

Analysis of Electrical Charge Distributions and Free Energy of DNA Molecule

-- Basic research for DNA molecular motor function.

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Mathematical computations were performed for potential evoked by the DNA molecules. The theoretical background was founded on the Debye-Huckel electrolyte theory and continuum theory. The DNA molecule was described by the cylindrical coordinate which was composed of three layers, inner region where the Phosphate negative charges exist, the local middle layer and the outer layer at which the ionic atmosphere exist. The electro static behaviors of these three regions were expressed by Laplace and Poisson equations. The unknown coefficients of the Potentials were determined by the Dirichlet and Neumann boundary conditions. The parameters were utilized from the reported experimental data. The present investigation is available for evaluating the electro and motor functions of DNA molecules.

DNA micro dynamics. DNA motor. Debye-Huckel electrolyte theory. Poisson equation.

DNA の電荷分布および自由エネルギー解析

分子モーターの基礎的研究

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DNA分子の動力学および分子モーター機能を分析するためDebye-Huckel 理論と連続体理論に基づいて、DNA分子が有するポテンシャルおよび、円周方向の力を算出する方法を報告し、一部計算結果を示した。DNA分子は円筒座標系で表わし、これにDebye-Huckel 理論とを適用し、最内層、中間層、外層の3層とした。最内層にはリン酸による電荷が存在するとした。最内層、中間層の静電場はラプラス方程式で、外層は対イオンが存在する外部環境であるためポアソン方程式で記述した。それぞれの層間で、ポテンシャルの連続条件をDirichlet型と Neumann 型で記述した。ベッセル関数をさらに級数展開することで未定係数を決定した。実験で報告されている分子間距離を代入してポテンシャルを計算した。本研究は、DNA分子の電氣的動力学を解析するうえで有用である。

DNA分子動力学. 分子モーター機能. Debye-Huckel 理論. 連続体理論. ラプラス方程式

1. Introduction.

The characteristics of all the biological systems are determined ultimately by the genes, functional groups of some DNA. Recently, numerous investigations have been disclosed the minute structures and information contents involved in the genes. These works have contributed to the analysis of pathogenesis of diseases, prediction of the diseases and gene recombination. Hence the analysis of DNA will be essential for creating artificial life. The molecular structure of DNA as a macro molecule has been identified in detail with precise spatial configuration of base pairs-phosphates-sugar complex composing the nucleic acid. The structure is strictly determined by the electrical factors having discrete distribution of the charges on the species composing the DNA strand. The geometry of charge distribution, its electrical potential, resulting forces and the Helmholtz free energy play the most important role in the molecular conformation. Thus, an electrical approach for the molecular structural stability of DNA is fundamental key issue in relation to the various conformations of the nucleic acid and replication of DNA double strand.

Nucleic acids work in poly-anionic form in neutral pH solution where negative charges situated in the phosphate groups on the backbone of the molecule. This electric feature of nucleic acid plays an important role for the mutual repulsions of the phosphate groups to achieve stable state of the DNA molecule. For preventing these repulsive effects, introduction of salt (counter ion) into a nucleic acid solution screen such repulsions. Such consideration is supported by the fact that increasing the salt concentration in a DNA solution increases the melting temperature T_m at which half the base pairs of DNA are in helix region, namely pre-replication state. Since many diseases occur at the replication stage, analysis of the interaction between salt and stability of DNA is important. This also extends to the creation of the artificial life.

In the present paper, we introduce a method for computing the potentials, forces and Helmholtz free energy of DNA by coaxial cylindrical modeling of the DNA based on Debye-Huckel dielectric continuum theory. We show three dimensional distributions of potentials and forces of at inner and local regions and geometric dependence of Helmholtz free energy.

Fig 3

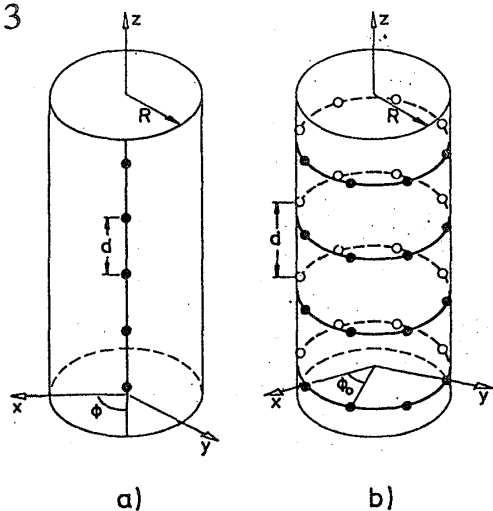


Fig 1

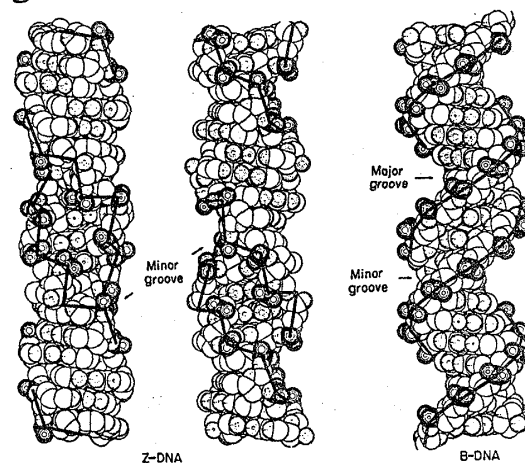


Fig 2

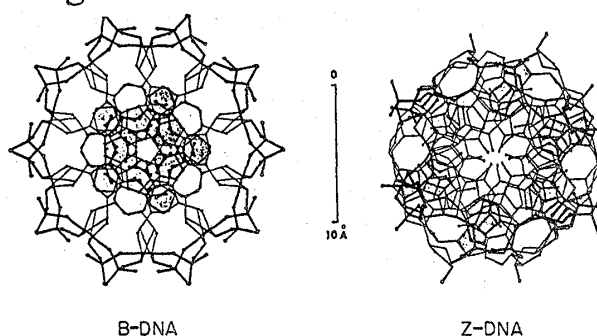
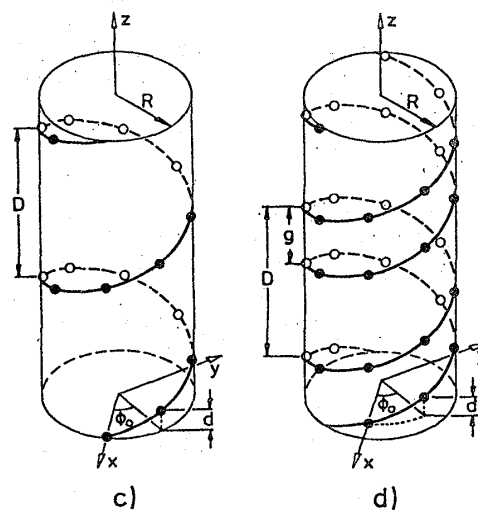


