Minimization of Gibbs free energy as thermodynamical variational principle in TGD framework

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Abstract

Minimization of Gibbs free energy is applied routinely in bio-chemistry as a thermodynamical variational principle. I have however not applied thermodynamical variational principles systematically in TGD inspired quantum biology. My excuse could be that it is not clear whether dark matter as $h_{eff} = n \times h_0$ phases is in thermal equilibrium with the ordinary matter. Therefore the arguments have been based mostly on energy minimization and make sense thermodynamically at zero temperature limit. In this article I introduce the minimization of Gibbs free energy via an interesting example related to the understanding of the thermal stability of DNA double strand and apply it to water understood as a system involving dark matter as $h_{eff} = n \times h_0$ phases.

1 Introduction

Minimization of Gibbs free energy is applied routinely in bio-chemistry as a thermodynamical variational principle. I have however not applied thermodynamical variational principles systematically in TGD inspired quantum biology. My excuse could be that it is not clear whether dark matter as $h_{eff} = n \times h_0$ phases is in thermal equilibrium with the ordinary matter. Therefore the arguments have been based mostly on energy minimization and make sense thermodynamically at zero temperature limit.

This article was inspired by highly interesting findings related to the stability of DNA double strand. It has been thought that hydrogen bonds between the bases of the two strands are responsible for the stability. This explanation has been challenged (for a popular article see http://tinyurl.com/yyvkeq8y). According to the article [I1] (see http://tinyurl.com/y5kwo5b4) of Bobo Feng et al, the experimental findings support the proposal that hydrophobic forces are actually responsible for the stability. The function of hydrogen bonds would be to take care of correct base pairing rather than stabilization.

In passive state DNA strands would bind together by hydrophobic forces keeping water out of the interior of DNA double strand forming a kind of dry pocket. When DNA is active - say replication or transcription is occurring - an appropriate enzyme opens DNA by splitting the hydrogen bonds and the interior parts get in contact with water. This process requires energy provided by ATP. After than the process could proceed in TGD Universe as discussed in [L8].

The attempt to gain an improved understanding of hydrophobic interactions led to the realization that I have not been considered the possibility that Gibbs free energy might provide a thermodynamical variational principle applicable also to dark matter as $h_{eff} = n \times h_0$ phases, in particular allowing to get a quantitative grasp on the model of water as a multi-phase system involving magnetic flux tubes with various values of h_{eff} [L7].

2 TGD based view about hydrophobia

Hydrophobic interactions play fundamental role in biology, and there are good motivations for gaining some understanding about the thermodynamics involved. Here the appropriate variational principle is minimization of Gibbs free energy G.

2.1 One hydrophobic in water

While reading the popular article I realized that my understanding about hydrophobic forces is rather limited. I decided to go to web and an found a rather nice article about hydrophobic forces (see `http://tinyurl.com/yyerhvte`).

1. Consider first what hydrophobia at molecular level means. Hydrophobic molecules do not dis-solve in water. When this kind of molecule is put into water, a water a chlathrate gage surrounding it is formed. Hydrogen bonds between water molecules surrounding the molecule are split and new hydrogen bonds giving rise to the chlathrate are created. Splitting requires heat energy which corresponds to a decrease of a thermodynamical function of state known as enthalpy: $\Delta H < 0$ (the formation of hydrogen bonds occurs spontaneously and must release energy). When the temperature is above $T = 0$, also entropy matters. Now entropy decreases since order is created in the formation of chlathrate.

2. Physicists and chemists love variational principles. Now the thermodynamical variational principle is minimization of Gibbs free energy G. Process occurs spontaneously if the change ΔG of Gibbs free energy in the process is negative: $\Delta G < 0$.

   One has $\Delta G = \Delta H - T\Delta S$, where ΔS is the change of entropy. $\Delta H < 0$ is known to be small in the recent case but ΔS is large and negative due to the formation of the chlathrate cage generating order order. Hence one has $\Delta G > 0$ and the hydrophobic molecule does not dis-solve to water. Hydrophilic molecules in turn are polar and form bonds with water and dissolve.

3. Organic molecules tend to turn their polar parts towards water and non-polar parts (say long hydrocarbon sequences) inwards to form dry pockets. Double lipid layer giving rise to cell membrane is a good example. The lipids turn their charged ends to the water in the interior and exterior of cell and the hydrocarbon sequences of lipids reside in the interior layer containing no water. Protein folding in turn leads to a situation in which hydrophobic parts of protein are directed towards interior of the folded protein and hydrophilic parts bind with the surrounding water by hydrogen bonds.

