A Method for Computing the Potentials in a DNA by a Concentric Cylinder Model.

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あらまし　　A method was introduced for computing the three dimensional distribution of the free energy and electro static force in a DNA molecules that has been proposed by Bailey (1976). A DNA molecule was modeled by a cylinder composed of three regions, inner region in which there is no ion, the intermediate region where the ions interact on the basis of screening effects of Debye-Huckel theory. These two regions were described by the Laplace equation. The outer region was described by the Poisson equation due to the surrounding ions atmosphere. The coefficients of the equations were determined by the continuity across the two boundaries of the three regions. The potentials and forces heavily depended on the circumferential angles. The present method, when it was improved, will be available for evaluating the free energy and potential of the DNA molecule.

和文キーワード　　DNA free energy, Electrical charge, Electrical Force. Screening effects, Debye-Huckel theory.

連続体円筒モデルによる有機分子としてのDNA のポテンシアル計算。

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Abstract

DNA分子を自由エネルギ-の視点から解析する方法をBailey (1976)らの研究にもとずいて紹介し、DNA を構成するリン酸による負の電荷分布によるポテンシアルと静電力の三次元分布を計算した。DNA分子は円筒状とし、電荷（イオン）が存在しない内相とイオン同士が相互干渉しあう中間領域および外部電場を設定した。これらに対して、それぞれ、ラプラス方程式およびポアソン方程式を設定し２つの境界での連続性を境界条件として、Green 関数を用いて、円筒座標系におけるポテンシアルを求めた。また円周方向に微分することで、静電力を算出し、それぞれの３次元分布をもとめた。ポテンシアルはDNAの円周方向で明確に変化した。静電力はそれより複雑な挙動をしめした。 本研究を発展させることでDNA分子の自由エネルギーを計算することが可能である。

英文 key words　　DNA分子自由エネルギ-. 電荷分布. ポテンシアル. 静電力. Debye-Huckel 理論 .

1. Introduction.

Characterization of DNA has been progressed for these two decades. Precise molecular structure has been reported particularly in their geometry. Fig 1 shows the configuration of the DNA molecule showing the double helix strand (Fig 1-a) . The Top view (Fig 1-b) shows how the phosphate charges are organized along the helical line with equivalent spacing. There are ten phosphates for each helical return with raise angle of 32 degree. Fig 1-c shows schematically the spatial positioning of the electrical charges around the modeled DNA cylinder. L is the length of the inter helical interval. ϕ is the latitudinal angle around the circular cross sectional plane of the DNA. Since the DNA molecule is consisted of neatly arranged charges, there is reasonable necessity to analyze the potential and electrical force derived from them so as to evaluate the dynamical behaviors of the DNA.

The present work introduce a method proposed by Bailey (1976) for computing the potential and force in DNA.
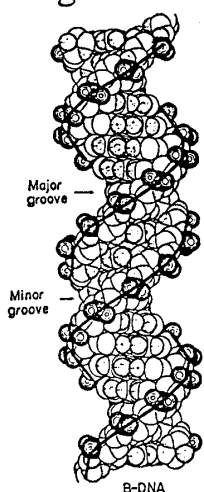
Fig 1-a　　　Fig 1-b

Major groove
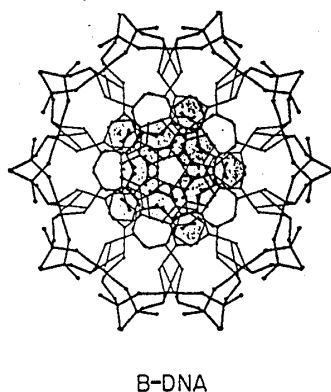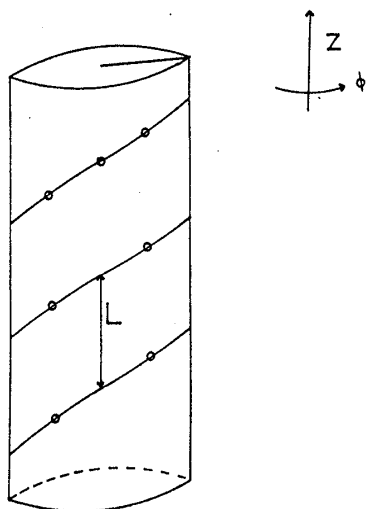
Minor groove

B-DNA

B-DNA

Fig 1-c

L

z

ϕ

2. Assumptions.

1. DNA helix is a long cylinder which is impermeable to the screening ions.
2. Phosphate charges locate along the helix.
3. The position of the charge is expressed

$$z_j = z_{oj} + kL \qquad \text{--------(1)}$$

where z_j is the axial position of the j th charge, k is an integer, L is the periodic length of the helical charge distribution. For circumferential direction

$$\phi_j = \phi_{oj} + k2\pi \qquad \text{--------(2)}$$

where ϕ_j is the circumferential angle of the j th charge. The radial coordinate of the j th charge is ρ_j.

4. For the simplicity, the inter molecular interaction derives from screening ions and the DNA helix.
5. The distribution of the screening ions is the linearized Poisson Boltzmann distribution on the basis of the Debye-Huckel theory.

The region I is the DNA cylinder with a radius b and dielectric constant Dh. The points of discrete charge originated from phosphate locate in this region. Region II is the area of the closest approach of the screening ions which range $b < \rho < d$. (d - b) is the radius of the screening ions. Region III is the region to which the screening ions can approach. Their distribution can be given by the Debye-Huckel theory. The dielectric constants for region II and II are assumed to be the same D which is the constant of the bulk solution.

We have to solve the Poisson equation in all of these regions under the adequate boundary conditions.