Fig 1 shows Van der Waals side views of Z-DNA and B-DNA. Two views of Z-DNA are shown which are 30 deg apart in orientation about the axis of helix. The irregularity of the Z-DNA backbone is indicated by the heavy lines. They direct from phosphate to phosphate residues along the DNA chain. B-DNA has a smooth line that connects the phosphate groups and two grooves. They do not extend to the axis of the helix. Fig 2 shows the end views of B-DNA and Z-DNA. The Guanine residues of one strand have been shaded. The B-DNA represents one full helix turn. In contrast to Z-DNA, the Guanine residues in B-DNA are located closer to the center of the molecules and the phosphates are on the outside.

Fig 3 shows configurations of discrete polyelectrolyte models. Each dot represents a point charge. (d) is the plectonemic double-helical lattice.



2. Physical consideration.

The present theory basis on the Debye-Huckel theory and linear Poisson Boltzmann equation. The main effect of introduced salt (counter ion) is the screening of the phosphate-phosphate repulsions. This screening can be treated in the Debye-Huckel theory. The distribution of the screening ions is given by the Boltzmann distribution forming a charge density

$$\rho = Nq(e^{-\epsilon\psi/kT} - e^{\epsilon\psi/kT}) \quad \text{----(1)}$$

where ρ is charge density, k is the Boltzmann constant, T is absolute temperature, ϵ is the electronic charge and N is the bulk ionic concentrations in ions per cubic centimeter. The Poisson equation for the potential ψ is

$$\nabla^2 \psi = -4\pi\rho/D$$

$$= -4\pi N/D(e^{-\epsilon\psi/kT} - e^{\epsilon\psi/kT}) \quad \text{----(2)}$$

D is the dielectric constant of the corresponding region. By the Taylor expansion for the exponential terms, the Equation (2) can be linearized to

$$\nabla^2 \psi = \kappa^2 \psi \quad \text{----(3)}$$

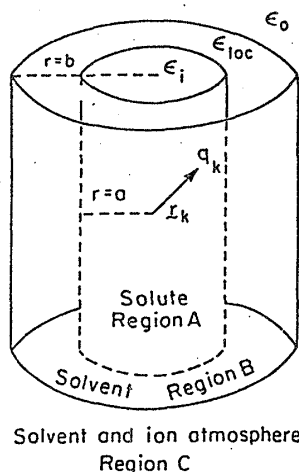
$\kappa^2 = 8\pi\epsilon^2 N M / (1000 D k T)$: N is the Avogadro's number, M is the molarity of the monovalent counter ion. κ is the Debye inverse length parameter which order is Angstrom. The vector form of solution of Equation (3) is

$$\psi(\mathbf{r}) = \epsilon/D \sum_j e^{(-\kappa|\mathbf{r}-\mathbf{r}_j|)} / |\mathbf{r}-\mathbf{r}_j| \quad \text{----(4)}$$

giving the basic terms for the potential of the DNA in any coordinate system. The potential at the position of \mathbf{r} can be regarded as the result of screened repulsions from all the phosphate charges. In the present paper, we assumed that the DNA helical strand is impermeable to screening ions. The dielectric constant of the inner region of the DNA differs from the outer region where the bulk solvent distributes to constitute the ion atmosphere. The electro static contribution to the free-energy relates to the electro static potential ψ by

$$Ael = 1/2 \sum_i \psi_i q_i \quad \text{----(5)}$$

Fig 4



3. Modeling

3-1. General Theory

Fig 2 shows the generalized model of DNA. The coaxial cylindrical system consisted of three regions. Only the phosphate coordinates were used. The charges are represented by only the DNA phosphate groups and assumed to locate by discrete positions. The inner region (Region A) describes a cylindrical cavity with L height, $r=a$ radius and a dielectric constant ϵ_i . The solute charges are located at sites r_k .

Region B is a local region extending radially from $r=a$ to $r=b$. This region describes the first shell of the solute and contains solvent of dielectric constant ϵ_{loc} . Region B constitute the ion exclusion zone. According to the Debye-Huckel theory, region B is the area of the closest approach of the screening ions (counter ions). There is no charge in this region. The spatial distributions of the potentials in these regions is given by the Laplace equation.

$$\Delta \phi = 0 \quad \text{----(6)}$$

Region C is the outer region which ranges from $r=b$ to $r=\infty$. This region contains solvent of dielectric constant ϵ_o and ion atmosphere including counter ion and co-ions. The ion atmosphere enters into modeling through the Debye inverse length parameter κ . This area is completely accessible to the screening ions and its distribution is given by the Debye-Huckel theory. The dielectric constants in regions B and C are those of the bulk solution. The spatial distribution of the potential of this region satisfies the linearized Poisson-Boltzmann equation

$$(\Delta - \kappa^2) \phi = 0 \quad \text{----(7)}$$

The general solutions for regions A and B are

$$\phi_i \text{ and } \phi_{loc} = \sum_{k=1} B_k / |\mathbf{r} - \mathbf{r}_k| \quad \text{----(8)}$$

and for region C.

$$\phi_o = \sum_{k=1} (A_k \exp(-\kappa|\mathbf{r} - \mathbf{r}_k|) / |\mathbf{r} - \mathbf{r}_k| + B_k \exp(-\kappa|\mathbf{r} - \mathbf{r}_k|) / |\mathbf{r} - \mathbf{r}_k|) \quad \text{----(9)}$$

ϕ_i and ϕ_{loc} contain the Coulombic potential due to the discrete charge distribution. ϕ contains screened Debye potential. r_k represents the Cartesian coordinates of the k th charge. Modifications to the Coulombics due to the presence of dielectric boundaries are introduced via the constants A_k and B_k . They are determined by adequate boundary conditions.

Fig 4 shows the definition of the parameters for the coaxial cylindrical di-electric continuum problem. q_k is the k th electrical charge at the discrete point in the inner region of the DNA. This three layers model imposes two boundary conditions at $r=a$ and $r=b$.

3-2. Configuration of charge distribution.

According to the molecular configuration analysis, the phosphate charges locate periodically along the helix of the DNA.

3-2-1. Circumferential direction.

