About mRNA folding, quenching, blackhole-like objects and universal genetic code

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Matti Pitkänen

orcid:0000-0002-8051-4364.
email: matpitka6@gmail.com,
url: http://tgdtheory.com/public_html/,
address: Valtatie 8, as. 2, 03600, Karkkila, Finland.

Contents

Abstract

This article was inspired by a discussion related to a model mRNA folding by assuming a given mRNA strand, whose nucleotides (A,U,C,G) and their order is known. The folding corresponds to the energy minimum.

The computational problems arise from the fact that mRNA strands can have very many shapes. The constraints are that the length of the strand is fixed and the lengths assignable to nucleotides are constant. The hope is that quantum computing using so called quenching would make the process sufficiently fast.

In the TGD framework mRNA has monopole flux tubes as a counterpart. In the case of blackhole-like objects the non-intersecting flux tubes would fill the entire volume and an attractive proposal is that the dark protons filling the flux tube can be assigned to the points of a lattice so that the energy minima could corresponds to a Hamilton cycle(s). This would mean enormous simplification. Same proposal might work for the energy minima in protein folding.

Contents

1 Introduction

We had a highly interesting discussion with Tuomas Sorakivi, a member of our Zoom group. The topic was the attempt to model mRNA folding by assuming a given mRNA strand, whose nucleotides (A,U,C,G) and their order is known. The folding corresponds to the energy minimum.

The computational problems arise from the fact that mRNA strands can have very many shapes. The constraints are that the length of the strand is fixed and the lengths assignable to nucleotides are constant. The hope is that quantum computing would make the process sufficiently fast.

1.1 Formulation of the problem

mRNA is single stranded but can fold back to itself and involves secondary structure related to base pairing and also 3-dimensional tertiary structures. Folding depends on mRNA sequence. mRNA sequence is charged since there is negative charge per every nucleotide. This causes self-repulsion. Local charge neutralization by ions can affect and control the folding. Also the interactions of mRNA with water are involved. This brings in the dependence on temperature and pH.

1. The folded RNA strand should minimize energy. In the more general case (temperature above T=0 K) free energy F is minimized instead of energy. F=E-TS includes energy E as well as -TS term from entropy. Energy minimization and entropy maximization compete.

2. In the models considered it is assumed that, as a good approximation, free energy is quadratic in observables, which include the orientation angles of the segments formed by two nucleotides in the mRNA chain. The total energy contains the sum of energies that depend on the orientation angles between the nucleotide and its successor and predecessor. A further simplification is to limit the strand to a plane.

3. What makes the situation non-trivial is that there can be segments in the mRNA strand that are conjugates of mirror images of each other. Conjugation means the replacement A$\leftrightarrow$U, C$\leftrightarrow$G. These segments tend to undergo base-pairing just like in the DNA double helix. This reduces the total energy and has a stabilizing effect.

   The first task is to identify such segment pairs and to process all possible configurations involving them to find the energetically most promising configuration and minimize the energy of the remaining part of the strand.

4. The model considered is as simple as possible and quadratic in the observables, which include the orientation angles between the two nucleotides. One can of course ask whether codons can be treated as linear units of three nucleotides, i.e. codons would not bend.

5. The first step is to consider only planar configurations. The natural assumption is that the mRNA chain has no self intersections. In a plane, this assumption is very strong.

   One can also consider configurations which define closed 2-surfaces such as Platonic solids. Maximal symmetry is highly suggestive and an interesting possibility is provided by Hamiltonian cycles or paths at the sphere, which go through every vertex without intersections. Also torus topology allowing lattice-like structure is interesting and one can consider even knotted tori for both DNA, RNA and proteins.

6. In the 3-D case, one can imagine that the paired segments can even have portions, which are double helices like DNA (and also RNA). Protein folding gives some hint of what might happen. Protein involves 3-D helical structures (1-D aperiodic lattices deformed to a helical shape, two-dimensional planar lattice-like pieces in which the protein travels back and forth in a single direction, plus random sequences. The inactive state of protein is essentially 3-dimensional cluster-like configuration. Parameters like temperature and pH determine which kind of structures appear.

1.2 How to calculate?

Although the quadratic model is in principle extremely simple and computable, the actual calculation is difficult. Part of the reason is the large number of codons and the base-pairing. The situation is the same for proteins.

Quantum computing raises the hope that folding could be predicted even when the number of mRNA codons is large. Quenching is the method used in the work that we discussed.

1. The energy landscape of the system can be assumed to be fractal. There are potential wells inside potential wells. Spin glass is the standard term used for these kinds of systems.

2. The straightforward energy minimization by moving in the direction in which the energy decreases maximally leads to a lower well, which is hardly an absolute minimum. It is

necessary to get out of it and therefore thermal energy must be fed into the system by using a suitable perturbation. After this one can try again. In this way, by gradually reducing the heating energy, it is hoped to end up to an absolute minimum.

