Interaction of macromolecules injected into a liquid crystal

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(Submitted 25 January 1978)
Zh. Eksp. Teor. Fiz. **25**, 361–367 (July 1978)

This article is concerned with the problem of the interaction with each other of foreign molecules injected into a liquid-crystal medium. It is very probable that such interactions play an important role in biochemical reactions that occur in biological systems. An injected molecule produces in the liquid-crystal medium distortions whose dimensions considerably exceed its own dimensions; and another injected molecule, if it enters the distorted region, will interact effectively with the first. Nematic and smectic liquid crystals are considered. Expressions are obtained for the asymptotic value of the interaction energy in the limit of large distances between the injected molecules. In the large-distance limit, the interaction energy decreases according to a power law. For typical biological macromolecules, with distances of hundreds of angstroms between them, the energy of interaction through the medium considerably exceeds the van der Waals energy.

PACS numbers: 61.30.Cz, 87.15.Kg

INTRODUCTION

There has now accumulated a quite large body of experimental material indicating that the interaction between molecules of substances dissolved in a liquid—which may under certain conditions exist in the form of a liquid crystal—is strongly dependent on whether the solvent is in the isotropic or in the liquid-crystal phase. Thus in a number of cases[1, 2] a transition of the solvent to the liquid-crystal phase leads to considerable increase of the rates of reaction of the dissolved substances. This circumstance is the more interesting, because it is known that there are biochemical reactions that occur under natural conditions in a phase very reminiscent in its properties of a liquid-crystal phase.[1]

The principal difference of liquid crystals from ordinary isotropic liquids consists, as is well known, of the fact that over a certain temperature range, there are in these substances long-range correlations in the orientations of the molecules. It is therefore natural to suppose that a transition of the solvent to the liquid-crystal phase leads to the appearance of a new form of interaction between molecules injected into such a liquid: through long-range orientational order. Specifically: an injected molecule produces around it a region of distortion of the liquid crystal, which may occupy a volume considerably exceeding the size of this molecule; another molecule, if it is in a state to react somehow to this distortion, will thus effectively interact with the first. Our aim is to construct a phenomenlogical theory of such interaction. Nematic and smectic liquid crystals are considered in this article. Formulas are obtained for the interaction energy of molecules located at sufficiently large distances from each other.

It should be noted that it is quite easy to change, by external actions, the interaction parameters of molecules of a dissolved substance; this opens up, in principle, a possibility for direct test of the theory set forth in this article. The effect of external factors is considered in the example of a liquid crystal located in a constant, uniform external magnetic field.

1. INTERACTION OF MOLECULES INJECTED INTO A NEMATIC LIQUID CRYSTAL

The free energy of a nematic liquid crystal, as is well known,[3, 4] can be written in the form

$$F=\int \{F_0+{}^1/_2[a_1(\operatorname{div}\mathbf{n})^2+a_2(\mathbf{n}\operatorname{rot}\mathbf{n})^2+a_3((\mathbf{n}\nabla)\mathbf{n})^2]\}\,dv. \tag{1}$$

Here $\mathbf{n}(\mathbf{r})$ is the director, which defines the orientation of the molecules; a_1, a_2, and a_3 are temperature-dependent coefficients.

We consider a large[1)] molecule located in the liquid crystal. If we suppose that the interaction energy of each section of the molecule depends on the direction of the director at the place where this section is located, then the total interaction energy can be expressed in the form

$$\mathscr{E}_{int}=\int g(\mathbf{r};\mathbf{n})\,dv, \tag{2}$$

where $g(\mathbf{r};\mathbf{n})$ is interaction-energy density. Since in liquid crystals replacement of $\mathbf{n}$ by $-\mathbf{n}$ changes nothing physically, we may write

$$g(\mathbf{r},\mathbf{n})\equiv g(\mathbf{r};-\mathbf{n}). \tag{3}$$

We consider the case in which the perturbations of the director field caused by the presence of the inhomogeneity of the foreign molecule are sufficiently small. In this case we have

