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Nematic fluid at a hard wall in the mean field approximation

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In the framework of a field theoretical approach we study Maier-Saupe nematogenic fluid in contact with a hard wall. The pair interaction potential of the considered model consists of an isotropic and an anisotropic Yukawa terms. In the mean field approximation the contact theorem is proved. For the case of the nematic director being oriented perpendicular to the wall, analytical expressions for the density and order parameter profiles are obtained. It is shown that in a certain thermodynamic region the nematic fluid near the interface can be more diluted and less orientationally ordered than in the bulk region.

Key words: *Maier-Saupe nematogenic fluid, field theoretical approach, interface, contact theorem*

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Due to orientational ordering, nematic fluids near a surface show richer behavior than in the case of simple fluids. Among them are the anchoring phenomena, whereby the surface induces a specific orientation of the nematic director with respect to the surface [1]. In order to understand this phenomenon, during the past decade the Henderson-Abraham-Barker (HAB) approach [2, 3], previously developed in the theory of isotropic fluids in contact with solid surfaces [4], has been employed. In this approach, the description of the fluid density profile reduces to the solution of the Ornstein-Zernike (OZ) integral equation for the fluid particle-wall distribution function calculated from the known fluid particle distribution function in the bulk. In the framework of the HAB approach, the application to the bulk of the nematic model, analytically solvable at the level of the mean spherical approximation (MSA) [5], makes it possible to investigate the role of orientational-dependent molecular interactions with the surface in anchoring phenomena [2, 3]. However, in the MSA, this approach does not take into account the contribution from long-range molecular interactions and, as a result, does not satisfy the exact relation known as the contact theorem [6, 7]. According to this theorem, the contact value of the particle density near a hard wall for a neutral fluid is determined by the pressure of the fluid in the bulk volume.

Recently, the density field theory, previously developed for ionic fluids near a hard wall [8–10], has been applied to the description of simple fluids with Yukawa-type interactions near a hard wall [11]. In both cases, the developed approach yielded correct results. In this theory, the contributions from the mean field and from the fluctuations are separated. In [11], it was shown that the mean field treatment of a Yukawa fluid near a wall reduces to solving a non-linear differential equation for the density profile while the treatment of fluctuations reduces to the OZ equation with the Riemann boundary condition.

In this paper, the density field theory, developed in [11] for simple fluids at a hard wall, will be generalized to nematic fluids at a hard wall. To this end, we consider Maier-Saupe nematogenic fluid model [12, 13] as one of the simplest models that account for the isotropic-nematic phase transition. For simpli-

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fication we consider a fluid of point uniaxial nematogens interacting through the pair potential

$$v(r_{12},\Omega_1\Omega_2) = v_0(r_{12}) + v_2(r_{12})P_2(\cos\theta_{12}), \tag{1}$$

where the first term $v_0(r_{12}) = (A_0/r_{12})\exp(-\alpha_0 r_{12})$ describes the isotropic repulsion and the second term with $v_2(r_{12}) = (A_2/r_{12})\exp(-\alpha_2 r_{12})$ describes the anisotropic attraction between particles ($A_0 > 0$, $A_2 < 0$), r_{12} denotes the distance between particles 1 and 2, $\Omega = (\theta,\phi)$ are orientations of particles, $P_2(\cos\theta_{12}) = (3\cos^2\theta_{12} - 1)/2$ is the second order Legendre polynomial of the relative orientation θ_{12}.

The application of the density field theory to the description of bulk properties of such nematic fluids was considered in [14, 15]. It was shown that beyond the mean field approximation, the repulsive isotropic term in (1) is very important for the description of the nematic phase. Within the field-theoretical formalism, the Hamiltonian is a functional of the density field and can be written as the sum of entropic and interaction terms

$$\begin{aligned}\beta H[\rho(\mathbf{r},\Omega)] = &\int \rho(\mathbf{r},\Omega)\left[\ln(\rho(\mathbf{r},\Omega)\Lambda_R\Lambda_T^3) - 1\right]\mathrm{d}\mathbf{r}\mathrm{d}\Omega \\ &+ \frac{\beta}{2}\int v(r_{12},\Omega_1\Omega_2)\rho(\mathbf{r_1},\Omega_1)\rho(\mathbf{r_2},\Omega_2)\mathrm{d}\mathbf{r_1}\mathrm{d}\mathbf{r_2}\mathrm{d}\Omega_1\mathrm{d}\Omega_2\,,\end{aligned} \tag{2}$$