3. The hardening of a scythe (I am a farmer's son) is a concrete example and is called quenching. First the scythe is forged and then cooled in a water tank. Then it is heated again and the same step is repeated. The amount of heating is reduced gradually. Finally, the energy minimum is obtained, which means the scythe is very hard.

2 The TGD analog for the mRNA folding problem

The mRNA folding problem has a very general counterpart in TGD [L11, L12].

1. Now the folding and tangling occurs for monopole flux tubes [K1] [L6, L7], and the many-sheeted space-time makes cross-bonds between flux tubes portions as analogs of base pairing possible.

   Also now modelling as a spin glass [L4] is natural in ZEO. One can ask whether classical action rather than energy is a more natural quantity to be minimized. The slight failure of determinism in holography= holomorphy vision [L8, L13, L14, L15] implies that spin glass property is extended to time direction in a discrete way. If the classical action reduces to Kähler action, the non-determinism is huge.

2. The scale of the flux tube tangles varies from the elementary particle level [K3, K4], through nuclear physics [K5], molecular physics and biology [L1, L2, L3, L5] to astrophysics and cosmology [L9].

The black hole, which in TGD generalizes to an entire hierarchy of black hole-like objects, serves as a good example.

1. For the TGD equivalent of a black hole, the flux tube tangle fills the entire volume [L10]. The quantized thickness of the flux tube is the basic parameter labelling an entire hierarchy of blackhole-like objects. Even the solar core could be a blackhole-like object in this generalized sense. For the TGD counterpart of the ordinary black hole, the thickness would correspond to the Compton wavelength of a nucleon.

2. What is important is that a 3-D lattice structure can be attached to the system, each point of which corresponds to one neutron in the flux tube. If the flux tube cannot intersect itself, then it corresponds to a Hamiltonian path and Hamiltonian cycle when the path is closed. This means a huge reduction in the number of degrees of freedom but could be favored by energy minimization.

3. The first task is to determine all Hamiltonian paths/cycles. This is a purely geometric, well-known mathematical problem. One can find the cycle which minimizes the energy or free energy. The separation of energetics/thermodynamics from the geometry simplifies the situation dramatically.

2.1 From black holes to mRNA and universal genetic code

Hamiltonian paths/cycles could also be considered in the case of mRNA.

1. The size of the codon/nucleotide is constant so it is natural to assign a lattice to the system. Also now can find Hamiltonian paths/cycles by purely geometric arguments and the calculation is dramatically simplified.

2. Quite concretely, the simplification means that the orientation angle for two nucleotides/codons takes only a few values corresponding to the nearest neighbors. For a cubic lattice there are only 6. This prediction should be testable. Even if not exact energy minima, these configurations could be excellent approximations to them. Note however, that minima favor symmetries and lattice symmetry is this kind of symmetry.

As a matter of fact, Hamilton cycles on the icosahedron and tetrahedron, which are finite lattices on a sphere, are essential in the TGD-based model of the genetic code. One cannot exclude the possibiblity that these cycles correspond to closed monopole flux tubes.

1. The essential point is that icosa- and tetrahedral Hamilton cycles can be classified by using their symmetry group as a subgroup of the icosahedral or tetrahedral symmetries. Symmetry determines how many DNA codons code for a given amino acid and the model predicts correctly these numbers [K2] [L2, L5]. If the genetic code is universal, these symmetries might play an essential role even in systems with an astrophysical size.

2. TGD indeed predicts that genetic code is universal and based on the completely unique icosa tetrahedral tessellation of the hyperbolic 3-space [L3, L5] playing a central role in TGD (mass shell, light-cone proper time constant surace). This tessellation would have tetrahedra, octahedra, and icosahedra, which are Platonic solids having triangles as faces, as basic building bricks. Does universality imply that both the notions of DNA, RNA and amino acids, or rather, their dark variants realized in terms of flux tubes carrying dark nucleons, are universal? This leads to ask whether 2- and 3-D realizations of the counterpart of dark DNA are possible. Even cell membrane could provide such a realization.

3. With motivation coming from the numerous anomalies related to the physics of the Sun, TGD suggests a model for the Sun [L10] as a living system analogous to a cell or cell nucleus and perhaps realizing the universal genetic code. Could the Hamiltonian paths or cycles, defined by the monopole flux tube tangles and associated with the icosa tetrahedral tessellation, give rise to the analogs of DNA strands? If so, the Sun could be an extremely intelligent conscious entity, something totally different from a mere fusion reactor. In fact, the TGD view of the Sun proposes that the solar wind and solar radiation is produced at the surface layer of the Sun and that new physics predicted by TGD is involved.

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