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The thermal denaturation of the Peyrard–Bishop model with an external potential

A Sulaiman[1,2,4], **F P Zen**[1,4], **H Alatas**[3,4] and **L T Handoko**[5,6]

[1] Theoretical Physics Laboratory, THEPI Research Division, Institut Teknologi Bandung, Jl. Ganesha 10, Bandung 40132, Indonesia
[2] Badan Pengkajian dan Penerapan Teknologi, BPPT Bld. II (19th floor), Jl. M H Thamrin 8, Jakarta 10340, Indonesia
[3] Theoretical Physics Division, Department of Physics, Bogor Agricultural University, Jl. Meranti, Kampus IPB Darmaga, Bogor 16680, Indonesia
[4] Indonesia Center for Theoretical and Mathematical Physics (ICTMP), Jl. Ganesha 10, Bandung 40132, Indonesia
[5] Group for Theoretical and Computational Physics, Research Center for Physics, Indonesian Institute of Sciences, Kawasan Puspiptek Serpong, Tangerang 15310, Indonesia
[6] Department of Physics, University of Indonesia, Kampus UI Depok, Depok 16424, Indonesia

E-mail: albertus.sulaiman@bppt.go.id, fpzen@fisika.itb.ac.id, alatas@ipb.ac.id and handoko@teori.fisika.lipi.go.id

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Abstract

The impact of various types of external potentials on the Peyrard–Bishop DNA denaturation is investigated through the statistical mechanics approach. The partition function is obtained using the transfer integral method, and the stretching of hydrogen bonds is calculated using the time-independent perturbation method. It is shown that all types of external potentials accelerate the denaturation processes at lower temperature. In particular, it is argued that the Gaussian potential with infinitesimal width reproduces a constant force at one end of the DNA sequence as was already done in some previous works.

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1. Introduction

It is known that the base-pairs of a double-helix break up and dissociate from each other to form two separated random coils when a solution of DNA macromolecules is heated up to 80°C. This phenomenon is referred to as DNA denaturation or thermal DNA melting ([1] and references therein). On the other hand, at lower temperature before melting two strands of DNA can also be separated by applying an oppositely directed force on two strands at the DNA terminal point. This is known as the force-induced DNA melting [1]. Theoretically, the phenomena has been discussed in many works, for example the work by Hanke *et al* [2] on the denaturation of stretched DNA. Also using the worm-like chain, the opened double-stranded DNA can be explained by a force exceeding a certain critical value [3, 4]. On the other hand, the study of shear effect of the pulling force shows that the shear unzipping of a heteropolymer would be similar to the unzipping in a tensile mode with sequence heterogeneity [5, 6].

It has been shown that a random external force would drastically change the phase diagram, while the ground state develops bubbles with various lengths when the random force fluctuation is increased. The fluctuating force denaturates the DNA by a gradual increase of bubble sizes. This suggests the possibility of opening up local bubbles in the selective regions without breaking the whole DNA [7]. Denaturation at lower temperature is realized by enzymes, protein and so forth [8]. The effects are influenced by many factors such as the alkaline compound filling up a cell. Some works also investigated other effects, for example the phase transition in a short DNA using the Peyrard–Bishop (PB) with an additional delta function potential [9]. The paper argued that denaturation is a localization–delocalization transition process. In the case of no external force, denaturation is a second-order transition, whereas under an external force it becomes a first-order one [1]. On the same lines, this paper deals with external potentials interacting with DNA within the PB model and investigates its effects on the denaturation process.

This paper is organized as follows. First of all, the PB model with various external potentials is briefly introduced. It is then followed by the statistical mechanics formulation on the partition function of the Hamiltonian under consideration. Before ending the paper with a summary, the detailed calculation of hydrogen bond stretching using first-order time-independent perturbation and its thermal behavior are presented in sections 3 and 4.

2. The model

Following the original PB model, the motion of DNA molecules is represented by transversal displacement, u_n and v_n, corresponding to the base displacement from their equilibrium position along the direction of hydrogen bonds that is represented by the Morse potential to connect two bases in a pair [10].

