variety of process types can be expressed in terms of a master equation of the form

$$d\Psi_{\ell'}(t)/dt = \sum_{\ell} H_{\ell'\ell}\, \Psi_{\ell}(t). \quad (\#)$$

The idea about the underlying process types is comparatively simple: If $x_i(t)$ is the number of objects of type *i* at time t, and a transition between states of the system destroys m_i objects and creates n_i of them, the respective rate equations can be written as

$$dx_i/dt = r\,(n_i - m_i)\, x_1^{m1} \dots x_k^{mk},$$

where the somewhat complicated product shows up because a transition occurs at a rate which is proportional to the product of numbers of objects it takes as inputs. The reaction rate is r here. With an appropriate vectorial notation, this can be alternatively written in the form

$$dx/dt = r\,(n - m)\, x^{m}.$$

As to a master equation for these rate equations, we have to bear in mind that the probability that a given transition occurs within a time Δt is approximately the rate constant for that transition times Δt times the number of ways the transition can occur. Now, obviously, the number of ways to choose M distinguishable things from a collection of L is the falling power of the kind

$$L^{M} = L\,(L - 1) \dots (L - M + 1).$$

Take a stochastic Petri net now with k species (types) and one transition with rate constant r such that the *i-th* species appears m_i times as input and n_i times as output. We introduce a *labelling* which is a k-tuple of natural numbers $\ell = (\ell_1 \dots \ell_k)$ saying how many things (objects) are in each species. Let $\Psi_{\ell}(t)$ be the probability that the labelling is ℓ at time t, then we arrive at the above master equation (#). The matrix H gives all possible transitions among what we can practically call *states* (ℓ', ℓ) of the system in question. Note that we come back to the vectorial terminology (and thus skip indices in the preceding), then we have a master equation of the form

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[68] Ibid., 553.

[69] Ibid., 562.

[70] John C. Baez, Jacob D. Biamonte: A Course on Quantum Techniques for Stochastic Mechanics. www.arxiv.org/pdf/1209.3632 (2012). – I reproduce here a number of pages from my book on systems: Metaphysics of Emergence, op. cit., 107 sqq.

$$d\Psi/dt = H\,\Psi.$$

Obviously, the interesting point is here that the equation looks very much like Schrödinger's equation. The difference is that in the classical case described, Ψ is actually a probability (and a *real number* as to that), while in quantum mechanics it is only a probability amplitude so that the full probability is given by the expression $|\Psi|^2$ (whilst Ψ itself is a *complex number*). Before discussing this result further, let us shortly recall what a Petri net actually is:

Definition (Petri nets): These consist of a set S of species and a set T of transitions, together with a function $i: S \times T \rightarrow N$, saying how many copies of each species show up as *input* for each transition, and a function $o: S \times T \rightarrow N$, saying how many copies show up as *output*, respectively.

However, usually, the transitions take place in a *stochastic* fashion. We have thus a generalized definition:

Definition (stochastic Petri nets): These are Petri nets, together with a function $r: T \rightarrow (0, \infty)$, giving the *transition rate* (the rate for each transition which can be taken to be a constant).

In other words, we have a *rate equation*, telling us how the *expected number of objects* (copies) of each species changes with time. More interesting however is the *master equation*, telling us how the *probability that we have a given number of objects* (copies) of each species changes with time. In a sense, the rate equation is deterministic, but approximate – however, if the expected value of the numbers involved is large and the standard deviation is small, then it is quite a good approximation after all.

It is very useful now to choose Petri nets having the category formalism in mind in order to clarify the difference between objects and morphisms. In fact, in the case of Petri nets, species and transitions take the latter. The idea is that they express the relevant interactions between species (earlier called vertices here) with respect to their outcome: In the traditional networks of interactive type, the vertices are visualized as operators or agents, actively acting upon other vertices, while the quality of the interaction is depicted by the labelling of edges among vertices. As to Petri nets we have to bear in mind two important aspects: On the one hand, they are exclusively *active* networks in the sense that they always describe interactions of agents rather than passive layouts of networks (such as unutilized bridges or streets) that *could be* eventually utilized by agents whilst fulfilling their tasks. Hence, on the other hand, the transition box in the various diagrams (of which we display only one here) represent not just the fact of a particular interaction which takes place between two agents, but instead, is rather showing the *result* of the interactions involved such that the initial state of the agents involved is altered. A simple example would be the creation of a chemical compound consisting of two types of reactants: Say, we have atoms of type H and atoms of type O, then a more or less complex series of interactions results in molecules of the type H_2O. This outcome is thus the result of two interacting species (objects) and a number of associated transitions (morphisms).

