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Physica A 290 (2001) 203–210

PHYSICA A

www.elsevier.com/locate/physa

Application of the theory of stochastic processes to the configuration of biological systems

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Received 24 July 2000

Abstract

In this work we extend the framework of the stochastic processes to describe the properties of the DNA chain near its melting temperature. To achieve this goal, we focus our attention on the renaturation process; it is conceived as a one-dimensional random walk which depends on time and temperature. The fundamental units in the DNA performing during the process are the base pairs adenine–thymine (A–T) and cytosine–guanine (C–G). The main result in this report is a theoretical framework that allows us to predict an important empirical relation between the melting temperature and the concentration of base pairs C–G for oligonucleotides.

1. Introduction

One of the most important contributions in the field of biological science has been the discovery of the secondary structure of the DNA-B chain by Watson and Crick. They proposed a tridimensional model of the DNA taking into account the basic chemical units [1]. The basic structure which they deduced was a large molecule with a high molecular weight, which contains two long polynucleotide chains wound around each other to give a double helix. Each of the strands is made of units called nucleotides, formed by a phosphate group, a sugar and a nitrogenous base. As is well known, normally only two types of nitrogenous bases are present in the DNA chain, purine and pyrimidine bases. Two purines and two pyrimidines are found in the DNA. The two purines are adenine (A) and guanine (G); the two pyrimidines are cytosine (C) and thymine (T). The polymeric strands are held together by phosphate groups joining

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0378-4371/01/$ - see front matter
PII: S0378-4371(00)00486-6

the sugar molecules of the nearest nucleotide in such a way that along the chain a sugar and a phosphate group alternate with each other. Therefore, the DNA-B consists of a double helix of antiparallel sugar–phosphate chains with approximately 10 base pairs per turn of 34 Å and with all the bases perpendicular to the helix axis.

According to the chemical and physical properties of the nitrogenous bases these units are inter-connected as follows: a cytosine joins only with the guanine (C–G), and thymine joins with adenine (A–T), by three and two hydrogen bonds, respectively. These predominant bonds between nucleotides leads us to explain the empirical Chargaff's rules which have been observed in many biological species [2,3]. Chargaff found that the concentration of adenine [A] is approximately equal to thymine concentration [T] for many organisms and the same occurs with the [C] and [G] bases. A direct consequence of this observation is that the ratios [G+A]/[C+T] and [G+T]/[A+C] are close to unity [4,5].

In this work we focus our attention to describe the renaturation process of DNA molecule. For such a molecule, that has been thermally denaturated previously, this process consists in the gradual joining of the two complementary strands of polynucleotides to form the double chain of DNA. The renaturation process has interesting characteristics from the physical point of view. Particularly, it takes place in a narrow region of temperature close to a characteristic temperature T_m which identifies the transition coil–helix. This T_m is called the melting temperature [2,3], and it is defined as the temperature where half of the total base pairs are unbonded. In essence, the renaturation consists in the joining process between nucleotides, A–T and C–G, in complementary strands. This effect can be observed by changing the temperature, the salt concentration or the pH in the solution [6].

The experimental research made in short chains of DNA has stressed the influence that factors such as the length of the chain and the concentration of cytosine–guanine base pairs have on renaturation [6]. The knowledge of how the DNA behaves during melting, taking into account the previous factors, has important implications in the fields of molecular biology and biotechnology [7]. Consequently, in the literature we can find many empirical expressions relating the melting temperature with the length of the chain, the number of units that confirm it, the concentration of cytosine–guanine base pairs [C+G], and the interaction with the properties of the environment [6]. From a theoretical point of view, the statistical and thermodynamic properties of the DNA chain in the transition helix–coil at the premelting and melting temperature, have been studied in terms of the Ising model [8]. All theoretical approaches investigating the helix–coil transition in DNA employ the same fundamental model.

2. Theory and results

In this work we suggest a statistical mechanical framework to justify an experimental relation found in renaturation process for oligomers. To achieve this goal the description