3. Geometric consideration for the discrete distribution of the point charges due to phosphate groups.

1. Circumferential direction.

There are ten phosphates which are arranged helically around the central axis of the DNA cylinder. Since they are equally spaced along the helical pathway, each electrical charge makes $\phi = 2\pi/10$. The k th charges has
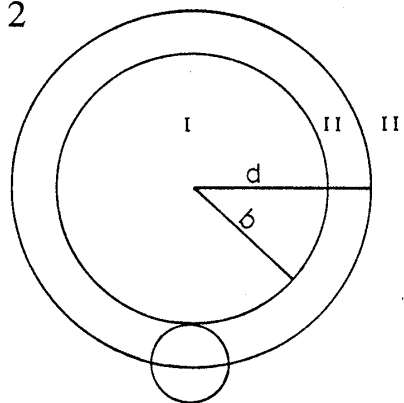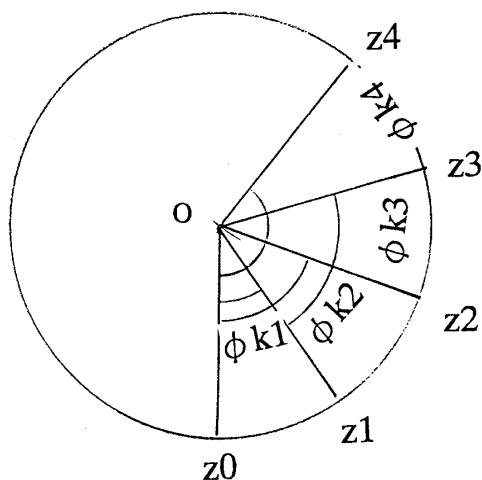
Fig 2

I　　II　III

d

ϕ

Fig 3 -a

Fig 3-a. Circumferential positions of charges.

Fig 3 -a is the top view of DNA molecule showing the circumferential positions of the Phosphate charges on the horizontal cross sectional plane of the DNA helix. Each position was denoted by z_0, z_1, z_2, z_3 --. The circumferential angle between charges at z_0 and z_1 is expressed by ϕk_1. The angle from z_0 to z_2 is ϕk_2, from z_0 to z_3 is ϕk_3 and to z_4 , ϕk_4. Since all the phosphate charges occupied their spatial positions in equivocal distances, we set all the circumferential angles between two neighboring charges $\phi km = \phi k$.
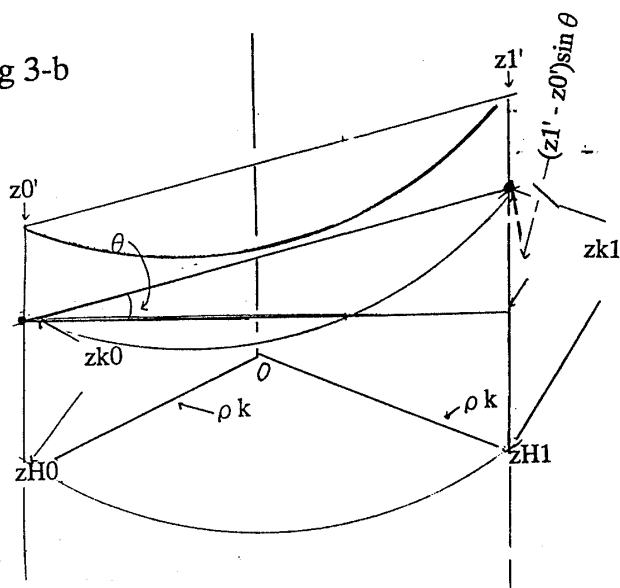
Fig 3-b

Fig 3-b. Axial positions of charges.

Fig 3 -b is the side view of DNA molecule showing the axial positions of the phosphate charges. O is the center of the cylinder. $O\text{-}zH_0\text{-}zH_1$ is the horizontal cross sectional plane on which phosphate charges positioned at z_0' and z_1' on the helical curve were projected vertically. In this figure, " ' " denotes the position of an electrical charge on the helical curve and H denotes the charge position projected on the horizontal plane.

zk_0 is the axial distance of the 0 th charge from reference horizontal cross sectional plane $O\text{-}zH_0\text{-}zH_1$ and zk_1 is the axial distance of 1 th charge from the same plane. The rise angle between two neighboring phosphate charges are , thus $\cos\theta = (zH_1 - zH_0)/(z_1' - z_0')$.

Since all the phosphate charges are arranged in parallel, the axial rise of charge position at z_1' from that at z_0' is $(z_1' - z_0') \sin\theta$. Thus the axial distance of the 1 th charge from the horizontal plane zk_1 is expressed by zk_0
$$zk_1 = zk_0 + (z_1' - z_0') \sin\theta .$$
By this recurrent formula, all the axial positions can be expressed.
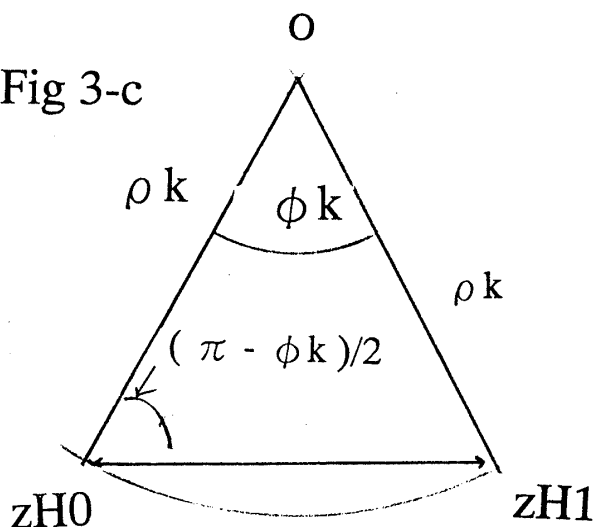
Fig 3-c

Fig3-c. Horizontal position of charge.

