Quasi-Continuum Models of Low-Frequency Oscillators in DNA Using the Morse Potential*

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We calculate the wavenumbers for A, B, and Z-DNA using the Morse Potential expanded up to second order (harmonic approach) ill tlie quasi-continuum model. The results are compared with available experimental data.

I. Introduction

In the last decade there have been many on preliminary effects that could be important to understand tlie transcriptiori of DNA. Essentially, these works describe some dynamic aspects related to local denaturationm[1], drug intercalation[2] and the acoustic and optical low-frequency modes[3−6]. Prohosfsky and coworkers[7], for example, have used the self consistent phonon approximation to describe the optical low-frequency spectra. The main ingredient of their model was tlie non harmonic behavior of the Morse Potential

$$V_M(y) = D[1 - \exp(-\alpha y)],\qquad (1)$$

where y is tlie distance between the base-pair in DNA. The parameters a and D found by these authors have evolved as a more elaborated model proposed or by confrontation with experimental data. To describe thermal denaturation, Bishop and Peyrard[8] used the same potential in a discrete model for DNA.

The aim of the present work is to use a quasi-continuum model, previously introduced by Chou et al.[9], to study the distribution of low frequency modes in DNA, with the a and D parameters obtained by Bishop and I'eyrard which correspond to mean values for N-H...-H and N-H...-O bonds in A-T and G-C base-pairs. This approach is different from the one proposed in refs. [9-10] where each H-bond is treated separately.

Therefore we explore the harmonic part of the Morse potent al to obtain information about the DNA. First, we expand the potential up to second order and use the quasi-continuum model, that describes the DNA

as double ribbons joined together by hydrogen-bonds (H-bonds). We get the main peaks of low-frequency spectra of some oligomers of DNA. The results are compared with experimental values.

The basic idea involved in this work is to treat DNA in two regions. First, when the non-harmonic part of the potential is predominant, e.g., at high temperatures (this is the case studied in ref. [8]). In the second region studied here (at low temperature) the harmonic part of the potential becomes more important. In this case, we study the potential around its stable minimum and the mathematical tool used was the quasi-continuum model.

We could identify two distinguished regions in the Morse potential that simulated H-bond interaction, as indicated in Fig. *1*. The region *A* would correspond to the important region of melting and the potential allows to break the H-bond. The region B, around the stable minimum, would be responsible for the collective oscillations and can be treated by the quasi-continuum model. These comments supply a qualitative picture of the idea presented in this paper.

II. Quasi-continuum model

The quasi-continuum model, proposed by Chou et al.[9], treats DNA as two ribbons of uniformly distributed mass joined by springs and allows two kinds of collective oscillations: the twist-like and accordion-like motions. The equality of the maximum kinetic and potential (harmonic) energy, in a classical approach, provide us with the values for the wavenumbers associated to the main peak, given by
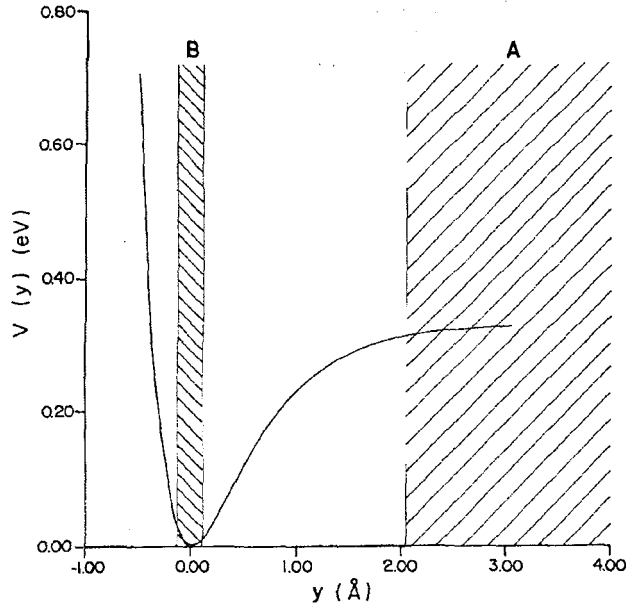
Figure 1: Morse Potential with D = 0.33 eV and α = 1.8 $\mathring{A}^{-1}$. Tlie region A is important to study melting and tlie region B is used to apply tlie quasi-continuum model.

$$\nu_t = \frac{sen\ (\xi/2)}{\pi^2 c}$$
$$\times \sqrt{\frac{3k}{<m>\left[1 + \frac{3}{\pi^2}g^2(n)\right]}}\,g(n), \qquad (2)$$

and

$$\nu_\alpha = \frac{sen\ (\xi/2)}{\pi^3 c}\left(\frac{H}{2r}\right)$$
$$\times \sqrt{\frac{3k}{<m>\left[1 + \frac{3}{\pi^4}\left(\frac{H}{2r}\right)^2 g^2(n)\right]}}\,g(n), \quad (3)$$

where ν_t and v, are tlie twist-like and accordion-like wavenumber oscillations, respectively. ξ is the difference between the phase angles of two ribbons, c is the velocity of light, k is tlie spring constant, $<m>$ is tlie mass of the DNA molecule divided by tlie number of base-pairs, H is the pitch of tlie helical ribbon, r is tlie radius of tlie virtual cylinder made by double-helical, $g(n) = H/L$ (L is the length of the DNA segment). The numerical values for the structural parameters of DNA are given in the appendix. The complete deduction of eq. (2) and (3) is presented in detail in ref. [9].

Table I - Wavenumbers of the twist-like and accordion-lilíe motions calculated for A, B and Z-DNA (in cm^{-1}).

