A Note on Self-Replicating Information Yielding the Chemical Origin of Life

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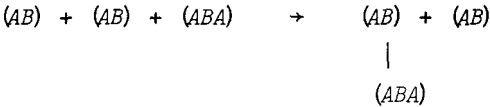
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Abstract   Stabilization in the length of growing polymers, starting from small constituents via self-replicating information, isobtained through the analogy between laser crossing threshold and critical phenomena.

The question of cooperative effects and self-organization plays nowadays a central role in theoretical biology[1-3].   Its formulation on mathematical grounds, as suggested by Haken[4], comes from laser theory[5-7] extended to biology. In fact, both laser and biological systems areopen systems far from thermal equilibrium.

The fields under investigation to which laser theory concepts and techniques may be applied are mainly (i) ecology (population-dynamics), (ii) evolutionof species and (iii) morphogenesis.   In thefirst case, the question to be understood is basically the distribution and abundance of species (e.g., population of different butterflies in certain areas). The parameters that determine the sizeof a population and the different species which can coexist are some of the correlated questions in this field. Due to the high complexity of biological systems, incomparison to physical systems, its description in terms of a microscopic is a hopeless task. Since Oparin[8] there has been some attempts to explain the process which leads from inanimate matter to life.   Recently some authors[3,10] have shown that starting with 'small fragments' (monomers, dimers, trimers, etc.) one can account for the growth of apolymer, with a biologically promising sequence of oligomers, through condensation reactions which are catalysed by fragments complementary to the original ones . A simplified model considers the formation of a linear macromolecule, as the sequence: $ABABAB...$, where A and B represent oligomers as purine and pyrimidine in DNA and the growth is assumed to be catalysed by complementary oligomers, such as ABA, as follows:

$$(AB) + (AB) + (ABA) \quad \rightarrow \quad (AB) + (AB)$$
$$|$$
$$(ABA)$$

$$\rightleftarrows (AB)\,(AB) \quad \rightleftarrows \quad (ABAB) \quad \rightleftarrows \quad (ABAB) + (ABA)\ .$$
$$|\ \ || \qquad\qquad |\,|\,|$$
$$(A\ \ BA) \qquad\quad (ABA)$$

In the above diagram the vertical lines represent chemical bonds between complementary fragments and they play a crucial role in the process. A configuratiorial analysis[10] of growing polymers, using the renormalization group (RG) concept, leads to a critical point k^* for the equilibrium constant k (fugacity) and also to two (stables) fixed points: k=O (corresponding to a lack of growth) and $k\rightarrow\infty$ (corresponding to infinite growth) .

The relevant result obtained from the treatment rnentioned above is the existence of a critical point $k=k^*$. This shows that the transition from inanimate matter to life can be looked at as a critical phenomenon[10]. However, although it supplies the critical point k^*, this technique does not take care of the stabilization in the length of growing polymers. Therefore, mechanism that tends to stop the growth when a convenient length is attained is not included in this treatment.

In order to explain the polymer growth and its properties, alternative treatments in terms of the polymerization-degree parameter can be used as, for example, in the model of self-avoiding random walk[11] (SAW). Treatments that follow the models for magnetic systems are also investigated[12]. In this paper we employ a different (though phenomenological) procedure following the laser analogy: we assume the same growth-model of ref. 10, but adopt the length $L(t)$ of a growing polymer as the desired variable. We set $L(t) = N(t)L_0$, where $N(t)$ is the polymerization-degree parameter[11], as appears for example in

$$[- (AB) -]^N$$

and L, is the length of the small constituent as AB. Typically, $L_0 \approx 5\text{Å}$; $N \simeq 10^4$, which gives L $\simeq 10^4$ L, $\simeq 5 \times 10^4$Å.