Fig 3 -c is phosphate charges projected on the horizontal plane. They make the angle ϕk with the center of cylinder O. On this horizontal plane, the distance $O\text{-}zH_0$ and $O\text{-}zH_1$ is equal to ρk, the trigonometric relation $I\ zH_{n-1} - zH_n\ I\ /\sin\phi k = \rho n / \sin((\pi - \phi k)/2)$ holds.

circumferential angle of

$$\phi_k = 2\pi k/10 \qquad \text{--------(3)}$$

2. Arrangement along the axial direction.

Denoting z_k is the distance of the k th charge from the horizontal plane position z_{H1} of the DNA helix to the position on the helical pathway $z_{k'}$ (Fig 2).

$$z_k = z_{k-1} + I z_{k'} - z_{k-1'} I \sin\psi \qquad \text{---------(4)}$$

ψ is the rise angle.

3. Relative positional arrangement between the adjacent charge.

Since the relation between

$$\cos\psi = I z_{Hk} - z_{Hk-1} I / I z_{k'} - z_{k-1'} I \qquad \text{--------(5)}$$

$$I z_{Hk} - z_{Hk-1} I /\sin(\phi_k) = \rho_k /\sin((\pi - \phi_k)/2) \qquad \text{-------(6)}$$

Hence
$$\cos\psi = \rho_k \sin(\phi_k) /\sin((\pi - \phi_k)/2) / I z_{k'} - z_{k-1'} I \text{---(7)}$$

Thus
$$I z_{k'} - z_{k-1'} I = \rho_k \sin(\phi_k) /\sin((\pi - \phi_k)/2)* 1/\cos\psi \qquad \text{--(8)}$$

Hence the k th position on the axial direction is

$$z_k = z_{k-1} + I z_{k'} - z_{k-1'} I \sin\psi$$
$$= z_{k-1} + \rho_k \sin(\phi_k) /\sin((\pi - \phi_k)/2) \tan\psi$$
$$= k \rho_k \sin(\phi_k) /\sin((\pi - \phi_k)/2) \tan\psi \qquad \text{----------(9)}$$

From the reported measured data, we have

$$\psi = 32° \quad \text{and} \quad \phi_k = 36° \qquad \text{-----------(10)}$$

4. Mathematical description of the system.

Phosphate groups produces a charge density on the region I which is a sum of delta functions

$$\rho_I(r) = \sum_j \varepsilon_j \delta(r - r_j) \qquad \text{--------(11)}$$

The sum is all over the points of discrete charge. Then the Poisson equation is

$$\nabla^2 \psi_I(r) = -4\pi/Dh \, \rho_I(r) \qquad \text{--------(12)}$$

and the related Laplace equation is

$$\nabla^2 \psi_I(r) = 0 \qquad \text{--------(13)}$$

The related particular equation is

$$\nabla^2 \psi_p(r) = -4\pi/Dh \sum_j \varepsilon_j \delta(r - r_j) \qquad \text{--------(14)}$$

The particular solution can be obtained by the Green function

$$\nabla^2 G(r,r') = -4\pi \delta(r-r') = -4\pi/\rho \, \delta(\rho - \rho') \, \delta(z - z')$$
$$\delta(\phi - \phi') \qquad \text{--------(15)}$$

where
$$\delta(z-z') = 1/2\pi \int_{-\infty}^{-\infty} d\lambda \exp(i\lambda(z-z')) \qquad \text{--------(16)}$$

$$\delta(\phi - \phi') = 1/2\pi \sum_{m=-\infty}^{m=\infty} \exp(im(\phi - \phi')) \qquad \text{--------(17)}$$

By these expressions, the Green function is

$$G(r,r') = 1/4\pi^2 \int d\lambda \exp(i\lambda(z-z')) \{ \sum_{m=-\infty} \exp(im(\phi$$
$$-\phi')) \, gm(\rho, \rho') \} \qquad \text{--------(18)}$$

where gm is the radial Green function that satisfies

$$1/\rho \, \partial/\partial \rho [\rho \, \partial gm/\partial \rho] -(\lambda^2 + (m/\rho)^2) gm$$
$$= -4\pi/\rho \, \delta(\rho - \rho') \qquad \text{---------(19)}$$

which is obtained by the ortho gonarity of the delta function. gm gives

$$gm(\rho, \rho') = = 4\pi/[\rho \, W(\psi_1, \psi_2)] \psi_1(\rho>) \psi_2(\rho<) \qquad \text{---------(20)}$$

where $\rho>$ defines larger of ρ and ρ'. $\psi_1(\rho>)$ is a solution of equation (15) that satisfies all the boundary conditions when $\rho > \rho'$. $\psi_2(\rho<)$ is a solution that satisfies all the boundary conditions for $\rho < \rho'$. W is the Wronskian of $\psi_1(\rho>) \psi_2(\rho<)$. Utilizing these expressions for the radial Green function, the particular solution is

$$\psi_p(\rho,z,\phi) = 1/(\pi^2 Dh) \sum_j \varepsilon_j \int_0 d\lambda \cos(\lambda(z-z_j))$$
$$\{ \sum_{m=1} \cos(m(\phi-\phi_j)) gm(\rho, \rho_j) + go(\rho, \rho_j)/2 \} \qquad \text{---------(21)}$$

for $\lambda \neq 0$, the Green function is
$$gm(\rho, \rho_j) = 4\pi \, Im(\lambda \rho_j) Km(\lambda \rho)$$
$$go(\rho, \rho_j) = 4\pi \, Io(\lambda \rho_j) Ko(\lambda \rho) \qquad \text{---------(22)}$$

and for $\lambda = 0$, the radial Green function is
$$gm(\rho, \rho_j) = \pi/m (\rho_j/\rho)^m$$
$$go(\rho, \rho_j) = 2\pi \log(1/\rho) \qquad \text{---------(23)}$$

