# Calculated enhancement of open base pair probability downstream of a $(TATA)_2$ box

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ABSTRACT The modified self-consistent phonon approximation is generalized to calculate the open base pair probability of a $(TATA)_2$ insert between two semi-infinite poly(d*A*–d*C*) · poly(d*G*–d*T*) helices. An iterative method based entirely on the Green's function method is developed to compute the open interbase hydrogen bond probability of the insert and near bases versus temperature. The open interbase hydrogen bond probability is calculated for two temperatures and compared with perfect homopolymer open base pair probabilities at room temperature. The probability of opening is enhanced by a factor of two for the major groove bond of the AT pair at the transcriptional downstream end of the $(TATA)_2$ insert. The total base pair opening probability of that pair is enhanced by 54%. The probability of the next inline GC base pair to be open is increased by a factor of ten.

## INTRODUCTION

Back in 1910 Lindeman (1) first correlated melting with thermal vibrational motion in his published melting formula. The generalization, the Lindeman criterion has remained a valid phenomenological predictor of melting ever since. The essence of the criterion is that all solids melt when the vibrational amplitude of a bond between atoms reaches ≈ 10% of the bond length. This implication is that thermal motion ultimately leads to atoms escaping the binding associated with rigidly bound structures.

We have developed a quantitative theory for bond breaking and melting of the DNA helix. We do find that the interstrand hydrogen bonds are disrupted when the thermal motion along these bonds reaches ≈ 10% of the total hydrogen bond length. This bond separation is not to be confused with helix unwinding which obviously requires additional motion. The melting we refer to is just the breakdown of the rigid bonding associated with the structural models of DNA. This type of DNA melting seems not to be unique in any way and is in line with observations on other materials and the Lindeman criterion.

There have been many observations by both Raman scattering and infrared radiation (i.r.) absorption of vibrational motion assigned to motion along the interbase hydrogen bonds (2–5). The principal such band ≈ 85 $cm^{-1}$ has been shown to be intrahelical as the Raman curves are identical for DNA ranging from those dissolved in dilute solution, fibers with widely ranging hydration levels, nucleosome core particles, to unseparated chromatin (6). The band is seen to soften with increasing temperature and disappear at the melting temperature (2). The band is resonant (not overdamped) and its lifetime has been studied in some detail based on observed line widths (7).

In line with these observations of resonant bands in DNA we have developed an effective harmonic theory of vibrational motion for the DNA helix. The theory is based on a modified self-consistent phonon approximation (MSPA) (8). The method predicted the 85-$cm^{-1}$ band (9) and predicts its observed temperature dependence from liquid helium temperatures to melting temperatures (10). Because melting involves displacements up to ≈ 10% of bond lengths simple harmonic theories are inappropriate. The MSPA effective force constants, calculated for the interaction between atoms across the hydrogen bonds, are not constant nor are they the small displacement force constants of traditional harmonic theory. They are thermodynamic parameters that themselves depend on the thermal motion. The parameter can be used however, to give solutions of problems involving H-bond stretch. The functional form for determining the effective force comes from a free energy minimization (8). Such an effective force constant can be compared to an analogous parameter, the compressability of a gas used in calculations of acoustic propagation. That too is a thermodynamic effective parameter that is appropriate to solutions of acoustic problems. The origin of the compressability is quite complex and also depends on thermal motion. The hydrogen bond thermal motion that leads to melting is calculated by this approach. All the earlier applications have dealt with systems with helical symmetry (11, 12). This work applies the bond breaking theory to a system with a specific symmetry breaking base sequence. The results of the earlier work have been in agreement with the


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observation of fluctuational opening in the premelting region (11) and has shown the proper cooperative behavior in the critical transition region (12).

A Green's function technique (13) has been modified to study the vibrational properties of DNA polymers with broken helical symmetry and has been applied to several examples of DNA double helix. These include the junction of AT/GC helices (14), the terminus of a DNA homopolymer (15), a junction of DNA double helix and single strands (16), and defect-mediated melting of DNA homopolymers (8). In these examples, the alterations in interactions between atoms from those of the perfect helix are treated as defects. The presence of such defects breaks the helical symmetry thereby making the description of the normal modes much more difficult. However, for situations of interest, such defects usually exist in a finite region of the polymer and involve a relatively small number of atoms. The problem is then conveniently solved by the Green's function technique.