This paper adopts the PB model with an additional external potential V that has the same direction as the Morse potential:

$$H = \sum_n \frac{1}{2M}\dot{u}_n^2 + \frac{\kappa}{2}(u_n - u_{n-1})^2 + \sum_n \frac{1}{2M}\dot{v}_n^2 + \frac{\kappa}{2}(v_n - v_{n-1})^2 + \frac{D}{2}\left(\mathrm{e}^{-\alpha/2\sqrt{2}(u_n - v_n)} - 1\right)^2 + V(u_n - v_n). \tag{1}$$

Performing a transformation into the center of mass coordinate representing the in-phase and out-phase transversal motions, one can define $X_n = (u_n + v_n)/\sqrt{2}$ and $Y_n = (u_n - v_n)/\sqrt{2}$. Then, it yields the PB Hamiltonian [10]

$$H = \sum_n \frac{1}{2M}p_n^2 + \frac{\kappa}{2}(X_{n+1} - X_n)^2 + \sum_n \frac{1}{2M}P_n^2 + \frac{\kappa}{2}(Y_{n+1} - Y_n)^2 + \frac{D}{2}\left(\mathrm{e}^{-\alpha/2\,Y_n} - 1\right)^2 + V(Y_n), \tag{2}$$

where D and α are the depth and the inverse width of the potential, respectively. $p_n = M\dot{X}_n$, $P_n = M\dot{Y}_n$ and κ is the spring constant.

It should be remarked that some previous works have suggested that the nth nucleotide in one strand might preferably interact with the $(n \pm h)$th nucleotides in another strand with $h = 4$ or 5 [11–13]. However, for the sake of simplicity, throughout the paper let us consider the original PB model with taking into account only the nearest-neighbor nucleotides of another strand. Extension to the cases of $h \neq 1$ requires extensive numerical studies that is beyond our current interest. The variable X_n is decoupled from Y_n corresponding merely to the linear chain, while Y_n represents the stretching motion that is of our main interest. So, from now on, let us ignore the X_n part in further calculations.

3. Mechanical statistics calculation

Now let us calculate the mechanical statistics behavior of the current system using the transfer integral method. Given a certain Hamiltonian of an equilibrium system, one can extract some physical observables through the statistical mechanics approach. The approach is particularly suitable for investigating the dynamics of DNA with thermal fluctuations, since the exact solution to its equation of motion never exists [14]. Within the PB model, DNA denaturation and its melting temperature have previously been studied in terms of temperature [10, 12]. It was argued that denaturation can be induced by energy localization due to nonlinear effects, and should be highly influenced by external interactions such as V_n in the present case.

Using the Hamiltonian in equation (2), one can consider the partition function to further calculate some thermodynamic variables. In [10, 14], the calculation has been performed using the transfer integral method for $V = 0$. This paper follows the same procedure. In the canonical ensemble the partition function density is related to the Hamiltonian by $Z \propto \exp(\beta H)$. For the present case it reads

$$Z = \int\!\!\int \prod_{n=1}^{N} \prod_{n=0}^{N} \mathrm{d}P_n\, \mathrm{d}Y_n \exp\left\{-\beta\left[\sum_n \frac{P_n^2}{2M} + \frac{\kappa}{2}(Y_n - Y_{n-1})^2 + \frac{D}{2}\left(\mathrm{e}^{-\alpha/2\,Y_n} - 1\right)^2 + V(Y_n)\right]\right\} \delta(Y_N - Y_0), \tag{3}$$

where $\beta = 1/kT$ with k being the Boltzmann constant. It can further be decomposed into its momentum and coordinate spaces, $Z = Z_P Z_Y$, with

$$Z_P = \int \prod_{n=1}^{N} \mathrm{d}P_n \exp\left(-\beta \sum_n \frac{P_n^2}{2M}\right), \tag{4}$$

$$Z_Y = \int \prod_{n=0}^{N} \mathrm{d}Y_n\, \delta(Y_N - Y_0) \exp\left\{-\beta\left[\frac{\kappa}{2}(Y_n - Y_{n-1})^2 + \frac{D}{2}\left(\mathrm{e}^{-\alpha/2\,Y_n} - 1\right)^2 + V(Y_n)\right]\right\}. \tag{5}$$

The Gaussian integration in equation (4) yields

$$Z_P = \left(\sqrt{\frac{2\pi M}{\beta}}\right)^N. \tag{6}$$

On the other hand, equation (5) reads

$$Z_Y = \int \prod_{n=0}^{N} \mathrm{d}Y_n\, \delta(Y_N - Y_0) \prod_{n=1}^{N} \mathrm{e}^{-\beta\Theta(Y_n, Y_{n-1})}, \tag{7}$$

where

$$\Theta(Y_n, Y_{n-1}) = \frac{\kappa}{2}(Y_n - Y_{n-1})^2 + \frac{D}{2}(\mathrm{e}^{-\alpha/2Y_n} - 1)^2 + V(Y_n). \tag{8}$$

This can be solved using the transfer integral method.

