Primordial synthesis machines and the origin of the genetic code

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Abstract

We characterize the dynamics of primitive molecular synthesis machines operating in outer space on quasi-one-dimensional channels where polymers interact with fixed particles. We show that a generic property of particle/polymer electrostatic interactions is an average three monomer spacing between consecutive interaction potential minima. We exhibit that this property translates into locomotion regularities with a slowing down every three monomers. We argue that this transport property may be at the origin of the three base codon composition of the genetic code. We relate these findings to present day protein synthesis mechanisms. © 1998 Elsevier Science B.V. All rights reserved.

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1. Introduction

A fundamental question that arises when dealing with the genetic code is the understanding of why the basic coding units for protein synthesis, codons, consist of three elements. In previous work [1], which we shall refer to as (I) we related this feature to the dynamical properties of primitive molecular machines operating in outer space. Here we elaborate on this proposition by characterizing in more detail the dynamics of these machines.

Our starting point is that important steps of the prebiotic synthesis took place in the interstellar medium and in comets. This proposal is backed by the presence of a variety of organic compounds in the interstellar medium, comets and meteorites [2–4]. Furthermore, the recent evidence for life on Earth 3870 million years ago [5],
has introduced severe doubts on the likelihood that all the prebiotic and protobiotic processes took place on the Earth due to the short time gap for the adequate temperature conditions.

In the synthesis scenario we are contemplating polymerization is enhanced by taking place on the surface of channels or filaments which are present in interstellar and cometary material. On these surfaces organic monomers would adsorb and evaporate. Ultraviolet radiation could ionize the monomers and long wave electromagnetic radiation force them to oscillate, collide and form \( n \)-mers from free radical covalent bonding. The polymers would also have interactions with particles in the channels mainly of an electrostatic nature. In general the monomer charge distribution would be non-uniform giving rise to particle/\( n \)-mer asymmetric interaction potentials. In (I) we showed that the average distance between the consecutive minima of such potentials is generically close to three monomers. Under these circumstances we have a ratchet type nanomachine which can present an effective drift [6–8]. The polymer slows down every three monomers allowing for deposition of other molecular compounds along exposed channel segments. We believe that this is a basic mechanism at the origin of the three base codon structure.

2. Model

Let us consider a model consisting of a polymer built from \( N \) monomers which can be of \( m \) different types, sequenced with a random composition. The polymer will be on the surface of a channel where a fixed particle is present. Polymer and particle are separated by a transversal distance \( h \); we assume that the monomers have an extended charge density and, for simplicity, that they are of equal length \( l \) (Fig. 1a). The particle will interact with the different monomers of the polymer through a short range interaction. The intensity of the particle–monomer interaction will depend on the type of monomer, but it will have the same functional shape.

The passage of the polymer at the particle position in the high friction limit can be to a first approximation described by the following Langevin equation [9]:

\[
- \gamma \frac{dx}{dt} - \nabla U(x) + F(t) + f(t) = 0,
\]

where \( x \) is the distance measured from the polymer origin to the particle position, \( \gamma \) is the friction coefficient, \( U(x) \) the particle/polymer potential, \( F(t) \) is an external driving force and \( f(t) \) a noise contribution.

Within the outer space low temperature context we consider \( f(t) \) negligible, the potential of an electrostatic nature and associate \( F(t) \) with an oscillating electromagnetic force. In (I) we exhibited basic transport mechanisms, considering monomers with non-uniform charges equally oriented. If we have a constant unidirectional forcing term or a long period oscillating forcing term, the asymmetry is not required for the study of the locomotion regularities we are interested in. Here we consider such a forcing term, we relax the asymmetry requirement and go beyond the “toy model” approach.
The potential we work with comes from the interaction of uniformly charged monomers with polarizable fixed particles along the channel. Such a choice, besides being physically appealing, yields feasible parameter values.

In Fig. 1b we represent the nth monomer as a uniformly charged rod of length $l$ inducing a dipolar moment on a particle placed at a perpendicular distance $h$. The expression for the interaction potential is

$$U_n(x) = -K^2 \lambda_n^2 x \left\{ 1/r_{n2}(x) - 1/r_{n1}(x) \right\}^2 + \frac{1}{h^2} \left( \cos \theta_{n1}(x) + \cos \theta_{n2}(x) \right)^2,$$

where $K$ is Coulomb’s constant, $\lambda_n$ the nth monomer linear charge density, $x$ the fixed particle polarizability and $x$ is the particle–polymer relative position. The complete potential $U(x)$ is the sum over all the monomers of $U_n(x)$.

