

Von Neumann Entropy and Evolution

Richard D Bateson

Cavendish Laboratory, Cambridge, CB3 0HE, UK.
Email: rb2009@cam.ac.uk

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Abstract

In this paper I outline a hypothesis where quantum information in the form of von Neumann entropy provides a universal driving force for increasing complexity of systems and for evolutionary processes. Interference between quantum states of interacting systems allows storage of free energy that can be used to overcome kinetic barriers and accelerate reactions. This informational work cycle is analogous to entanglement in quantum Carnot engines where energy is stored as phase or so-called phaseonium fuel. The von Neumann entropy subadditivity and Araki-Lieb inequality properties of combined states can lower effective entropy and favour routes to increasing complexity of systems. It is proposed that observed macroscopic evolutionary processes are the emergent manifestation of this microscopic informational drive to complexity.

1 Introduction

Evolution of biological organisms is well studied since Charles Darwin [1] and the role of genetic modification for variation and heredity is firmly established. Recently, the evolutionary key principles of variation and natural selection via so-called “survival of the fittest” have been extended to non biological systems in the hope that a universal theory of evolution can be discovered [2,3]. This involves identifying conceptual evolutionary equivalence between systems ranging from stellar evolution and nucleosynthesis to mineral evolution and biological evolution.

The major processes in such a proposed theory are (i) component diversity where each system is formed from numerous interacting units that can provide many configurations, (ii) component exploration where ongoing processes can generate large numbers of configurations and (iii) selection where some configurations due to stability or other competitive advantage persist due to selection by function. The selection proposed can range from kinetic stability to dynamic stability such as homeostasis and novelty search.

The degree of function in the model of Wong [3] is defined as the measure of a configurations ability to perform a function. In analogy with information theory the functional information (in bits) of a configuration is given as the logarithm of the fraction of configurations that can exceed a certain threshold of function. In the model a law of increasing functional information is proposed where any mechanism that selects from a population of states, based on greater degrees of function, will lead to increased functional information with respect to the selected function.

Thus, as with conventional biological evolution selection pressure is viewed as the sufficient condition for increasing complexity of systems. However, in complex systems often selection pressure occurs at a macroscopic level whereas the variation and increasing complexity arise at smaller

or microscopic scales such as atomic positions, molecular arrangements and in sequences of macromolecules such as proteins and DNA.

An obvious question is does there exist a physical “driving force” at the microscopic level for increasing complexity of systems? If this were the case, then selection processes are merely screening an increasing expanding lexicon of system configurations for those best adapted for the macroscopic environment [4]. If this the case then observed evolutionary processes are the emergent manifestation of this universal underlying drive to complexity.

In this paper I outline a route where quantum information in the form of von Neumann entropy [5] provides a possible universal driving force for increasing complexity of systems. Interference between quantum states of interacting systems allows storage of free energy that can be used to overcome kinetic barriers and accelerate reactions. This storage of free energy is analogous to entanglement in quantum Carnot engines where energy is stored as phase or so-called phaseonium fuel [6,7,8]. The von Neumann entropy subadditivity and triangle inequality properties of combined states, relative to classical Shannon entropy [9], can favour routes to increasing complexity of systems. Facilitating increased complexity at a microscopic quantum level would then promote observable evolutionary processes. A simple model shows that since the work per entanglement cycle is proportional to the entropy or information content, this can lead to exponential rises in complexity of systems over many cycles.

2 Classical and Quantum Entropies

An informational view of entropy is as measure of complexity or information contained in a system. The Shannon entropy [9] of a system is the average over the microstates for a variable X . The dimensionless form assuming units of Boltzmann constant $k_B = 1$ and temperature $T = 1$ is

$$H(X) = - \sum_{x \in X} p(x) \log p(x) \quad (1)$$

Usually the logarithm is 2 so the entropy is measured in bits.

The analogous quantum entropy is the von Neumann entropy [5] calculated from the density matrix ρ

$$S(\rho) = -Tr(\rho \log \rho) \quad (2)$$

and is measured in quantum bits (qubits). The density matrix contains all the state information of a system with the off diagonal terms containing phase information. In general for a mixed quantum state

$$S(\rho) \leq H(X) \quad (3)$$

so a quantum system due to interference can encode or compress more information.

3 Classical and Quantum Work

The thermodynamic work that can be extracted from a state can be evaluated from the first law of thermodynamics [10,11]. For a classical system with an n-bit random variable X the amount of work is the change of entropy of the state

$$W_C = n - H(X) \quad (4)$$

The higher the entropy of the state the less work that can be extracted. The similar quantum system consisting of n qubits of state ρ is given as

$$W_Q = n - S(\rho) \tag{5}$$

In the above C denotes classical information systems and Q the analogous quantum system. The first term of n in Eq. (4) is the finite work of writing or erasing a bit of information [12,13] and the second term is the relevant entropy. A consequence of Eq.(3) is that a quantum system can perform more work than a classical system.