Shifting the operator $Y_{n-1} \to Y_n$ and defining an eigenfunction $\phi(Y_n)$ that satisfies [14]

$$\int \mathrm{d}Y_{n-1}\, \mathrm{e}^{-\beta\Theta(Y_n,Y_{n-1})}\phi_i(Y_{n-1}) = \mathrm{e}^{-\beta E_i}\phi_i(Y_n), \tag{9}$$

equation (7) becomes

$$Z_Y = \int \prod_{n=0}^{N} \mathrm{d}Y_n\, \delta(Y_N - Y_0)\, \mathrm{e}^{-\beta E_i}\phi_i(Y_n). \tag{10}$$

Since $\delta(Y_N - Y_0) = \sum_i \phi_i^*(Y_N)\phi_i(Y_0)$ and taking the normalization $\int \mathrm{d}Y\, \phi^*\phi = 1$, one obtains

$$Z_Y = \sum_i \mathrm{e}^{-\beta N E_i}. \tag{11}$$

Let us find the eigenfunction $\phi(y)$ and the eigenvalue E of equation (9). First of all, in the continuum limit, $Y_{n-1} \sim x$ and $Y_n \sim y$, equation (9) reads

$$\int \mathrm{d}x\, \phi(x) \exp\left\{-\beta\left[\frac{\kappa}{2}(y-x)^2 + \frac{D}{2}\left(\mathrm{e}^{-\alpha/2\, y} - 1\right)^2 + V(y)\right]\right\}$$
$$= \mathrm{e}^{-\beta E}\,\phi(y). \tag{12}$$

Now assuming that the harmonic term is dominant, $x = y + z$ can be expanded as a Taylor series in powers of z. Expansion up to the second order yields

$$\int \mathrm{d}z\, \mathrm{e}^{-\beta\kappa/2z^2}\left[\phi(y) + \frac{\mathrm{d}\phi}{\mathrm{d}y}z + \frac{1}{2}\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2}\right]$$
$$= \exp\left\{-\beta\left[E - \frac{D}{2}\left(\mathrm{e}^{-\alpha/2\, y} - 1\right)^2 + V(y)\right]\right\}\phi(y). \tag{13}$$

Again, this is just the Gaussian integration and the result is [15]

$$\begin{aligned}\phi(y) + \frac{1}{2\beta\kappa}\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} &= \exp\left\{-\beta\left[E + \frac{1}{2\beta}\ln\left(\frac{2\pi}{\beta\kappa}\right)\right.\right.\\ &\quad \left.\left.-\frac{D}{2}\left(\mathrm{e}^{-\alpha/2\, y} - 1\right)^2 + V(y)\right]\right\}\phi(y)\\ &\approx \left[1 - \beta E - \frac{1}{2}\ln\left(\frac{2\pi}{\beta\kappa}\right)\right]\phi(y)\\ &\quad + \beta\left[\frac{D}{2}\left(\mathrm{e}^{-\alpha/2\, y} - 1\right)^2 + V(y)\right]\phi(y).\end{aligned} \tag{14}$$

This is nothing else than the Schrödinger-like equation

$$-\frac{1}{2m_0}\frac{\mathrm{d}^2\phi}{\mathrm{d}y^2} + \frac{D}{2}\left[\mathrm{e}^{-\alpha/2\, y} - 1\right]^2\phi + V(y)\phi = \bar{E}\phi, \tag{15}$$

where $m_0 = \kappa\beta^2$ and $\bar{E} = E + 1/(2\beta)\ln[2\pi/(\beta\kappa)]$. The problem is therefore turned into finding the eigenvalue of equation (15).

Equation (15) then yields an eigenequation $H\phi_m = \bar{E}_m\phi_m$ with the Hamiltonian

$$H = \frac{1}{2m_0}\frac{\mathrm{d}^2}{\mathrm{d}y^2} + \frac{D}{2}\left[\mathrm{e}^{-\alpha/2\, y} - 1\right]^2 + V(y), \tag{16}$$

and m is an integer. For a constant force V_0, $V(y) = V_0 y$, the transformation $\phi = \exp(\beta V_0 y)\psi$ reproduces the Schrödinger equation with the Morse potential [16]. Unfortunately, the equation can be solved only for a few special cases. Generally, the solution can be obtained perturbatively by assuming that the potential $V(y)$ is small enough compared to the Morse potential. Under this assumption, the eigenequation can be solved using time-independent perturbation theory in standard quantum mechanics. However, it should be emphasized that the problem remains a classical one, and the quantum mechanics is borrowed only for technical reasons since the calculation yields the Schrödinger equation.

