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STATISTICAL DESCRIPTION OF AN ENSEMBLE OF DNA MOLECULES

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A statistical description of an ensemble of DNA molecules in an electrolyte solution has been developed. Radial distribution functions for all the components of the system and a single-particle distribution function for the elements of a molecule and its orientation elastic moduli have been calculated on this basis.

Among the biological materials characterized by the liquid-crystalline order [1], ensembles of DNA molecules are of primary importance [2, 3]. In the last sixty years, its has been established by investigating a number of important biological objects such as chromosomes, certain viruses and bacteriophages, and spermatozoon nuclei that they represent ordered phases formed of DNA molecules which are both in linear and annular closed forms and stay in certain solvents. These phases found both *in vivo* and *in vitro* possess a liquid-crystalline structure [1–3].

We will assume that DNA molecules whose elements carry a negative charge are in the solution of a strong NaCl-type electrolyte. Therefore, their statistical description is complicated, among other things, by the presence of a long-range Coulomb interaction. The solution of such a problem will be subdivided into two steps. First we consider the problem of isotropic Coulomb interaction between all the elements of the system and thereafter use these results in allowing for the nonisotropic interaction between the elements of a DNA molecule.

If the influence of the solvent is allowed for only by the dielectric constant ξ, the system will be three-component even in this case and its description will require six binary distribution functions. Let there be N_1 positive ions carrying a charge e, N_2 ions having a charge $-e$, and N_3 ions having a charge pe (p is the integer) in the system. The total number of particles is equal to $N = N_1 + N_2 + N_3$, and they occupy volume V. The condition of electroneutrality of such a system has the form

$$N_1 e - N_2 e + N_3 pe = 0 , \tag{1}$$

or

$$n_1 - n_2 + n_3 p = 0 , \tag{2}$$

where $n_\mu = N_\mu/N$, $\mu = 1$, 2, and 3. Since we have

$$n_1 + n_2 + n_3 = 1 , \tag{3}$$

one parameter n_μ remains free.

In any method of closing a chain of equations for partial distribution functions, the binary functions are determined by the expressions

$$g_{\mu\nu} = \exp\left[-\beta\left(\Phi^s_{\mu\nu} + \Phi^c_{\mu\nu} + \omega_{\mu\nu}\right)\right] , \tag{4}$$

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where $\beta = 1/(k_B T)$ and Φ^s, Φ^c, and ω are the short-range, Coulomb, and average-force potentials respectively. It follows from the last expression that the correct behavior of the binary functions at infinity can be ensured and consequently the thermodynamic quantities themselves, by which they are determined, can exist only in the case where the sum of the Coulomb potential and the average-force potential will be short-range. We denote it by $\Omega = \Phi^c + \omega$. For functions of this kind, we have obtained earlier [4] the following system of nonlinear integral equations:

$$\Omega_{\mu\nu}(1,2) + \frac{1}{2}\sum_{\lambda} \rho_\lambda \int d3 \left[\Phi^c_{\mu\lambda}(1,3)\,\Omega_{\nu\lambda}(2,3) + \Omega_{\mu\lambda}(1,3)\,\Phi^c_{\nu\lambda}(2,3)\right] =$$

$$= \Phi^c_{\mu\nu}(1,2) - \sum_{\lambda} \rho_\lambda \int d3\, h_{\mu\lambda}(1,3)\, h_{\nu\lambda}(2,3)\,. \tag{5}$$

Here we have

$$\rho_\lambda = n_\lambda\, \rho = n_\lambda N/V\,; \tag{6}$$

$$h_{\mu\lambda} = \exp\left[-\left(\Phi^s_{\mu\lambda} + \Omega_{\mu\lambda}\right)\right] - 1\,; \tag{7}$$

all the potentials are dimensionless (due to the multiplication of dimensional quantities by β); the sorts of particles are denoted by the Greek letters and their coordinates are denoted by the figures.

Equations (5) contain the Coulomb potential

$$\Phi^c_{\mu\nu}(r) = \frac{\beta e_\mu e_\nu}{\varepsilon r}\,, \tag{8}$$

leading to a divergence of integrals because of its too slow decrease at large distances (integration in (5) is over the entire space) if the equations are used in reduced form. This problem is characteristic of systems with Coulomb interaction and is eliminated in different manners.