The advantage of what Baez and Biamonte offer us is that we can utilize the methods from the field of quantum field theory in order to understand the classical stochastic processes better: The first, very useful probability distribution that can be discussed in terms of Petri nets is the *Poisson distribution* well-known from many fields in physics and elsewhere. The idea is the following: The probability for one fish (say!) caught within time Δt is $r\,\Delta t$. The probability for n fish being caught is $\Psi(n, t)$ accordingly. All such probabilities can be summarized in terms of a power series of the form

$$\Psi(t) = \sum_0^\infty \Psi(n, t)\, z^n,$$

where we call z the *generating function*. Now, recall that the master equation can be written in a form which is similar to Schrödinger's equation. Traditionally, we call H the *Hamilton operator* (or: Hamiltonian). In our case here, this equation describes how the probability of having caught any given number of fish changes with time. However, in quantum physics we discuss the creation and annihilation of particles. Thinking of fish instead, we can express the fact that we can be sure at time t to have n fish by writing

$$\Psi = z^n.$$

Creation of particles is given by the creation operator of the form $a^\dagger \Psi = z \Psi$. Hence, one more fish is consequently expressed by

$$a^\dagger \Psi = z^{n+1}.$$

And the probability of having caught n fish by time t is given by the distribution

$$[(rt)^n/n!] \exp(-rt),$$

which is called *Poisson distribution*. We find that this result is compatible with choosing the Hamiltonian such that $H = r(a^\dagger - 1)$. This also solves the master equation whose general solution is $\Psi(t) = \exp(t H)\, \Psi(0)$ with $\Psi(0) = 1$. Remember that the Hamiltonian for macroscopic everyday problems is actually a matrix.

Comparing then stochastic (macroscopic) dynamics with quantum dynamics, we realize that in probability theory, the passage of time is described by a map that sends probability distributions to other probability distributions. This can be described by a *stochastic operator* of the form

$$U: L^1(X) \to L^1(X)$$

which is linear such that $\int U \Psi = \int \Psi$ and $\Psi \geq 0$, $U \Psi \geq 0$. While in quantum physics the passage of time is described by a map that sends wave-functions to wave-functions, which can be expressed in terms of an *isometry*

$$U: L^2(X) \to L^2(X)$$

that is also linear in the sense that $< U \Psi, U \Phi> = <\Psi, \Phi>$. If these isometries have inverses, they are called *unitary* operators. (Time evolution in quantum physics is usually reversible. In probability theory it is usually not.)[71]

In quantum physics, the solution of the Schrödinger equation is mainly expressed by the term $\exp(-i t H)$, and a Hamilton operator that makes this term unitary for all t is one which is *self-adjoint*: $<H \Psi, \Phi> = <\Psi, H \Phi>$. So what properties should a Hamilton operator possess in order to make $\exp(t H)$ stochastic? Now what we find is that we must have

$$\int \exp(t H)\, \Psi = \int \Psi.$$

We can also recognize that the condition $\Psi \geq 0 \Rightarrow \exp(t H)\, \Psi \geq 0$ is satisfied, if we introduce the concept of an *infinitesimally stochastic matrix* H: This is one whose columns sum to zero and whose off-diagonal elements are non-negative.

Let us come back now to our general (and sufficiently abstract) objects: In a given population of objects, we call Ψ_n the probability of having n of them. We utilize then the power series expansion of the form

$$\Psi = \sum_0^\infty \Psi_n z^n.$$

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[71] We use here Dirac's bracket notation and come back to that later. The full bracket is a scalar product.

So what we do here is essentially to sum over all possible probabilities. The advantage is in the fact that we can define creation and annihilation operators on formal power series such that

$$a\,\Psi = d/dz\,\Psi,$$

$$a^{\dagger}\,\Psi = z\,\Psi,$$

where the first expression gives the *annihilation operator* and the second the *creation operator*. The annihilation procedure is a little more complicated, because we have to think of the n ways we could pick an object and make it disappear. We have thus:

$$a\,\Psi = n\,z^{n-1}.$$

Note that we have also

$$(aa^{\dagger} - a^{\dagger}a)\,\Psi = d/dz\,(z\,\Psi) - z\,d/dz\,\Psi = \Psi,$$

hence, creation and annihilation operators do not commute: $[a, a^{\dagger}] = 1$. This essentially means that there is one more way to put an object into the population, and then take one out, than to take one out and then put one in. Clearly, the evolution of the probabilities summarized in Ψ follows the rate of change of Ψ according to $d/dt\,\Psi = H\,\Psi$. The details depend on the situation chosen. If we solve now the master equation accordingly such that we have $\Psi(t) = e^{tH}\,\Psi(0)$, then we can utilize the fact that