In quantum mechanics the perturbation is applied by expanding the Hamiltonian (H) in the form of $H = H_0 + \epsilon V$ with H_0 being the Hamiltonian in equation (16) without the potential, while ϵ is a small parameter. According to the time-independent perturbation theory, the eigenvalue and its eigenfunction can be written as [17]

$$\bar{E}_m = \bar{E}_m^{(0)} + \epsilon\bar{E}_m^{(1)} + \epsilon^2\bar{E}_m^{(2)} + \cdots, \tag{17}$$

$$\phi_m(y) = \phi_m^{(0)}(y) + \epsilon\phi_m^{(1)}(y) + \epsilon^2\phi_m^{(2)}(y) + \cdots. \tag{18}$$

The eigenvalue for H_0 is determined by $H_0\phi^{(0)} = \bar{E}_0^{(0)}\phi^{(0)}$, that is,

$$-\frac{1}{2m_0}\frac{\mathrm{d}^2\phi^{(0)}}{\mathrm{d}y^2} + \frac{D}{2}\left(\mathrm{e}^{-\alpha/2\, y} - 1\right)^2\phi^{(0)} = \bar{E}^{(0)}\phi^{(0)}, \tag{19}$$

where $\bar{E}^{(0)} = E^{(0)} + 1/(2\beta)\ln[2\pi/(\beta\kappa)]$. The equation is just the well-known Schrödinger equation with the Morse potential and the solution has been derived in [14]. Substituting $y' = (1/2)\alpha y$, $\lambda = 2\sqrt{m_0 D}/\alpha$, $\mathcal{E}^{(0)} = 8m_0/\alpha^2\bar{E}^{(0)}$ and $z = 2\lambda\exp(-y')$, one arrives at the eigenvalue problem for $\beta\sqrt{\kappa D}/\alpha > 1/2$ as [17, 18]

$$-\frac{\mathrm{d}^2\phi^{(0)}}{\mathrm{d}y'^2} + \lambda^2\left(\mathrm{e}^{-2y'} - 2\mathrm{e}^{-y'}\right)\phi_m^{(0)} = \mathcal{E}_m^{(0)}\phi_m^{(0)}. \tag{20}$$

The eigenvalue and its eigenfunction are

$$\mathcal{E}_m^{(0)} = -\left(\lambda - m - \tfrac{1}{2}\right)^2, \tag{21}$$

$$\phi_m^{(0)} = N_m z^{b_m}\,\mathrm{e}^{-z/2}\,L_m^{2b_m}(z), \tag{22}$$

where $b_m = \lambda - m - 1/2$ and $N_m = m![\Gamma(m+1)\Gamma(2\lambda - m)]^{-1/2}$ with Γ being the Gamma function. $L_m^{2b_m}(z) = (z^{-2b_m}\mathrm{e}^z/m!)(\mathrm{d}^m(\mathrm{e}^{-z}z^{m+2b_m})/\mathrm{d}z^m)$ is the associated Laguerre polynomial or generalized Laguerre polynomials.

Based on these transformations, using the standard procedure in quantum mechanics, one obtains the solution up to first order [17]:

$$\mathcal{E}_m = \mathcal{E}_m^{(0)} + \epsilon\mathcal{E}_m^{(1)}, \tag{23}$$

$$\phi_m(y') = \phi_m^{(0)}(y') + \epsilon\phi_m^{(1)}(y'), \tag{24}$$

where

$$\mathcal{E}_m^{(1)} = \int \mathrm{d}y'\, \phi_m^{(0)*}(y')V(y')\phi_m^{(0)}(y'), \tag{25}$$

$$\phi_m^{(1)}(y') = \sum_{k\neq m} \frac{\int \mathrm{d}y'\, \phi_k^{(0)*} V(y')\phi_m^{(0)}(y')}{\mathcal{E}_m^{(0)} - \mathcal{E}_k^{(0)}}\phi_k^{(0)}(y'). \tag{26}$$

