Parameters describing the H bond in DNA

Elso Drigo-Filho
Instituto de Biociências, Letras e Ciências Exatas/UNESP, Rua Cristovão Colombo 2265, 15055 São José do Rio Preto, São Paulo, Brazil and Instituto de Física Teórica/UNESP, Rua Pamplona 145, 01405 São Paulo, São Paulo, Brazil

J. R. Ruggiero
Instituto de Biociências, Letras e Ciências Exatas/UNESP, Rua Cristovão Colombo 2265, 15055 São José do Rio Preto, São Paulo, Brazil
(Received 8 July 1991)

We analyze the parameters present in the Morse potential and van Zandt potential to describe the hydrogen bonds in DNA using the quasicontinuum model applied to the low-frequency vibrational modes.

PACS number(s): 87.15.By, 87.15.He

Recently, van Zandt [1,2] and Techera, Daemen, and Prohofsky [3] have diverged about the realism of the parameters of the potential used in Ref. [1] to describe the hydrogen bonds in the DNA molecule. One of the major disagreements is in regard to the depth of the potential and the dynamical behavior around the stable minimum.

In this Brief Report we use the quasicontinuum model [4] to study the low-frequency motions in DNA and analyze the parameters used by those authors.

The quasicontinuum model uses the harmonic approach of the H-bond vibrations. In this way, we expand the potentials around the stable minimum and calculate some wave numbers of low-frequency oscillations. The results are compared with some experimental data; in this respect caution is needed because the low-frequency motions are treated in a very simple way. We must keep in mind that, doing that, the quasicontinuum model can lead to an unrealistic picture. There are more elaborate models to study the low-frequency motions that give us a more realistic scheme for DNA (e.g., Refs. [5–7]). However, the results of Ref. [4] are in reasonable agreement with the experimental data and it is this aspect that we will explore in this paper.

Techera, Daemen, and Prohofsky [3] use the Morse potential

$$V_M(y)=V_0(1-e^{-\alpha y})^2 \tag{1}$$

and the harmonic approach is given by

$$V_M(y)=\frac{2V_0\alpha^2}{2}y^2 , \tag{2}$$

where $\alpha=\sqrt{2}$. 2.5 Å^{-1} [2,8] and $V_0=0.06$ eV [3] for a single hydrogen bond.

The van Zandt potential [1,2] and its harmonic approach is written as

$$V_z(y)=\frac{\sigma}{42\alpha^2}\left[1-\frac{1+7\alpha y}{(1+\alpha y)^7}\right]=\tfrac{1}{2}\sigma y^2 \tag{3}$$

with $\sigma=1.05$ eV/Å^2. (This value can be computed, for example, by the relation $\sigma/V_0=42$ Å^{-2} with $V_0=0.025$ eV given in Ref. [2].)

In the quasicontinuum model the DNA double helix is described by two ribbons linked by springs, with the same force constant k_s. We have two kinds of vibrations: twistlike and accordionlike oscillations. The frequency of oscillations are as follows [4]:

$$\nu_t=\frac{\sin(\xi/2)}{\pi^2 c}\left[\frac{3k_s}{\langle m\rangle[1+(3/\pi^2)g^2(n)]}\right]^{1/2} g(n) \tag{4}$$

and

$$\nu_a=\frac{\sin(\xi/2)}{\pi^3 c}\left[\frac{H}{2r}\right] \times\left[\frac{3k_s}{\langle m\rangle[1+(3/\pi^4)(H/2r)^2g^2(n)]}\right]^{1/2} g(n) , \tag{5}$$

where ξ is the difference between the phase angles of the ribbons (for A-DNA we get $\xi=0.972\pi$ and for B-DNA we get $\xi=0.783\pi$); c is the velocity of light; $\langle m\rangle$ is the total mass of DNA molecule divided by the total number of its base pairs ($\langle m\rangle=1.0224\times10^{-21}$ g); n is the number of base pairs and $g(n)$, H, and r are related to the form of the DNA [for A-DNA$\rightarrow g(n)=11/n$ and $H/2r=1.49$, for B-DNA$\rightarrow g(n)=10/n$ and $H/2r=2.06$]. In these equations the subindices stand for twistlike and accordionlike modes.

We have, in our approach, the spring constant for one H bond given by

$$k_M=2V_0\alpha^2=1.50 \text{ eV/Å}^2=0.240\times10^5 \text{ erg/cm}^2 , \tag{6}$$

$$k_z=\sigma=1.05 \text{ eV/Å}^2=0.168\times10^5 \text{ erg/cm}^2 \tag{7}$$

for the Morse and van Zandt potentials, respectively. Using the values in Eqs. (4) and (5) we obtain the wave numbers for segments of DNA. In the quasicontinuum model the large segment of DNA has the wave number given by $n=24$. This number corresponds to a typical intact segment of DNA. The theoretical results and the experimental data are shown in Table I.