The position of each phosphate rotates around the Helical axis with the equivocal latitudinal angle ϕ . The one helical turn can be achieved by p number of the phosphates. Hence,

$$2\pi/p = \phi. \quad \text{---(10)}$$

As a result, the circumferential position is the n th charge is given by

$$\phi_n = \phi_0 + n * \phi \quad \text{---(11)}$$

where ϕ_0 is the reference circumferential position.

3-2-2. Axial direction. Fig

We define that θ is the angle between the helix of the DNA and the Horizontal axis of the co axial cylinder. On the helix curve, we denote the n th position of the discrete charge by z_n' while along the axial coordinate in z direction, we denote by z_n where n is an integer satisfying $0 < n < p+1$. Increasing number of n indicates that the the position of a charge climbs along the helix curve. The vertical shift along the helical axis of the DNA between the $n-1$ th and n th charge is

$$(z_n' - z_{n-1}') \sin \theta. \quad \text{---(12)}$$

Hence, the axial shift (z direction) from the central horizontal axis of the DNA for the n th charge can be expressed by the recurrent formula

$$z_n = z_{n-1} + (z_n' - z_{n-1}') \sin \theta. \quad \text{---(13)}$$

Then, the axial (z direction) position of each charge from the horizontal axis of the DNA is

$$z_1 = z_0 + 1 * (z_1' - z_0') \sin \theta$$

$$z_2 = z_0 + 2 * (z_2' - z_1') \sin \theta$$

$$z_3 = z_0 + 3 * (z_3' - z_2') \sin \theta$$

**

$$z_n = z_0 + n * (z_n' - z_{n-1}') \sin \theta$$

$$z_{p-1} = z_0 + (p-1) * (z_p' - z_{p-1}') \sin \theta \quad \text{---(14)}$$

where z_0 is the reference axial position. These relations basis on the equivalent separation between the adjacent phosphate.

3-2-3. Solid relation between two adjacent charge.

$$\cos \theta = |z_{Hn-1} - z_{Hn}| / |z_{n-1}' - z_n'| \quad \text{---(15)}$$

where $|z_{Hn-1} - z_{Hn}|$ is the distance along the horizontal direction between the $n-1$ th and n th charges. On the horizontal plane, the circumferential angle ϕ is the right angle constituted of z_{Hn-1} , z_{Hn} across the central axis

of the DNA. By assuming that the all the charges exist on the same radial position with the distance from the central axis of the DNA by ρ_n , the trigonometric relations results in

$$|z_{Hn-1} - z_{Hn}| / \sin \phi = \rho_n / \sin((\pi - \phi)/2) \quad \text{---(16)}$$

Hence

$$\cos \theta = \rho_n * \sin \phi / \sin((\pi - \phi)/2) * 1 / |z_{n-1}' - z_n'| \quad \text{---(17)}$$

As a result,

$$|z_{n-1}' - z_n'| = \rho_n \sin \phi / \sin((\pi - \phi)/2) * 1 / \cos \theta \quad \text{---(18)}$$

Finally, we characterize the axial position of n th charge by

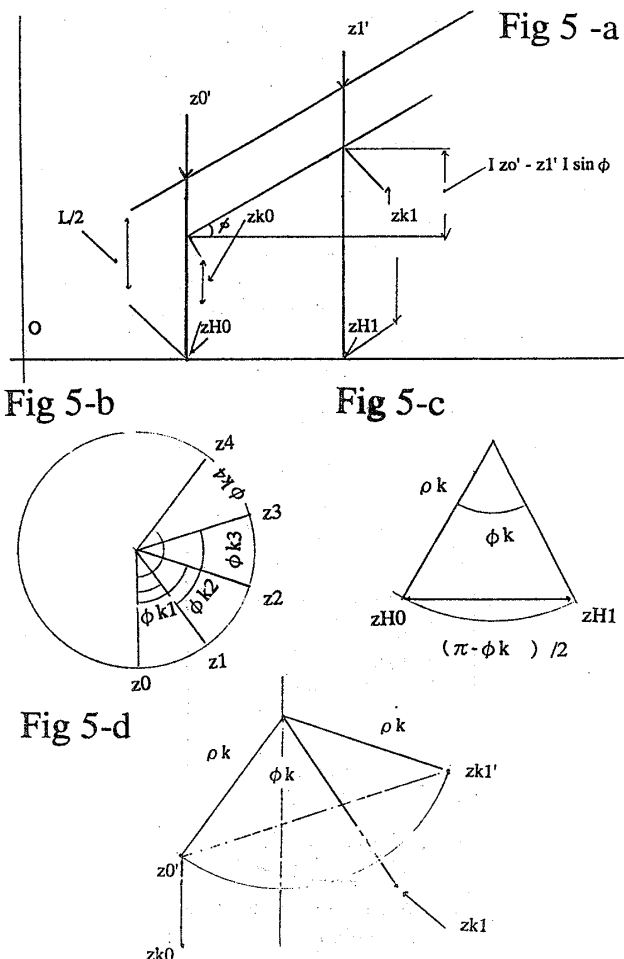
$$z_n = z_0 + n \sin \theta \rho_n \sin \phi / \sin((\pi - \phi)/2) * 1 / \cos \theta \quad \text{---(19)}$$

According to the molecular conformational analysis, the parameters of structure has been strictly determined as

$$p=10, \quad \phi = \pi/5 \text{ and } \theta = 8/9 \phi \quad \text{---(20)}$$

The most potent inter molecular interactions operate between the screening ions and the DNA helix.

Fig 5 shows the coordinates and configurations.



3-3. Solutions of the Electrical potential field.

The general solutions for the regions A, B and C in cylindrical coordinates are

$$\phi_i = 1/\varepsilon_i \sum_{k=1} [-2q_k/L \log(\omega_k) + B_k + F_k + \sum_{n=1} \{B_{nk} \text{Io}(\lambda \omega_k) + F_{nk} \text{Io}(\lambda \omega_k) + 4q_k/L \text{Ko}(\lambda \omega_k)\} \cos(\lambda(z-z_k))] \quad \text{---(21)}$$

$$\phi_{loc} = 1/\varepsilon_{loc} \sum_{k=1} [-G_k \log(\omega_k) + F_k + \sum_{n=1} \{F_{nk} \text{Io}(\lambda \omega_k) + G_{nk} \text{Ko}(\lambda \omega_k)\} \cos(\lambda(z-z_k))] \quad \text{---(22)}$$

and

$$\phi_o = 1/\varepsilon_o \sum_{k=1} [C_k \text{Ko}(\kappa \omega_k) + \sum_{n=1} \{C_{nk} \text{Ko}(\lambda' \omega_k)\} \cos(\lambda'(z-z_k))] \quad \text{---(23)}$$

where $\text{Ko}(s)$ and $\text{Io}(s)$ are the modified Bessel functions of zero order. The terms in B_k originate in the polarization of the local dielectric. Terms in F_k originate in the polarization of the bulk dielectric continuum. The cylindrical coordinates of the k th charge are described by ρ_k , ϕ_k and z_k . In addition

$$\omega_k = [\rho^2 + \rho_k^2 - 2\rho \rho_k \cos(\phi - \phi_k)]^{1/2} \quad \text{---(24)}$$

$$\lambda = 2\pi/L, \quad \lambda' = (\lambda^2 + \kappa^2)^{1/2} \quad \text{---(25)}$$