Finally, the partition function of y is given by

$$Z_y = \sum_m \mathrm{e}^{-\beta N E_m}, \tag{27}$$

with the eigenvalue

$$E_m = \frac{\alpha^2}{8\kappa\beta^2}\mathcal{E}_m + \frac{1}{2\beta}\ln\left(\frac{\beta\kappa}{2\pi}\right). \tag{28}$$

4. Thermal denaturation

One of the relevant parameters in the study of DNA denaturation is the mean stretching, $\langle y_n\rangle$, of the hydrogen bond. It is defined as

$$\langle y_n\rangle = \frac{1}{Z}\int \mathrm{d}y_n\,\mathrm{d}p_n \prod_{n=1}^{N} y_n\,\mathrm{e}^{-\beta H}. \tag{29}$$

The average value of hydrogen bond stretching can be calculated through

$$\langle y\rangle = \frac{\sum_{i=1}^{N}\langle\phi_i(y)\mid y\mid\phi_i(y)\rangle \mathrm{e}^{-N\beta\bar{E}_i}}{\sum_{i=1}^{N}\langle\phi_i(y)\mid\phi_i(y)\rangle \mathrm{e}^{-N\beta\bar{E}_i}}. \tag{30}$$

In the limit of large N, $\langle y\rangle$ is dominated by the ground state [14], that is, $\langle y\rangle = \int \mathrm{d}y(\phi_0(y))^* y\phi_0(y)$. Up to the leading term of perturbation, i.e. $\phi_0(y) = \phi_0^{(0)}(y) + \epsilon\phi_0^{(1)}(y)$, equation (30) reads

$$\langle y\rangle = \int \mathrm{d}y\,\phi_0^{(0)*}(y)y\phi_0^{(0)}(y) + \epsilon\left[\int \mathrm{d}y\,\phi_0^{(0)*}(y)y\phi_0^{(1)}(y) + \int \mathrm{d}y\,\phi_0^{(1)*}(y)y\phi_0^{(0)}(y)\right]. \tag{31}$$

The higher order of eigenvalue and eigenfunction are given by

$$\mathcal{E}_0^{(1)} = \int \mathrm{d}y\phi_n^{(0)*}(y)V(y)\phi_n^{(0)}(y) \tag{32}$$

and

$$\begin{aligned}\phi_0^{(1)}(y) &= \sum_{k\neq 0}\frac{\int \mathrm{d}y\,\phi_k^{(0)*}V(y)y\phi_0^{(0)}(y)}{\mathcal{E}_0^{(0)} - \mathcal{E}_k^{(0)}}\phi_k^{(0)}(y)\\ &= \frac{\int \mathrm{d}y\,\phi_1^{(0)*}V(y)\phi_0^{(0)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}}\phi_1^{(0)}(y)\\ &\quad + \frac{\int \mathrm{d}y\,\phi_2^{(0)*}V(y)\phi_0^{(0)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}}\phi_2^{(0)}(y) + \cdots.\end{aligned} \tag{33}$$

Then equations (22)–(26) yield

$$\begin{aligned}\langle y\rangle = I_{(00)} + \epsilon\Bigg[&\frac{I_{(10)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}}\int \mathrm{d}y\,\phi_0^{(0)*}(y)y\phi_1^{(0)}(y)\\ &+\frac{I_{(10)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}}\int \mathrm{d}y\,\phi_1^{(0)*}(y)y\phi_0^{(0)}(y)\\ &+\frac{I_{(20)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}}\int \mathrm{d}y\,\phi_0^{(0)*}(y)y\phi_2^{(0)}(y)\\ &+\frac{I_{(20)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}}\int \mathrm{d}y\,\phi_2^{(0)*}(y)y\phi_0^{(0)}(y) + \cdots\Bigg] + O(\epsilon^2),\end{aligned} \tag{34}$$

where

$$I_{00} = \int \mathrm{d}y\,\phi_0^{(0)*}(y)V(y)\phi_0^{(0)}(y), \tag{35}$$

$$I_{10} = \int \mathrm{d}y\,\phi_1^{(0)*}(y)V(y)\phi_0^{(0)}(y), \tag{36}$$

$$I_{20} = \int \mathrm{d}y\,\phi_2^{(0)*}(y)V(y)\phi_0^{(0)}(y), \tag{37}$$

while the eigenvalues and eigenfunctions are given by

$$\mathcal{E}_0^{(0)} = -\left(\lambda - \frac{1}{2}\right)^2, \tag{38}$$

$$\mathcal{E}_1^{(0)} = -\left(\lambda - \frac{3}{2}\right)^2, \tag{39}$$

$$\mathcal{E}_2^{(0)} = -\left(\lambda - \frac{5}{2}\right)^2, \cdots. \tag{40}$$