where $\beta = 1/k_\mathrm{B}T$ is the inverse temperature, $\mathrm{d}\Omega = (1/4\pi)\sin\theta\mathrm{d}\theta\mathrm{d}\phi$ is the normalized angle element, $\rho(\mathbf{r},\Omega)$ is particle density per angle, so that $\int\rho(\mathbf{r},\Omega)\mathrm{d}\Omega = \rho(\mathbf{r})$, Λ_T is the thermal de Broglie wavelength of the molecules, the quantity Λ_R^{-1} is the rotational partition function for a single molecule [16].

In this paper, we will restrict our consideration to the mean field approximation (MFA) which is the lowest order approximation for the partition function. In the canonical formalism it corresponds to fixing the Lagrange parameter λ, so that the following relation is true for the singlet distribution function

$$\left.\frac{\delta\beta H[\rho(\mathbf{r},\Omega)]}{\delta\rho(\mathbf{r},\Omega)}\right|_{\rho^{\mathrm{MFA}}} = \lambda. \tag{3}$$

As a result,

$$\rho(\mathbf{r}_1,\Omega_1) = \rho^{\mathrm{bulk}}(\Omega_1)\exp\left\{-\beta\int v(r_{12},\Omega_1\Omega_2)\left[\rho(\mathbf{r}_2,\Omega_2) - \rho^{\mathrm{bulk}}(\Omega_2)\right]\mathrm{d}\mathbf{r_2}\mathrm{d}\Omega_2\right\}, \tag{4}$$

where

$$\rho^{\mathrm{bulk}}(\Omega) = \rho_\mathrm{b}\exp\left[-\left(\varkappa_2^2 S_\mathrm{b}/\alpha_2^2\right)P_2(\cos\theta)\right]\Big/\int\limits_0^1 \mathrm{d}\cos\theta\exp\left[-\left(\varkappa_2^2 S_\mathrm{b}/\alpha_2^2\right)P_2(\cos\theta)\right] \tag{5}$$

is the singlet distribution function for the bulk nematic in the MFA defined in the framework of the Maier-Saupe theory [14, 15], $\varkappa_2^2 = 4\pi\rho_\mathrm{b}\beta A_2$, ρ_b is the bulk value of the fluid density, $S_\mathrm{b} = (1/\rho_\mathrm{b})\int_0^1 P_2(\cos\theta)\rho^{\mathrm{bulk}}(\Omega)\mathrm{d}\cos\theta$ is the bulk value of the orientational order parameter.

In order to integrate with respect to the angle in (4), we should separate the angle Ω_{in} between the particles and the director and the angle Ω_{nw} between the nematic director and the surface. To this end, we express the Legendre polynomial in the potential $v(r_{12},\Omega_1\Omega_2)$ in terms of spherical harmonics $Y_{2m}(\Omega)$ as $P_2(\cos\Omega_{12}) = (1/5)\sum_m Y_{2m}^*(\Omega_{1n})Y_{2m}(\Omega_{2n})$. As a result,

$$\frac{\rho(\mathbf{r}_1,\Omega_{1n},\Omega_{wn})}{\rho^{\mathrm{bulk}}(\Omega_{1n})} = \exp\left\{-\left[V_0(\mathbf{r}_1,\Omega_{wn}) - V_0^\mathrm{b}\right] - \frac{1}{\sqrt{5}}\sum_m Y_{2m}(\Omega_{1n})\left[V_{2m}(\mathbf{r}_1,\Omega_{wn}) - V_{2m}^\mathrm{b}\right]\right\}, \tag{6}$$

where the mean field potentials

$$V_0(\mathbf{r}_1,\Omega_{wn}) = \beta\int v_0(r_{12})\rho(\mathbf{r}_2,\Omega_{wn})\mathrm{d}\mathbf{r}_2\,, \tag{7}$$

$$V_{2m}(\mathbf{r}_1,\Omega_{wn}) = \beta\int v_2(r_{12})S_{2m}(\mathbf{r}_2,\Omega_{wn})\mathrm{d}\mathbf{r}_2\,. \tag{8}$$