The constants B, F, G and C are determined by the boundary conditions. The reaction potential is

$$\phi_R = 1/\varepsilon_i \sum_{k=1} [B_k + F_k + \sum_{n=1} \{(B_{nk} + F_{nk}) \text{Io}(\lambda \omega_k)\} \cos(\lambda(z-z_k))] \quad \text{---(26)}$$

The electric Helmholtz free energy of the charge distribution is

$$\text{AeL} = 1/2 \sum_{\nu=1} q_\nu \phi_R(r_\nu) \quad \text{---(27)}$$

$\phi_R(r_\nu)$ is the reaction potential at the charged site r_ν of charge q_ν . The matching conditions for this problem are that the potential and dielectric displacement across the boundaries be continuous. This requires

$$(\phi_i)_{\rho=a} = (\phi_{loc})_{\rho=a} \quad \text{---(28)}$$

$$(\phi_{loc})_{\rho=b} = (\phi_o)_{\rho=b} \quad \text{---(29)}$$

$$\varepsilon_i (d\phi_i/d\rho)_{\rho=a} = \varepsilon_{loc} (d\phi_{loc}/d\rho)_{\rho=a} \quad \text{---(30)}$$

$$\varepsilon_{loc} (d\phi_{loc}/d\rho)_{\rho=b} = \varepsilon_o (d\phi_o/d\rho)_{\rho=b} \quad \text{---(31)}$$

In applying these boundary conditions

$$\log(1/\omega_k) = \log(1/\rho) + \sum_{m=1} 1/m (\rho < \rho_k)^m \cos(m(\phi - \phi_k)) \quad \text{---(32)}$$

$$\text{Ko}(\lambda \omega_k) = \text{Io}(\lambda \rho) + \text{Ko}(\lambda \rho_k) + 2 \sum_{m=1} \cos(m(\phi - \phi_k)) \text{Im}(\lambda \rho) \text{Km}(\lambda \rho_k) \quad \text{---(33)}$$

$$\text{Io}(\lambda \omega_k) = \text{Io}(\lambda \rho) + \text{Io}(\lambda \rho_k) + 2 \sum_{m=1} (-1)^m \cos(m(\phi - \phi_k)) \text{Im}(\lambda \rho) \text{Im}(\lambda \rho_k) \quad \text{---(34)}$$

Utilizing these expressions, the reaction potential can be

$$\begin{aligned} \phi_R(r_k) = 1/\varepsilon_i \sum_{k=1} [B_k + F_k + \sum_{m=1} \cos(m(\phi - \phi_k)) (B_{mk} + F_{mk}) \rho^m/m + \sum_{n=1} \{(B_{nk} + F_{nk}) \text{Io}(\lambda \rho_k) \text{Io}(\lambda \rho) \cos(\lambda(z-z_k)) + 2 \sum_{m=1} \cos(m(\phi - \phi_k)) (-1)^m \sum_{n=1} (B_{mnk} + F_{mnk}) \text{Im}(\lambda \rho_k) \text{Im}(\lambda \rho) \cos(\lambda(z-z_k))\}] \quad \text{---(35)} \end{aligned}$$

Using the equations (5) to (8), (12) to (18), the coefficients in (19) are

$$B_k = 2q_k/(L \varepsilon_b) (1 - \varepsilon_a)/\varepsilon_a \{ \text{Ko}(\kappa b)/(\kappa b \text{K}_1(\kappa b)) + \varepsilon_b \log(b/a) \} \quad \text{---(36)}$$

$$F_k = 2q_k/(L \varepsilon_b) \{ \text{Ko}(\kappa b)/(\kappa b \text{K}_1(\kappa b)) + \varepsilon_b \log(b) \} \quad \text{---(37)}$$

$$B_{mk} = 2q_k/L (1 - \varepsilon_a)/\varepsilon_a (\rho_k^m/a^{2m}) [1 + (a/b)^{2m} \{ (m \text{Km}(\kappa b) + \varepsilon_b \kappa b \text{Km}'(\kappa b))/ (m \text{Km}(\kappa b) - \varepsilon_b \kappa b \text{Km}'(\kappa b)) \}] \quad \text{---(38)}$$

$$F_{mk} = 2q_k/L (\rho_k^m/b^{2m}) [\{ (m \text{Km}(\kappa b) + \varepsilon_b \kappa b \text{Km}'(\kappa b))/ (m \text{Km}(\kappa b) - \varepsilon_b \kappa b \text{Km}'(\kappa b)) \}] \quad \text{---(39)}$$

$$B_{mnk} = (-1)^m 4q_k/L (\varepsilon_a' - 1) \text{Km}'(\lambda a)/\text{Im}'(\lambda a) \quad \text{---(40)}$$

$$F_{mnk} = (-1)^m 4q_k/L \varepsilon_a' \theta \quad \text{---(41)}$$

$$B_{nk} = B_{nk}^0 \quad \text{and} \quad F_{nk} = F_{nk}^0 \quad \text{---(42)}$$

$$\theta = [(\varepsilon_b \lambda' \text{Km}'(\lambda' b) \text{Km}(\lambda b) - \lambda \text{Km}(\lambda' b) \text{Km}'(\lambda b))/(-\varepsilon_b \lambda' \text{Km}'(\lambda' b) \text{Im}(\lambda b) + \lambda \text{Km}(\lambda' b) \text{Im}'(\lambda b))] \quad \text{---(43)}$$

$$\varepsilon_a' = \varepsilon_a/(\lambda a) 1/[(1 - \varepsilon_a) \theta \text{Im}(\lambda a) \text{Im}'(\lambda a) + \text{Km}(\lambda a) \text{Im}'(\lambda a) - \varepsilon_a \text{Km}'(\lambda a) \text{Im}(\lambda a)] \quad \text{---(44)}$$

$$\varepsilon_a = \varepsilon_{loc}/\varepsilon_i \quad \text{and} \quad \varepsilon_b = \varepsilon_o/\varepsilon_{loc} \quad \text{---(45)}$$