In this case, we use the fact that all the integrals in (5) are the convolutions of two functions. This enables us to apply the Fourier transformation to both sides of (5) to obtain a system of linear algebraic equations for the Fourier transforms of the quantities Ω on the left-hand side of the system of integral equations in question. Determining the Fourier transformation by the relation

$$\tilde{\Omega}(k) = \int d^3 r\, \Omega(r) \exp(i\mathbf{k}\cdot\mathbf{r})\,, \tag{9}$$

we obtain

$$\tilde{\Omega}_{\mu\nu} + \frac{1}{2}\sum_{\lambda} \rho_\lambda \left(\tilde{\Phi}^c_{\mu\lambda}\,\tilde{\Omega}_{\nu\lambda} + \tilde{\Phi}^c_{\nu\lambda}\,\tilde{\Omega}_{\mu\lambda}\right) = \tilde{\Phi}^c_{\mu\nu} - \tilde{B}_{\mu\nu}\,, \tag{10}$$

where the notation

$$\tilde{B}_{\mu\nu} = \sum_{\lambda} \rho_\lambda \tilde{h}_{\mu\lambda}\, \tilde{h}_{\nu\lambda} \tag{11}$$

is introduced to shorten the notation and the dependence of the Fourier transforms on k is not indicated (since all the functions in (5) are dependent only on the corresponding distances, their Fourier transforms are functions of the modulus of the vector $\mathbf{k}$).

All the quantities in (10) are symmetric about the rearrangement of the Greek subscripts; therefore, it is only $\tilde{\Omega}_{11}$, $\tilde{\Omega}_{12}$, $\tilde{\Omega}_{13}$, $\tilde{\Omega}_{22}$, $\tilde{\Omega}_{23}$, and $\tilde{\Omega}_{33}$ that will be independent. Then the system of equations (10) in expanded form will appear as

$$(1+\rho_1\tilde{\Phi})\,\tilde{\Omega}_{11}-\rho_2\tilde{\Phi}\tilde{\Omega}_{12}+\rho_3 p\tilde{\Phi}\tilde{\Omega}_{13}=\tilde{\Phi}-\tilde{B}_{11}\,, \tag{12}$$

$$-\frac{1}{2}\rho_1\tilde{\Phi}\tilde{\Omega}_{11}+\left(1+\frac{\rho_1+\rho_2}{2}\tilde{\Phi}\right)\tilde{\Omega}_{12}-\frac{1}{2}\rho_3 p\tilde{\Phi}\tilde{\Omega}_{13}-\frac{1}{2}\rho_2\tilde{\Phi}\tilde{\Omega}_{22}+\frac{1}{2}\rho_3 p\tilde{\Phi}\tilde{\Omega}_{23}=-\tilde{\Phi}-\tilde{B}_{12}\,, \tag{13}$$

$$\frac{1}{2}\rho_1 p\tilde{\Phi}\tilde{\Omega}_{11}-\frac{1}{2}\rho_2 p\tilde{\Phi}\tilde{\Omega}_{12}+\left(1+\frac{\rho_1+\rho_3 p^2}{2}\tilde{\Phi}\right)\tilde{\Omega}_{13}-\frac{1}{2}\rho_2\tilde{\Phi}\tilde{\Omega}_{23}+\frac{1}{2}\rho_3 p\tilde{\Phi}\tilde{\Omega}_{33}=p\tilde{\Phi}-\tilde{B}_{13}\,, \tag{14}$$

$$-\rho_1\tilde{\Phi}\tilde{\Omega}_{12}+(1+\rho_2\tilde{\Phi})\,\tilde{\Omega}_{22}-\rho_3 p\tilde{\Phi}\tilde{\Omega}_{23}=\tilde{\Phi}-\tilde{B}_{22}\,, \tag{15}$$