$$\mathbf{n}=\mathbf{n}_0+\mathbf{v}(\mathbf{r}), \tag{4}$$

where $\mathbf{n}_0 \perp \nu(r)$ and $|\nu| \ll 1$. The total free energy, with allowance for interaction with the injected molecule, can be represented in the form

$$F=\int \{F_0+g(\mathbf{r};\mathbf{n}_0)\}\,dv$$
$$+\int {}^1/_2\{[a_1(\operatorname{div}\mathbf{v})^2+a_2(n_0\operatorname{rot}\mathbf{v})^2+a_3((n_0\nabla)\mathbf{v})^2]+\mathbf{b}(\mathbf{r})\mathbf{v}\}\,dv; \tag{5}$$

0038-5646/78/070180-04$02.40

$$\mathbf{b}(\mathbf{r})=\frac{\partial g}{\partial n_x}\mathbf{i}+\frac{\partial g}{\partial n_y}\mathbf{j}+\frac{\partial g}{\partial n_z}\mathbf{k} \quad \text{at} \quad \mathbf{n}=\mathbf{n}_0. \tag{6}$$

It can be shown that when we consider the problem of interaction of molecules at large distances and close to the molecules, the condition $|\boldsymbol{\nu}| \ll 1$ is violated; but if we renormalize $\mathbf{b}(\mathbf{r})$ appropriately, then even for this case it is possible to represent the free energy in the form (5).

We consider an unconstrained molecule. In the zeroth approximation with respect to $\boldsymbol{\nu}$, the variation of $\int g(\mathbf{r};\mathbf{n}_0)dv$ with respect to possible rotations of the molmolecule as a whole must vanish. But rotations of the molecule are equivalent to rotations of $\mathbf{n}_0$. We have

$$\delta\int g(\mathbf{r};\mathbf{n}_0)\,dv=\delta\mathbf{n}_0\int \mathbf{b}(\mathbf{r})\,dv=0. \tag{7}$$

Hence we find that the vector

$$\mathbf{p}=\int \mathbf{b}(\mathbf{r})\,dv \tag{8}$$

is parallel to $\mathbf{n}_0$.

We consider two molecules. Their interaction energy can be represented in the form

$$\mathscr{E}=-2\int \mathbf{b}_2^*(\mathbf{r})\hat{G}(\mathbf{r}-\mathbf{r}')\mathbf{b}_1(\mathbf{r}')\,d\mathbf{r}\,d\mathbf{r}', \tag{9}$$

where $\mathbf{b}_1(\mathbf{r})$ refers to the first molecule, $\mathbf{b}_2(\mathbf{r})$ to the second; $\hat{G}(\mathbf{r}-\mathbf{r}')$ is Green's function. The equation for $\hat{G}_{ij}(\mathbf{r}-\mathbf{r}')$ can be obtained from (5) by setting $\mathbf{b}(\mathbf{r}) =\mathbf{b}_1\,\delta(\mathbf{r}')$ in it and varying with respect to $\delta\boldsymbol{\nu}$.

We transform to the k representation:

$$\mathscr{E}=-\frac{2}{(2\pi)^3}\int \mathbf{b}_2^*(\mathbf{k})\hat{G}(\mathbf{k})\mathbf{b}_1(\mathbf{k})\,d\mathbf{k}, \tag{10}$$

$$\mathbf{b}(\mathbf{k})=\int \mathbf{b}(\mathbf{r})e^{-i\mathbf{k}\mathbf{r}}\,d\mathbf{r}, \quad G_{ij}(\mathbf{k})=\int G_{ij}(\mathbf{r})e^{-i\mathbf{k}\mathbf{r}}\,d\mathbf{r}. \tag{11}$$