Substituting above constants in (19) and (11), the electrostatic free energy is obtained as

$$\begin{aligned} \text{AeL} = \sum_{L=1} \sum_{k=1} [q_L q_k/(L \varepsilon_b \varepsilon_i) \{ (1 - \varepsilon_a)/\varepsilon_a \{ \text{Ko}(\kappa b)/(\kappa b \text{K}_1(\kappa b)) + \varepsilon_b \log(b/a) \} + (\text{Ko}(\kappa b)/(\kappa b \text{K}_1(\kappa b)) + \varepsilon_b \log(b)) \} + q_L q_k/(L \varepsilon_i) \sum_{m=1} \cos(m(\phi_L - \phi_k))/m \{ ((1 - \varepsilon_a)/\varepsilon_a \{ 1 + (a/b)^{2m} \{ (m \text{Km}(\kappa b) + \varepsilon_b \kappa b \text{Km}'(\kappa b))/ (m \text{Km}(\kappa b) - \varepsilon_b \kappa b \text{Km}'(\kappa b)) \} \} + 1/b^{2m} \{ (m \text{Km}(\kappa b) + \varepsilon_b \kappa b \text{Km}'(\kappa b))/ (m \text{Km}(\kappa b) - \varepsilon_b \kappa b \text{Km}'(\kappa b)) \} \} \rho_k^m \rho^L/m \} \end{aligned}$$

$$\begin{aligned}
& + 2 q_L q_k / (L \varepsilon_i) \sum_{n=1} \{ ((1 - \varepsilon''_a) K_1(\lambda a) / I_1(\lambda a) + \varepsilon''_a \theta^{m=0}_{nk}) I_0(\lambda \rho k) I_0(\lambda \rho L) \cos(\lambda(z_L - z_k)) \\
& + 4 q_L q_k / (L \varepsilon_i) \sum_{m=1} \cos(m(\phi_L - \phi_k)) \sum_{n=1} ((\varepsilon'_a - 1) K_m'(\lambda a) / I_m'(\lambda a) + \varepsilon'_a \theta) I_m(\lambda \rho k) I_m(\lambda \rho L) \cos(\lambda(z_L - z_k)) \} \quad \text{---(46)}
\end{aligned}$$

where

$$\theta^{m=0}_{nk} = [(-\varepsilon_b \lambda' K_1(\lambda' b) K_0(\lambda b) + \lambda K_0(\lambda' b) K_1(\lambda b)) / (\varepsilon_b \lambda' K_1(\lambda' b) I_0(\lambda b) + \lambda K_0(\lambda' b) I_1(\lambda b))] \quad \text{---(47)}$$

$$\varepsilon''_a = \varepsilon_a / (\lambda a) 1 / [(1 - \varepsilon_a) \theta^{m=0}_{nk} I_0(\lambda a) I_1(\lambda a) + K_0(\lambda a) I_1(\lambda a) + \varepsilon_a K_1(\lambda a) I_1(\lambda a)] \quad \text{---(48)}$$

Putting

$$\alpha = (m K_m(\kappa b) + \varepsilon_b \kappa b K_m'(\kappa b)) / (m K_m(\kappa b) - \varepsilon_b \kappa b K_m'(\kappa b)) \quad \text{---(49)}$$

The potential in the inner region is

$$\begin{aligned}
\phi_i = & \sum_{k=1} 2 q_k / (L \varepsilon_i) \left[\text{Log}(1/\rho) + \varepsilon_i / \varepsilon_o \{ K_0(\kappa b) / (\kappa b K_1(\kappa b)) \} + \varepsilon_i / \varepsilon_{loc} \log(b/a) + \log(a) \right] \\
& + \sum_{m=1} \cos(m(\phi - \phi_k)) / m \{ 1 + ((1 - \varepsilon_a) / \varepsilon_a) (\rho/a)^{2m} \{ 1 + (a/b)^{2m} \alpha \} + (\rho/a)^{2m} \alpha \} \rho k^m / \rho^m \\
& + 2 \sum_{n=1} \{ ((1 - \varepsilon''_a) K_1(\lambda a) / I_1(\lambda a) + \varepsilon''_a \theta^{m=0}_{nk}) I_0(\lambda \rho k) I_0(\lambda \rho) + I_0(\lambda \rho k) K_0(\lambda \rho) \} \cos(\lambda(z - z_k)) \\
& + 4 \sum_{m=1} \cos(m(\phi - \phi_k)) \sum_{n=1} ((\varepsilon'_a - 1) K_m'(\lambda a) / I_m'(\lambda a) + \varepsilon'_a \theta) I_m(\lambda \rho k) I_m(\lambda \rho) + I_m(\lambda \rho k) K_m(\lambda \rho) \} \cos(\lambda(z - z_k)) \} \quad \text{---(50)}
\end{aligned}$$

For the Local potential

$$G^{m=0}_{nk} = [[\varepsilon_{loc} / \varepsilon_i 4 q_k / L [[K_0(\lambda a) + \{ (1 - \varepsilon''_a) K_1(\lambda a) / I_1(\lambda a) + \varepsilon''_a \theta^{m=0}_{nk} \} I_0(\lambda a)]] - F^{m=0}_{nk} I_0(\lambda a)]] / K_0(\lambda a) \quad \text{---(51)}$$

$$G^{m}_{nk} = [[\varepsilon_{loc} / \varepsilon_i 4 q_k / L [[K_m(\lambda a) + \{ (\varepsilon'_a - 1) K_m'(\lambda a) / I_m'(\lambda a) + \varepsilon'_a \theta \} I_m(\lambda a)]] - F^{m}_{nk} (-1)^m I_m(\lambda a)]] / K_m(\lambda a) \quad \text{---(52)}$$

$$G^m_k = 2 q_k / L [1 + (a/b)^{2m} \alpha] \quad \text{---(53)}$$

$$G^{m=0}_k = - [[2 \varepsilon_{loc} q_k / L [1 / \varepsilon_o K_0(\kappa b) / (\kappa b K_0(\kappa b)) + 1 / \varepsilon_{loc} \log(b/a)] - F_k]] / \log(a) \quad \text{---(54)}$$