$$\frac{1}{2}\rho_1 p\tilde{\Phi}\tilde{\Omega}_{12}-\frac{1}{2}\rho_1\tilde{\Phi}\tilde{\Omega}_{13}+\left(1+\frac{\rho_2+\rho_3 p^2}{2}\tilde{\Phi}\right)\tilde{\Omega}_{23}-\frac{1}{2}\rho_3 p\tilde{\Phi}\tilde{\Omega}_{33}=-p\tilde{\Phi}-\tilde{B}_{23}\,, \tag{16}$$

$$\rho_1 p\tilde{\Phi}\tilde{\Omega}_{13}-\rho_2 p\tilde{\Phi}\tilde{\Omega}_{23}+(1+\rho_3 p^2\tilde{\Phi})\,\tilde{\Omega}_{33}=p^2\tilde{\Phi}-\tilde{B}_{33}\,. \tag{17}$$

Here the Fourier transform of the Coulomb interaction between oppositely charged monovalent ions is denoted by $\tilde{\Phi}$.

Further computations are carried out for the case $p = -2$. The determinant of system (12)–(17) has the form

$$\Delta=\left(1+\frac{1+3n}{2}\rho\tilde{\Phi}\right)\left\{1+\frac{3}{2}(1+3n)\,\rho\tilde{\Phi}+\frac{1}{2}[1+n\,(8+11n)]\,(\rho\tilde{\Phi})^2+\frac{1}{2}n\,(1+n)\,(1+5n)\,(\rho\tilde{\Phi})^3\right\}, \tag{18}$$

where it is taken into account that, because of conditions (2) and (3), we have

$$n_1=\frac{1}{2}(1+n)\,,\quad n_2=\frac{1}{2}(1-3n)\,, \tag{19}$$

and n_3 is denoted by n.

The solution of the above system of linear equations is very cumbersome; therefore, we write it in compact form:

$$\tilde{\Omega}_{\mu\nu}=\left[-\tilde{B}_{\mu\nu}+\tilde{a}_{\mu\nu}\,\rho\tilde{\Phi}+\tilde{b}_{\mu\nu}\,(\rho\tilde{\Phi})^2+\tilde{c}_{\mu\nu}\,(\rho\tilde{\Phi})^3+\tilde{d}_{\mu\nu}\,(\rho\tilde{\Phi})^4\right]/\Delta\,, \tag{20}$$

where $\tilde{\alpha}_{\mu\nu}$, $\tilde{b}_{\mu\nu}$, $\tilde{c}_{\mu\nu}$, and $\tilde{d}_{\mu\nu}$ represent the linear combinations of $\tilde{B}_{11}$, $\tilde{B}_{12}$, $\tilde{B}_{13}$, $\tilde{B}_{22}$, $\tilde{B}_{23}$, and $\tilde{B}_{33}$ with coefficients determined by the quantity n, rather than give it completely.

Next we must perform the inverse Fourier transformation

$$\Omega_{\mu\nu}(r)=\frac{1}{(2\pi)^3}\int d^3k\,\tilde{\Omega}_{\mu\nu}(k)\exp(-i\mathbf{k}\cdot\mathbf{r})\,, \tag{21}$$

whose realizability is determined by the analytical properties of the integrand, mainly by the behavior of the functions $\tilde{\Omega}(k)$ determined by expression (20) for $k \to \infty$. In explicit form, the dependence of these functions on k is found in terms of the Fourier transform of the Coulomb potential