In explicit form, on choosing the direction of the x axis along $\mathbf{n}_0$, of the y along $\mathbf{k}$, and of the z along $\mathbf{n}_0 \times\mathbf{k}$, we have

$$G_{yy}(\mathbf{k})=-\frac{1}{(a_1\mathbf{k}_\perp^2+a_3k_\parallel^2)}, \quad G_{zz}(\mathbf{k})=-\frac{1}{(a_2\mathbf{k}_\perp^2+a_3k_\parallel^2)},$$
$$G_{yz}=G_{zy}=G_{xx}=G_{xy}=G_{yx}=G_{xz}=G_{zx}=0. \tag{12}$$

Here $\mathbf{k}=\mathbf{k}_\perp+k_\parallel\mathbf{n}_0$. We can write

$$\mathbf{b}_2^*(\mathbf{k})\hat{G}(\mathbf{k})\mathbf{b}_1(\mathbf{k})=-\frac{(\mathbf{k}_\perp\mathbf{b}_2^*)(\mathbf{k}_\perp\mathbf{b}_1)}{\mathbf{k}_\perp^2(a_1\mathbf{k}_\perp^2+a_3k_\parallel^2)}+\frac{(-1)([\mathbf{n}_0\mathbf{k}_\perp]\mathbf{b}_2^*)([\mathbf{n}_0\mathbf{k}_\perp]\mathbf{b}_1)}{\mathbf{k}_\perp^2(a_2\mathbf{k}_\perp^2+a_3k_\parallel^2)}. \tag{13}$$

In the process of motion of the molecules, the vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ change. We shall assume that conformational transitions are absent. The condition (8) fixes the axis of the molecule around which it might rotate freely. We introduce $\mathbf{b}(\mathbf{r})$ in a system of coordinates attached to the molecule. We denote it, in distinction from the $\mathbf{b}(\mathbf{r})$ of the laboratory system, by $\mathbf{b}'(r)$. We have

$$\mathbf{b}_{1;2}(\mathbf{k})=e^{-i\mathbf{k}\mathbf{R}_{1;2}}\hat{A}(\varphi_{1;2})\mathbf{b}'(\hat{A}(-\varphi_{1;2})\mathbf{k}). \tag{14}$$

Here $\mathbf{R}_{1;2}$ is the radius vector that describes the position of the center of mass of the molecules, and $\hat{A}(\varphi)$ is the operator of rotation of a vector through angle φ about an axis directed along $\mathbf{n}_0$. On subsituting (14) in (13) and then in (10), we get

$$\mathscr{E}=\frac{2}{(2\pi)^3}\int\Big\{\frac{(\mathbf{k}_\perp\hat{A}(\varphi_2)\mathbf{b}_2'^*(\hat{A}(-\varphi_2)\mathbf{k}))(\mathbf{k}_\perp\hat{A}(\varphi_1)\mathbf{b}_1'(\hat{A}(-\varphi_1)\mathbf{k}))}{k_\perp^2(a_1\mathbf{k}_\perp^2+a_3k_\parallel^2)}$$
$$+\frac{([\mathbf{n}_0\mathbf{k}_\perp]\hat{A}(\varphi_2)\mathbf{b}_2'^*(\hat{A}(-\varphi_2)\mathbf{k}))([\mathbf{n}_0\mathbf{k}_\perp]\hat{A}(\varphi_1)\mathbf{b}_1'(\hat{A}(-\varphi_1)\mathbf{k}))}{k_\perp^2(a_2\mathbf{k}_\perp^2+a_3k_\parallel^2)}\Big\}$$
$$\times\exp\{i\mathbf{k}(\mathbf{R}_2-\mathbf{R}_1)\}\,d\mathbf{k}. \tag{15}$$

The component of the vectors $\mathbf{b}'$ along $\mathbf{n}_0$, as was to be expected, makes no contribution to the energy.