A variety of realistic DNA molecules can be treated using this technique, including those with structural disorder, such as terminal regions, irregular base pair sequences, and various linking arrangements involving DNA double helices or single strands which occur during DNA replication, recombination, RNA transcription, and other biological processes. These defects are believed to play an important role in the melting of the DNA double helix. It has been found that localized modes can exist around defects in DNA polymers, which enhance the vibrational fluctuations in the hydrogen bonds that link the two complimentary strands of the DNA double helix. This can initiate melting of the DNA double helix around the defects (8, 14–16). It is also found experimentally that the stability of a portion of DNA helix can be influenced by the nucleotide sequence of adjacent regions (17, 18). Hence, alterations in the nucleotide sequence in regions adjacent to an actual DNA-protein interaction site could influence the recognition of that site, particularly if fluctuations to a transitory open state of the helix is important for protein binding and initiation of the biological process. It is also believed that A-T rich regions should melt at lower temperatures than G-C rich regions, and this can lead to an initiation of melting from the AT rich sites. Such open regions offer a potential interaction site.

In this paper, we apply the Green's function technique to study vibrational properties of a DNA double helix which has a finite region containing base pairs different from the rest of the helix. Breathing modes of the hydrogen bonds are of particular interest as discussed earlier. The Green's function method is used to study the thermal fluctuation in the average hydrogen bond stretch and lead to calculations of the probability of interbase hydrogen bond disruption. The calculation is carried out for a DNA double helix in the B conformation which has $(TATA)_2$ base pair box in between two semi-infinite poly(d$A$–d$C$) · poly(d$G$–d$T$) helices. One side of $(TATA)_2$ has a GC base pair next to the insert and the other, the downstream side, has an AT base pair next to the insert. This gives rise to a TATAA region that corresponds more closely to the consensus inserts (19, 20). Open base pair probability is calculated for the insert base pairs and for five base pairs on both sides of the insert and compared with those of poly(d$A$–d$C$) · poly(d$G$–d$T$) and poly(d$T$–d$A$) · poly(d$T$–d$A$) in the same conformation.

## FORMALISM

We construct the helix system starting with a perfect double helix (B poly(d$A$–d$C$) · poly(d$G$–d$T$)) and a finite section ($2N$ base pairs) of double helix with the same conformation but different base pairs $(TATA)_2$. Then we replace $N$ consecutive cells of the perfect helix by the finite section. This is achieved by setting the force constants linking the atoms across cell boundary to zero at two junctions $N$ cells apart in the infinite helix and adding corresponding forces to connect the finite section to the two semi-infinite strands as shown in Fig. 1. We choose to cut the O5-C5 bond so that the number of valence forces involved is a minimum. The nonbonded stacking forces are also cut (21).

The perfect helix system, consisting of an infinite double helix and a finite section of helix of different base pairs, is described by the eigen problem:

$$(\mathbf{F} - \omega^2\mathbf{I})\mathbf{q} = 0, \tag{1}$$

where $\mathbf{F}$ is the force constant matrix, $\mathbf{I}$ is a unitary matrix, $\omega$ and $\mathbf{q}$ are eigenvalues and eigenvectors in the mass weighted Cartesian (MWC) coordinates. The infinite helix eigenvalues and eigenvectors are solved by helical lattice methods (22). The finite helix section can be solved exactly if the number of cells, $N$, is small. To avoid the complexity added due to end effects of the finite section that ultimately go away and to reduce the computing time for large $N$, we approximate the eigenfrequencies and eigenvectors for the finite segment by those extracted from the eigen values and eigen vectors of the corresponding infinite double helix for only the following $\theta$ values:

$$\theta = -\pi + \frac{2\pi n}{N}, \quad n = 1, 2, 3, \ldots, N.$$

For a finite $(TATA)_2$ section four base pairs long (two unit cells long), the eigenvalues and eigenvectors corresponding to $\theta = 0$, and $\pi$ from those of B poly(d$T$–d$A$) · poly(d$T$–d$A$) are used. These two $\theta$ values for each band of the periodic helix give the correct number of states associated with a two unit cell section.