The bulk values of these quantities are $V_0^{\mathrm{b}} = \varkappa_0^2/\alpha_0^2$, $V_{20}^{\mathrm{b}} = \varkappa_2^2 S_{\mathrm{b}}/\alpha_2^2$, $V_{2m}^{\mathrm{b}} = 0$ for $m \neq 0$, where $\varkappa_0^2 = 4\pi\rho_{\mathrm{b}}\beta A_0$,

$$\rho(\mathbf{r},\Omega_{wn}) = \int \rho(\mathbf{r},\Omega_{1n},\Omega_{wn})\mathrm{d}\Omega_{1n} \tag{9}$$

is the density profile. The property

$$S_{2m}(\mathbf{r},\Omega_{wn}) = \frac{1}{\sqrt{5}}\int \rho(\mathbf{r},\Omega_{1n},\Omega_{wn})\,Y_{2m}(\Omega_{1n})\mathrm{d}\Omega_{1n} = \rho(\mathbf{r},\Omega_{wn})\,S_{2m}^{*}(\mathbf{r},\Omega_{wn}), \tag{10}$$

where $S_{2m}^{*}(\mathbf{r},\Omega_{wn})$ are the order parameter profiles. Far from the wall $S_{20}^{*}(\mathbf{r},\Omega_{wn}) \to S_{\mathrm{b}}$, $S_{2m}^{*}(\mathbf{r},\Omega_{wn}) \to 0$ for $m \neq 0$.

Taking the gradient of equation (6) we have

$$\frac{1}{\rho(\mathbf{r},\Omega_{1n},\Omega_{wn})}\boldsymbol{\nabla}\rho(\mathbf{r},\Omega_{1n},\Omega_{wn}) = \mathbf{E}_0(\mathbf{r},\Omega_{wn}) + \frac{1}{\sqrt{5}}\sum_m Y_{2m}(\Omega_{1n})\mathbf{E}_{2m}(\mathbf{r},\Omega_{wn}), \tag{11}$$

where we define an equivalent of the electric field by

$$\mathbf{E}_0(\mathbf{r},\Omega_{wn}) \equiv -\boldsymbol{\nabla} V_0(\mathbf{r},\Omega_{wn}), \qquad \mathbf{E}_{2m}(\mathbf{r},\Omega_{wn}) \equiv -\boldsymbol{\nabla} V_{2m}(\mathbf{r},\Omega_{wn}). \tag{12}$$

Due to the properties of the Yukawa potential

$$\left(\Delta - \alpha_0^2\right) V_0(\mathbf{r},\Omega_{wn}) = -4\pi\beta A_0\rho(\mathbf{r},\Omega_{wn}), \tag{13}$$

$$\left(\Delta - \alpha_2^2\right) V_{2m}(\mathbf{r},\Omega_{wn}) = -4\pi\beta A_2 S_{2m}(\mathbf{r},\Omega_{wn}). \tag{14}$$

Due to the translational invariance parallel to the wall, the functions considered depend only on the distance z to the wall, and replacing (13) and (14) into (11), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{\rho(z,\Omega_{wn})}{\rho_{\mathrm{b}}} + \frac{\alpha_0^2}{2\varkappa_0^2}V_0^2(z,\Omega_{wn}) - \frac{1}{2\varkappa_0^2}E_0^2(z,\Omega_{wn}) + \sum_m\left(\frac{\alpha_2^2}{2\varkappa_2^2}V_{2m}^2(z,\Omega_{wn}) - \frac{1}{2\varkappa_2^2}E_{2m}^2(z,\Omega_{wn})\right)\right] = 0. \tag{15}$$