The boundary conditions at $\rho = b$

$$\psi_I(\rho = b) = \psi_{II}(\rho = b) \qquad \text{--------(24)}$$

$$\varepsilon_1 \, \partial \psi_I/\partial \rho = \partial \psi_{II}/\partial \rho \qquad \text{--------(25)}$$

The eigen values are set as

$$\alpha(n)^2 = n^2 c^2 + \kappa^2 \qquad \text{---------(26)}$$

By setting the following coefficients,

$$Qnm1 = 8 \varepsilon_o/(L \, Dh) [nc \, Km(\alpha(n)d) \{ Im-1(ncd)$$
$$+ Im+1(ncd) \}/2$$
$$-\alpha(n) \{ Km-1(\alpha(n)d) + Km+1(\alpha(n)d) \}/2 Im(ncd)] \qquad \text{---------(27-a)}$$

$$Qnm2 = -(Dh - D) Km(ncb) \{ Km-1(ncb) + Km+1(ncb) \}/2 \qquad \text{---------(27-b)}$$

$$Qnm3 = - \varepsilon o / (L Dh) [n c Km(\alpha(n) b) \{ Km_{-1}(n c b)$$
$$+ Km_{+1}(n c b) \}/2$$
$$+ \alpha(n) Km(nc b) \{Km_{-1} (\alpha(n) b) + Km_{+1}(\alpha(n) b) \}/2]$$
$$\text{--------(27-c)}$$

$$Qnm4 = -Dh \ Im(n c d) \{ Km_{-1}(n c d) + Km_{+1}(nc d) \}/2$$
$$+ D \{ Im_{-1}(n c d) + Im_{+1}(n c d) \}/2 Km(n c d)$$
$$\text{--------(27-d)}$$

$$Qnm5 = Dh \ Km(n c b) \{ Im_{-1}(n c b) + Im_{+1}(n c b) \}/2$$
$$- D \{ Km_{-1}(n c b) + Km_{+1}(n c b) \}/2 Im(n c b)$$
$$\text{-------(27-e)}$$

$$Qnm6 = (Dh - D) Im(n c d) \{ Im_{-1}(n c d)$$
$$+ Im_{+1} (n c d) \}/2$$
$$\text{--------(27-f)}$$

$$Qnm = (Qnm1 \ Qnm2 + Qnm3 \ Qnm4)$$
$$/(Qnm1 \ Qnm5 + Qnm3 \ Qnm6)$$
$$\text{--------(27-g)}$$

$$Sm1 = \varepsilon o / (L Dh) (D + Dh) /d^m [- \kappa \{ Km_{-1}(\kappa d)$$
$$+ Km_{+1}(\kappa d) \}/2 \ - m/d \ Km(\kappa d)]$$
$$\text{--------(28-a)}$$

$$Sm2 = \varepsilon o / (L Dh) (D + Dh)d^m/b^{2m} [- \kappa \{ Km_{-1}(\kappa d)$$
$$+ Km_{+1}(\kappa d) \}/2 \ + m/d \ Km(\kappa d)]$$
$$\text{--------(28-b)}$$

$$Sm3 = (D + Dh)d^m/ \rho o^m [- \kappa \{ Km_{-1}(\kappa d)$$
$$+ Km_{+1}(\kappa d) \} /2 \ + m/d \ Km(\kappa d)]$$
$$\text{--------(28-c)}$$

$$Sm4 = (D - Dh)b^{2m}/(d^m \rho o^m) [- \kappa \{Km_{-1}(\kappa d)$$
$$+ Km_{+1}(\kappa d) \} /2 \ - m/d \ Km(\kappa d)]$$
$$\text{--------(28-d)}$$

$$Sm = (Sm1 + Sm2) /(Sm3 + Sm4)$$
$$\text{--------(29)}$$

Then,we have the potential for the inner region. ψ I

$$\psi I = \sum_{j} \sum_{n=1} \sum_{m=1} Qnm \cos(n c (z - zoj)) \cos[m(\phi - \phi oj)]$$
$$* Im(n c \rho o) Im(n c \rho)$$
$$+ \sum_{j} \sum_{m=1} Sm \cos[m(\phi - \phi oj)] \rho^m/m$$
$$+ \varepsilon \ Ko(\kappa d) / [L D \kappa d K1(\kappa d)]$$
$$+ \varepsilon /(L D) \log (d/b) + z /(L Dh) \log(b) + \psi p \text{--------(30)}$$

The characteristic potential is ψ p

$$\psi p = 8 \varepsilon o / (L Dh) \sum_{j} \sum_{n=1} \cos(n c (z - zoj)) \{ Io(n c \rho o)$$
$$Ko(nc \rho)/2 + \sum_{m=1} \cos[m(\phi - \phi oj)] Im(n c \rho o) Km(nc \rho) \}$$
$$+ \varepsilon o/(L Dh) \sum_{j} \sum_{m=1} \cos[m(\phi - \phi oj)] 1/m \ \rho^m/ \rho o^m$$
$$+ \varepsilon \log(1 / \rho) /(L Dh) \text{--------(31)}$$