The altered helix system is described by a similar eigen equation (23):

$$(\mathbf{F} - \omega^2\mathbf{I} + \mathbf{C} + \bar{\mathbf{C}})\mathbf{q} = 0, \tag{2}$$

where $\mathbf{F}$ is the force constant matrix for the unperturbed system. $\omega$ and $\mathbf{q}$ are the new eigenvalues and eigenvectors. The alteration matrix, $\mathbf{C}$, is the change in $\mathbf{F}$ necessary to bring about the severing of the infinite helix and the joining of the two semi-infinite helices created, to the finite section. $\bar{\mathbf{C}}$ is the matrix due to the anharmonicity of the hydrogen bonds which soften as the temperature rises or as the thermal motion

increases for any reason. Differences in motion are introduced by the C factors. The $\bar{\mathbf{C}}$ will act synergistically to enhance the altered motion arising from C, i.e., the structural defects. The finite alteration C breaks the helical symmetry. The normal mode calculation can no longer use helical lattice methods as these depend on symmetry. However, because C is a matrix of relatively low dimensionality, Eq. 2 can be solved in terms of Green's function of the unperturbed system.

The hydrogen bond mean square amplitudes may be directly calculated from normal mode analysis. In the current problem, however, the harmonic approximation fails because any analysis of hydrogen bond disruption necessarily involves large displacement of the hydrogen bonds. In the MSPA theory, an iterative method is introduced to compute the above quantities self-consistently for a Morse-like hydrogen bond potential. In this paper, an initial set of force constants are obtained by fitting to the Lippincott-Schroeder potential (24) for all hydrogen bonds. Then the secular equation is solved for the copolymers. The normal mode frequencies and eigenvectors are used to obtain anharmonic force constants from a Morse potential. For all future calculations, the Morse potential is used to calculate force constants appropriate to the degree of thermal fluctuation at a given temperature. These new force constants are used to calculate a new set of normal mode frequencies and eigenvectors which are used to reevaluate the force constants. This process is repeated until it reaches self-consistency, which is indicated by a convergence in the force constant for each hydrogen bond into a stable value (8).

In our approach, the double helix can be described by Eq. 1 and $\bar{\mathbf{C}}$ is the only matrix that depends on temperature. We may define a Green's function for the system at a fixed temperature with only structural defects (i.e., $\bar{\mathbf{C}} = 0$).

$$\mathbf{G} = (\omega^2\mathbf{I} - \mathbf{F} - \mathbf{C})^{-1}, \tag{3}$$

and a Green's function for the complete system, with thermal effects,

$$\bar{\mathbf{G}} = (\omega^2\mathbf{I} - \mathbf{F} - \mathbf{C} - \bar{\mathbf{C}})^{-1}. \tag{4}$$

It can be shown that (25):

$$\bar{\mathbf{G}} = \mathbf{G} + \mathbf{G}\bar{\mathbf{T}}\mathbf{G}, \tag{5}$$

where

$$\bar{\mathbf{T}} = (\bar{\mathbf{C}}^{-1} - \mathbf{G})^{-1}. \tag{6}$$

The Green's function G is temperature independent except for the Bose Einstein weight factor and needs to be calculated only once from the initial helix system. Then, Eqs. 5 and 6 can be used to compute the Green function $\bar{\mathbf{G}}$ of the complete system at any iterative step for a set of trial hydrogen bond force constants and only this calculation is done iteratively to self-consistency.

The inband thermal mean-squared vibrational amplitude for the $m$th hydrogen bond may be obtained by (14):

$$D^m(\omega) = \frac{\hbar}{\pi}\,\mathrm{Im}\,[\overline{G_{ss}^{mm}}(\omega^2)]\,\coth\left(\frac{\hbar\omega}{2kT}\right). \tag{7}$$

In calculating the total $D$ we integrate over $\omega$. The result is correct for a noncoherent set of contributions from all modes that have some projection on hydrogen bond stretch. It is not just the contribution from one coherent oscillation. The lifetime of the modes involved does not effect this result. The total integrated contribution from a mode is independent of lifetime for the same reason that the total integrated intensity of an absorption band is independent of mode lifetime and width, i.e., what is missed at one frequency is picked up elsewhere. The calculation related to an equilibrated system with some thermodynamic fluctuations.