We consider the case in which the distance $|\mathbf{R}_2-\mathbf{R}_1|$ between the molecules is much larger than the characteristic dimensions R' of the molecules. We can in principle expand $\mathscr{E}$ as a series in the small parameter $R'/|\mathbf{R}_2-\mathbf{R}_1|$. For this purpose it is most convenient to expand $\mathbf{b}'(\mathbf{k})$, in (15), as a series in powers of k:

$$\mathbf{b}'(\mathbf{k})=\mathbf{b}_0+i\hat{p}\mathbf{k}+O(\mathbf{k}^2), \tag{16}$$

where $\hat{p}$ is a tensor with components

$$p_{ij}=-\int b_i'(\mathbf{r})x_j\,d\mathbf{r}. \tag{17}$$

It follows from (8) that $\mathbf{b}_0 \parallel \mathbf{n}_0$, and therefore $\mathbf{b}_0$ makes no contribution to $\mathscr{E}$. In order to obtain the first term of the expansion, one must substitute $\mathbf{b}(\mathbf{k})$ in (15) in the form $i\hat{p}\mathbf{k}$, rejecting terms of order $\mathbf{k}^2$ and higher.

Thus all information about molecules interacting at large distances is contained in their tensors $\hat{p}$. In general, however, the expression for $\mathscr{E}$ in terms of the components p_{ij} turns out to be very cumbersome. We shall consider a special case: molecules possessing cylindrical symmetry. Through linear terms (dropping $\mathbf{b}_0$), one can write

$$\mathbf{b}_{1;2}'(\mathbf{k})=i(f_{1;2}^{(0)}\mathbf{k}_\perp+p_{1;2}^{(0)}[\mathbf{n}_0\mathbf{k}_\perp]). \tag{18}$$

Here $f_{1;2}^{(0)}$ and $p_{1;2}^{(0)}$ are coefficients characteristic of the molecules. On substituting (18) in (15), we get

$$\mathscr{E}=f_1^{(0)}f_2^{(0)}Q(a_1;a_3;\mathbf{R}_2-\mathbf{R}_1)+p_1^{(0)}p_2^{(0)}Q(a_2;a_3;\mathbf{R}_2-\mathbf{R}_1), \tag{19}$$

$$Q(a;a_3;\mathbf{R})=8\pi(aa_3)^{-1/2}\left(\frac{a_3}{aR_\parallel^2+a_3\mathbf{R}_\perp^2}\right)^{3/2}\left(\frac{3aR_\parallel^2}{aR_\parallel^2+a_3\mathbf{R}_\perp^2}-1\right). \tag{20}$$

In the large-distance limit, as is shown by formulas (19) and (20), $\mathscr{E}$ decreases as R^{-3}. We shall estimate $\mathscr{E}$ in order of magnitude. Let the molecules be close to each other. The energy $\mathscr{E}'$ of the perturbed liquid crystal is $aV/R'^2 \sim aR'$, where a is of the order of magnitude of the coefficients a_1, a_2, and a_3. For $a \sim 10^{-6}$ dyn and $R' \sim 100$ Å, $\mathscr{E}' \sim 1$ eV; the interaction energy decreases as R^{-3}, starting with distances of the order of the radii of the molecules. When $R/R' \sim (\mathscr{E}'/T)^{1/3}$, the interaction energy is comparable with the thermal energy. For $\mathscr{E}'$

~1 eV and $T\sim 300$ K, the distance R turns out to be of the order of 300 Å.

We shall now consider the effect of a magnetic field on $\mathscr{E}$. In the presence of a magnetic field $\mathbf{H}$ directed along $\mathbf{n}_0$, we must add to the parentheses in the numerators of (15) a term of the form $\chi_a H^2$, where χ_a is the magnetic susceptibility. For the case considered above, we have

$$Q(a;a_3;\mathbf{R})=8\pi(aa_3)^{-1/2}\left(\frac{a_3}{aR_\parallel^2+a_3R_\perp^2}\right)^{3/2}$$
$$\times\exp\left\{-\left[\frac{\chi_a H^2(aR_\parallel^2+a_3\mathbf{R}_\perp^2)}{aa_3}\right]^{1/2}\right\}\left\{\left(\frac{3aR_\parallel^2}{aR_\parallel^2+a_3\mathbf{R}_\perp^2}-1\right)\right.$$
$$\left.-\left[\chi_a H^2-\frac{(aa_3\chi_a H^2)^{1/2}}{(aR_\parallel^2+a_3\mathbf{R}_\perp^2)^{1/2}}\right]\frac{\mathbf{R}_\perp^2}{a}+\frac{2(\chi_a H^2)^{1/2}}{(aa_3)^{1/2}}(aR_\parallel^2+a_3\mathbf{R}_\perp^2)^{1/2}\right\}. \quad (21)$$