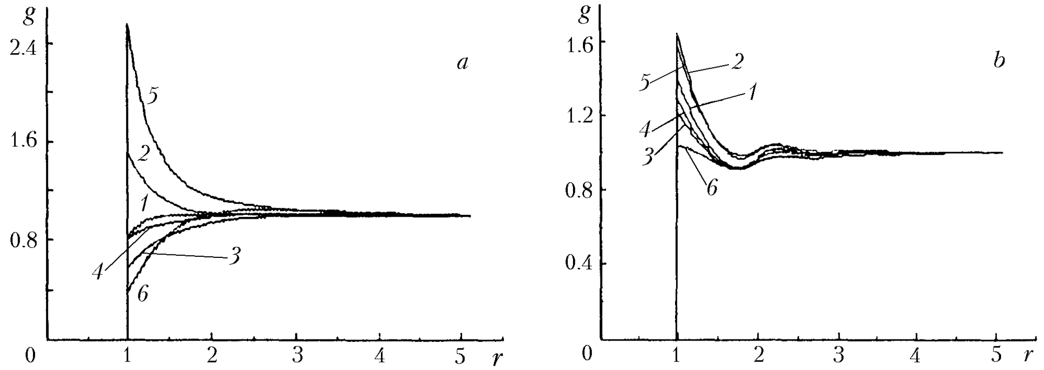

Fig. 1. Radial functions for low ($\rho = 0.1$) (a) and high ($\rho = 0.6$) (b) densities: 1) g_{11}, 2) g_{12}, 3) g_{13}, 4) g_{22}, 5) g_{23}, and 6) g_{33}.

$$\rho\tilde{\Phi}(k) = \frac{4\pi\beta\rho e^2}{\varepsilon k^2} = \frac{\kappa^2}{k^2}, \tag{22}$$

where $k = \sqrt{4\pi\beta\rho e^2/\varepsilon}$ is the Debye parameter. The substitution of (22) into (20) leads to the explicit dependence of the $\tilde{\Omega}$ functions on k:

$$\tilde{\Omega}_{\mu\nu}(k) = \frac{-\tilde{B}_{\mu\nu}k^8 + \tilde{a}_{\mu\nu}\kappa^2k^6 + \tilde{b}_{\mu\nu}\kappa^4k^4 + \tilde{c}_{\mu\nu}\kappa^6k^2 + \tilde{d}_{\mu\nu}\kappa^8}{(k^2 + a\kappa^2)(k^6 + 3a\kappa^2k^4 + b\kappa^4k^2 + c\kappa^6)}, \tag{23}$$

where

$$a = (1 + 3n)/2\,; \quad b = [1 + n(8 + 11n)]/2\,; \quad c = n(1 + n)(1 + 5n)/2\,. \tag{24}$$

Formally, expression (23) appears as the ratio of the polynomials of the eighth degree in k, but the coefficients of the numerator are functions of this variable and the most leading of them — $\tilde{B}_{\mu\nu}$ — may act as the Fourier transform of the Coulomb potential (22) in the most unfavorable case; therefore, the degree of the polynomial in the numerator is less than the degree of the denominator at least by two, which ensures a decrease in $\tilde{\Omega}(k)$ at infinity.

The value of the integral (21) is determined by the zeros of the denominator of (23). The investigations carried out have shown that the roots of this denominator are imaginary for all the permissible values of n. Closing the integration contour in the upper half-plane, for the integral (21) we obtain

$$\Omega_{\mu\nu}(r) = \frac{1}{4\pi^2 ir}\int_{-\infty}^{\infty} dk k\tilde{\Omega}_{\mu\nu}(k)\exp(ikr) = \frac{1}{2\pi r}\sum_{n=1}^{4}\lim_{k\to ik_n} k\tilde{\Omega}_{\mu\nu}(k)\exp(ikr)(k - ik_n)\,, \tag{25}$$

where k_n are the moduli of the roots of the denominator of (23).

It follows from dependence (25) that all the residues of the integrand are in proportion to $\exp(-k_n r)$; therefore, the inverse transforms of the average-force potentials will contain factors $\exp(-k_n r)/r$, because of which the correlation functions (7) will turn out to be short-range: after the transformations carried out, the Coulomb interaction appearing in (5) has turned out to be represented in shielded form.

The actual determination of the values of $\Omega(r)$ involves the necessity of solving a system of nonlinear equations. Such a system is expression (25), since all the coefficients of the numerator in (23) are functions of Ω and can be found only numerically. Figure 1 gives the calculated radial functions with a solid-sphere potential as a short-range part. When the densities are low, their behavior resembles Debye behavior, but when the density is high, they become liquid-like, which points to the occurrence of an efficient attraction between charged objects of all types under such conditions.