The force constant corresponding to the hydrogen bond with this mean square stretch amplitude is then calculated from reference 26 as:

$$\phi_i = \frac{\int_{-h_i}^{\infty} du e^{-u^2/2D_i}\dfrac{d^2V_i}{du^2}}{\int_{-h_i}^{\infty} du e^{-u^2/2D_i}}, \tag{8}$$

where

$$V(u) = V_0(e^{-2a(\langle R\rangle+u)} - 2e^{-a(\langle R\rangle+u)}) \tag{9}$$

is the Morse potential. Here $V_0$ and $a$ are parameters that characterize the potential, $\langle R\rangle$ is the thermal expanded mean hydrogen bond length and is the centroid of the distribution function $\exp(-u^2/2D)$ used in Eq. 8. It is a function of the mean square stretch amplitude. The determination of $\langle R\rangle$ is shown in earlier publications (26). The effective force constant $\phi$ depends on the mean square fluctuation of the hydrogen bond length $D$ and therefore depends on temperature. $D$ in turn depends on the eigenvalues and eigenvectors of the system which are functions of the force constant matrix which contains $\phi$. $\phi$, $\langle R\rangle$, and $D$ are all solved iteratively until a self-consistent set of values are obtained.

The probability of a single hydrogen bond, being disrupted in the premelting state, is then given by MSPA theory (11, 12) as

$$P_i = C_i \int_{L_i^{\max}}^{\infty} du \exp\,(-(u - \langle R_i\rangle)^2/2D_i), \tag{10}$$

where

$$C_i^{-1} = \int_{-h_i}^{\infty} \mathrm{du}\, e^{-u^2/2D_i}. \tag{11}$$

Here, $C_i$ is the normalization factor for the $i$th hydrogen bond. $L_i^{\max}$ is the maximum value of stretch before the $i$th hydrogen bond is considered in the open state. $D_i$ is the thermal mean fluctuation square stretch of the $i$th hydrogen bond. $\langle R_i\rangle$ is the equilibrium length of the $i$th hydrogen bond. $h_i$ is determined from the relation given below (11, 12):

$$V(\langle R_i\rangle - h_i) = V(\infty) = 0. \tag{12}$$

The probability that a given base pair is in the open state is the probability that all the hydrogen bonds of that pair are disrupted simultaneously and in our mean field approximation that is the product of the open probabilities of the individual hydrogen bonds. The Morse parameters and maximum length of all the hydrogen bonds used in this calculation are shown in Table 1 and Table 2 for Adenosine-Thymine and Guanine-Cytosine base pairs, respectively (10, 23). $R_0$ is the position of the minimum of the Morse potential and is equal to $\langle R\rangle$ at $T = 0$. The values for the Morse parameters used here give rise to mode calculations that fit the observed spectra (27) and fit

**TABLE 1 The Morse parameters of AT base pairs**

| Bond | $a$ Å$^{-1}$ | $R_0$ Å | $V_0$ mdyn Å | $L_{\max}$ Å |
|---|---|---|---|---|
| N(1)—H—N(3) | 2.402 | 2.782 | 0.01702 | 3.158 |
| N(6)—H—O(4) | 2.713 | 2.698 | 0.01959 | 3.146 |

TABLE 2 **The Morse parameters of GC base pairs**

| Bond | $a$ Å$^{-1}$ | $R_0$ Å | $V_0$ mdyn Å | $L_{max}$ Å |
|---|---|---|---|---|
| N(1)—H—N(3) | 2.349 | 2.805 | 0.0184 | 3.043 |
| O(6)—H—N(4) | 2.884 | 2.693 | 0.0257 | 3.020 |
| N(2)—H—O(2) | 2.784 | 2.706 | 0.0249 | 3.043 |

the temperature dependence of the 85-cm$^{-1}$ mode (9) which are derived by Chen, Y. Z., et al. (29).