In the bulk, when $z \to \infty$, we have $\rho(z,\Omega_{wn}) \to \rho_{\mathrm{b}}$, $E_0(z,\Omega_{wn}) \to 0$, $E_{2m}(z,\Omega_{wn}) \to 0$, $V_0(z,\Omega_{wn}) \to V_0^{\mathrm{b}}$, $V_{20}(z,\Omega_{wn}) \to V_{20}^{\mathrm{b}}$ and $V_{2m}(z,\Omega_{wn}) \to 0$ for $m \neq 0$. From Equation (15) we see that the quantity in brackets is constant regardless of the angle Ω_{wn} between the director and the wall, and, therefore, it can be evaluated, for instance, in the bulk as the reduced pressure $\beta P/\rho_{\mathrm{b}}$ within MFA [15]:

$$\frac{\beta P}{\rho_{\mathrm{b}}} = 1 + \frac{\varkappa_0^2}{2\alpha_0^2} + \frac{\varkappa_2^2}{2\alpha_2^2}S_{\mathrm{b}}^2. \tag{16}$$

Outside the system, where there are no particles, we have another invariant which is simply

$$\frac{\alpha_0^2}{2\varkappa_0^2}V_0^2(z,\Omega_{wn}) - \frac{1}{2\varkappa_0^2}E_0^2(z,\Omega_{wn}) + \sum_m\left[\frac{\alpha_2^2}{2\varkappa_2^2}V_{2m}^2(z,\Omega_{wn}) - \frac{1}{2\varkappa_2^2}E_{2m}^2(z,\Omega_{wn})\right], \tag{17}$$

its value is zero far from the interface and, therefore, it is zero at the interface as well. From the continuity of the potential and its derivative due to equation (13) and (14), we see that this is also true at the wall just inside the system $z = 0_+$. Thus,

$$\frac{\rho(0_+,\Omega_{wn})}{\rho_{\mathrm{b}}} + \frac{\alpha_0^2}{2\varkappa_0^2}V_0^2(0_+,\Omega_{wn}) - \frac{1}{2\varkappa_0^2}E_0^2(0_+,\Omega_{wn}) + \sum_m\left[\frac{\alpha_2^2}{2\varkappa_2^2}V_{2m}^2(0_+,\Omega_{wn}) - \frac{1}{2\varkappa_2^2}E_{2m}^2(0_+,\Omega_{wn})\right] = \frac{\rho(0_+,\Omega_{wn})}{\rho_{\mathrm{b}}}. \tag{18}$$

Since this quantity is constant, we obtain the so-called contact theorem

$$\beta P = \rho(0_+, \Omega_{wn}). \tag{19}$$

We should note that the contact theorem was usually proved for isotropic fluids near a hard wall [6, 7]. The result obtained here is probably the first verification of the contact theorem for anisotropic fluids at a hard wall.

From equations (10)-(14) we have a set of six differential equations for unknown functions $\rho(\mathbf{r}, \Omega_{1n}, \Omega_{wn})$, $S_{2m}(\mathbf{r}, \Omega_{wn})$, $E_0(\mathbf{r}, \Omega_{wn})$, $E_{2m}(\mathbf{r}, \Omega_{wn})$, $V_0(\mathbf{r}, \Omega_{wn})$, $V_{2m}(\mathbf{r}, \Omega_{wn})$. We note that in the case when the director is oriented perpendicular to the wall, $\Omega_{wn} = 0$, the singlet distribution function is axially symmetric. Consequently, in the equations considered only the terms with $m = 0$ will be present. In this paper, we will restrict our further consideration to this special case and consider the solution of the obtained differential equations in the linear approximation. Far from the wall $\rho(\mathbf{r}, \Omega) \to \rho^{\text{bulk}}(\Omega)$. After linearization of expression (6)

$$\rho'(z, \Omega) = [E_0(z) + E_{20}(z) P_2(\cos\theta)]\, \rho^{\text{bulk}}(\Omega) \tag{20}$$

and we have the following system of equations

$$\rho'(z) = [E_0(z) + S_\mathrm{b} E_{20}(z)]\, \rho_\mathrm{b}\,, \tag{21}$$

$$S'_{20}(z) = \left[E_0(z) S_\mathrm{b} + E_{20}(z) \frac{1}{5} \langle Y_{20}^2 \rangle_\Omega \right] \rho_\mathrm{b}\,, \tag{22}$$

$$V'_0(z) = -E_0(z), \qquad V'_{20}(z) = -E_{20}(z)\,, \tag{23}$$

$$E'_0(z) = -\alpha_0^2 V_0(z) + (\varkappa_0^2 / \rho_\mathrm{b})\, \rho(z)\,, \tag{24}$$