Thus, we have

$$\begin{aligned}
\phi_{loc} = & \sum_{k=1} [[- G_k \log(\rho) + F_k] \\
& + \sum_{m=1} [[G^{m=0}_k (1/m) (\rho k / \rho)^m \cos(m(\phi - \phi_k))
\end{aligned}$$

$$\begin{aligned}
& + \sum_{n=1} [[F^{m=0}_{nk} I_0(\lambda \rho k) I_0(\lambda \rho) + G^{m=0}_{nk} I_0(\lambda \rho k) K_0(\lambda \rho)] \cos(\lambda(z - z_k))]] \\
& + 2 \sum_{n=1} \sum_{m=1} [[(-1)^m F^{m}_{nk} I_m(\lambda \rho k) I_m(\lambda \rho) + G^{m}_{nk} I_m(\lambda \rho k) K_m(\lambda \rho)] \cos(m(\phi - \phi_k))]] \cos(\lambda(z - z_k))]] \quad \text{---(55)}
\end{aligned}$$

For the outer potential

$$C^{m}_{nk} = \varepsilon_o / \varepsilon_{loc} [(-1)^m F^{m}_{nk} I_m(\lambda b) + G^{m}_{nk} K_m(\lambda b)] I_m(\lambda \rho k) \cos(\lambda(z - z_k)) / [I_m(\lambda' \rho k) K_m(\lambda' b) \cos(\lambda'(z - z_k))] \quad \text{---(56)}$$

$$C^{m=0}_{nk} = \varepsilon_o / \varepsilon_{loc} [F^{m=0}_{nk} I_0(\lambda b) + G^{m=0}_{nk} K_0(\lambda b)] I_0(\lambda \rho k) \cos(\lambda(z - z_k)) / [I_0(\lambda' \rho k) K_0(\lambda' b) \cos(\lambda'(z - z_k))] \quad \text{---(57)}$$

$$C^{m=0}_k = [[\varepsilon_o / \varepsilon_{loc} G^{m=0}_k 1/m (\rho k/b)^m]] / [2 I_m(\kappa \rho k) K_m(\kappa b)] \quad \text{---(58)}$$

$$C^0_k = \varepsilon_o / \varepsilon_{loc} [- G_k \log(b) + F_k] / [I_0(\kappa \rho k) K_0(\kappa b)] \quad \text{---(59)}$$

Thus, we have

$$\begin{aligned}
\phi_{out} = & 1 / \varepsilon_o \sum_{k=1} [C^0_k I_0(\lambda' \rho k) K_0(\lambda' \rho) \\
& + 2 \sum_{m=1} [[C^m_k I_m(\lambda' \rho k) K_m(\lambda' \rho) \cos(m(\phi - \phi_k)) \\
& + \sum_{n=1} [[C^{m=0}_{nk} I_0(\lambda' \rho k) K_0(\lambda' \rho)] \cos(\lambda(z - z_k))] \\
& + 2 \sum_{n=1} \sum_{m=1} [[C^m_{nk} I_m(\lambda' \rho k) K_m(\lambda' \rho)] \cos(m(\phi - \phi_k)) \cos(\lambda(z - z_k))]]] \quad \text{---(60)}
\end{aligned}$$

In calculating the potentials, we set following parameters for DNA strands.

$\phi_k = 36 \text{ deg}$, $\psi_k = 32 \text{ deg}$
 ρ_k for inner region = $8 \cdot 10^{-8} \text{ } \rho_k$ for reaction potential
 $= 8 \cdot 10^{-8} \text{ } \rho_k$ for local region = $11 \cdot 10^{-8} \text{ } \rho_k$ for outer region = $15 \cdot 10^{-8} \text{ (cm)}$
 κ the Debye inverse length parameter $\kappa = 1/8 \cdot 10^{-8}$

4. Results.

Fig 6 shows the potential at the inner region (expressed by 10^{-5}) and Fig 7 shows the local potential (expressed by 10^{-7}) as functions of the axial positions $(z_{kn-1} + z_{kn})/2$ and circumferential angles $(\phi_{kn-1} + \phi_{kn})/2$. The inner potential showed a peak at the middle of the entire circumference. The local potential increased as the axial position increased. The present method will be available for evaluating the potentials and resulting forces of DNA motors.

Fig 6

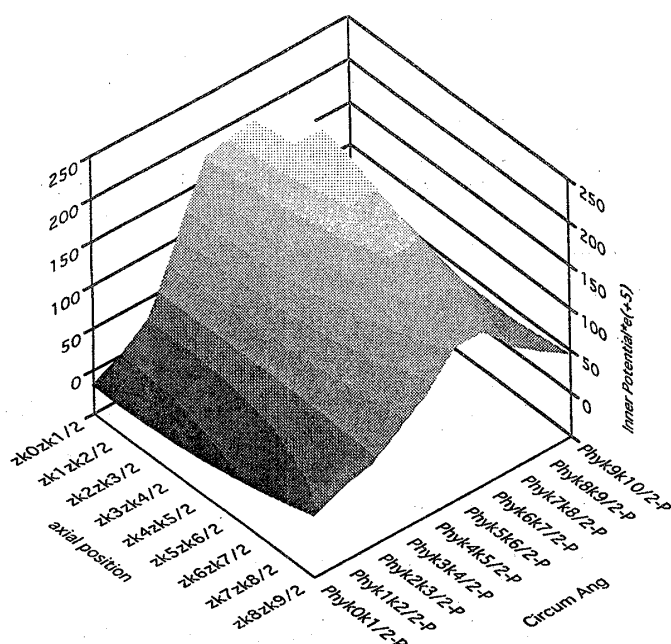
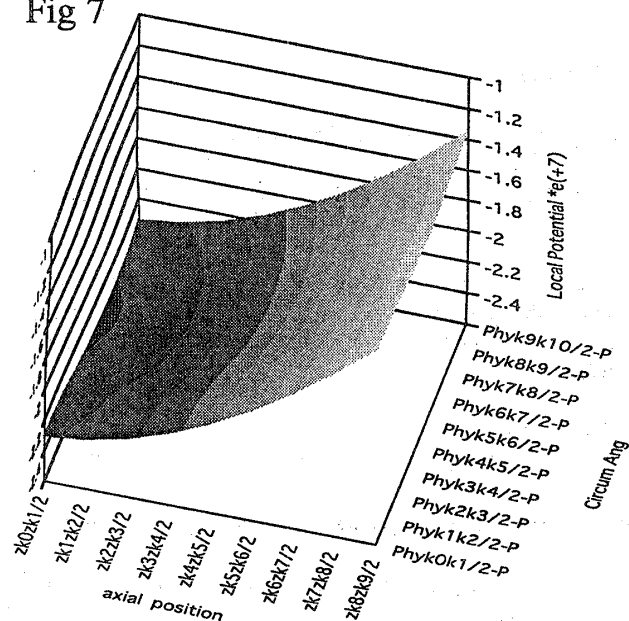


Fig 7



5. References

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APPENDIX.1. Solutions for Helmholtz equations.