$$e^{tH} = 1 + t\,H + (t\,H)^2/2! + \ldots$$

to multiply this with $\Psi(0)$ to get $\Psi(t)$ altogether. All the possible products involved can be drawn as Feynman-like diagrams, or to be more precise: as a sum of Feynman diagrams. Now, the interesting point is that the type of stochastic mechanics (or dynamics rather) we have discussed so far admits an *analogue of Noether's theorem*. In particular, this is true for *Markov processes* in general, of which stochastic Petri nets turn out to be a special case. If we consider a set of states X, then a Markov process is described by a real matrix $H = (H_{ij})$, $i,j \in X$. If we assume that the system is in state i, then the probability of being in some state j after some time changes with time, and the H_{ij} is defined to be the time derivative of this probability. From here, we can easily motivate again the introduction of "infinitesimal stochasticity": Given a finite set X, a matrix of real numbers H is *infinitesimally stochastic*, if $i \neq j \Rightarrow H_{ij} \geq 0$, and $\sum_i H_{ij} = 0$ for all $j \in X$. A Noether theorem applied to Markov processes tells us now that an observable commutes with the Hamiltonian if and only if (*iff*) the expected values of that observable and its square do not change with time. Or in other words, if O is the observable,

$$[O, H] = 0 \textit{ iff } d/dt \int O\,\Psi = 0 \textit{ and } d/dt \int O^2\,\Psi = 0,$$

for all Ψ that satisfy the master equation. (In a sense, it looks remarkable that we have to take care of the square of O here, not only of O itself. But this is due to the difference we have already noticed when comparing stochastic mechanics with quantum mechanics. We leave out the proof here and instead refer back to our primary source.)

In order to directly compare the Noether theorem versions in question here, we state the quantum version and the stochastic version one after the other:

Theorem A: Let X be a finite set. Suppose H is a self-adjoint operator on $L^2(X)$, and let O be an observable. Then $[O, H] = 0$ iff for all states Ψ satisfying Schrödinger's equation such that $d/dt\,\Psi = -\,i\,H\,\Psi$, the expected value of O in state Ψ does not change with time t.

Theorem B: Let X be a finite set. Suppose H is an infinitesimally stochastic operator on $L^1(X)$, and let O be an observable. Then [O, H] = 0 if for all states Ψ satisfying the master equation such that d/dt Ψ = H Ψ, the expected values of O and O^2 in the state Ψ do not change with time t.

Hence, in principle, what we do here is to compare approaches that rely on self-adjoint operators (in the case of quantum mechanics) and on infinitesimally stochastic operators (in the case of stochastic mechanics), respectively. This turns out to be very important for network theory, because there is a class of operators that combines both properties: Such operators are called *Dirichlet operators*. Hence, the operator H is said to be *self-adjoint*, if it equals the conjugate of its transpose: $H_{ij} = \bar{H}_{ji}$. And the operator H is said to be *infinitesimally stochastic,* if its columns sum to zero and its off-diagonal elements are non-negative. So H is a Dirichlet operator, if it is both self-adjoint and infinitesimally stochastic. We can formulate the following then:

Theorem C: Any finite simple graph with edges labelled by positive numbers gives a Dirichlet operator, and conversely.

It is interesting now to apply the insight gained to reaction networks of various kinds, particularly of chemical type. We take a simple reaction as an example:

$$A \to B,$$

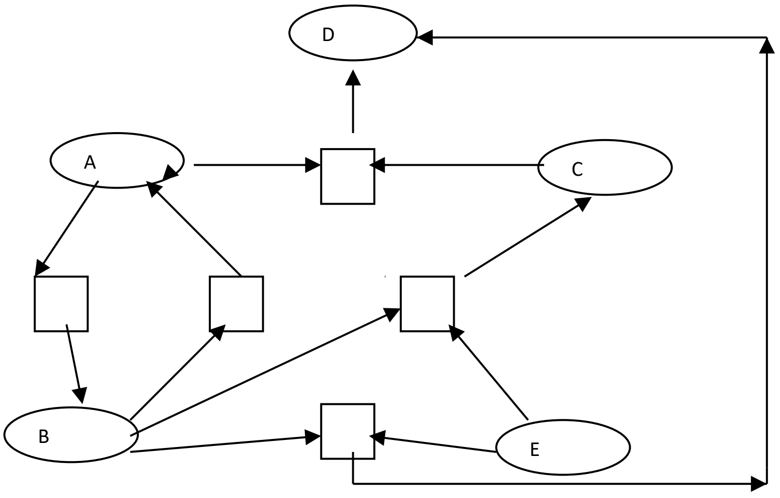
$$B \to A,$$

$$A + C \to D,$$

$$B + E \to A + C,$$

$$B + E \to D.$$

Equivalently, this can be visualized in terms of a Petri net of the following kind:



We have replaced here lines and arrows for the block arrows used earlier. Obviously, each reaction corresponds to a transition of this Petri net. We recognize the complexes here in which each species shows up several times. Hence, essentially, *a reaction network is a graph whose vertices are labelled by complexes*. On the other hand, a reaction network can also be visualized as a set of species together with a directed multi-graph whose vertices are labelled by complexes of those species. In this sense, it is also the generator of a Petri net and vice-versa. And if each reaction is labelled by a rate constant, the reaction network is said to be stochastic. (We can realize here the relevance of category theory again, because we can define suitable morphisms that map one type of network onto the other.)

Let us now define the *deficiency* of a network: This is the number of vertices minus the number of connected components minus the dimension of the stoichiometric subspace. Note that two vertices lie in the same connected component, iff you can get from one to the other by a path that is direction-independent. (In our example, there are five vertices and two connected components, depicted in the following fashion:

$$A \Leftrightarrow B$$

$$\begin{tikzcd}
A + C \arrow[r, Rightarrow] & D \\
B + E \arrow[u, Rightarrow] \arrow[r, Leftrightarrow, "id"] & B + E \arrow[u, Rightarrow]
\end{tikzcd}$$

The lower arrow is the identity here.)

The stoichiometric subspace of a reaction network is the subspace Stoch $\subseteq R^S$ spanned by vectors of the form x – y where x and y are complexes connected by a reaction. In our example, each complex can be seen as a vector in R^S which is a space whose basis can be visualized as A […] E. So each reaction gives a difference of two vectors with respect to the complexes: The top reactions give B – A and A – B, respectively. The central part gives D – A – C. The lower part gives on the left-hand-side A + C – B – E, while the right-hand-side gives D – B – E. These five vectors span the stoichiometric subspace. But because these vectors are linearly dependent, the subspace is three-dimensional rather than five-dimensional. Hence, in a sense, *the stoichiometric subspace is the space of ways to move in R^S that are allowed by the reactions in the given network*. So in the end, we find that the deficiency of our network example is 5 – 2 – 3 = 0.

Now then, we call a network *weakly reversible*, if whenever there is a reaction going from a complex x to a complex y, there is also a path going back from y to x. Hence, our network example is not weakly reversible, because we can go from A + C to D, but not back (and so forth). So we formulate the

Theorem D: Given a network with a finite set of species S. Suppose its deficiency is zero. Then:

(1) If the network is not weakly reversible and the rate constants are positive, the rate equation does not have a positive equilibrium solution.

(2) If the network is not weakly reversible and the rate constants are positive, the rate equation does not have a positive periodic solution.

(3) If the network is weakly reversible and the rate constants are positive, the rate equation has exactly one equilibrium solution in each positive stoichiometric compatability class. This equilibrium is complex balanced. Any sufficiently nearby solution that starts in the same stoichiometric compatability class will approach this equilibrium as t goes to infinity. There are no other positive periodic solutions.

In other words: The interesting dynamics happens in networks that have not deficiency zero. The first condition of part (3) is a consequence of the fact that if Stoch $\subseteq R^S$ is a stoichiometric subspace, and x(t) $\in R^S$ is a solution of the rate equation, then x(t) always stays within the set x(0) + Stoch. This is called the *stoichiometric compatibility class* of x(0). While the complex balance entails that we can turn the equilibrium solutions of the rate equation into those of the master equation. If we would prefer to have a compact version of what we have done so far, we could introduce a very compact diagram that summarizes the information in a stochastic reaction. Take the map Y: K $\to N^S$ sending each complex to the linear combination of species that it is composed of. Then the required diagram is of the form

$$(0, \infty) \xleftarrow{r} T \overset{s}{\underset{t}{\rightrightarrows}} K \xrightarrow{Y} N^S.$$

We have utilized here the definition of a reaction network in a more formal fashion, namely as a triple $(S, s, t: T \rightarrow K)$ such that S is a finite set of species, T a finite set of transitions, and K a finite set of complexes, together with source and target maps s and t. In particular, each transition τ gives a vector

$$\partial\tau = t(\tau) - s(\tau) \in R^K$$

that tells us what change in complexes it actually causes. In fact, ∂ can be extended (as all the other maps) to a linear map so that we can follow the mathematicians and call it *boundary operator*. Note that a reaction network has deficiency zero, iff $Y(\partial\rho) = 0 \Rightarrow \partial\rho = 0$ for every $\rho \in R^T$. (And it actually follows that the deficiency of a reaction network is the dimension of $\mathrm{im}\partial \cap \ker Y$. Indeed, $\mathrm{im}Y\partial$ is nothing but the stoichiometric subspace mentioned above.) We can compute the deficiency then by the number of vertices in the network minus the number of connected components minus the dimension of $\mathrm{im}Y\partial$. We know that for our last example, this is just zero. We can then also give the

<u>*Theorem E*</u>: A weakly reversible network with zero deficiency given. Then for any choice of rate constants there is an equilibrium solution of the rate equation where all species are present in nonzero amounts.

