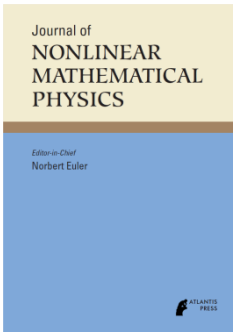


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# ON THE PSEUDO-SCHRÖDINGER EQUATION APPROXIMATION OF THE TRANSFER-INTEGRAL OPERATOR FOR 1-DIMENSIONAL DNA MODELS

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The Transfer-Integral (TI) operator is a powerful method to investigate the statistical physics of 1-dimensional models, like those used to describe DNA denaturation. At the cost of a certain number of approximations, the TI equation can be reduced to a Pseudo–Schrödinger Equation (PSE), according to which the DNA sequence is equivalent to a point particle moving in a potential well. In this paper, I check the validity of the standard PSE approximation for two different 1-dimensional DNA models, and show that it fails to provide correct results for both of them. I then propose a generalized PSE, which works well for one of the two models. Finally, I discuss the particle description of DNA denaturation that is derived from this generalized PSE.

*Keywords*: DNA denaturation; transfer-Integral operator; pseudo-Schrödinger equation.

2000 Mathematics Subject Classification: 92D20, 82B21, 41A58

## 1. Introduction

As is well known, DNA consists of two entangled long polymers of simple units. The polymers are called the strands and the monomer units the nucleotides. Each monomer consists of a phosphate group, a sugar group, and a base. The backbones of the strands are made of alternating phosphate and sugar groups connected by ester bonds. A base is attached to each sugar. There are four different types of bases, namely cytosine (C) and thymine (T), which are monocyclic, and guanine (G) and adenine (A), which are bicyclic. The genetic information is encoded in the succession of the various A, T, G and C bases that constitute a specific DNA sequence. The corresponding list of A, T, G and C letters is known as the primary structure (or genome) of the DNA. At physiological temperatures, DNA is essentially observed in the double-stranded structure, which results, as shown by Watson and Crick, from the hydrogen bonds that are formed selectively between A and T and between G and C. The association of the two strands due to base pairing is commonly referred to as the secondary structure of DNA. In addition, DNA sequences also have well-defined

higher order conformations, like the B-, A-, and Z- double helix forms, and they eventually further combine with histone proteins to form chromatin. In this paper, we are however only interested in the secondary structure of DNA and not in higher order conformations.

The two strands of DNA separate upon heating [1–4], a phenomenon called "denaturation" or "melting". Homogeneous DNA sequences denaturate abruptly at a precise temperature, while the denaturation of inhomogeneous sequences occurs through a series of steps, which can be monitored by UV absorption spectroscopy [5, 6]. At each step, large portions of the inhomogeneous DNA sequence separate over narrow temperature intervals, so that the whole denaturation process looks like a chain of sharp, first order-like phase transitions.

Following the pioneering work of Poland and Scheraga [7, 8], the simplest models for denaturation assume, in analogy with the Ising model, that a base pair is either open or closed and that its evolution can be depicted by a two-state variable (see for example [9–14]). Some of these statistical models are still used nowadays to compute rapidly denaturation curves of long DNA sequences that are in good agreement with experimental results.

While such statistical models were specifically derived to describe DNA melting, dynamical models (that is, models based on a Hamiltonian function of continuous variables) are in principle able to describe the whole dynamics of DNA, from small amplitude oscillations at low temperature to large amplitude motions close to denaturation. The first dynamical model was developed to investigate the properties of solitons in the DNA double strand. In 1980, hydrogen-deuterium exchange experiments indeed evidenced the propagation of base pair openings along the chain in a manner that resembles that of solitons [15]. In the same work, the authors proposed a Hamiltonian for describing DNA, in which the degrees of freedom are the rotation angles of the bases around the strand axes. This first model is quite simple, but more complex models have been proposed since that time and the corresponding solitonic solutions have been investigated (see for example [16–21]). These models are, however, not aimed at describing DNA denaturation, and cannot be used to investigate it, because denaturation involves essentially the stretching of the base pairs rather than the rotation of the bases around the strands.

To the best of my knowledge, the first dynamical model of DNA that depends on the distance between paired bases and might therefore be expected to describe DNA denaturation correctly was proposed by Prohofsky and co-workers [22, 23]. However, Dauxois, Peyrard and Bishop later realized that this original model predicts a denaturation transition that is much too smooth compared to experiments [24, 25]. They furthermore showed that the use of an anharmonic stacking potential instead of a harmonic one leads to denaturation curves that are in much better agreement with experiments [26–28]. More recently, other variants of the model of Prohofsky and co-workers were proposed and shown to display the correct sharp behaviour at denaturation (see for example [29, 30]).

All the dynamical models discussed above are mesoscopic 1-dimensional models, in the sense that they describe DNA as a ladder, whose rungs are the paired bases, and one coordinate is sufficient to describe the relative motion of paired nucleotides. Of course, there exist more elaborate models. For example, the model proposed in [31] is very appealing. This is indeed a mesoscopic model (6 sites, that is 18 coordinates, are used to model one base pair and the associated sugar and phosphate groups), so that standard workstations are sufficient to investigate DNA dynamics at relatively long times. Still, and in contrast with one-dimensional models, the double helix (tertiary structure) is properly taken into account