$$E'_{20}(z) = -\alpha_2^2 V_{20}(z) + (\varkappa_2^2 / \rho_\mathrm{b})\, S_{20}(z)\,, \tag{25}$$

where the prime denotes a derivative by z and $\langle Y_{20}^k \rangle_\Omega = (1/\rho_\mathrm{b}) \int_0^1 Y_{20}^k(\Omega) \rho^{\text{bulk}}(\Omega) \mathrm{d}\cos\theta$ $(k = 1, 2)$. This system reduces to two second order differential equations for $E_0(z)$ and $E_{20}(z)$

$$E''_0(z) = E_0(z) \left(\varkappa_0^2 + \alpha_0^2\right) + E_{20}(z) \varkappa_0^2 S_\mathrm{b}\,, \tag{26}$$

$$E''_{20}(z) = E_0(z) \varkappa_2^2 S_\mathrm{b} + E_{20}(z) \left[\alpha_2^2 + (\varkappa_2^2/5) \langle Y_{20}^2 \rangle_\Omega \right], \tag{27}$$

which can be solved with the boundary condition that should include the contact theorem (19). Thus,

$$\begin{aligned} \frac{\rho(z)}{\rho_\mathrm{b}} = 1 &- \frac{\lambda_0^2 - \alpha_2^2 - \frac{1}{5}\varkappa_2^2 \left(\langle Y_{20}^2 \rangle_\Omega - \langle Y_{20} \rangle_\Omega^2\right)}{\varkappa_2^2 S_\mathrm{b}} B_1 \mathrm{e}^{-\lambda_0 z} \\ &- \frac{\lambda_2^2 - \alpha_2^2 - \frac{1}{5}\varkappa_2^2 \left(\langle Y_{20}^2 \rangle_\Omega - \langle Y_{20} \rangle_\Omega^2\right)}{\varkappa_2^2 S_\mathrm{b}} B_2 \mathrm{e}^{-\lambda_2 z}, \end{aligned} \tag{28}$$

$$\frac{S_{20}(z)}{\rho_\mathrm{b} S_\mathrm{b}} = 1 - \frac{\left(\lambda_0^2 - \alpha_2^2\right)}{\varkappa_2^2 S_\mathrm{b}} B_1 \mathrm{e}^{-\lambda_0 z} - \frac{\left(\lambda_2^2 - \alpha_2^2\right)}{\varkappa_2^2 S_\mathrm{b}} B_2 \mathrm{e}^{-\lambda_2 z}, \tag{29}$$

where

$$\lambda_{0,2}^2 = \frac{1}{2} \left[\varkappa_0^2 + \alpha_0^2 + \frac{\varkappa_2^2}{5} \langle Y_{20}^2 \rangle_\Omega + \alpha_2^2 \pm \sqrt{\left(\varkappa_0^2 + \alpha_0^2 - \frac{\varkappa_2^2}{5} \langle Y_{20}^2 \rangle_\Omega - \alpha_2^2\right)^2 + 4 \varkappa_0^2 \varkappa_2^2 S_\mathrm{b}^2}\, \right], \tag{30}$$

$$B_1 = \frac{\varkappa_2^2 S_\mathrm{b}}{2\left[\lambda_0^2 - \lambda_2^2\right]} \left[-\frac{\varkappa_0^2}{\alpha_0^2} + \frac{\lambda_2^2 - \alpha_2^2 - (\varkappa_2^2/5) \langle Y_{20}^2 \rangle_\Omega}{\alpha_2^2}\right], \qquad B_2 = -\frac{\varkappa_2^2 S_\mathrm{b}}{2\alpha_2^2} - B_1\,. \tag{31}$$

The values of parameters λ_0 and λ_2 coincide with similar parameters obtained in the bulk case after