The following forms are solutions for the Helmholtz equation which satisfy the Poisson equation by replacing ik for k .

1. Expansion by Legendre spherical functions and Cylindrical functions

$$\frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|} = \pm \frac{ik}{4\pi} \sum_{n=0}^{\infty} (2n+1) P_n(\cos \gamma) \tilde{Y}_n^{(c)}(kr') h_n^{(c)}(kr) \quad (r > r'; r \leftrightarrow r') \quad (3.2.24)$$

γ is an angle by the vectors r and r' . h_n is the Hankel function.

$$\begin{aligned} \frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|} &= \pm \frac{ik}{4\pi} \sum_{n=0}^{\infty} (2n+1) \sum_{m=-n}^n \frac{(n-m)!}{(n+m)!} \\ &\times P_n^m(\cos \theta) P_n^m(\cos \theta') e^{im(\varphi-\varphi')} j_n(kr') h_n^{(c)}(kr) \\ &= \pm \frac{ik}{4\pi} \sum_{n=0}^{\infty} (2n+1) \sum_{m=0}^n \epsilon_m \frac{(n-m)!}{(n+m)!} \cos m(\varphi-\varphi') \\ &\times P_n^m(\cos \theta) P_n^m(\cos \theta') j_n(kr') h_n^{(c)}(kr) \quad (r > r'; r \leftrightarrow r') \quad (3.2.25) \end{aligned}$$

where

$$\epsilon_m = 2 - \delta_{m0} = \begin{cases} 1 & (m=0) \\ 2 & (m=1, 2, \dots) \end{cases} \quad (3.2.26)$$

For the cylindrical coordinates (ρ, φ, z)

$$\begin{aligned} \frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|} &= \pm \frac{i}{4\pi} \int_{W^{(c)}} H_0^{(c)}(\pm i\sqrt{\lambda^2 - k^2} |\rho - \rho'|) \cos \lambda(z-z') d\lambda \\ &= \pm \frac{i}{4\pi} \int_0^\infty H_0^{(c)}(\sqrt{k^2 - \lambda^2} |\rho - \rho'|) \cos \lambda(z-z') d\lambda \\ \frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|} &= \pm \frac{i}{4\pi} \sum_{m=0}^{\infty} \epsilon_m \cos m(\varphi-\varphi') \int_0^\infty H_m^{(c)}(\rho\sqrt{k^2 - \lambda^2}) \\ &\times J_m(\rho'\sqrt{k^2 - \lambda^2}) \cos \lambda(z-z') d\lambda \quad (\rho > \rho'; \rho \leftrightarrow \rho') \\ \frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|} &= \frac{1}{4\pi} \int_{W^{(c)}} J_0(\lambda|\rho - \rho'|) e^{-\sqrt{\lambda^2 - k^2}|z-z'|} \frac{\lambda d\lambda}{\sqrt{\lambda^2 - k^2}} \\ &= \frac{1}{4\pi} \int_0^\infty J_0(\lambda|\rho - \rho'|) e^{-\sqrt{\lambda^2 - k^2}|z-z'|} \frac{\lambda d\lambda}{\sqrt{\lambda^2 - k^2}} \\ \frac{e^{\pm ik|r-r'|}}{4\pi|r-r'|} &= \frac{1}{4\pi} \int_{W^{(c)}} \sum_{m=0}^{\infty} \epsilon_m J_m(\lambda\rho) J_m(\lambda\rho') \cos m(\varphi-\varphi') \\ &\times e^{-\sqrt{\lambda^2 - k^2}|z-z'|} \frac{\lambda d\lambda}{\sqrt{\lambda^2 - k^2}} \quad (3.2.35) \end{aligned}$$

$$\frac{1}{4\pi|r-r'|} = \frac{1}{4\pi} \sum_{n=0}^{\infty} P_n(\cos \gamma) \frac{r'^n}{r^{n+1}} \quad (r > r'; r \leftrightarrow r') \quad (3.2.36)$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^n \frac{\epsilon_m (n-m)!}{4\pi (n+m)!} P_n^m(\cos \theta) P_n^m(\cos \theta') \cos m(\varphi-\varphi') \frac{r'^n}{r^{n+1}} \quad (r > r'; r \leftrightarrow r') \quad (3.2.37)$$

$$= \frac{1}{2\pi^2} \int_0^\infty K_0(\lambda|\rho - \rho'|) \cos \lambda(z-z') d\lambda \quad (3.2.38)$$

$$= \sum_{m=0}^{\infty} \frac{\epsilon_m}{2\pi^2} \cos m(\varphi-\varphi') \int_0^\infty K_m(\lambda\rho) J_m(\lambda\rho') \cos \lambda(z-z') d\lambda \quad (\rho > \rho'; \rho \leftrightarrow \rho') \quad (3.2.39)$$

$$= \frac{1}{4\pi} \int_0^\infty J_0(\lambda|\rho - \rho'|) e^{-\lambda|z-z'|} d\lambda \quad (3.2.40)$$

$$= \sum_{m=0}^{\infty} \frac{\epsilon_m}{4\pi} \cos m(\varphi-\varphi') \int_0^\infty J_m(\lambda\rho) J_m(\lambda\rho') e^{-\lambda|z-z'|} d\lambda$$

For the two dimensional system in which the eigen values are discrete.

$$\frac{\pm i}{4} H_0^{(\epsilon)}(k|\rho - \rho'|) = \frac{\pm i}{4} \sum_{m=0}^{\infty} \epsilon_m \cos m(\varphi - \varphi') H_m^{(\epsilon)}(k\rho) J_m(k\rho') \quad (\rho > \rho'; \rho \leftrightarrow \rho') \quad (3.2.42)$$

c) The cylindrical boundary.

