Melting behavior and different bound states in three-stranded DNA models

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Thermal denaturation of DNA is often studied with coarse-grained models in which native sequential base pairing is mimicked by the existence of attractive interactions only between monomers at the same position along strands (Poland and Scheraga models). Within this framework, the existence of a three-stranded DNA bound state in conditions where a duplex DNA would be in the denaturated state was recently predicted from a study of three directed polymer models on simplified hierarchical lattices ($d > 2$) and in $1 + 1$ dimensions. Such a phenomenon which is similar to the Efimov effect in nuclear physics was named Efimov-DNA. In this paper we study the melting of the three-stranded DNA on a Sierpinski gasket of dimensions $d < 2$ by assigning extra weight factors to fork openings and closings, to induce a two-strand DNA melting. In such a context we can find again the existence of the Efimov-DNA-like state but quite surprisingly we discover also the presence of a different phase, to be called a mixed state, where the strands are pair-wise bound but without three chain contacts. Whereas the Efimov DNA turns out to be a crossover near melting, the mixed phase is a thermodynamic phase.

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I. INTRODUCTION

A loosely bound state of a triple-stranded DNA when no two are bound was recently found with a theoretical approach and named Efimov-DNA [1–3]. It occurs at and above the melting point of a double-stranded DNA (dsDNA) [4–8], and is reminiscent of the Efimov effect in quantum mechanics [9,10]. In fact, the sequential base pairing of a DNA opens up a path to make a formal connection between a quantum problem and the DNA thermodynamics, with thermal fluctuations playing the role of quantum fluctuations. Owing to this quantum analogy, an Efimov-DNA could be an affordable system in the domain of classical biology for studying aspects of the quantum Efimov physics. In this paper we widen the scope of the Efimov physics by establishing the presence of the effect in certain classes of low-dimensional DNA models by staying purely in the classical domain of statistical mechanics. We also show that the same cause that produces the Efimov-like effect in DNA can lead to a new phase in triple-stranded DNA, a phase we call a *mixed phase*.

In 1970, a novel phenomenon in quantum mechanics, the Efimov effect [9,10], was discovered, which resembled the by-then-forgotten Thomas effect of the 1930s [11]. Three nucleons with a critical short range pair potential become bound due to an emergence of a long range interaction. The result was a tower of an infinite number of bound states right at the critical threshold of the two-body binding. As one moves away from the critical point the number of bound states decreases and vanishes at a particular strength. This three-body bound state has a size much larger than the range of the short range pair potential. Such a loose three-body bound state is named the quantum Efimov state.

The paths of particles in quantum mechanics (QM), in the path integral formalism, are analogous to Gaussian polymers under an imaginary time transformation; the time of quantum mechanics maps on to the contour length of the polymers. In QM, along the paths of two interacting particles, the interactions are strictly at the same time only. This maps nicely onto the sequential base pairing of a dsDNA. The excursions of the quantum particles in the classically forbidden region because of quantum fluctuations correspond to the bubbles on a DNA generated by thermal fluctuations. The infinite time limit in QM corresponds to an infinitely long DNA, a necessity for a phase transition. For the case of base pairing as the only form of mutual interaction, the melting is equivalent to the unbinding transition of a pair of particles in quantum mechanics when the bound state energy approaches zero by tuning the potential. This basic connection prompts the similarities between the Efimov problem in QM and a tsDNA.

Triple-stranded DNA (tsDNA) is well known in biology [12,13]. The base sequence of a double-stranded DNA (dsDNA) allows a third strand to bind via the Hoogsteen or the reverse Hoogsteen pairing to form a triple helix [14,15]. There are evidences, from NMR, of Hoogsteen pairing formed dynamically (1% of time) even in a normal DNA [16]. The triplex helix can also be formed with DNA-RNA [17] and DNA-peptide nucleic acid (PNA), whose uncharged peptide backbone helps in the stabilization of the triplet structure [18–21]. A triple helix formation controls the gene expression, which may be of use in antibiotics [22], and therapeutic applications like targeting a specific sequence in gene therapy [23–25]. All of these involve tightly bound states of a size determined by the hydrogen bond length. The Efimov-DNA however is not a tight bound state like these triple helices and one does not need any special pairing for its formation.

The nature of dsDNA melting depends on many factors and could either be an all-or-none process or be mediated by

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