A magnetic field can produce a peculiar shielding of the interaction. The characteristic shielding distance L is $(a/\chi_a H^2)^{1/2}$. For example, for $a\sim 10^{-6}$ dyn, $\chi_a\sim 10^{-5}$, and $H\sim 3.10^5$ the characteristic distance $L\sim 100$ Å.

Since strong magnetic fields affect the interaction energy, there is in principle a possibility of using them to change the rates of chemical reactions occurring in liquid crystals.

INTERACTION OF MOLECULES INJECTED INTO A SMECTIC LIQUID CRYSTAL

As is well known,[3,4] in the simplest case smectic crystals form a layered structure, consisting of planes located at equal distances from one another, and capable of moving comparatively freely with respect to one another. We shall suppose that the unperturbed layers are parallel to the yz plane. A perturbation can be specified by the x component $u_x(\mathbf{r})$ of the displacement of points of a layer. By use of $u_x(\mathbf{r})$, the free energy can be represented in the form

$$F=F_0+\int\frac{1}{2}\left\{\bar{B}\left(\frac{\partial u_x}{\partial x}\right)^2+K_1\left(\frac{\partial^2 u_x}{\partial y^2}+\frac{\partial^2 u_x}{\partial z^2}\right)^2\right\}dv, \quad (22)$$

where F_0 is the part of the free energy that is independent of the perturbations; $\bar{B}$ and K_1 are coefficients.

If the perturbations produced by a large foreign molecule, injected into the smectic crystal, are small, then, just as for nematic liquid crystals the interaction energy is represented in the form $\int \mathbf{b}\boldsymbol{\nu}\,dv$, so in the present case we can represent it as

$$\mathscr{E}_{int}=\int P(\mathbf{r})u_x(\mathbf{r})\,d\mathbf{r}. \quad (23)$$

Here $P(\mathbf{r})$ is a function characteristic of the injected molecule.

On varying the sum of (22) and (23) with respect to δu_x, we get

$$-\bar{B}\frac{\partial^2 u_x}{\partial x^2}+K_1\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)^2 u_x+P=0. \quad (24)$$

We transform to the k representation:

$$u_x(\mathbf{k})=\int u_x(\mathbf{r})e^{-i\mathbf{k}\mathbf{r}}\,d\mathbf{r}, \quad (25)$$
$$P(\mathbf{k})=\int P(\mathbf{r})e^{-i\mathbf{k}\mathbf{r}}\,d\mathbf{r}. \quad (26)$$

We have

$$u_x(\mathbf{k})=-P(\mathbf{k})/(\bar{B}k_\parallel^2+K_1k_\perp^4). \quad (27)$$

We note that $P(0)=0$. In fact, a displacement of the molecule as a whole along x causes a change of energy

$$\delta\mathscr{E}_{int}=\int P(\mathbf{r})\,\delta u_x\,dv, \quad (28)$$

where δu_x is a constant defining the displacement. But the molecule is located at a position of equilibrium. Therefore $\delta\mathscr{E}_{int}/\delta u_x=0$. From this it follows directly that $P(0)=\int P(\mathbf{r})\,dv=0$. If we consider in analogous fashion a variation $\delta\mathscr{E}_{int}$ with respect to rotations of the molecule as a whole, we can derive

$$\int P(\mathbf{r})\mathbf{r}_\perp\,dv=0. \quad (29)$$

We consider two molecules. Their interaction energy can be represented in the form

$$\mathscr{E}=\frac{2}{(2\pi)^3}\int\frac{P_2^*(\mathbf{k})P_1(\mathbf{k})}{\bar{B}k_\parallel^2+K_1k_\perp^4}\,d\mathbf{k}. \quad (30)$$