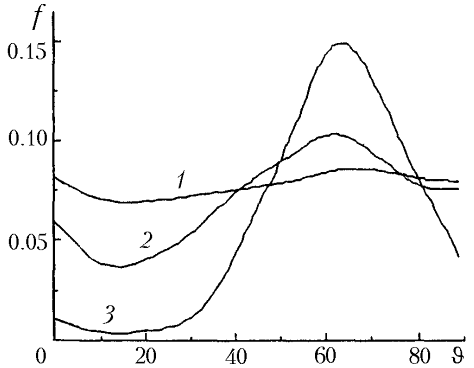

Fig. 2. Single-particle distribution function for different densities: 1) $\rho = 0.1$; 2) 0.2; 3) 0.3.

It is problematic to allow for the anisotropic short-range interaction at the level of binary functions because of the too large number of variables determining the states of particles. The manner in which Eqs. (5) should be treated is unclear, since all the transformations described above are inapplicable in this case. Therefore, we restrict our consideration to single-particle functions describing the behavior of the elements of a DNA molecule in the ionic environment presented above. An equation for the single-particle function has the form [5]

$$\varphi(1) = -A \int d2 \exp[-\varphi(2)] \left\{ -\Phi^{s}(1, 2) - \Omega(1, 2)] - 1 \right\}. \tag{26}$$

Here φ is the average-force potential determining the single-particle distribution function

$$f(1) = A \exp[-\varphi(1)]; \tag{27}$$

Ω is the binary average-force potential which is the solution of the system of equations considered above, and Φ^{s} is the noncentral short-range potential of direct interaction of the elements. As the latter, we have selected the Gay–Berne potential [6] used in liquid-crystalline models. The nonlinear integral equation (26) has been solved numerically. Figure 2 gives the dependences (calculated for different densities) of the single-particle distribution function on the angle between a certain fixed direction and the long axis of an ellipsoid of revolution modeling molecular elements. It is seen in the figure that in the case of a low density a nearly uniform distribution is transformed toward increasing values of this angle with growth in the density.

The single-particle distribution function found enables us to calculate the orientation elastic moduli, i.e., the Franck moduli of a DNA molecule, considering it from the viewpoint of a nematic liquid crystal. For this purpose we use results of the statistical theory developed earlier and computational formulas [7] for the Franck moduli.

The Franck moduli are determined by the expressions

$$K_{11} = Ls^2 \left[\frac{1-\chi}{2\chi} (\langle \cos^2 \vartheta \rangle - \langle \cos^4 \vartheta \rangle) + \frac{3}{4} (\langle \cos^2 \vartheta \rangle - 2 \langle \cos^4 \vartheta \rangle + \langle \cos^6 \vartheta \rangle) \right] (\langle \cos^2 \vartheta \rangle - \langle \cos^4 \vartheta \rangle), \tag{28}$$

$$K_{22} = Ls^2 \left[\frac{1-\chi}{\chi} (\langle \cos^2 \vartheta \rangle - \langle \cos^4 \vartheta \rangle) + \frac{1}{4} (\langle \cos^2 \vartheta \rangle - 2 \langle \cos^4 \vartheta \rangle + \langle \cos^6 \vartheta \rangle) \right] (\langle \cos^2 \vartheta \rangle - \langle \cos^4 \vartheta \rangle), \tag{29}$$

$$K_{33} = Ls^2 \left[\frac{1-\chi}{2\chi} (\langle \cos^2 \vartheta \rangle - \langle \cos^4 \vartheta \rangle) + (\langle \cos^4 \vartheta \rangle - \langle \cos^6 \vartheta \rangle) \right] (\langle \cos^2 \vartheta \rangle - \langle \cos^4 \vartheta \rangle), \tag{30}$$

$$L = 3\pi M b^2 \rho^2 \sigma_0^3 \chi^3 \left(1 + \frac{3}{14} \chi^2 \right) \Big/ \beta (1-\chi)^2, \tag{31}$$

$$b = 4\pi\rho\sigma_0^3 m\chi^2 \left(1 + \frac{3}{14}\chi^2\right) / 3\,(1 - \chi)\,, \tag{32}$$

$$s = \langle P_2 \rangle = \int\limits_{\Omega} d\Omega P_2\,(\vartheta)\, f\,(\Omega)\,, \tag{33}$$