Here, the important (and sufficiently innovative) aspect is that the rate equation for a reaction network looks like

$$dx/dt = Y\, H\, x^Y,$$

where Y is a matrix now such that the equation becomes non-linear! The equilibrium would be given by $dx/dt = 0$ so that we should look for a solution of $H\, x^Y = 0$. This is mainly achieved by finding all solutions of $H\, \Psi = 0$ first, and then also those for which $\Psi = x^Y$. The relevant information for doing so is contained in the sequence shown above so that we get the finite sets of transitions (T), complexes (K), species (S) plus the rate constant for each transition given by r, the source and target maps s, t, as well as the injection Y which tells us how each complex is made of species. Utilizing some knowledge from the handling of sequences (of which we will leave out the details here[72]), we can actually reproduce the desired equation of the indicated type. By replacing addition by multiplication and multiplication by exponentiation, we also achieve a generalized type of matrix operations such that we can write:

$$x^Y = (x_1, \dots x_k)^{\begin{pmatrix} Y_{11} & \dots & Y_{1\ell} \\ \dots & & \dots \\ Y_{k1} & \dots & Y_{k\ell} \end{pmatrix}}$$

so that $x^Y = (x_1^{Y11} \dots x_k^{Yk1}, \dots, x_1^{Y1\ell} \dots x_k^{Yk\ell})$. The entries of the matrix Y tell us how many times each species shows up in each complex. Or in general: If you have a certain number of things of each species, then we can list these numbers such that the matrix formed describes in how many ways one can built up each complex from the available things. We can still show the equivalence of three expressions:

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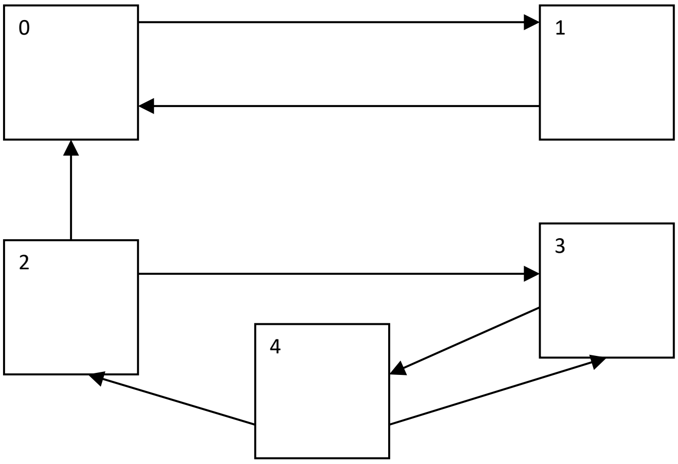
[72] But see Baez and Biamonte, op. cit., 207–209.

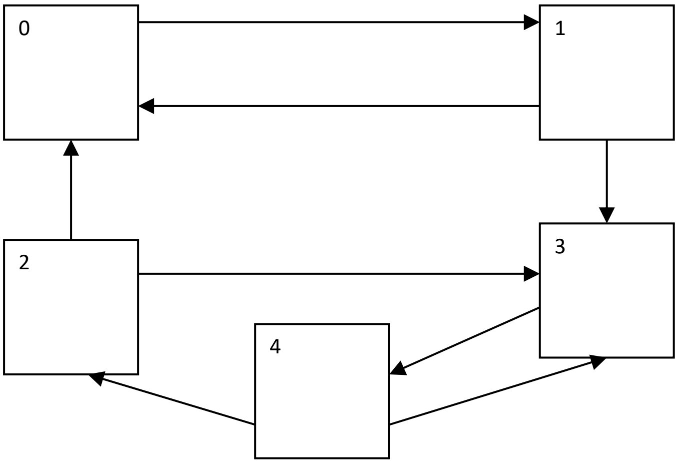
$$dx/dt = Y \sum_{\tau\in T} r(\tau)\, (t(\tau) - s(\tau))\, x^{Ys(\tau)} = Y\, (t - s)\, s^{\dagger}\, x^{Y} = Y\, H^{Y}.$$

It is important to remark that these relationships fall into a field that is closely related to category theory. In fact, the mappings involved can be visualized as arising from a pair of adjoint functors.