## RESULTS AND DISCUSSION

We carried out the calculation for an infinite DNA double helix in the B conformation, which has $(TATA)_2$ base pairs in the middle and poly(d$A$–d$C$) · poly(d$G$–d$T$) base pairs for the rest of it. We have found that breathing modes exist around 85 wave numbers in both homopolymers (28). We scanned through the entire spectra of both poly(d$T$–d$A$) · poly(d$T$–d$A$) and poly(d$A$–d$C$) · poly(d$G$–d$T$) and found that the average hydrogen bond stretch amplitude is significant only for a few branches of the perfect helix dispersion curves between 5 and 300 cm$^{-1}$. Therefore, only this frequency range is considered in studying the breathing modes of the altered helix.

The open hydrogen bond probability is given in Table 3 for temperatures $T$ = 293 and 310 K. The hydrogen bond numbers refer to the numbers seen at the bottom of Fig. 1. The open hydrogen bond probability ($P_i$) for the hydrogen bonds upstream of the insert except for hydrogen bond number 4 are smaller than the perfect open hydrogen bond probability ($P$(per)). Inside the insert the open hydrogen bond probabilities are lower than the perfect AT copolymer open hydrogen bond probability. This is because the C-G base pairs now included on both sides of the insert tend to increase the stability of the insert and lower the open hydrogen bond probability. The open hydrogen bond probabilities are dramatically increased for the hydrogen bonds downstream the insert for number 14 at $T$ = 293 K. The effect of the particular sequence studied is to stabilize the base pair bonding to one side of the insert (the upstream side) and to destabilize the base pair bonding on the other side (downstream side). Downstream is the direction that RNA transcription occurs with respect to the $(TATA)_2$ insert in many studied initiation sites. The pair opening probability for AT pairs is farily large. The likely critical element in initiating or elongating an open state, necessary for transcription to occur, is to open the GC pairs. They would form the bottleneck to open state elongation. The first GC pair downstream of the insert is an order of magnitude more likely to fluctuate to an open state than a GC pair in the original perfect copolymer. It is 110 times more likely to open than the first GC pair upstream to the $(TATA)_2$ insert.

TABLE 3 **Insert open base pair probabilities**

| H Bond$_i$ | $P$(per) $T$ = 293 | $\Pi_i P$(per) $T$ = 293 | $P_i$ $T$ = 293 | $\Pi_i P_i$ $T$ = 293 | Ratio | $P_i$ $T$ = 310 |
|---|---|---|---|---|---|---|
| 1 | 0.0758 | 0.00488 | 0.0680 | 0.00391 | 0.80 | 0.0774 |
| 2 | 0.0644 | | 0.0576 | | | 0.0649 |
| 3 | 0.0226 | | 0.0047 | | | 0.0064 |
| 4 | 0.0230 | 0.00019 | 0.0336 | 0.000002 | 0.09 | 0.0390 |
| 5 | 0.0369 | | 0.0108 | | | 0.0131 |
| 6 | 0.0692 | 0.00527 | 0.0579 | 0.00215 | 0.41 | 0.0639 |
| 7 | 0.0761 | | 0.0372 | | | 0.0440 |
| 8 | 0.0692 | 0.00527 | 0.0060 | 0.00020 | 0.03 | 0.0078 |
| 9 | 0.0761 | | 0.0337 | | | 0.0407 |
| 10 | 0.0692 | 0.00527 | 0.0154 | 0.00064 | 0.12 | 0.0208 |
| 11 | 0.0761 | | 0.0419 | | | 0.0515 |
| 12 | 0.0692 | 0.00527 | 0.0615 | 0.00296 | 0.56 | 0.0685 |
| 13 | 0.0761 | | 0.0482 | | | 0.0563 |
| 14 | 0.0758 | 0.00488 | 0.0592 | 0.00748 | 1.54 | 0.0647 |
| 15 | 0.0644 | | 0.1264 | | | 0.1328 |
| 16 | 0.0226 | | 0.0624 | | | 0.1287 |
| 17 | 0.0230 | 0.000019 | 0.0696 | 0.00019 | 10.0 | 0.0828 |
| 18 | 0.0369 | | 0.0455 | | | 0.0887 |

Column 1 is H-bond number. Column 2 is open probability for each H-bond at 293 K, for the perfect system, i.e., the separate homopolymers. Column 3 is the probability of a base pair being open at 293 K for the perfect system. Column 4 is the individual H-bond open probability for the new structure with insert at 293 K. Column 5 is the open base probability for the new structure. Column 6 is the ratio of open base probability for new structure to perfect system. Column 7 is the H-bond open probability at 310 K.