We introduce the function $P'_{1;2}(\mathbf{r})$, which is $P_{1;2}(\mathbf{r})$ calculated in a specially chosen system of coordinates attached to the molecule. By use of $P'_{1;2}(\mathbf{r})$, (30) can be expressed in the form

$$\mathscr{E}=\frac{2}{(2\pi)^3}\int\frac{P_2'^*(\hat{A}(-\varphi_2)\mathbf{k})P_1(\hat{A}(-\varphi_1)\mathbf{k})}{\bar{B}k_\parallel^2+K_1k_\perp^4}\exp\{i\mathbf{k}(\mathbf{R}_2-\mathbf{R}_1)\}\,d\mathbf{k}. \quad (31)$$

The function $P'_{1;2}(\mathbf{r})$ can be rewritten

$$P'_{1;2}(\mathbf{r})=R_{1;2}^{(0)}+R_{1;2}^{(1)}e^{i\varphi}+R_{1;2}^{(-1)}e^{-i\varphi}+R_{1;2}^{(2)}e^{2i\varphi}+\ldots, \quad (32)$$

where $R_{1;2}^{(i)}$ depend on $|\mathbf{r}_\perp|$ and on x. We have $(R_{1;2}^{(i)})=(R_{1;2}^{(-i)})^*$. We introduce

$$Z_{1;2}^{(m)}(k_\parallel;k_\perp)=2\pi(-1)^m i^m\int_{-\infty}^{\infty}\int_0^{\infty}R_{1;2}^{(-m)}J_m(k_\perp r_\perp)\exp(-ik_\parallel x)r_\perp\,dr_\perp\,dx. \quad (33)$$

By use of this expression, (30) can be put into the form

$$\mathscr{E}=\frac{2}{(2\pi)^2}\sum_{m;l}\int_{-\infty}^{\infty}\int_0^{\infty}i^m\frac{(Z_2^{(l)})^*(Z_1^{(l+m)})}{\bar{B}k_\parallel^2+K_1k_\perp^4}$$
$$\times\exp\{i(m+l)\varphi_1-il\varphi_2+ik_\parallel(x_2-x_1)\}J_m(k_\perp|(\mathbf{R}_2-\mathbf{R}_1)_\perp|)\,k_\perp\,dk_\perp\,dk_\parallel. \quad (34)$$

We consider the case of large distances between the molecules. In the linear approximation with respect to k, only one of all the $Z_{1;2}$ remains:

$$Z_{1;2}^{(0)}=-2\pi ik_\parallel\int_{-\infty}^{\infty}\int_0^{\infty}R_{1;2}^{(0)}\,xr_\perp\,dr_\perp\,dx\equiv ik_\parallel\varkappa_{1;2}. \quad (35)$$

On substituting (35) in (34), we get

$$\mathscr{E}=\frac{\varkappa_1\varkappa_2}{4\pi(\bar{B}K_1)^{1/2}(x_1-x_2)^2}\left(\frac{\bar{B}(\mathbf{R}_2-\mathbf{R}_1)_\perp^2}{4K_1^{1/2}|x_1-x_2|}-1\right)\exp\left\{-\frac{\bar{B}^{1/2}(\mathbf{R}_2-\mathbf{R}_1)_\perp^2}{4K_1^{1/2}|x_1-x_2|}\right\}. \tag{36}$$