$$M = -\int\limits_0^{\infty} y^4 c\,(y)\, dy\,, \tag{34}$$

$$m = -\int\limits_0^{\infty} y^2 c\,(y)\, dy\,, \tag{35}$$

where $c(y)$ is the direct correlation function for the system of spherical particles and σ_0 and χ are the parameters of the Gay–Berne potential [6]. The angle brackets mean averaging using the single-particle distribution function $f(\vartheta)$ obtained in solving Eq. (26). Introducing the average value

$$K = \frac{1}{3}\,(K_{11} + K_{22} + K_{33})\,, \tag{36}$$

we can determine the dimensionless elastic moduli

$$k_{11} = \frac{K_{11}}{K}\,, \quad k_{22} = \frac{K_{22}}{K}\,, \quad k_{33} = \frac{K_{33}}{K}\,. \tag{37}$$

Expressions (34) and (35) involve the direct correlation function which can be found using the Ornstein–Zernicke equations if we know the total correlation functions (7). For a multicomponent system, it becomes the system of equations

$$h_{\mu\nu}\,(r) = c_{\mu\nu}\,(r) + \sum_{\lambda} \rho_\lambda \int d^3t c_{\mu\lambda}\,(t)\, h_{\nu\lambda}\,(|\mathbf{r} - \mathbf{t}|)\,. \tag{38}$$

Since the integrals are convolutions here, we use a technique based on the Fourier transformation. We obtain the following system of linear equations for the Fourier transforms:

$$\tilde{h}_{\mu\nu} = \tilde{c}_{\mu\nu} + \sum_{\lambda} \rho_\lambda \tilde{c}_{\mu\lambda} \tilde{h}_{\mu\lambda}\,, \tag{39}$$

or, in detailed representation,

$$\tilde{h}_{11} = \tilde{c}_{11}\,(1 + \rho_1 \tilde{h}_{11}) + \rho_2 \tilde{c}_{12} \tilde{h}_{12} + \rho_3 \tilde{c}_{13} \tilde{h}_{13}\,, \tag{40}$$

$$\tilde{h}_{12} = \tilde{c}_{11} \rho_1 \tilde{h}_{12} + \tilde{c}_{12}\,(1 + \rho_2 \tilde{h}_{22}) + \rho_3 \tilde{c}_{13} \tilde{h}_{13}\,, \tag{41}$$

$$\tilde{h}_{13} = \tilde{c}_{11} \rho_1 \tilde{h}_{13} + \rho_2 \tilde{c}_{12} \tilde{h}_{23} + \tilde{c}_{13}\,(1 + \rho_3 \tilde{h}_{33})\,, \tag{42}$$

$$\tilde{h}_{22} = \tilde{c}_{12} \rho_1 \tilde{h}_{12} + \tilde{c}_{22}\,(1 + \rho_2 \tilde{h}_{22}) + \rho_3 \tilde{c}_{23} \tilde{h}_{23}\,, \tag{43}$$

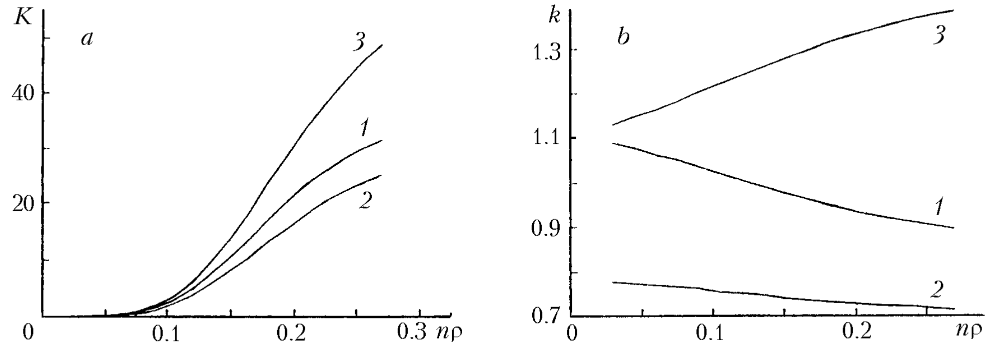

Fig. 3. Orientation elastic moduli (a) [1) K_{11}, 2) K_{22}, and 3) K_{33}] and their dimensionless values (b) [1) k_{11}, 2) k_{22}, and 3) k_{33}].