TABLE I. Wave numbers of twistlike and accordionlike motions calculated for *A*- and *B*-DNA and the experimental data [9].

	Morse potential				van Zandt potential				Experimental data	
	A-DNA		*B*-DNA		*A*-DNA		*B*-DNA			
n	ν_t	ν_a	ν_t	ν_a	ν_t	ν_a	ν_t	ν_a	*A*-DNA	*B*-DNA
poly-$(\text{C-G})_8$[a]	53.7	30.1			44.9	25.2			22±2	
poly-$(\text{mix})_{12}$[b]			32.0	22.1			26.7	18.6		18±2
poly-$(\text{mix})_{24}$	19.9	9.7	17.1	11.4	16.6	8.1	14.3	9.5	15	12

[a]Reference [10].
[b]Reference [11].

Table I shows that the low-frequency vibrations in the quasicontinuum model with the parameter σ used by van Zandt [1,2] describe approximately the experimental results. Raman measurements on poly-d$(\text{G-C})_8$ *A*-DNA and poly-$(\text{mix})_{12}$ *B*-DNA showed that the low-frequency resonances were at 22±2 and 18±2 cm^{-1}, respectively, while the corresponding values for the accordionlike modes calculated with the van Zandt model leads to $\nu_a=25.2$ and 18.6 cm^{-1}. Two other low-frequency modes $\nu_t=14.3$ and 16.6 cm^{-1} can be obtained with these modes, corresponding to the 12- and 15-cm^{-1} bands observed experimentally for *B*-DNA and *A*-DNA, respectively. These results should be improved if we take a small value for σ ($\sigma \cong 0.81$ eV/Å^2).

On the other hand, the parameters used in the Morse potential (α and V_0) are not appropriate to describe these oscillations. In Ref. [3] the authors point out $V_0=0.044$ eV ($k_M=1.1$ eV/Å^2) as the value indicated by experience. This number greatly improves the results. We obtained $\nu_a=25.7$ cm^{-1} for poly$(\text{C-G})_8$ *A*-DNA, $\nu_a=18.9$ cm^{-1} for poly$(\text{mix})_{12}$ *B*-DNA and when $n=24$ we got $\nu_t=17.0$ and 14.6 cm^{-1} for *A*- and *B*-DNA, respectively. We notice that these values are approximately the same as those obtained with the van Zandt potential.

Then, the quasicontinuum model allows us to conclude that the Morse potential with $V_0=0.04$ eV and $a=\sqrt{2}$ 2.5 Å^{-1} and the van Zandt potential with $\sigma=1.05$ eV/Å^2 yields, practically, the same values for the low-frequency motions, at least when we treat the harmonic approximation. This conclusion corroborates van Zandt's argumentation in Ref. [2] about the dynamical behavior around the stable minimum of these potentials. We also notice that $V_0=0.06$ eV is not a good value to describe the low-frequency motions in this way, which agrees with the experimental arguments used in Ref. [3]. Finally, the present study points out that the model would be improved by increasing the parameters of the potentials.

However, these conclusions are constrained to the simple quasicontinuum model, and it would be interesting to do other tests to confirm the tendency observed here.

One of the authors (E.D.F.) acknowledges partial support form CAPES, Brazil.

[1] L. L. van Zandt, Phys. Rev. A **40**, 6134 (1989).
[2] L. L. van Zandt, Phys. Rev. A **42**, 5036 (1990).
[3] M. Techera, L. L. Daemen, and E. W. Prohofsky, Phys. Rev. A **42**, 5033 (1990).
[4] K. C. Chou, G. M. Maggiora, and B. Mao, Biophys. J. **56**, 295 (1989).
[5] L. Young, V. V. Prabhu, E. W. Prohofsky, and G. S. Edwards, Phys. Rev. A **41**, 7020 (1990).
[6] J. W. Powell, G. S. Edwards, L. Genzel, F. Kramer, A. Wittlin, W. Kubasek, and W. L. Peticolas, Phys. Rev. A **35**, 3929 (1987).
[7] V. K. Saxena, B. H. Dorfman, and L. L. van Zandt, Phys. Rev. A **43**, 4510 (1991).
[8] M. Techera, L. L. Daemen, and E. W. Prohofsky, Phys. Rev. A **40**, 6636 (1989).
[9] These experimental results are given in Ref. [4] and are based on the data of O. P. Lamba, A. H. J. Wand, and G. J. Thomas, Jr., Biopolymers **28**, 667 (1989) and S. M. Lindsay, J. W. Powell, and A. Rupperecht, Phys. Rev. Lett. **53**, 1853 (1984).
[10] Poly(C-G) segment has three H bonds (spring constant $=3k_s$).
[11] Poly(mix) segment has an equal number of A-T and C-G base pairs (spring constant $=2.5k_s$).