In this approximation, the energy $\mathscr{E}$ differs significantly from zero only when

$$|(\mathbf{R}_2-\mathbf{R}_1)_\perp|\leqslant(K_1/\bar{B})^{1/4}|x_1-x_2|^2\sim\lambda^{1/2}|x_1-x_2|^{1/2},$$

where λ is the distance between layers in the smectic. But in this range, where $|(\mathbf{R}_2-\mathbf{R}_1)_\perp|\ll|x_1-x_2|$, the linear approximation with respect to k proves insufficient. It is necessary to take account of terms of order $k_\perp^2 r_\perp^2$. We have

$$\begin{gathered}Z_{1;2}^{(0)}=ik_\parallel\varkappa_{1;2}-2\pi\int\limits_{-\infty}^{\infty}\int\limits_{0}^{\infty}R_{1;2}^{(0)}\frac{k_\perp^2r_\perp^3}{4}dr_\perp\,dx=ik_\parallel\varkappa_{1;2}+\beta_{1;2}k_\perp^2,\\ Z_{1;2}^{(2)}=(Z_{1;2}^{(-2)})^*=-2\pi\int\limits_{-\infty}^{\infty}\int\limits_{0}^{\infty}R_{1;2}^{(-2)}\frac{k_\perp^2r_\perp^3}{8}dr_\perp dx=k_\perp^2|s_{1;2}|\exp(-i\theta_{1,2}).\end{gathered} \tag{37}$$

The interaction energy can now be represented as the sum of three expressions:

$$\mathscr{E}=\mathscr{E}_1+\mathscr{E}_2+\mathscr{E}_3; \tag{38}$$

$\mathscr{E}_1$ is the expression (36) with $\varkappa_1\varkappa_2$ replaced by

$$(\operatorname{sign}(x_2-x_1)\varkappa_2+(\bar{B}/K_1)^{1/2}\beta_2)(\operatorname{sign}(x_2-x_1)\varkappa_1-(\bar{B}/K_1)^{1/2}\beta_1)$$
$$-2\frac{\bar{B}}{K_1}|s_1s_2|\cos(2\varphi_1-2\varphi_2+\theta_2-\theta_1);$$

for $\mathscr{E}_1$ and $\mathscr{E}_2$ we have

$$\begin{gathered}\mathscr{E}_2=-\frac{\bar{B}}{8\pi K_1^2}\left[|s_2|\left(\beta_1-\left(\frac{K_1}{\bar{B}}\right)^{1/2}\operatorname{sign}(x_2-x_1)\varkappa_1\right)\cos(2\varphi_2-\theta_2)\right.\\ \left.+|s_1|\left(\beta_2+\left(\frac{K_1}{\bar{B}}\right)^{1/2}\operatorname{sign}(x_2-x_1)\varkappa_2\right)\cos(2\varphi_1-\theta_1)\right]\frac{(\mathbf{R}_2-\mathbf{R}_1)_\perp^2}{|x_1-x_2|^3}\\ \times\exp\left\{-\frac{\bar{B}^{1/2}(\mathbf{R}_2-\mathbf{R}_1)_\perp^2}{4K_1^{1/2}|x_1-x_2|}\right\},\end{gathered} \tag{39}$$

$$\mathscr{E}_3=\frac{8|s_1s_2|\cos(2\varphi_1+2\varphi_2-\theta_1-\theta_2)}{\pi(\bar{B}K_1)^{1/2}(\mathbf{R}_2-\mathbf{R}_1)_\perp^4}\gamma\left(4;\frac{\bar{B}^{1/2}(\mathbf{R}_2-\mathbf{R}_1)_\perp^2}{4K_1^{1/2}|x_1-x_2|}\right). \tag{40}$$

Here γ is the incomplete gamma function.

Formulas (38)–(40) show that the interaction energy of molecules lying in a plane parallel to the planes of the smectic decreases as the inverse fourth power of the distance. If, however, the molecules are located on a line perpendicular to these planes, the interaction energy varies as x^{-2}, where x is the distance between them.

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1) A "large" molecule here means one whose dimensions are much larger than the intermolecular distances in the liquid crystal, so that the liquid crystal, in its interactions with the molecule, can be treated in the continuous-medium approximation.

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Translated by W. F. Brown, Jr.