$$\tilde{h}_{23} = \tilde{c}_{12}\rho_1\tilde{h}_{13} + \rho_2\tilde{c}_{22}\tilde{h}_{23} + \tilde{c}_{23}\,(1 + \rho_3\tilde{h}_{33})\,, \tag{44}$$

$$\tilde{h}_{33} = \tilde{c}_{13}\rho_1\tilde{h}_{13} + \rho_2\tilde{c}_{23}\tilde{h}_{23} + \tilde{c}_{33}\,(1 + \rho_3\tilde{h}_{33})\,. \tag{45}$$

In this case $\tilde{c}_{33}$, i.e., the Fourier transform of the direct correlation function of the elements of a DNA molecule, is of interest:

$$\begin{aligned}
\tilde{c}_{33} = \frac{1}{\Delta}\Big\{&(1 + \rho_2\tilde{h}_{22})\,[2\rho_1\rho_2\tilde{h}_{12}\tilde{h}_{13}\tilde{h}_{23} - \rho_2\tilde{h}_{23}^2\,(1 + \rho_1\tilde{h}_{11}) - \rho_1\tilde{h}_{13}^2\,(1 + \rho_2\tilde{h}_{22}) +\\
&+ \tilde{h}_{33}\,(1 + \rho_1\tilde{h}_{11} + \rho_2\,(\tilde{h}_{22} - \rho_1\,(\tilde{h}_{12}^2 - \tilde{h}_{11}\tilde{h}_{22})))] +\\
&+ \rho_2^2\tilde{h}_{33}\,(\tilde{h}_{33} - \rho_2\,(\tilde{h}_{23}^2 - \tilde{h}_{22}\tilde{h}_{33}))\,[\tilde{h}_{33}\,(1 + \rho_1\tilde{h}_{11} + \rho_2\,(\tilde{h}_{22} - \rho_1\,(\tilde{h}_{22}^2 - \tilde{h}_{11}\tilde{h}_{22}))) +\\
&+ \tilde{h}_{13}\,\rho_2\tilde{h}_{23}\,(\rho_1\,(\tilde{h}_{12} - \tilde{h}_{11}) - 1) + \rho_1\tilde{h}_{13}\,(\rho_2\,(\tilde{h}_{12} - \tilde{h}_{22}) - 1)] +\\
&+ \rho_3\,[2\tilde{h}_{33}^2\,(1 + \rho_2\tilde{h}_{22})\,(1 + \rho_1\tilde{h}_{11} + \rho_2\,(\tilde{h}_{22} - \rho_1\,(\tilde{h}_{12}^2 - \tilde{h}_{11}\tilde{h}_{22}))) +\\
&+ \rho_2\tilde{h}_{13}\tilde{h}_{23}\,(\rho_2\tilde{h}_{23}^2\,(1 + \rho_1\,(\tilde{h}_{11} - 2\tilde{h}_{12})) + 2\rho_1\tilde{h}_{13}\tilde{h}_{23}\,(1 - \rho_2\tilde{h}_{22}) - \rho_1\tilde{h}_{13}^2\,(1 + \rho_2\tilde{h}_{22})) +\\
&+ \tilde{h}_{33}\,\rho_1\tilde{h}_{13}^2\,(\rho_2\,(\tilde{h}_{12} - \tilde{h}_{22}) - 2)\,(1 + \rho_2\tilde{h}_{22}) - \rho_2\tilde{h}_{13}\tilde{h}_{23}\,(1 + \rho_1\,(\tilde{h}_{11} - 3\tilde{h}_{12}))\,(1 + \rho_2\tilde{h}_{22}) -\\
&- \rho_2\tilde{h}_{23}^2\,(2\,(1 + \rho_1\tilde{h}_{11} + \rho_2\tilde{h}_{22} + \rho_1\rho_2\tilde{h}_{11}\tilde{h}_{22}) - \rho_1\rho_2\tilde{h}_{12}^2)]\Big\}\,,
\end{aligned} \tag{46}$$