The potential $U(x)$ for a uniform random choice of $\lambda_n$ (corresponding to charges ranging from 1 to 4 electron charge units, i.e., an $m=4$ case) is shown in Fig. 2a. An amplification of this potential is given in Fig. 2b. Notice the appearance of two types of neighboring minima: small ripples, related to structures smaller than the monomer length, superimposed as a small perturbation on a larger scale minima structure. The average distance between the neighboring large scale minima $\delta_{\text{min}}$ is in the vicinity of 3. In (1) we showed that for random step function potentials with $m$ different values, $\delta_{\text{min}} = 6m(1 - (1/m)^N)/(2m - 1)$, which for large $N$ reduces to $6m/(2m - 1)$ and hence for $m = 4$, $\delta_{\text{min}} = 3.428$. This result holds for general $1/r^h$ potentials with $h \geq 1$ if $h$ is small enough since the step function case is attained in the $h \to 0$ limit (in this limit the above small scale perturbation disappears). The distribution corresponding to the potential of Fig. 2a for $N = 10,000$ is shown in Fig. 2c. Though $\delta_{\text{min}} = 3.367$, the most probable value is 2.
3. Dynamics

We shall now look into the dynamical behavior of Eq. (1) with the potential of Eq. (2), \( f(t) = 0 \) and \( F(t) = F_0 \cos(\omega t) \), with \( w^{-1} \) sufficiently large to guarantee the long forcing period mentioned above. Fig. 3a is a plot of the velocity \( v(x) = dx/dt \) resulting from a Runge–Kutta solution of Eq. (1). Fig. 3b is the graph of the local transit times defined as the inverse of the velocity. We should emphasize that the parameter values used for the determination of these graphs are physically meaningful: 
\[ \alpha = 10^{-41} \text{ J}^{-1} \text{ C}^2 \text{ m}^2, \quad \lambda_n = \beta_n \times 5 \times 10^{-11} \text{ C m}^{-1}, \quad \beta_n = 1, 2, 3, 4; \quad \gamma = 6 \times 10^{-11} \text{ kg s}^{-1}, \]
$N = 500, \ l = 1 \text{nm}$. With this set of parameters, the resulting intensity of the forcing electric field is $16 \text{V m}^{-1}$ with a frequency of $5.4 \text{kHz}$.

In Fig. 3c we show the power spectrum of the transit times. The peak at 2.05 corresponds to a spatial Fourier component of period 3.06, i.e., the polymer has a maximum transit time nearly every three monomers.

We should remark that the above behavior is not restricted to a particular choice of electrostatic potential, the same result is obtained so long as short range interactions are being considered. In Fig. 4 this genericity is shown explicitly by plotting in Fig. 4a a Coulomb $1/r$ potential for the same polymer configuration of Fig. 2b. Notice that the minima distribution is practically identical except for the ripples. Fig. 4b shows the transit time power spectra for the $1/r$ potential, which again selects the 3.06 period of Fig. 4c.
4. Ribosomal synthesis

The considerations we have put forth for the primordial synthesis machines are of such a general nature that it is tempting to explore whether similar features are encountered in present day synthesis machines, namely, in the ribosome dynamics. So far we have shown that for random potentials the average of the distance $\delta$ between neighboring minima is near to 3, however, the most probable value is close to 2. One could expect that due to selective adaptation, coding sequences would exhibit deviations from randomness in order to have the maxima of the distribution for $\delta$ in the vicinity of 3. Furthermore, these deviations should be related to physicochemical properties of the
RNA and not necessarily be present for DNA since the latter is geared fundamentally
towards the replication and transcription processes instead of ribosomal translation.
In Figs. 5 and 6 we show the histogram $H(\delta)$ of the distance between consecutive
dimer interaction minima of various coding sequences, using the DNA [10] and the
Notice that for the RNA histograms the values of $H(\delta)$ for $\delta = 2$ and $\delta = 3$ approach
Fig. 6. Same as Fig. 6 for anabaena (archaeabacteria) and salmonela (bacteria) genes.

each other. This flattening of $H(\delta)$ in $\delta = 2$, which closes the gap between the most probable and the average values of $\delta$ is not present for the DNA and random table histograms. In this respect the DNA shows a stronger resemblance to random behavior.

5. Discussion

The scheme we have developed here should be visualized as a first step; the analysis of polymer chain interactions with several particles viewed as a collective phenomena
is called for. Our main result here is to have uncovered the generality of the spatial regularities in a wide class of potentials and related them to dynamical regularities which are of consequence in coding processes. This approach can also be useful in the study of primitive replication mechanisms by considering channel branching.

So far we have not considered in detail the effect of noise. The noise contribution is important if we look into processes operative in outer space that could further develop in the transition to Earth conditions. The recent progress in the study of nano-machines subject to a variety of potentials, forcing terms and stochastic environments, provides a promising tool in this respect. It would also be interesting to explore the possibility of some chemically activated energy pump realizable in the interstellar medium and relate it to the ones operating presently.

One of the objectives of this work is to point out how relevant dynamics can be in our understanding of the genetic code. We believe this to be a promising line of thought.

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References