2.2 Two hydrophobics in water

What happens when one puts two hydrophobics in water? It is easy to guess if one takes seriously what phobia means.

1. Hydrophobics are like two sociophobics in a big celebration. They seek protection from the crowd and can provide it to each other. Two hydrophobics in water come as close to each other as possible so that there is no water between them anymore. As they bind together, hydrogen bonds in the interior of the volume possessed by them are split. This requires energy ($\Delta H > 0$) but the entropy increases in the reduction of the size of the chlathrate area and the net effect is $\Delta G = \Delta H - T\Delta S < 0$ so that the process occurs spontaneously implying that hydrophobic substance does not dissolve.

One can apply this picture in order to understand the formation DNA double strand.

1. The formation of DNA double strands would be a process in which the hydrophobic sides of the strands become in a close contact and exclude the water from the interior of DNA. This would give rise to the helical double strand. The hydrogen bonds connecting the strands would not be responsible for the binding. Their formation generates order and the corresponding reduction of entropy should be smaller than the increase of entropy due to the splitting of hydrogen bonds of DNA strands with water.

2. The hydrophilic parts of DNA codons are directed towards the surrounding water. To open the double strand metabolic energy is needed. Also an enzyme catalyzing the process is needed but this is different story in which TGD view about quantum theory predicting mechanisms for how the reacting bio-molecules can find each other in the molecular crowd and how the potential wall making the reaction extremely slow can be overcome.

Is hydrophobia enough for the stability? My strong personal suspicion is that the stability of DNA is far from understood in bio-chemistry approach. In vitro DNA is unstable. The reason is that DNA nucleotides have negative charge and could cause instability of strands and double strand. In TGD based model the negatively region around DNA would be exclusion zone and represent ordered water. The model brings in dark matter as dark nuclei identified as dark proton sequences at flux tubes and generated in Pollack effect requiring metabolic energy feed.

The great surprise was that in a simple model for dark nuclei, the states of dark proton triplets correspond to DNA,RNA,tRNA, and amino-acids and vertebrate genetic code emerges [L5, L8]. Genetic code could be realized already at the level of water. In TGD framework the pairing of DNA strand with dark DNA strands carrying dark proton sequences with 3 proton units and charge of +3 units in 1-1 correspondence with DNA codons with total charge of -3 units could induce the stability. The formation of DNA could involve Pollack effect [L1] causing charge separation and forming negatively charged regions: part of protons would transform to dark protons at flux tubes.

3 Minimization of Gibbs free energy and TGD view about the role of water in life

Coherence of bio-matter is one of the characteristic of the living systems having no explanation in life-as-mere- bio-chemistry approach. The TGD based view of about water and its role in biology relies on the presence of long magnetic flux tubes containing dark protons as $h_{eff} = n \times h_0$ phases making possible quantum coherence in long scales. Flux tubes with varying values of h_{eff} would form a master-slave hierarchy having ordinary matter at the bottom. The quantum coherence of the master would induce the coherence of the ordinary matter serving as a slave.

All self-organizing systems generate long range correlations and an energy feed is necessary for the self-organization. Could they all be quantum critical with h_{eff} phases realizing the quantum criticality? If so, the energy feed would be needed to preserve the distribution of large h_{eff} phases: dark matter would be directly visible in the physics of every-day life [L11]!

3.1 Water as multiphase system

This picture suggests that water involves several phases [L7]. These phases would correspond to the presence of long flux tubes characterized by the values of $h_{eff} = n \times h_0$ and n can have several values: already water would be a living system [L10], and dark proton sequences at the flux tubes might realize genetic code [L5]. Interesting questions relate to the description of the proposed long flux tubes perhaps giving also rise to long variants of hydrogen bonds having non-standard effective value $h_{eff} = n \times h_0$ of Planck constant.

1. Could one apply thermodynamical considerations to the situation? This would require that dark protons and dark ions at the flux tubes are in thermal equilibrium with ordinary matter. Assume that this is the case. Under what conditions one has $\Delta G = \Delta H - T\Delta S < 0$ so that the formation of dark flux tube network is possible thermodynamically?