The potential for the intermediate region ψ II is

$$\psi II = \sum_{j} \sum_{m=0} \sum_{n=1} Qnm \cos(n c (z - zoj)) \cos[m(\phi - \phi oj)]$$
$$*[AII \ Im(n c \rho) + FII \ Km(n c \rho)]$$
$$+ \sum_{j} \sum_{m=1} [BII \ \rho^m + GII / \rho^m] \cos[m(\phi - \phi oj)]$$
$$+ TII + HII/(c \rho) \text{--------(32)}$$

$$FII = b [[(1 - \varepsilon 1 / \varepsilon 2) Qnm \ Im(n c \rho o) DInmb$$
$$* Im(n c b) + 8 \varepsilon o / (L Dh) Im (n c \rho o)$$
$$\{ Km(n c b)*DInmb - \varepsilon 1 / \varepsilon 2 DKnmb* Im(n c b)]]$$
$$\text{--------(33)}$$

$$AII = 1/Im(n c b) [[Qnm \ Im(n c \rho o) Im(n c b)$$
$$+ 8 \varepsilon o / (LDh) Im (n c \rho o)Km(n c b) - FII \ Km(n c b)]]$$
$$\text{--------(34)}$$

where
$$DInmb = n c \ \partial Im(z) \ \partial z (z =b)$$
$$DKnmb = n c \ \partial Km(z) \ \partial z (z =b) \text{--------(35)}$$
and
$$GII = 1/m [[(1- \varepsilon 1 / \varepsilon 2) Snm \ b^m + (1- \varepsilon 1 / \varepsilon 2) \varepsilon o$$
$$/(L Dh) \ \rho o^m/b^m]]$$
$$\text{--------(36)}$$

$$BII = 1/b^m [[(Snm \ b^m + \rho o^m/b^m) /m - GII /b^m]]$$
$$\text{--------(37)}$$

$$HII = c b \ \varepsilon 1 / \varepsilon 2 \ \varepsilon /(L Dh) \text{--------(38)}$$

$$TII = \varepsilon /(L Dh) \ \log(1/b) - HII /(c b) + \psi Ic \text{--------(39)}$$

The potential for the external region ψ III is

$$\psi III = \sum_{j} \sum_{n=1} \sum_{m=0} FIII \cos(n c (z + r \ \pi /2)) \cos[m(\phi$$
$$+ r \ \pi'/2)] * Km(\alpha(n) \ \rho)$$

$$= \sum_{j} \sum_{m=0} \sum_{n=1} FIII' \cos(n c (z + r \ \pi /2)) \cos[m(\phi$$
$$+ r \ \pi'/2)] * Km(\alpha(n) \ \rho)$$
$$+ \sum_{j} \sum_{m=1} FIII'' \cos[m(\phi + r \ \pi'/2)] * Km(\alpha(n=0) \ \rho)$$
$$+ FIII''' (n=0,m=0)/Ko(\alpha(n=0) d) \text{--------(40)}$$

$$FIII' (m=0,n=1 \text{ loop}) =[AII \ Im(n c d) + FII \ Km(n c d)]$$
$$/ Km(\alpha(n) d) \text{--------(41)}$$

$$FIII'' (n=0, m \text{ loop}) =[BIId^m + GII/d^m] / Km(\alpha(n=0) d)$$
$$\text{--------(42)}$$

$$FIII''' (n=m=0 \text{ loop}) = [TII + HII/(c d)] /Ko(\alpha(n=0) d)$$
$$\text{--------(43)}$$

To describe the three dimensional distribution of potentials and forces at the inner and middle regions, we computed for circumferential direction every $n \pi /6$ for n=1 to 6. For axial direction, we computed them at z=2,4,6,8 and $10 \ 10^{-8}$ cm. For the bio physical parameters, we set

$$L = 5 \ 10^{-8} \quad \kappa = 10 \ 10^{-8} \quad b = 10 \ 10^{-8}$$
$$\rho o = 9 \ 10^{-8} \quad d = 12 \ 10^{-8}$$

For the inner region , we took $\rho = 9.5 \ 10^{-8}$ and for the intermediate region, $\rho = 11 \ 10^{-8}$. In the following figures, potentials were timed by the factor 10^{-8} and forces by the factor 10^6, the axial positions were timed by the factor 10^{-8}.