4 Combining and Entangling Quantum States

If we combine two systems A and B the combined entropy and hence available work can be calculated. For a classical system the Shannon entropy has a lower bound such that the combined system contains at least as much information as its components

$$H_{AB} \geq \max(H_A, H_B) \tag{6}$$

The result for the quantum system is given by the Araki-Lieb inequality [14]

$$S_{AB} \geq |S_A - S_B| \tag{7}$$

This combined with sub-additivity gives the triangle relation for the combined quantum entropy

$$|S_A - S_B| \leq S_{AB} \leq S_A + S_B \tag{8}$$

Remarkably this implies that the combined quantum system can have less entropy than either of its components and indeed for $S_A = S_B$ the entropy can even attain zero. This is a result of quantum interference of the entangled states and the off diagonal components of the density matrix. The quantum work available from the combined system can thus have a maximum value of

$$W_{Q,AB,Max} = n_A + n_B - |S_A - S_B| \tag{9}$$

which can be higher than the equivalent maximum classical work

$$W_{C,AB,Max} = n_A + n_B - \max(H_A, H_B) \tag{10}$$

and higher than the sum of the work of the separated quantum systems

$$W_{Q,A} + W_{Q,B} = n_A + n_B - S_A - S_B \tag{11}$$

The difference between Eq (9) and Eq. (11) provides the maximum work available via the entropy term through quantum entanglement.

$$\Delta W_{Q,AB,Max} = S_A + S_B - |S_A - S_B| \tag{12}$$

A cycle of entanglement and decorrelation can store and release energy. Defining a degree of correlation attained as

$$\alpha = \frac{S_A + S_B - S_{AB}}{S_A + S_B - |S_A - S_B|} \tag{13}$$

The general energy stored by entanglement capable of work is

$$\Delta W_{Q,AB} = \alpha \Delta W_{Q,AB,Max} \tag{14}$$

5 Evolutionary Cycles

The combined entangled quantum system leads to the possibility of an energetically favourable process to develop complexity. A quantum system A and system B, when entangled, can effectively store free energy to overcome kinetic barriers to form a new combined system C. The kinetic barriers to forming C may involve for example involve creation of chemical bonds and molecular structural rearrangements.

Importantly, the free energy stored in the entangled system is taken from the environment, for example a heat bath, and the laws of thermodynamics are not violated [7,12]. An analogy is the charging of a battery or a capacitor to enable work when required. By gradually storing energy in the entanglement cycle the system can deploy the energy in a reaction at the opportune moment.

In conventional reaction kinetics the Arrhenius equation has an exponential form for the reaction rate constant based on the activation energy E_a .

$$k = Ae^{-E_a} \quad (15)$$

assuming units of $k_B = 1$ and $T = 1$ as before. In an isothermal system, where energy has been accumulated through increased quantum entanglement, the effective activation energy can be lowered or overcome entirely through the available work $\Delta W_{Q,AB}$ and consequent entropy increase of the system.

$$k = Ae^{-E_a + \Delta W_{Q,AB}} \quad (16)$$

These forms are however based on statistical theory and in a quantum reaction the barrier could be viewed as an absolute threshold or quantum tunnelling could be effective if energies are below the activation energy. For the quantum system very low entropies or so-called neg entropies are available mathematically through the $|S_A - S_B|$ term in Eq. (7) which are not available classically. The proposed process can be a many stage cycle if the system C is itself a potential quantum system that can be subsequently entangled with new units. The above model is essentially a model of non equilibrium thermodynamics. In a thermodynamic sense the system is non ergodic since the kinetic barriers provide islands of ergodicity in phase space.

This mechanism is similar to extracting work in a quantum Carnot engine [6,7,8,12] where quantum coherence can provide fuel to run faster or more efficiently. Since this fuel is obtained from the phase information in the density matrix it is often termed phaseonium fuel. A conventional Carnot cycle requires the existence of two heat reservoirs at different temperatures since the Carnot efficiency for converting heat into work is given by the relation $\eta = (1 - T_{source}/T_{sink})$ where heat is extracted from the bath at temperature T_{source} and transferred to the low temperature sink T_{sink} . Importantly, a quantum Carnot cycle still can function when there is only one reservoir or $T_{source} = T_{sink}$. Thus in a quantum entanglement cycle the system can be in contact with a single temperature source and still store and later release energy.