Now, if we introduce graphs that are weakly reversible, i. e. such that for every edge τ: i → j, there is a directed path going back from j to i, meaning that we have edges τ_1: j → j_1, … τ_n: j_{n-1} → i. The advantage of the weakly reversible case is that we get one equilibrium solution of the master equation for each component of our graph, and all equilibrium solutions are linear combinations of these. Note that the following graph (where we use boxes for the acting complexes as an exception) is *not* weakly reversible while the second actually *is*:



We can label the edges with rate constants (from above: 1, 1, ½, ½, 1, ½, ½ , say). The second diagram is:



Here, the labels of the second edge from above and of the new one on the right-hand-side are ½ each. Utilizing this insight, we can re-phrase earlier results in the following way:

Theorem F: Let H be the Hamiltonian of a weakly reversible graph with rates

$$(0, \infty) \xleftarrow{r} T \Rightarrow_{t}^{s} K.$$

Then for each connected component $C \subseteq K$, there is a unique probability distribution $\Psi_C \in R^K$ that is positive on that component, zero elsewhere, and is an equilibrium solution of the master equation $H\Psi_C = 0$. Moreover, such distributions form a basis for the space of equilibrium solutions of the master equation. So, the dimension of this space is the number of components of K.

We also note from the above that we can formulate

Theorem G: The Hamiltonian for a graph with rates is given by $H = \partial s^{\dagger}$.

Note the universality of theorems A through G due to their sufficient abstractness that guarantees a wide variety of phenomena which can be covered by this approach – and in a classical manner that is nevertheless based on quantum mechanics. In other words: The former shows up here as an approximation to the latter such that the classical entities can be visualized as average view of superpositions of underlying quantum entities. For a discussion of processes on planetary surfaces it is necessary to also include the transition area between the one and the other.

5 Astrobiology Proper

From the abstract level of processes that lead to the emergent constitution of organized (ordered) systems given some suitable initial system (in our case the Universe altogether), it is difficult to find the appropriate link to ongoing research of a more empirical character (though of course, the top-down method of theoretical conceptualization is not really devoid of empirical insight). In principle, we have to differ between two types of approach then: There is the attempt to conceptualize evolution in the first place including its origin and global as well as local structure, on the one hand, and there is ongoing research about details of planetary evolution, of Earth, but especially with a view to the multitude of recently found exo-solar planets, on the other. To these two types of approach correspond two types of available literature, respectively.

Probably, one of the first unified conceptualization of the problems involved is given in the conference proceedings dating back to the ISES95 meeting in Vienna.[73] The contributions of Bruce Weber[74] and of Juan Alvarez de Lorenzana[75] are particularly interesting within our context chosen in this present paper. Another collection of fragments developed on the same line of argument, but visualized from a purely physical perspective, is given in the volume celebrating the life of John A. Wheeler published in 2004.[76] The approaches displayed range from information theory[77] via cosmology[78] and the problem of origins[79] up to autonomous agents.[80] All these contributions struggle in one way or another with the initiation of ordered structures. In a sense, they are dealing with the philosophical question: Why is there something rather than nothing? Although they do not answer this question in the strict sense, because there is no metaphysical embedding available for the physical discussion.

Even more abstract (because of its mathematical focus) is the volume edited by Luciano Boi published in 2005.[81] Included is the seminal paper by the editor himself on the interaction of physics and

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[73] Gertrudis Van de Vijver, Stanley N. Salthe, Manuela Delpos (eds.): Evolutionary Systems. Kluwer, Dordrecht, 1998.

[74] Bruce H. Weber: Emergence of Life and Biological Selection from the Perspective of Complex Systems Dynamics. In: Van de Vijver et al. (eds.), op. cit., 59–66.

[75] Juan M. Alvarez de Lorenzana: Self-Organization and Self-Construction of Order. In: Van de Vijver et al. (eds.), op. cit., 67–78.

[76] John D. Barrow, Paul C. W. Davies, Charles C. Harper jr. (eds.): Science and Ultimate Reality. CUP 2004.

[77] David Deutsch: It from Qubit. In: Barrow et al. (eds.), op. cit., 90–102.

[78] Andreas Albrecht: Cosmic Inflation and the Arrow of Time. In: Barrow et al. (eds.), op. cit., 363–401.

[79] Marcelo Gleiser: The Three Origins: Cosmos, Life, and Mind. In: Barrow et al. (eds.), op. cit., 637–653.

[80] Stuart Kauffman: Autonomous Agents. In: Barrow et al. (eds.), op. cit., 654–666.