Helmholtz Green

$$\frac{e^{\pm i k |r - r'|}}{4\pi |r - r'|} = \frac{\pm i}{4\pi} \sum_{m=0}^{\infty} \epsilon_m \cos m(\varphi - \varphi') \times \int_0^{\infty} H_m^{(\epsilon)}(\sqrt{k^2 - \lambda^2} \rho) J_m(\sqrt{k^2 - \lambda^2} \rho') \cos \lambda(z - z') d\lambda \quad (\rho > \rho'; \rho \leftrightarrow \rho') \quad (5.3.17)$$

The the discontinuity at $\rho = \rho'$

The reciprocal forms

$$\sum_{m=0}^{\infty} \cos m(\varphi - \varphi') \int_0^{\infty} F_m(\lambda) H_m^{(\epsilon)}(\sqrt{k^2 - \lambda^2} \rho) \times H_m^{(\epsilon)}(\sqrt{k^2 - \lambda^2} \rho') \cos \lambda(z - z') d\lambda \quad (5.3.18)$$

$$\sum_{m=0}^{\infty} \cos m(\varphi - \varphi') \int_0^{\infty} F_m(\lambda) J_m(\sqrt{k^2 - \lambda^2} \rho) \times J_m(\sqrt{k^2 - \lambda^2} \rho') \cos \lambda(z - z') d\lambda \quad (5.3.19)$$

They form the solutions for the simultaneous equations by setting some $F_m(\lambda)$ functions that are guaranteed of the convergency of summation and integration.

$$A \frac{\partial G(\mathbf{r}, \mathbf{r}')}{\partial \rho} + B G(\mathbf{r}, \mathbf{r}') = 0 \quad (\rho' = a) \quad (5.3.20)$$

For the outer region, $\rho > \rho'$ the Green function is

$$G(\mathbf{r}, \mathbf{r}') = \frac{i}{4\pi} \sum_{m=0}^{\infty} \epsilon_m \cos m(\varphi - \varphi') \int_0^{\infty} \left\{ J_m(\sqrt{k^2 - \lambda^2} \rho') - \frac{A\sqrt{k^2 - \lambda^2} J_m'(\sqrt{k^2 - \lambda^2} a) + B J_m(\sqrt{k^2 - \lambda^2} a)}{A\sqrt{k^2 - \lambda^2} H_m^{(1)}(\sqrt{k^2 - \lambda^2} a) + B H_m^{(1)}(\sqrt{k^2 - \lambda^2} a)} \right\} H_m^{(1)}(\sqrt{k^2 - \lambda^2} \rho) \cos \lambda(z - z') d\lambda \quad (\rho > \rho'; \rho \leftrightarrow \rho') \quad (5.3.21)$$

Direct differentiation $J_m'(\sqrt{k^2 - \lambda^2} a)$

$$(5.3.21) \quad G^{\infty}(\mathbf{r} - \mathbf{r}') + g(\mathbf{r}, \mathbf{r}')$$

Green (5.3.20)

For the inner $\rho' > \rho$, $H_m(\rho') J_m(\rho)$ in the (5.3.17)

$$G(\mathbf{r}, \mathbf{r}') = \frac{i}{4\pi} \sum_{m=0}^{\infty} \epsilon_m \cos m(\varphi - \varphi') \int_0^{\infty} \left\{ H_m^{(1)}(\sqrt{k^2 - \lambda^2} \rho') - \frac{A\sqrt{k^2 - \lambda^2} H_m^{(1)}(\sqrt{k^2 - \lambda^2} a) + B H_m^{(1)}(\sqrt{k^2 - \lambda^2} a)}{A\sqrt{k^2 - \lambda^2} J_m'(\sqrt{k^2 - \lambda^2} a) + B J_m(\sqrt{k^2 - \lambda^2} a)} \right\} J_m(\sqrt{k^2 - \lambda^2} \rho) \cos \lambda(z - z') d\lambda \quad (\rho' > \rho; \rho' \leftrightarrow \rho) \quad (5.3.22)$$

For the Laplace equation, We have the following forms of the solutions of the simultaneous equations.

$$\sum_{m=0}^{\infty} \cos m(\varphi - \varphi') \int_0^{\infty} F_m(\lambda) K_m(\lambda \rho) K_m(\lambda \rho') \cos \lambda(z - z') d\lambda \sum_{m=0}^{\infty} \cos m(\varphi - \varphi') \int_0^{\infty} F_m(\lambda) I_m(\lambda \rho) I_m(\lambda \rho') \cos \lambda(z - z') d\lambda \int_0^{\infty} F(\lambda) I_0(\lambda |\rho - \rho'|) \cos \lambda(z - z') d\lambda \quad (5.3.26)$$

By utilizing these functions, we can have the Green functions that satisfies the circular cylindrical boundary conditions. The form for the outer region is

対象とするときは

$$G(\mathbf{r}, \mathbf{r}') = \sum_{m=0}^{\infty} \frac{\epsilon_m}{2\pi^2} \cos m(\varphi - \varphi') \int_0^{\infty} \left\{ I_m(\lambda \rho') - \frac{A\lambda I_m'(\lambda a) + B I_m(\lambda a)}{A\lambda K_m'(\lambda a) + B K_m(\lambda a)} K_m(\lambda \rho') \right\} K_m(\lambda \rho) \cos \lambda(z - z') d\lambda \quad (\rho > \rho'; \rho \leftrightarrow \rho') \quad (5.3.27)$$

For the inner region is

$$G(\mathbf{r}, \mathbf{r}') = \sum_{m=0}^{\infty} \frac{\epsilon_m}{2\pi^2} \cos m(\varphi - \varphi') \int_0^{\infty} \left\{ K_m(\lambda \rho') - \frac{A\lambda K_m'(\lambda a) + B K_m(\lambda a)}{A\lambda I_m'(\lambda a) + B I_m(\lambda a)} I_m(\lambda \rho') \right\} I_m(\lambda \rho) \cos \lambda(z - z') d\lambda \quad (\rho' > \rho; \rho' \leftrightarrow \rho) \quad (5.3.28)$$

APPENDIX.2

Putting the sum of the rotational factors by

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

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

$$z_j' = z_0^j + kL \quad \text{---(A2)}$$

$$\phi_j' = \phi_0^j + k2\pi \quad \text{---(A3)}$$

Using these relations and $\cos(x-y) = \cos x \cos y + \sin x \sin y$

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

Since

$$\sum_{k=-\infty} e^{i\lambda kL} = \sum_{k=-\infty} e^{ik[\lambda L - 2n\pi]} = 2\pi \delta(\lambda L - 2n\pi) \quad \text{---(A5)}$$

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

$$\sum_{k=-\infty} e^{i\lambda kL} = 2\pi/L \sum_{n=-\infty} \delta(\lambda - 2n\pi/L) \quad \text{---(A6)}$$

Thus,

$$S = \sum_{j=1} \cos(m(\phi - \phi_0^j)) \cos(\lambda(z - z_0^j)) = 2\pi/L \sum_{n=-\infty} \delta(\lambda - 2n\pi/L) \quad \text{---(A7)}$$