Here,

$$\phi_0^{(0)} = \frac{(2\lambda)^{\lambda-1/2}}{\sqrt{\Gamma(2\lambda)}}\,\mathrm{e}^{-\lambda\exp(-\alpha/2\,y)}\,\mathrm{e}^{-\alpha/2(\lambda-1/2)y}, \tag{41}$$

$$\begin{aligned}\phi_1^{(0)} = &\frac{2(2\lambda)^{\lambda-3/2}}{\sqrt{\Gamma(2)\Gamma(2\lambda-1)}}\,\mathrm{e}^{-\lambda\exp(-\alpha/2\,y)}\,\mathrm{e}^{-\alpha/2(\lambda-3/2)y}\\ &\times\left[-\lambda\mathrm{e}^{-\alpha/2\,y} + (\lambda-1)\right],\end{aligned} \tag{42}$$

$$\begin{aligned}\phi_2^{(0)} = &\frac{4(2\lambda)^{\lambda-5/2}}{\sqrt{\Gamma(3)\Gamma(2\lambda-2)}}\,\mathrm{e}^{-\lambda\exp(-\alpha/2\,y)}\,\mathrm{e}^{-\alpha/2(\lambda-5/2)y}\\ &\times\left[\lambda^2\,\mathrm{e}^{-\alpha y} - \lambda(2\lambda-3)\,\mathrm{e}^{-\alpha/2\,y} + \frac{1}{4}(2\lambda-3)(2\lambda-4)\right],\end{aligned} \tag{43}$$

where $\lambda = 2\sqrt{\kappa D}/(\alpha k_{\mathrm{B}}T)$.

Considering the case of the linear potential $V(y) = V_0 y$, the wave function is given by

$$\phi_0(y) = \phi_0^{(0)} + \epsilon\left[\frac{V_0\int \mathrm{d}y\,\phi_1^{(0)*}y\phi_0^{(0)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_1^{(0)}}\phi_1^{(0)}(y) + \frac{V_0\int \mathrm{d}y\,\phi_2^{(0)*}y\phi_0^{(0)}}{\mathcal{E}_0^{(0)} - \mathcal{E}_2^{(0)}}\phi_2^{(0)}(y) + \cdots\right]. \tag{44}$$

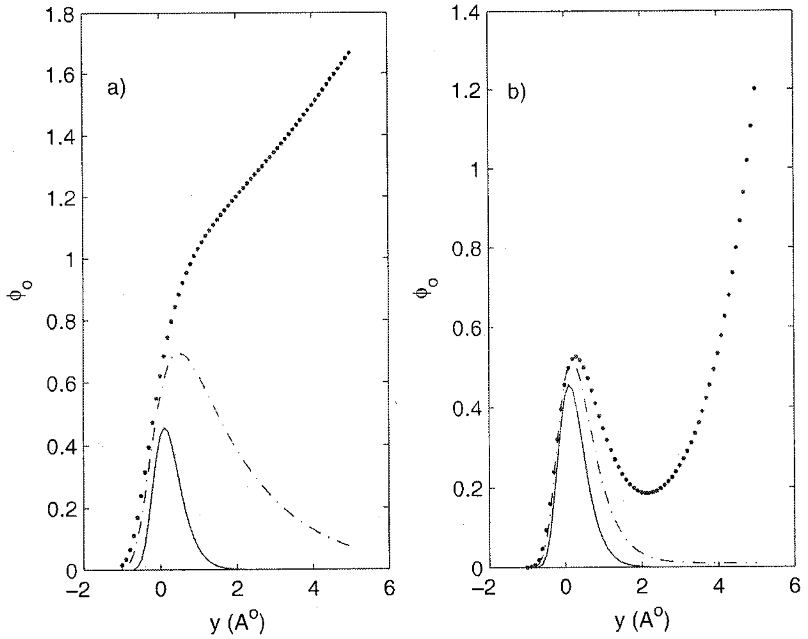

Figure 1. The eigenfunction without (left) and with (right) external linear potential as a function of the displacement in various temperatures: 100 K (solid line), 300 K (dashed-line) and 500 K (dotted-line) in the left; and 100 K (solid line), 150 K (dashed-line) and 200 K (dotted-line) in the right figures.