3. Results.

1. Distribution of potential at the inner region (Fig 4).

Fig 4-a is the top view of the three dimensional distribution of the inner potential. The potential slightly depended on the axial position at small circumferential angle. With an increase of the angle, the axial dependency became explicit. At the middle axial point $z = 6 \ 10^{-8}$, the potential seems to reach the local minimum. Fig 4-b emphasizes the dependency of the potential on the circumferential direction on the half plane of the cross sectional area. The potential monotonically increased until the contra lateral position.
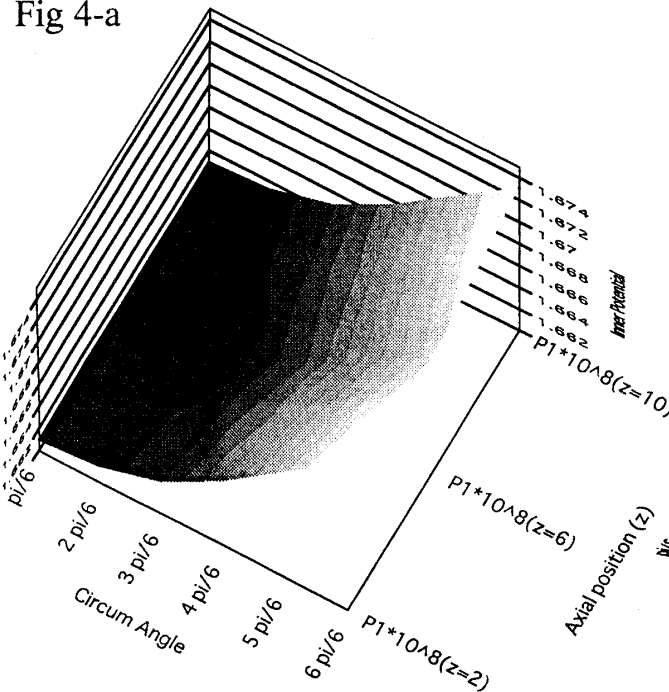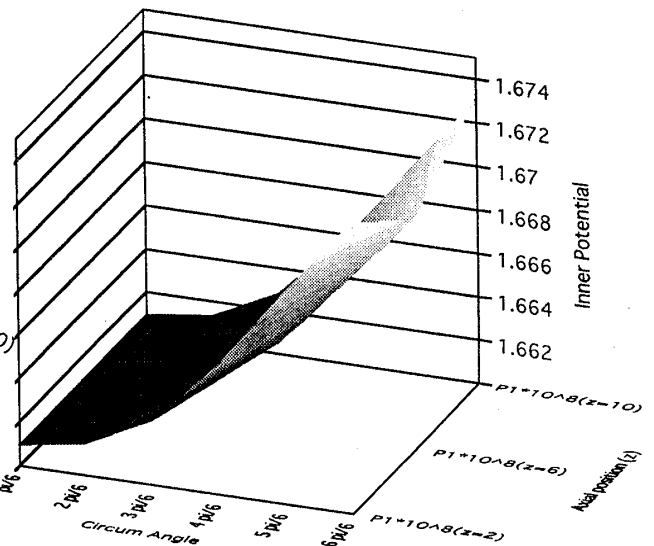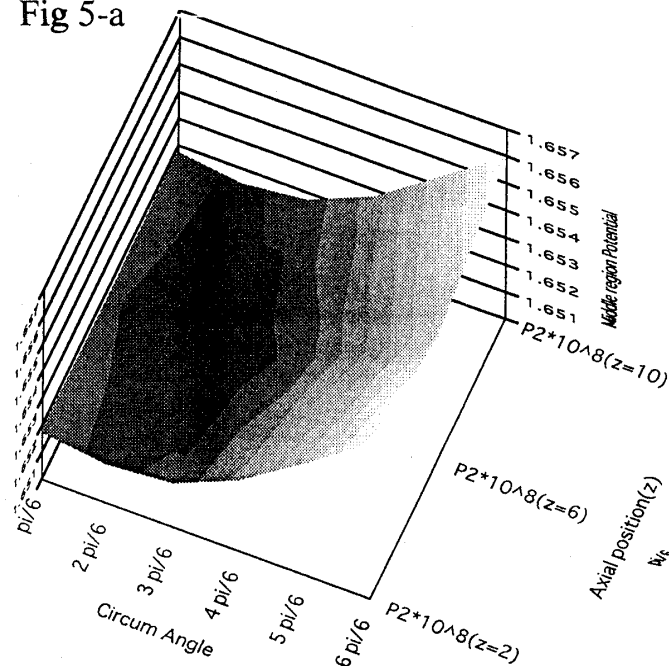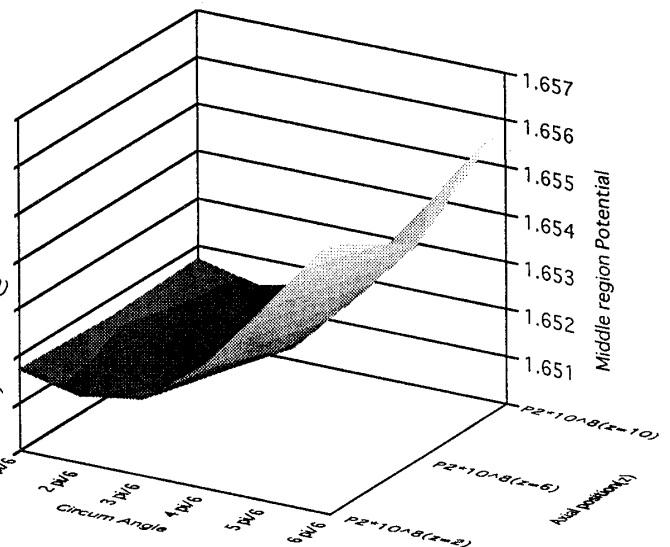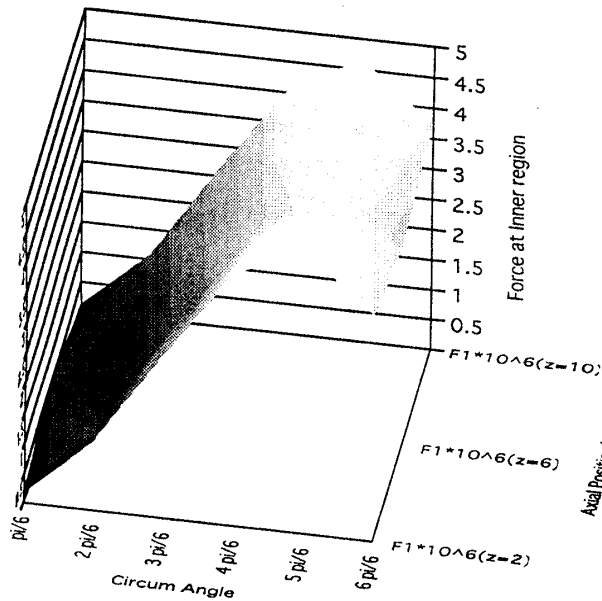
2. Distribution of the potential at the intermediate region (Fig 5).