[81] Luciano Boi (ed.): Geometries of Nature, Living Systems, and Human Cognition. World Scientific, Singapore etc., 2005.

biology.[82] Two aspects must be noticed here: On the one hand, biological models (drawing heavily on the results of Louis Kauffman's mathematical knot theory) start more or less with the existence of RNA and DNA structures or their constitution as to that. (As seen under our own perspective, this might be a stage too late for understanding the true origin of life.) On the other hand – and this is fairly innovative within these approaches – the conceptualization of the structure and evolution of Nature is given here in direct dependence of the properties of *human cognition*. This is an important point for us here, because as mentioned in the beginning, all what we do is to be valued in terms of a mapping procedure and produces pictures rather than true objects: "The world is not as we observe it."

More recently, another volume on the principles of evolution has been published within a more practical context.[83] Here, the physical aspects are being stressed, and networks come clearer into focus than ever.[84] In fact, Thurner's contribution comes nearest to what we have learned from the discussion in the lectures of Baez and Biamonte. Finally, the volume by Sara Walker and others is the most recent approach to the transition from matter as such up to forms of life.[85] Particularly interesting here the contribution by Anne-Marie Grisogono.[86]

Unfortunately, as it is very often the case in the sciences, research in the physical aspects of evolution, the biological aspects, and astrobiology proper, is if not diverging, but parallel and disjoint for most of the time. An early contribution to an empirically oriented study of life in the Universe is the book by Schulze-Makuch and Irwin which has been published in its third edition in 2018.[87] As far as I can realize, there is only one other book that has been published earlier.[88] While this is presenting a view onto the problem which is nearer to what we have discussed here, it is nevertheless very general and non-technically written, and cannot likewise display a similar amount of facts than Schulze-Makuch and Irwin have to offer in their book. Hence, the latter is a promising compilation of what we can know today on the technical aspects of the topic.

However, when looking into the large apparatus of references in this book covering roughly 45 pages with more than 1000 entries, we can only find sparse hints to a few of the protagonists mentioned above: Brian Goodwin, Stuart Kauffman, Lovelock and Margulis, Maturana and Varela. On the other hand, protagonists of the research about life on Earth and other various astrobiological approaches are actually displayed. Which is more than usual. Because sometimes, even terrestric biology and astrobiology are disjoint parts of ongoing research. This is probably due to the specialized origin of the respective protagonists as to their field background rather than due to the topical demands of the research involved.

The pioneering and otherwise instructive book by Gale[89] does not refer to any details of evolution, dynamical systems, or the initiation of order. The book of Cockell[90] deals mainly with the physical boundary conditions for life as we can observe it. Hence, this is about the outcome, not the origin of relevant processes of evolution. The most recent books have their focus on specialized details: Adam Frank's book[91] e.g. concentrates of aspects of what is called "anthropocene" dealing with the impact human existence has on the planet with a view to former events when a species was able to change the living conditions such as during the Great Oxidation Event. Recently, this has become a common topic in astrobiology, probably because it has straightforward implications for all those problems that

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[82] Luciano Boi: Topological Knots Models in Physics and Biology. In: id. (ed.), op. cit., 203–278.

[83] Hildegard Meyer-Ortmanns, Stefan Thurner (eds.): Principles of Evolution. Springer, Berlin, Heidelberg, 2011.

[84] Peter Schuster: Physical Principles of Evolution. In: Meyer-Ortmanns et al. (eds.), op. cit., 45–79. – Stefan Thurner: A Simple Generation Method of Evolutionary Dynamics. In: ibid., 119–144. – Sanjay Jain, Sandeep Krishna: Can We Recognize an Innovation? Perspective from an Evolving Network Model. In: ibid., 145–172.

[85] Sara Imari Walker, Paul C. W. Davies, George F. R. Ellis (eds.): From Matter to Life. Information and Causality. CUP 2017.

[86] Anne-Marie Grisogono: (How) Did Information Emerge? In: Walker et al. (eds.), op. cit., 61–96.

[87] Dirk Schulze-Makuch, Louis N. Irwin: Life in the Universe. Expectations and Constraints. Springer, Berlin, Heidelberg, 2004, 2008, 2018.

[88] James N. Gardner: Biocosm. Inner Ocean (!), Makawao, Maui, 2003.

[89] Joseph Gale: Astrobiology of Earth. OUP 2009.

[90] Charles S. Cockell: The Equations of Life. Basic Books, New York, 2018.