2. What ΔH is now? ΔH should contain the sum of magnetic and volume energy of the flux tube. Magnetic flux is quantized so that the magnetic energy in a simple model is proportional to L/S, L the length of the flux tube and S its transversal area taken to be non-dynamical. Volume energy is proportional to SL so that one has $E = aSL + bS/L$. In equilibrium L is fixed from energy minimization with respect to L as $L = \sqrt{b/a}$. The energy in equilibrium is given by $E = 2\sqrt{ab}S = 2aSL$. The local value of the length scale dependent cosmological constant determines the ratio $\sqrt{b/a} = L$.

   The naive expectation is that ΔH contains also the energy of dark matter at the flux tube. Quantum classical correspondence however suggests that classical energy equals to the energy of dark particles. For nuclei identified in TGD as nuclear strings [K1] this would mean that there is string tension which of order of m_p^2 (one proton mass m_p per proton Compton length $\hbar/m_p$). This is of same order of magnitude as hadronic string tension in the string model of hadrons. For dark proton sequences the tension would correspond to roughly one proton mass per electron Compton length: that this $2^{-11}m_p^2$.

3. There should be a contribution do the reduction of the total energy of the system due to the formation of the flux tube and this should win the energy of the flux tube. For instance, this energy could correspond to interaction energy of particles at the ends of the flux tube mediated by classical em fields along the flux tube.

   Coulomb energy between particles of opposite charge at the ends of the flux tube would be essentially that in 1-D world and proportional to the $q_1q_2L < 0$ and increase with the length of the flux tube. This would favor long flux tubes. The large interaction energy would be due to the channeling of the electric flux. There would be a competition between the negative Coulomb interaction energy and the energy of the flux tube. This energy should be included to the energy minimized and would modify the expression for the value of L obtained above to give $E = -Q^2e^2/L + S(aL + b/L)$. Energy minimum would correspond to $L = (b/(a + Q^2e^2/S))^{1/2}$. a is proportional to cosmological constant and b inversely proportional to Kähler coupling strength. a degreases as cosmological constant decreases so that also L increases. If volume energy is approximately constant ($SL = V_0 = constant$), one has $L^2a - bV_0 + L^3Q^2e^2 = 0$ in energy minimum and the term $Q^2e^2/S \propto L$ in the denominator reduces the value of L.

4. The naive and optimistic expectation is that one has $\Delta H < 0$ also for the formation of long flux tubes possibly accompanied by the analogs of hydrogen bonds so that the process would be energetically favourable at low enough temperatures and take place spontaneously.

5. ΔG contains also the competing contribution $-T\Delta S$ and the formation of flux tube structures brings in order so that this term is positive and tends to prevent this process. Could there be a critical temperature T_c above which this term wins and the formation of the flux tube network is not possible anymore? Could T_c be around the physiological temperature as biology and also the findings about thermodynamical anomalies of water would suggest

   Living matter stays conscious in a rather narrow temperature range. Where does the lower bound on temperature come from? Quantum criticality indeed suggests that there is also a lower bound for this temperature. Could it be that at temperatures near critical temperature the magnetic body of the system is maximally flexible and can change its structure. Residing at the border of order and chaos would make the cellular water very sensitive to external perturbations and provide its magnetic body with sensory and motor system. The biochemical realizations of sensory and motor systems would have emerged later.

3.2 Snow flakes and macroscopic quantum self-organization

Thanks for Nikolina Benedikovic for a link (see `http://tinyurl.com/rpvglge`) representing images of snowflakes. This led to a very interesting discussion generating new details to the view about self-organization in TGD Universe. Also phase transitions liberating heat as a new manner to generate dark matter in TGD sense in phase transition liberating heat energy suggest themselves and could provide a manner to generate artificial life in quantum sense.

The link told about snowflakes having incredibly precise symmetry. Their formation is still poorly understood and their precise symmetries remain a mystery. One would expect something like this in atomic length scales, where one has quantum coherence but certainly not in macroscopic scales. This inspires heretic questions. Could it be that the snowflakes reflect quantum coherence in their own size scale? Snowflakes are not macroscopically quantum coherent. What could be the quantum coherent system involved?

I can reveal my cards. This was mere rhetoric. I have made these questions 15 years ago but in different context. The outcome of these questions is TGD view about living matter and matter in general based now of adelic physics providing number theoretic vision about TGD [L4, L6] .

Magnetic body containing dark matter as $h_{eff} = nh_0$ phases ($h/h_0 = 6$ is a good guess [L2]) and inducing self-organization of ordinary matter with quantum coherence of dark matter inducing the ordinary long range coherence of ordinary matter. The relevance for quantum biology would be that the highly problematic quantum coherence of ordinary bio-matter would not be needed.