Fig 5-a is the top view of the potential at the intermediate region just emphasizing its dependency on the axial position. As in the inner region potential, there was local minimum at the middle axial position $z = 6 \ 10^{-8}$. Also this figure shows the local minimum at the circumferential angle of $2 \ \pi/6$ at any axial position. Fig 5-b shows the potential dependency on the circumferential angle. The potential decreased during $1 \ \pi/6$ to $2 \ \pi/6$, then increased monotonically until $6 \pi/6$.

Fig 4-a

Fig 4-b

Fig 5-a

Fig 5-b

3. Distribution of the force at the inner region (Fig 6)

The three dimensional distributions of the forces were more complicated than those of the potentials. Fig 6-a shows the force generated by the inner region potential. The potential increased along the circumferential direction until $5\pi/6$ then decreased slightly. The dependency on the axial position (Fig 6-b) is more complicated where there was a little oscillation of magnitude of the potential along the z axial distances.

4. Distribution of the force at the intermediate region.(Fig 7)

Fig 7-a shows the three dimensional distribution of the force generated by the potential at the intermediate region. The force has oscillated depending on the circumferential direction. The force also oscillated slightly as function of the axial distance z . (Fig 7-b).

4. Discussion.

The present investigation was founded on the Debye-Huckel theory. We give some explanations for the assumptions and approximations.
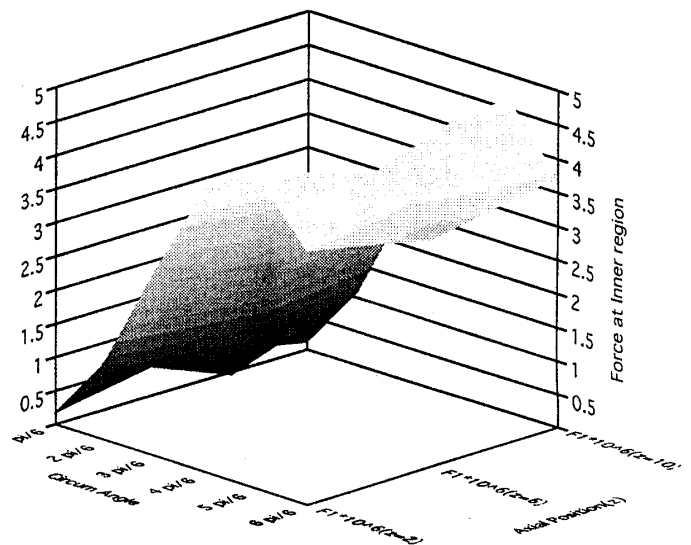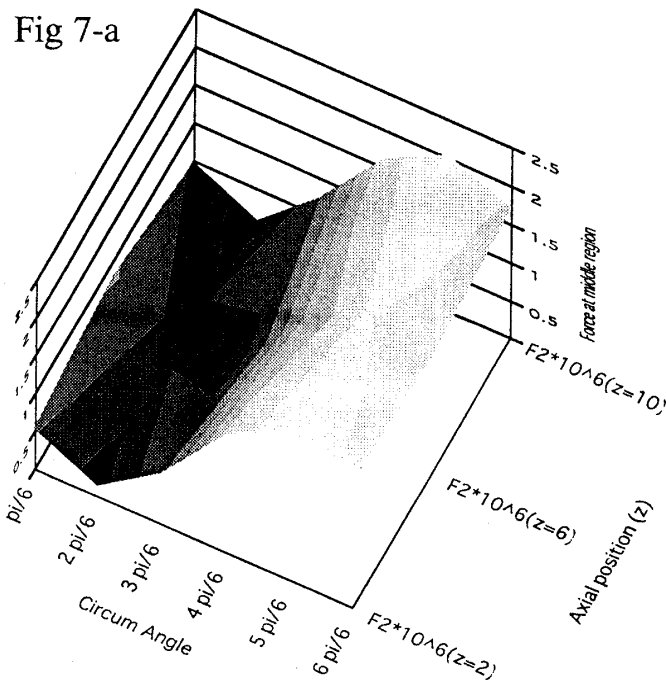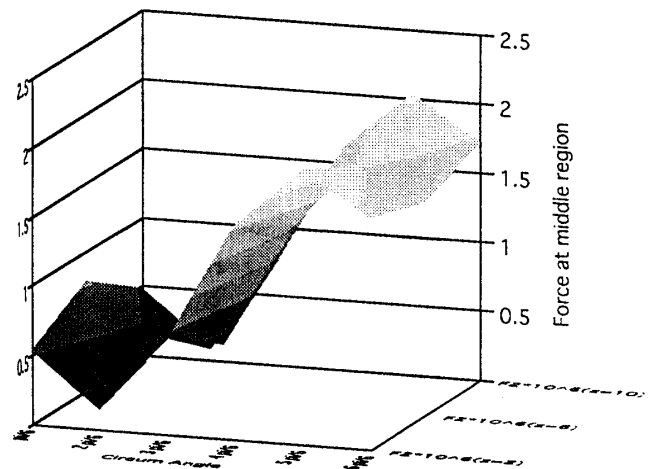
Fig 6-a

Fig 6-b

Fig 7-a

Fig 7-b

—43—

1. Assumption 1.

" Each spherical ion can be replaced by a point charge at its center ".

This assumption neglects ionic volumes and is only valid when the mean inter ionic distance is large compared with their sizes. This state is the dilute solution.

Around any ion of type j, the charge distribution is assumed to be spherically symmetrical. The charge density of the j ion $\rho_j(r)$ is

$$\int_a^\infty 4\,\pi\,r^2\,\rho_j(r)dr = -z_j\,e \qquad \text{-----(A-1)}$$

This expresses the electrical neutrality. The total charge of all the ions around the j th ion is equal and opposite to the charge on j th ion. a is the distance of the closest approach to the ion. It is equal to the sum of the radii a_i and a_j of the i th and j th ions. $a = a_i + a_j$

The sphere of radius a around ion j is the volume from which the centers of gravity of other ions are excluded. This approach corresponds to the assumption in the Debye-Huckel mode.