6 A Model for Exponential Complexity

The evolutionary model of Carter [15] proposes that evolution takes place through a series of low probability stages. In general, we might consider that each of these stages at a microscopic level requires a series of kinetic barriers to be overcome and the model presented will drive complexity at each stage of the evolutionary process allowing novel systems to be constructed and selected for fitness.

From Eq. (12) we can see that the larger the entropy or information of a system the larger the work available from entanglement. A more complex system can, when entangled, store more

energy to drive further increases in complexity. A simple mathematical model can be formed to demonstrate this process. To simplify assume all systems or building blocks have broadly similar complexity such that $S = S_A \approx S_B$. Then from Eq. (12) and Eq. (13)

$$\Delta W_{Q,AB} = 2\alpha S \quad (17)$$

Assume the cycle is charged via an external energy source. If a fraction β of the available work is permanent information gain ΔS over each cycle then the rate of entropy increase is

$$\Delta S = \beta \Delta W_{Q,AB} = 2\alpha\beta S \quad (18)$$

For a continuous process over N cycles we can integrate to have

$$S(N) = S(0)e^{2\alpha\beta N} \quad (19)$$

where $S(N)$ is the entropy after N cycles and $S(0)$ the starting entropy. Thus over time the system's information entropy or complexity will increase exponentially. As the information of the system increases more information can be incorporated at a faster pace leading to an rise in complexity. This idealistic model is of course predicated on several assumptions such as assuming units of similar complexity and constant levels of entanglement and retention of information.

7 Discussion

I have considered the quantum work of informational systems but applying the notion of informational thermodynamics to actual physical molecular and solid state systems remains an new field. Defining informational entropy of molecules is currently highly subjective. Entropy can arguably be estimated from structure and alignment of the individual atoms and can be extended to include entropy of rotational and vibrational states etc. Using graph techniques [16], the informational entropy of most simple organic molecules lies in the range 1 – 3 bits. For example the entropies of two isomers of C_2H_{12} pentane and neopentane are estimated to be 2.351 bits and 1.086 bits. The informational entropy changes for chemical reactions such as etherification are estimated to be lower at ≤ 0.2 bits.

If we consider classical probabilities uniformly distributed then $p(x) = 1/n$ and $H(X) = \log n$ so that Eq. (4) for available work is $W_C = n - \log n$. This is the classical maximum entropy case. Since n varies faster than $\log n$ we might expect the entropy term to only be relevant when n is small. At $n = 10$ the entropy contribution is 3.3 bits (33%) and by $n = 1000$ relatively smaller at around 10 bits or 1%. Thus storing free energy from quantum entanglement has a more significant effect relative to total available work in smaller systems compared with overall thermal energy. However, the quantum entanglement effect allows energy storage in a contained cycle that scales with the overall entropy of the system.

Thus, despite the current difficulties in quantifying informational entropy at a molecular level, it seems possible that for smaller molecules the free energy from entanglement is in the region of the number of bits that are required to influence chemical reactions. The possibility remains whether regions of larger molecules such as proteins or sections of DNA could be entangled to provide free energy for changes to amino acids or nucleotides that might be otherwise energetically unfavourable.

Whether a chemical reaction destroys quantum correlations and any phase information is not currently well determined experimentally. It may be that a chemical reaction is a form of quantum measurement process which leads to diagonalisation of the density matrix and selection of particular

states. However, the model presented here is agnostic in the destruction of phase information since new entanglement processes can be developed after a chemical reaction and bonding. New entanglement processes require energy input into the system.

It is worth noting, that Shannon information and the analogous quantum von Neumann entropy are not the only way of defining complexity of a system. The complexity can also be considered to be the shortest length of algorithm needed to construct a system as in Kolmogorov complexity. Evolutionary models based on Kolmogorov complexity were proposed by Chaitin [17], where the DNA is considered the software that is evolved by mutation. However, for simple, low complexity systems the expected Kolmogorov complexity is approximately the Shannon entropy.

8 Conclusion

Combining quantum systems through entanglement allows very low entropies or so-called “neg entropies” to be achieved mathematically through the $|S_A - S_B|$ Araki-Lieb inequality term. This allows greater work than what is available classically. By exploiting a quantum Carnot cycle to store energy a joint quantum entangled state can store energy like a battery or capacitor to overcome kinetic barriers. Since the size of the potential energy storage scales with the information or complexity of a system, over a period of many cycles large increases in complexity can be achieved. This production of complexity possibly provides the raw material for evolutionary selection at different length scales. The different complex combinations developed would be filtered for macroscopic suitability [4] or Darwinistic “survival of the fittest”. The informational entanglement cycle would then be the underlying driving force behind all emergent evolutionary processes.

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