Number of base pairs	A-DNA		B-DNA		Z-DNA	
n	$\tilde{\nu}_t$	$\tilde{\nu}_\alpha$	$\tilde{\nu}_t$	$\tilde{\nu}_\alpha$	$\tilde{\nu}_t$	$\tilde{\nu}_\alpha$
6	43.6	26.5	39.2	29.9	42.3	39.8
8	37.1	20.8	32.8	23.8	36.4	33.6
10	31.8	17.0	27.9	19.7	31.5	28.7
12	27.7	14.3	24.2	16.7	27.6	24.0
15	23.0	11.6	20.0	13.6	23.1	20.7
18	19.6	9.7	17.0	11.4	19.7	17.6
24	15.0	7.3	13.0	8.6	15.2	13.5
38	9.7	4.6	8.3	5.5	9.8	8.6
50	7.4	3.5	6.3	4.2	7.5	6.6

The spring constant is found expanding tlie Morse potential, eq. (1), up to second order (harmonic approach around tlie stable minimum) as

$$V_M(y) \simeq \frac{2D\alpha^2}{2}y^2 = \frac{K_M}{2}y^2, \qquad (4)$$

wliere y is tlie distance between the ribbons. We use D = 0.33 eV and $\alpha = 1.8\mathring{A}^{-1}$, which are tlie same values as used in ref. [8] to study melting. Then, we get

$$K_M = 2,138\frac{eV}{\mathring{A}^2} = 0.343 \cdot 10^5 \frac{erg}{cm^2}. \qquad (5)$$

It is important to note that this value is directly derived from the parameters in Morse's potential.

III. Results and Discussion

The wavenumbers obtained for twist-like and accordion-like oscillations are shown in Table I for A-, B- and Z-DNA with different numbers of base-pairs. A confrontation with the values obtained by Chou and co-workers[9] shows that our results are in agreement. However, they are systematically higher for poly(MIX)$_n$ DNA, wliere tlie number of A-T and G-C base-pairs are tlie same and correspond to the inean values used here.

The experimental results obtained through Raman spectroscopy[4] present a characteristic peak at (22 ± 2) cm^{-1} for poly(C-G)$_8$ A-DNA and (18 ± 2)

cm^{-1} for poly(MIX)$_{12}$ B-DNA. From Table I we note that tlie correspoiiding values obtained with tlie quasi-continuum model are v, $= 20,8$ cm^{-1} for A-DNA (n $= 8$) and v, $= 16,7$ cm^{-1} for B-DNA ($n = 12$). Tliese result; are in good agreement with tlie experimental ones. It is important to note that we do note that we do not distinguisli oligomers from non-oligomers DNA in tliis approach.

Lindsay et al.[5], using Raman spectroscopy, reported low-fiequency bands also at 15 cm^{-1} for A-DNA and 12 cm^{-1} for B-DNA. In tlie quasi-continuum model, these bands correspond to oscillations of intact segments in DNA containing all average of 24 base-pairs[6]. Our results to $n = 24$ in Table I are $\nu_t = 15,0cm^{-1}$ for A-DNA and $\nu_t = 13,0$ cm^{-1} for B-DNA. Tliese results again, agree with tlie experimental data.

For Z-DNA there is an experimental band[4] at 30 cm^{-1} for poly(G-C)$_6$ and our best result is $\nu_\alpha = 39,8$ cm^{-1}. This cifference between theoretical and experimental values also appears in the original work of Chou et al.[9], where tliat difference is related to tlie fact tliat in Z-DNA we do not have well defined geometric paraineters and because tlie DNA with n $= 6$ base-pairs would be too small to lse treated by this simple model. We believe tliat tlie discussion presented in ref. [9] is also applicabl: liere.

IV. Conclusion

We studied the harmonic approximation of Morse's potential in tlie quasi-continuum model aiid have obtained the lou-frequency oscillations of some segments of DNA. Tlie results are in reasonable agreement with experimental data avaliable and with otlier theoretical works[9]. Our results allow us to conclude that tlie parameters used (D and α) are sufficiently reliable to describe the harnonic dynamics of tlie hydrogen bonds, at least when we are interested in collective oscillations.

A word of caution must be said about the simplicity of the quasi-continuum model. Assuming the DNA as two ribbons of uniformly distributed masses, some intramolecular interations (e.g., base stacking, conformational rotations and electrostatic interactions) are neglected. For this reason, tlie present model describes only the main peaks of the low frequency spectrum. Recent models[11-13], based on lattice dynamics in which tlie electrostatic interactions are considered by an effective field apprcach, point out that the lower resonances

could be atributed only to motions of whole inolecule.

Finally, we emphasize tliat an other advantage of usiiig tlie Morse Potential is its broad applicability on studying other effects, such as denaturation[8] and non-linear excitations[14] (solitons). Tlie original quasi-continuum model[9], purely harmonic, does iiot permit to study tliese effects, it is confining (does iiot allow melting) and excludes tlie non-linear excitations.

Appendix: Structural Parameters

Tlie parameters used here are tlie same considered by Chou et al. in Ref.[9].

The total mass of tlie DNA molecule divicled by tlie total number of base-pairs is:

$$< m >= 1,0224 \times 10^{-21} g$$

and tlie otlier parameters are given in Table II.

Table II: Structural parameters to A, B and Z-DNA.

	ξ	$g(n)$	$H/2r$
A-DNA	0.972π	11/n	1.49
B-DNA	0.783π	10/n	2.06
Z-DNA	0.761π	12/11	2.76

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