The variation of the wave function with respect to temperature is depicted in figure 1 for the same parameters as in [12], i.e. $D = 0.04\,\mathrm{eV}$, $\alpha = 4.45\,\text{Å}^{-1}$, $\epsilon = 0.01$, $\kappa = 0.06\,\mathrm{eV}\,\text{Å}^{-2}$ and $V_0 = 15\,\mathrm{pN}$.

The ground state of the eigenfunction for the linear potential gives the weighting factor for the calculation of DNA displacement $\langle y\rangle$ [10]. The figure shows that at low temperature, the peak is close to the minimum of the Morse potential and decays exponentially as the displacement increases. Without the external potential, the eigenfunction increases drastically at the melting temperature, i.e. about 500 K, as was already pointed out in [12]. On the other hand, the same behavior occurs at lower temperature when an external potential is applied to the system, i.e. at about 200 K.

From equation (34), the influence of various external potentials in denaturation processes is depicted in figure 2 using the same parameters as in [12]. The figure describes the effects of the linear potential $V(y) = V_0 y$, the sinusoidal potential $V(y) = V_0 \sin(ay)$ and the Gaussian potential $V(y) = V_0\,\mathrm{e}^{-ay^2}$ with a being a constant. It should be noted that the result coincides with a previous work for zero external potential [12]. The figure shows that the critical temperature is approximately 400 K without an external potential and around 200 K with a constant external potential. Nevertheless, the critical temperature becomes around 350 K for a periodic sinusoidal force with $a = 2.5$. The same behavior of $\langle y\rangle$ for the non-forcing condition has been also obtained in [19] using the flexible chain model with the typical parameter $D = 0.25\,\mathrm{eV}$, $\alpha = 2.8\text{Å}^{-1}$ and numerical calculation of the stochastic description of flexible polymer models.

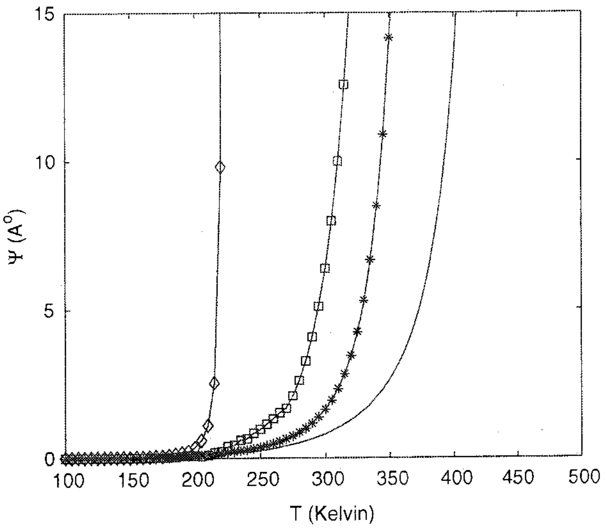

Figure 2. The hydrogen bond stretching as a function of melting temperature using the same parameters as in [12] for various potentials: $V(y) = 0$ (plain line), $V(y) = V_0 y$ (line with diamonds), $V(y) = V_0 \sin(2.5y)$ (line with squares) and $V(y) = V_0\,\mathrm{e}^{-10y^2}$ (line with stars).

5. Summary

The effect of an external potential on the PB DNA denaturation has been investigated for various types of potentials: linear potential $V(y) = V_0 y$, sinusoidal potential $V(y) = V_0 \sin(ay)$ and Gaussian potential $V(y) = V_0\,\mathrm{e}^{-ay^2}$ with a being a constant. The DNA denaturation and its melting temperature have been further studied in the framework of the statistical mechanics approach. The calculation of the partition function has been performed perturbatively using the transfer integral method to obtain analytically the mean stretching of hydrogen bonds.

This paper supports the results of previous works. In a cell, DNA strands can be separated by applying a certain external potential [20], or in chemical terms by enzymes whose interactions with DNA could make the strand separation thermodynamically favorable at ambient temperature [21]. It has been shown that two strands of double-stranded DNA can be separated by applying a $V_0 \sim$ 15 pN force at room temperature. The model also predicts that the DNA overstretching force should be a decreasing function of temperature; in other words, the melting temperature should be a decreasing function of the applied force [20, 22].

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