[91] Adam Frank: Light of the Stars. Norton, New York, London, 2018.

are immanent in the presence of our time (climate, food etc.). Hence, the recent talk given by Axel Kleidon on the Leibniz day celebration of the likewise named learned society in Berlin[92] centres mainly around the question of energy generation on Earth. Universality and necessity of life in the Universe are usually stressed in all these contributions, but little is said about foundations. Despite the absence of ideas as to the foundations, there are nevertheless very interesting offspring publications which might turn out to be helpful when the question of linking the fundamental and global perspective to the detailed local one is at issue.[93] This is also true for the December contribution of William Martin to another conference of the Leibniz learned society Berlin that dealt with the primordial origin of cell structures on Earth.[94]

The only exception within this inventory seems to be the volume of Lineweaver et al.[95] that assembles a variety of contributions bordering clearly on what we have mentioned here. In particular, the contributions of Seth Lloyd[96] and Marcelo Gleiser[97] are quite illuminating. And of course, we can always come back to the book of Smith and Morowitz, as we have already seen in this present paper. We can realize though that it is very promising to look for an adequate research methodology that might be able to unify the various viewpoints. Note by the way that this has nothing to do with any kind of "reduction". Instead, the ongoing conceptualizations refer to the *emergent paradigm* in the first place. And in the end then, a physical theory of the foundations of processes that lie at the roots of evolution is still *another type of mapping* that might offer us a picture which is more complete than what we have developed so far, but nevertheless it remains a picture after all. Hence, despite prevailing exuberance and optimism, modesty should always be inherent.

6 Preliminary Conclusions

In order to conclude now what we have done so far, we have to notice that this present paper should serve as a kind of quarry for further ideas rather than presenting already definite results on the topics outlined here. It is important to realize that questions concerning the origin, structure, and evolution of life are linked not only to their physical foundations, but also to the metaphysical origin of those (non-physical) foundations that found the former in turn. In other words: Looking backwards at what came "top-down", we deal with philosophy rather than with theoretical physics. On the other hand, looking into the forward direction of what comes "bottom-up", we have to find further links that lead down into the branching grove of phenomenological details that can be actually observed by means of experimental sciences. After having had a look at the current literature, we find that probably the book of Smith and Morowitz can provide a suitable starting point for this. The unifying concept which represents a continuous line of argument running through all of the fields involved may be that of networks treated in technical terms by means of mathematical graph theory. In fact, it is *the emergence of interacting networks and their agglomeration due to phase transitions triggered by a critical percolation of energy and information within systems* what might be the most promising agenda to

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[92] Axel Kleidon: Was leistet die Erde und was trägt die Menschheit dazu bei? Antworten aus der Thermodynamik des Erdsystems. Leibniz online 37 (2019) Cf. https://leibnizsozietaet.de/wp-content/uploads/2019/08/04_Kleidon_Vortrag_rh.pdf (10.01.20)

[93] Adam Frank, Marina Alberti, Axel Kleidon: Earth as a Hybrid Planet. The Anthropocene in an Evolutionary Astrobiological Context. Manuscript Version due to private communication. (2018) See also: Gavin A. Schmidt, Adam Frank: The Silurian Hypothesis. Int. J. Astrobiol. (CUP), 2018, 1–9. There is actually a possible application to urban spaces: Marina Alberti: Cities That Think Like Planets. University of Washington Press, Seattle, London, 2016.

[94] William Martin: Wie und wo lebten die ersten Zellen? Neue Erkenntnisse über den Ursprung des Lebens. Cf. https://leibnizsozietaet.de/event/dezember-sitzung-des-plenums-der-leibniz-sozietaet-der-wissenschaften-zu-berlin/ (10.01.20)

[95] Charles H. Lineweaver, Paul C. W. Davies, Michael Ruse (eds.): Complexity and the Arrow of Time. CUP 2013.

[96] Seth Lloyd: On the Spontaneous Generation of Complexity in the Universe. In: Lineweaver et al. (eds.), op. cit., 80–112.

[97] Marcelo Gleiser: Emergent Spatiotemporal Complexity in Field Theory. In: Lineweaver et al. (eds.), op. cit., 113–131.

look at in the near future. Obviously, fundamental physics, emergence, evolution and their philosophical conceptualization show up as the most basic components that constitute actuality.

Abstract

A research program is outlined concerning the physical foundations of astrobiology, a field that is not yet fully investigated and comprises a large number of knowledge gaps in an insufficiently continuous narrative about the becoming of structures within the Universe, starting from its initial states through to the concrete fine structure as presented by the variety of forms that we can actually observe within Nature. Problems and objectives are discussed within the framework of ongoing research looking for the possibility to eventually reconcile the various fields and the results generated within them which are topical in the sciences for a long while, although unfolding their respective activities in a rather disjoint fashion rather than unifying all the different aspects involved.

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