2. Assumption 2.

The variation in charge density $\rho_j(r)$ is assumed to follow the Boltzmann distribution law. This states that tyhe number n_i of ions around the ion j is given by

$$n_i = n_i{}^\circ\,exp\,[\,-w_{ij}(r)\,/(k_B\,T)\,] \qquad \text{-----(A-2)}$$

and hence

$$\rho_j(r) = \sum_i e\,z_i\,n_i = \sum_i n_i{}^\circ\,z_i\,exp\,[\,-w_{ij}(r)\,/(k_B\,T)\,] \qquad \text{-----(A-3)}$$

where $w_{ij}(r)$ is the potential energy corresponding to the mean force exerted between ions i and j. The number $n_i{}^\circ$ is effectively the concentration of the salt solution. The difference of $n - n_i{}^\circ$ is the average local excess or deficiency of an ion (cation or anion) at a point where the potential energy is $w_{ij}(r)$. The Boltzmann factor is the statistical weight multiplying the ionic concentration to account for mean local electrical interactions between ions.

3. Approximation 1.

The factor $w_{ij}(r)$ can be replaced by the potential energy of an ion i which locates at a point where there is a potential Ψ_j due to ion j. This is a mean energy because it corresponds to the force acting between i ion and j ion after averaging over N- 3 other ions in all possible positions. Thus, we can approximate

$$w_{ij}(r) \doteqdot z_i\,e\,\Psi_j(r) \qquad \text{-----(A-4)}$$

Combining (A-3) and (A-4) and using the spherical coordinate Laplacian expression to satisfy the symmetry assumption 1, we arrive the Poisson-Boltzmann equation

$$1/r^2\,d/dr\,(\,r^2\,d\Psi\,/\,dr\,) = 1/(\,\varepsilon_0\,\varepsilon\,)\sum_i e\,n_i{}^\circ\,z_i$$
$$exp\,[\,-\Psi_j(r)\,/(k_B\,T)\,]\,\text{--(A-5)}$$

4. Approximation2.

Equation (A-5) does not have an analytic solution. To obtain an analytic form, we approximate
$$exp(\,-y\,) = 1 - y\ \text{ for } y \ll 1.$$
This is equivalent to set

$$z_i\,e\,\Psi_j(r)\,/(k_B\,T) \ll 1.\,\text{------(A-6)}$$

This approximation is not made to satisfy the superposition theorem of electrostatics. The theorem depends on the linear form of equations and not on the linear relationship between ρ and Ψ.

The contradiction using the non linear Poisson- Boltzmann equation. Approximation 1 amounts to neglecting all interactions between groups of three, four et. ions and only considering those between pairs. This is only valid for very dilute state when the number of clusters of more than two ions are negligible.

The linearization of the Debye-Huckel theory, (A-6) is equivalent to assume that there is sufficient dilution to increase the mean distance between ions sufficiently to produce a low potential.

5. Conclusion.

1. A modeling theoretical method was proposed for analyzing the three dimensional potential and force distribution around the DNA molecule.

2. The potentials and forces at the inner and intermediate regions of DNA cylinder changed on the circumferential angles.

6. Reference.

1. Bailey, J.M. Biopolymers vol 12. pp 559-574. 1973.

APPENDIX.

Putting the sum of the rotational factors by

$$S = \sum_{j'=1} cos(\,m(\,\phi - \phi_{j'}\,)\,)\,cos(\,\lambda\,(\,z - z_{j'}\,)\,) \qquad \text{--(A1)}$$

By assuming that the DNA helix is an infinitely long cylinder, the position of a charge is given by specifying some unit cell and the position of the charge in that unit cell is given

$$z_{j'} = z_0{}^j + k\,L \qquad \text{---(A2)}$$
$$\phi_{j'} = \phi_0{}^j + k\,2\pi \qquad \text{---(A3)}$$

Using these relation and $cos(x-y) = cosx\,coy + sinx\,siny$

$$S = \sum_{k=-\infty}\sum_{j'=1} cos(\,m(\,\phi - \phi_0{}^j\,)\,)\,cos(\,\lambda\,(\,z - z_0{}^j\,)\,)\ cos\lambda k\,L$$

$$= \sum_{k=-\infty} e^{i\lambda k\,L}\sum_{j'=1} cos(\,m(\phi - \phi_0{}^j\,)\,)\,cos(\,\lambda\,(\,z - z_0{}^j\,)\,)e^{i\lambda k\,L} \qquad \text{---(A4)}$$

Since

$$\sum_{k=-\infty} e^{i\lambda k\,L} = \sum_{k=-\infty} e^{ik\,[\,\lambda L - 2n\,\pi\,]} = 2\,\pi\,\delta\,(\,\lambda\,L - 2n\,\pi\,) \qquad \text{---(A-5)}$$

where $n = 0, \pm 1, \pm 2, \pm 3$. Hence

$$\sum_{k=-\infty} e^{i\lambda k\,L} = 2\,\pi/L\sum_{n=-\infty} \delta\,(\,\lambda\, - 2n\,\pi/L\,) \qquad \text{---(A-6)}$$

Thus,

$$S = \sum_{j=1} cos(\,m(\,\phi - \phi_0{}^j\,)\,)\,cos(\,\lambda\,(\,z - z_0{}^j\,)\,)$$

$$*2\,\pi/L\sum_{n=-\infty} \delta\,(\,\lambda\, - 2n\,\pi/L\,) \qquad \text{---(A-7)}$$