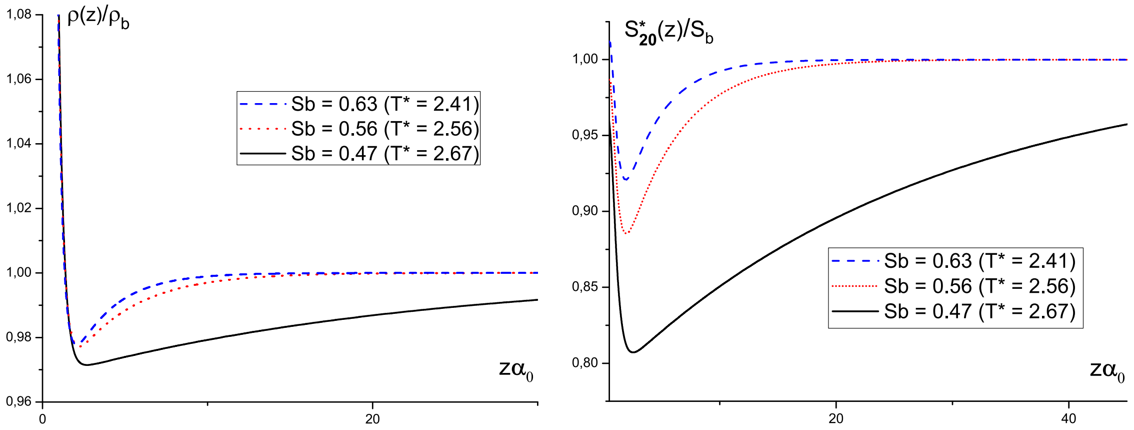

Figure 1. (Color online) The density and the order parameter profiles in the linearized approximation for $\rho_{\mathrm{b}}/\alpha_0^3 = 0.5$, $A_0/A_2 = 2.2$, $\alpha_0/\alpha_2 = 1.25$. Different lines correspond to different values of S_{b} [i.e., the reduced temperature $T^* = 1/(\beta A_2 \alpha_2)$].

including the Gaussian fluctuations [15]. Similarly to the bulk case, parameters λ_0 and λ_2 characterize the screening of the repulsive isotropic and the attractive anisotropic interactions, respectively. The density profile $\rho(z)$ and the order parameter profile $S_{20}^*(z) = S_{20}(z)/\rho(z)$ calculated from equations (28)–(29) are presented in figure 1. As we can see, both profiles have layer-like forms. At the surface, the fluid is more dense and orientationally ordered than in the bulk. But at higher distances there is a large region where the fluid is more diluted and less orientationally ordered than in the bulk. This result is obtained in the MFA. For isotropic fluids, as was shown in [11], the inclusion of fluctuation terms leads to the depletion effect. We can suppose that a similar effect will take place for the considered anisotropic fluid. It means that the inclusion of fluctuation terms does not change our conclusion drawn from figure 1 concerning the existence of a more diluted and less ordered region of the fluid near the surface compared to the bulk region.

Other interesting phenomena that can be observed within the framework of the formulated MFA approach are connected with the possibility that the angle between the nematic director and the surface can change near the surface. Consequently, phases with the order parameters $S_{2m}^*(z) = S_{2m}(z)/\rho(z)$ ($m \neq 0$) can appear near the surface. These phenomena will be investigated in a separate paper.

In conclusion, using the field theoretical approach we have formulated the mean field approximation as the first starting point for the description of a nematic fluid at a hard wall. For the first time, an exact derivation of the contact theorem for anisotropic fluids has been presented within the MFA. It has been shown that the contact value of the density profile is determined by the pressure of the fluid in the bulk volume and does not depend on the angle between the nematic director and the surface. For the case of the director being oriented perpendicular to the wall, in the linear approximation for the MFA, we have obtained analytical expressions for the density and order parameter profiles. It has been shown that at some values of the parameters of the model considered, the fluid near the surface can be more diluted and less orientationally ordered than in the bulk.

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Нематичний плин біля твердої поверхні у наближенні середнього поля

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В рамках теоретико-польового підходу вивчається нематогенний плин Майєра-Заупе біля твердої поверхні. У розглядуваній моделі парний потенціал взаємодії складається з ізотропного та анізотропного Юкавівських доданків. У наближенні середнього поля доведено контактну теорему. Для випадку, коли директор направлений перпендикулярно до стінки, отримано аналітичні вирази для профілів густини та параметра порядку. Показано, що у певній термодинамічній області нематичний плин поблизу поверхні може бути більш розрідженим і менш орієнтаційно впорядкованим, ніж в об'ємній області.

Ключові слова: *нематичний плин Майєра-Заупе, теоретико-польовий підхід, поверхня розділу, контактна теорема*