Could this explain snowflakes as impossibly perfect designs as self-organization patters forced in ordinary matter by quantum coherent magnetic body of water? I remember that some-one has said that snowflakes are like zoom-ups of atomic systems reflecting basic molecular symmetries.

They could be indeed analogous to zoom-ups of atomic systems with zooming factor given by n. Quite concretely, the lengths of hydrogen bonds would be scaled up by n.

Concerning a concrete model for snowflakes there is clear hint. The self-organization would increase the values of h_{eff} and this requires energy feed. Where does it come from?

Freezing of water liberates energy: this could serve as source of metabolic energy. More generally phase transitions liberating heat energy could generate h_{eff} ¿ h phases and generate highly ordered structures. Here might a possible method to create dark matter in TGD sense.

An interesting application is to the findings of Masaru Emoto [L13] that emotional expressions of humans seem to affect water at criticality for freezing. Angry voices are claimed to create ugly patterns and friendly voices beautiful ones. The metabolic energy needed to induce phase transition transforming ordinary matter to dark matter as exotic phase of water would come from the latent heat liberated in freezing. By macroscopic quantum coherence of MB the resulting dark parts of water's MB would be sensitive to human emotional expressions.

3.2.1 Could living systems utilize quantum critical phase transition liberating energy?

Wes Johnson commented about the ability of living systems to use heat as metabolic energy. Could phase transitions liberating heat produce this energy and lead to a generation of large h_{eff} phases?

1. In TGD Universe the efficiency of living matter to use heat as metabolic energy would a characteristic of not only life but all self-organizing systems. The distinction between living and in-animate would be only quantitative. The evolutionary aspect of self-organization would be generation of coherence in longer scales and would be induced by generation of large h_{eff} phases at magnetic body becoming thus quantum coherent in long scales. Energy feed would generate these phases and at criticality for a phase transition liberating heat energy (enthalpy) this is easy.

2. Living systems are conscious in a narrow temperature range. Perhaps this relates to the criticality for phase transition liberating energy in turn generating especially important h_{eff} phases. Water has special anomalies around the physiological temperature and looks like a two-phase system (at least). This kind of a phase transition of water could be fundamental for living matter.

   This could have a direct connection with the Pollack effect [**?**] creating charge separation: in TGD part of protons would become dark protons at magnetic flux tubes - dark nuclei providing a fundamental representation for genetic code [L8].

3. Carbohydrates are carriers of metabolic energy. Could this mean that they have molecular bonds (valence bonds) with non-standard value of Planck constant h_{eff} and that their energy is liberated when these bonds disappear in the splitting of these bonds or even in the reduction of h_{eff} , which would be basic element of bio-catalysis. I have indeed proposed a model for valence bonds in terms of dark flux tubes with $h_{eff} > h$ [L3]. The values of n involved would be relatively small and would correspond to the many-sheetedness for the space-time surface as covering of $H = M^4 \times CP_2$ coordinates would be n-valued. n would increase towards right end of the rows of the periodic end and this would explain the different roles of the molecules at opposite ends of the rows in biology.

3.2.2 The two aspects of self-organization

Note that these phase transitions producing phases with a non-standard value of h_{eff} represent evolution as a statistical increase of the dimension of extension of rationals and relying on "big" (ordinary) state function reductions (BSFRs). This active, evolutionary aspect could be seen as quantal aspect of self-organization.

There is also classical, passive, aspect assignable to the evolution of subsystem by "small" state function reductions (SSFRs) serving as counterparts of weak measurements. In TGD inspired theory of consciousness, motor-sensory duality corresponds to these two aspects. Motor actions correspond to BSFRs and sensory experience to SSFRs.

1. ZEO predicts that time reversal occurs in ordinary state function reductions (BSFRs) and that these reductions occur in all scales and look like ordinary classical evolutions leading to the final state smoothly and deterministically: this was discovered by Minev et all in atomic systems [L9]. This would remove the conflict between classicality and no-determinism at the level of conscious experience. Quantum systems would do their best to look like classical.

2. Self-organization as a generation of structures at space-time level (passive aspect) can be understood in terms of zero energy ontology (ZEO) alone [L12]. Self-organization (its sensory aspect) and metabolism (use of energy) could be seen as a dissipation in opposite direction of time: no separate models or mechanisms would be needed. Gradients would increase, structure would be generated. Basic biological processes at bio-molecular level would be controlled by magnetic bodies in time reversed states. The only challenge is to understand how living matter generates the sources of metabolic energy - how living system stores energy.

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