Equilibrium and Nonequilibrium Statistical Mechanics of a Nonlinear Model of DNA

Mario Techera
Max Planck Inst. For Biophysical Chemistry,
Dept. of Molecular Biology,
W-3400 Göttingen, Germany

L.L. Daemen
Theoretical Division, Los Alamos National Laboratory,
Los Alamos, New Mexico 87545

E.W. Prohofsky
Department of Physics, Purdue University,
West Lafayette, Indiana 47907

Experimental and theoretical studies indicate that the hydrogen bond stretch mode dominates DNA dynamics close to denaturation temperatures. We analyze a simplified model for DNA which retains only this (nonlinear) degree of freedom. The dynamics and thermodynamics of the system are discussed. In particular, the analytical and numerical results do not exhibit a melting transition but instead a state of pseudo-equilibrium distinct from the state expected from equilibrium thermodynamics. Finally numerical results show that energy transport is unlikely at biological temperatures.

I. THE MODEL

Deoxyribonucleic acid, or DNA, is conceivably the most important biomolecule. Its double stranded helical structure is of particular interest since the four bases (Adenine, Thymine, Guanine and Cytosine or A,T,G and C), whose sequence determines the genetic code, are projected inward toward the helix axis. On the outside of the double helix is found the backbone formed by two strands consisting of alternating phosphate groups and deoxyribose sugars. An excellent overview of DNA structure and function can be found in Saenger. As such, the geometry of the double helix requires that the two complementary strands come apart in order for the base sequence to be read by other molecules. This melting, or denaturation of DNA has been the study of intensive experimental and theoretical investigation because of its biological importance. In the present paper we present the motivation for a very simple model of DNA along with an analysis of its thermodynamics.

The infrared transmission spectrum of DNA has shown the existence of soft mode around 85 cm⁻¹. This mode is seen to drop in frequency as the melting temperature is approached. Using normal mode analysis Awati was able to characterize this mode as a collective motion of the bases that stretch the interbase hydrogen bonds (HBs). With the use of the Modified Self-Consistent Phonon Approximation, MSPA, he was able to predict the temperature dependence of this mode along with the fact that it also gained further HB stretch character as the melting temperature is approached.
The following simplified geometry is considered for DNA; the molecule is first un-twisted and each strand is then represented by a set of point masses (the nucleotides) connected by linear springs. The intrastrand interactions (i.e. the HBs between base pairs) are modeled by a Morse potential. Schematically this can be represented as in Fig. 1(a). The displacement from equilibrium of the \( n^{th} \) mass point is denoted by \( u_n \) (\( v_n \)) in the top (bottom) chain respectively. Only transverse motions are considered. The equations of motion for \( u_n \) and \( v_n \):

\[
m \ddot{u}_n = k(u_{n+1} + u_{n-1} - 2u_n) - \frac{\partial \phi}{\partial (u_n - v_n)},
\]

\[
m \ddot{v}_n = k(v_{n+1} + v_{n-1} - 2v_n) + \frac{\partial \phi}{\partial (u_n - v_n)},
\]

where \( \phi \) is the non-linear potential describing the HB interaction. At this point, it should be emphasized again that the source of the nonlinearity in the model lies in the coupling between the strands not between adjacent particles on the same strand.

![Figure 1(a)](image1)

Since the individual masses of the four different nucleotides differ by at most 13\%, the masses of the particles on each strand have been made equal in the above equations. Furthermore, for the sake of simplicity, it has been assumed that the force constants \( k \) are the same throughout the chain. These assumptions permit a transformation to center of mass coordinates:

\[
x_n = \frac{1}{\sqrt{2}}(u_n + v_n),
\]

\[
y_n = \frac{1}{\sqrt{2}}(u_n - v_n),
\]

Eqns. (1) and (2) become:

\[
m \ddot{x}_n = k(x_{n+1} + x_{n-1} - 2x_n),
\]

\[
m \ddot{y}_n = k(y_{n+1} + y_{n-1} - 2y_n) - \frac{\partial \phi}{\partial y_n}.
\]