Setting the equation of motion for $N(t)$ as:

$$\frac{dN}{dt} = (g-\ell)\ N\ ,\qquad\qquad (1)$$

where g is a gain parameter (due to all mechanisms that tend to increase the size of the polymers) and R is a loss parameter (due to mechanisms that act in opposition to the growth of the polymer). Eq. (1) can lead either to an exponential growth for $g > \ell$ (corresponding to the infinite growth for $k>k^*$ as mentioned in ref. 10), or to an exponential decay for $g < \ell$ (corresponding to the lack of growth for $k<k^*$ as also mentioned in ref. 10). There is a slight difference in ref. 10 where below threshold $(k<k^*)$ one finds a finite value $N(\infty) \propto (k-k)^{-\nu} \neq 0$ where ν is a critical exponent. This difference, however, can be easily circunvented by the substitution $N(t) \rightarrow \mathcal{N}(t) = N(t) - N(\infty)$.

The approximation described by eq. (1) gives the threshold condition: g-R=O (corresponding to the critical point $k=k^*$, of ref. 10). However, eq. (1) does not give an upper bound to the growth, since above threshold $(g>\ell)$ the length of growing polymers blows up.

In fact, eq. (1) corresponds to a linear approximation which is valid only for small values of $N(t)$. For large values of $N(t)$ the growing polymers become sensible to the presence of mechanisms that act in opposition to growth, leading to the stabilization in the length of the polymers. For example, we may have a saturation[14] in the gain parameter, as in lasers (see ref. 7, pg. 153), due to internal ' forces '. In this case, following the laser analogy, we would have a modification in the gain parameter, yielding $g \rightarrow g - \beta_1 N$. Alternatively, we could have a modification in the loss parameter, yielding $\ell \rightarrow \ell + \beta_2 N$, probably due to external 'forces' (e.g. collisions with neighboring molecules in Brownian movement). We assume that the saturation parameter $\beta = \beta_1 (\beta_2)$ is very small in such a way that $\beta_1 << g (\beta_2 << \ell)$. Therefore the nonlinear term $\beta_1 N (\beta_2 N)$ becomes significant only for $N(t) >> 1$ which leads to the stabilization in the length of polymers for large values of $N(t)$. Hence, whatever the nature of the mechanisms might be, instead of eq. (1), we set:

$$\frac{dN}{dt} = \gamma N - \beta N^2 \qquad\qquad (2)$$

where $\gamma = g - \ell$ is the effective gain parameter and $\beta = \beta_1 (\beta_2)$ is the gain (loss) saturation parameter. Eq. (2) is a nonlinear Bernoulli's equation.

Its general solution is easily found, but here we are only interested in its steady state solution $(N=N_S)$ which is obtained by setting $dN/dt = 0$, yielding

$$N_S = \gamma/\beta = (g-\ell)/\beta \ .\qquad(3)$$

Of course, the process is not deterministic as one would conclude from eq. (2). There are other complications due to the presence of thermal fluctuations which destroy the deterministic character of eq. (2). To take into account the random process, we add, by hand, a fluctuation term $F(t)$, with $<F(t)> = 0$, which leads to a more realistic equation:

$$\frac{dN}{dt} = \gamma N - \beta N^2 + F(t)\qquad(4)$$

which is a nonlinear Langevin-type equation[15]. Its solution, and the solution of its corresponding associated Fokker-Planck equation, can be found in the literature[16].

For the sake of completeness, we mention that the analogy of the present process with a phase transition phenomenon can also be established through a potential function[17] $G(N)$, given by:

$$G(N) = -\gamma N^2/2 + \beta N^3/3 \ ,\qquad(5)$$

satisfying the condition $dG/dN = -dN/dt$.

In conclusion, the presence of the nonlinear term in eq. (2) responds for the stabilization of the polymer growth. The procedure of ref. 10 would correspond, in a way, to the linear approximation of eq. (1). For complicated systems such as growing polymers, or even in recent more realistic laser models[18], the linear approximation is a first step in the direction of a complete treatment.

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Resumo

A estabilização no comprimento de polímeros que crescem a partir de pequenos constituintes, pelo mecanismo de auto-réplicas de informação, é obtido através da analogia entre o lazer atravessando o limiar e fenômenos críticos.