The actual numerical values of open bond probability

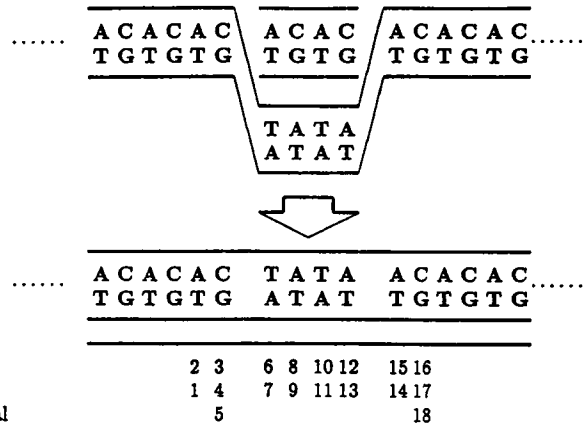


FIGURE 1 The double helix is constructed by cutting the perfect helix, and joining the finite section $(TATA)_2$ to the semi-infinite strands. The numbers at the bottom identify the hydrogen bonds of each base pair and are used in Table 3.

are strongly dependent on values chosen for $L_i^{max}$. Our choice of $L_i^{max}$s come from observation of the onset of anomalous behavior when exploring the thermal melting of homopolymer DNAs (29). The actual values would be determined by how hydrogen bonds are altered by the presence of solvent atoms and should be fit with greater care. The values chosen do however fit data of bond opening based on analysis of proton exchange for both amino and imino protons in DNA fairly well (11).