where

$$\begin{aligned}
\Delta = {}&(1 + n\rho\tilde{h}_{33})\,[1 + \rho_2\tilde{h}_{22} + n\rho\,(\tilde{h}_{33} - \rho_2\,(\tilde{h}_{23}^2 - \tilde{h}_{22}\tilde{h}_{33}))] \times\\
&\times \Big\{1 + \rho_2\,(\tilde{h}_{22} - \rho_1\tilde{h}_{12}^2) + n\rho\,(\tilde{h}_{33} + \rho_1\rho_2\tilde{h}_{13}\,(\tilde{h}_{12}\,(\tilde{h}_{13} + \tilde{h}_{23}) -\\
&- \tilde{h}_{13}\tilde{h}_{22}) + \rho_2\tilde{h}_{33}\,(\tilde{h}_{22} - \rho_1\tilde{h}_{12}^2) - \tilde{h}_{13}\,(\rho_1\tilde{h}_{13} + \rho_2\tilde{h}_{23})) +\\
&+ \rho_1\tilde{h}_{11}\,(1 + \rho_2\tilde{h}_{22} + n\rho\,(\tilde{h}_{33} - \rho_2\,(\tilde{h}_{13}\tilde{h}_{23} - \tilde{h}_{22}\tilde{h}_{33})))\Big\}\,.
\end{aligned} \tag{47}$$

Applying the inverse Fourier transformation to (46) with account for (47), we obtain the direct correlation function in direct space, using which we find the values of (34) and (35) and determine the orientation elastic moduli from formulas (28)–(33), (36), and (37). The calculated dependences on density at room temperature are presented in Fig. 3 (K and ρ are in the units of $\sigma_0 = 3.5$ Å and $n = 0.3$). It is seen that the rate of change in the Franck moduli becomes somewhat slower with growth in the density. All the results presented in the figures have been obtained for the first time.

NOTATION

A, normalization constant; a, b, and c, coefficients of the determinant of the system of linear algebraic equations; $c_{\mu\nu}$, direct correlation function for particles of the μ and ν sort; $\tilde{B}_{\mu\nu}$, quadratic forms of the Fourier transforms of total correlation functions; $\tilde{a}_{\mu\nu}$, $\tilde{b}_{\mu\nu}$, $\tilde{c}_{\mu\nu}$, and $\tilde{d}_{\mu\nu}$, linear combinations of $\tilde{B}_{\mu\nu}$; e, ionic charge, C; f, single-particle distribution function; $g_{\mu\nu}$, radial distribution function of the μ and ν sort; $h_{\mu\nu}$, total correlation function of the μ and ν sort; i, imaginary unit; $\mathbf{k}$, wave vector; k, wave-vector modulus; k_B, Boltzmann constant; K_{11}, K_{22}, and K_{33}, Franck moduli, pN; k_{11}, k_{22}, and k_{33}, dimensionless Franck moduli; m and M, second and fourth moduli of the direct correlation function; N_μ, number of particles of the μ sort; n_μ, concentration of particles of the μ sort; N, number of particles; p, charge multiplicity; P_2, second Legendre polynomial; r, distance between particles, m; s, order parameter; T, absolute temperature, K; V, volume, m^3; y_1, y_2, and y_3, roots of the cubic equation; $|y_1|$, $|y_2|$, and $|y_3|$, moduli of the roots of the cubic equation; β, inverse energy, 1/J; Δ, determinant of the system of linear equations; ε, dielectric constant; ϑ, angle, rad; κ, Debye parameter, m^{-1}; φ, single-particle average-force potential, J; ω, binary average-force potential, J; Ω, dimensionless average-force potential; ρ, average density of the medium, m^{-3}; ρ_μ, density of a component of the μ sort, m^{-3}; Φ^s, short-range interaction potential, J; Φ^c, Coulomb-interaction potential, J; $\tilde{\Omega}$, Fourier transform; σ_0, cross diameter of a molecule, m; χ, parameter of the Gay–Berne potential.

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