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## REFERENCES

1. Lindeman, F. 1910. Thermal melting law. *Phys. Z.* 11:609–611.
2. Urabe, H., and Y. Tominga, 1981. Low frequency Raman spectra of DNA. *J. Phys. Soc. Jpn.* 50:3543–3544.
3. Lamba, O. P., A. H. J. Wang, and G. J. Thomas, Jr. 1989. Low frequency dynamics and Raman scattering of crystals, of B-, A-, and Z-DNA and fibers of C-DNA. *Biopolymers.* 28:667–678.
4. Weidlich, T., and S. M. Lindsay. 1988. Counterion effects on the structure and dynamics of solid DNA. *Phys. Rev. Lett.* 61:1674–1677.
5. Powell, J. W., G. S. Edwards, L. Genzel, and A. Wittlin. 1987. Investigation of far-infrared vibrational modes in polynucleotides. *Phys. Rev. A.* 35:3929–3939.
6. Urabe, H., H. Hayashi, X. Tominga, Y. Nishimura, K. Kubota, and M. Tsuboi. 1985. Collective vibrational modes in molecular assembly of DNA and its applications to biological systems. Low frequency Raman spectroscopy. *J. Chem. Phys.* 82:531–535.
7. Tominga, Y., M. Shida, K. Kubota, H. Urabe, Y. Nishimura, and M. Tsuboi. 1985. Coupled dynamics between DNA helix and spectroscopy. *J. Chem. Phys.* 83:5972–5975.
8. Kim, Y., and E. W. Prohofsky. 1986. Defect-mediated hydrogen-bond instability of *poly(dG)·poly(dC)*. *Phys. Rev.* B33:5676–5681.
9. Eyster, J. M., and E. W. Prohofsky. 1974. Lattice vibrational modes of *Poly(rU)·Poly(rA)*. A coupled single-helical approach. *Biopolymers.* 13:2527–2543.
10. Kim, Y., and E. W. Prohofsky. 1987. Vibrational modes of a DNA polymer at low temperature. *Phys. Rev.* B36:3449–3451.
11. Chen, Y. Z., Y. Feng, and E. W. Prohofsky. 1991. Premelting thermal fluctuational base pair opening probability of *poly(dA)·poly(dT)* as predicted by the modified self-consistent phonon theory. *Biopolymers.* 31:139–148.
12. Chen, Y. Z., and E. W. Prohofsky. 1991. A self-consistent mean-field calculation of a homopolymer deoxyribose nucleic acid strand separation: bond breaking in a macromolecule. *J. Chem. Phys.* 94:4665–4667.
13. Lifshitz, I. M., and S. I. Pekar. 1955. Tamm connected states of electrons on the surface of a crystal and the surface oscillations of the atoms of a lattice. *Usp. Fiziol. Nauk.* 56:531–568.
14. Feng, Y., R. D. Beger, X. Hua, and E. W. Prohofsky. 1989. Breathing modes near a junction of DNA double helices. *Phys. Rev.* 40:4612–4619.
15. Putnam, B. F., L. L. Van Znadt, E. W. Prohofsky, and W. N. Mei. 1989. Resonant and localized breathing modes in terminal regions of the DNA double helix. *Biophys. J.* 35:271–287.
16. Putnam, B. F., and E. W. Prohofsky. 1983. Localized vibrational modes at a double-helix single strand junction. *Biopolymers.* 22:1759–1767.
17. Wells, R. D., R. W. Blakesley, S. C. Hardies, G. T. Horn, J. E. Larson, E. Selsing, J. F. Burd, H. W. Chan, J. B. Dodgson, K. F. Jensen, I. F. Nes, and R. M. Wartell. 1977. The role of DNA structure in genetic regulation. *CRC Critical Reviews in Biochemistry.* 305–340.
18. Burd, J. D., R. M. Wartell, J. B. Dodgson, and R. D. Wells. 1975. Transmission of stability (telestability) in deoxyribonucleic acid. *J. Biol. Chem.* 250:5109–5113.
19. Hawley, D. K., and W. R. McClure. 1983. Compilation and analysis of Escherichia coli promoter sequences. *Nucleic Acids Res.* 11:2237–2255.
20. Cho, K., and C. Yanofsky. 1988. Development of a trpE promoter-strength measuring system and its use in comparison of the trpEDCBA, trpR and aroH promoters. *J. Mol. Biol.* 204:41–50.
21. Putnam, B. F. 1981. Calculation of macromolecular force constants and vibrational properties of a semi-infinite strand of the DNA double helix. Ph.D. Thesis, Purdue University, West Lafayette, IN. 87–135.
22. Eyster, J. M. 1974. Normal modes of helical polymers of biological interest. Ph.D. Thesis, Purdue University, West Lafayette, IN. 47–85.
23. Feng, Y., W. Zhuang, and E. W. Prohofsky. 1991. Calculation of temperature dependence of interbase breathing motion of a guanine-cytosine DNA double helix with adenine-thymine insert. *Phys. Rev. A.* 43:1049–1053.
24. Schroeder, R., and E. R. Lippincott. 1957. Potential function model of hydrogen bonds. II. *J. Phys. Chem.* 61:921–928.
25. Bottger, H. 1983. Principles of the Theory of Lattice Dynamics. Physik-Verlag, Weinbeim, FRG. 87 pp.
26. Gao, Y., K. V. Prasad, and E. W. Prohofsky. 1984. A self-consistent microscopic theory of hydrogen bond melting with application to *poly(dG)·poly(dC)*. *J. Chem. Phys.* 80:6291–6298.
27. Devi-Prasad, K. V., and E. W. Prohofsky. 1984. Low-frequency mode predictions in A-DNA compared to experimental observations and significance for A-to-B. *Biopolymers.* 23:1795–1798.
28. Prohofsky, E. W. 1985. Biomolecular Stereodynamics IV, Proceedings of the Fourth Conservation in the Discipline Biomolecular Stereodynamics. Albany, NY. 21–46.
29. Chen, Y. Z., Y. Feng, and E. Prohofsky. 1990. Criteria of thermal denaturation for modified self-consistent-phonon-theory mean-field calculations in DNA polymers. *Phys. Rev.* B.42:11335–11338.