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A continuum theory for liquid crystals describing different degrees of orientational order

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Starting out with mesoscopic orientational balance equations for each orientational component of a liquid crystal which is described as a formal mixture, a set of independent macroscopic variables, the state space Z, is induced

$$Z:=\{\rho, \theta, \nabla\theta, \mathbf{D}, \omega, \mathbf{A}, \nabla\mathbf{A}, \nabla\nabla\mathbf{A}, \mathrm{D}_t^{(2)}\mathbf{A}, \Gamma\}(\mathbf{x}, t).$$

This set includes a second-order tensorial measure of alignment, called the alignment tensor $\mathbf{A}$, and its derivatives. In terms of these state space variables constitutive equations are proposed by exploiting the dissipation inequality due to Coleman and Noll. The constitutive equations around equilibrium are investigated. The results are compared in the case of total alignment to those of Ericksen and Leslie, who described the alignment in a liquid crystal with only a macroscopic unit director field $\mathbf{d}(\mathbf{x}, t)$ indicating the 'mean orientation' of the media. In a recent paper Ericksen introduced beside the macroscopic director an additional scalar order parameter $S(\mathbf{x}, t)$ and its derivatives (Maier–Saupe theory) which turns out to be the uniaxial case in the alignment tensor formulation. Also in this case the restrictions on the constitutive equations caused by the dissipation inequality are discussed and compared to Ericksen's results.

1. The mesoscopic concept

To describe the behaviour of a nematic liquid crystal a common model is used for the particles which are assumed to be rigid rods with fixed length [5]. Thus the orientation is given by a microscopic director $\mathbf{n}$ of unit length

$$\mathbf{n}^2=1, \quad \mathbf{n}\cdot\mathbf{u}=0 \quad \text{with} \quad \mathbf{u}:=\frac{d}{dt}\mathbf{n}. \tag{1}$$

Consequently each particle has a set of five independent coordinates (three in position space and two in orientation space). For simplicity we presuppose a head-tail symmetry for the particles—thus particles with orientation $\mathbf{n}$ and $-\mathbf{n}$ are indistinguishable—and that the particles are needle-shaped.

Then we combine this microscopic director approach with an orientation distribution function (ODF) in order to describe changes in orientational order. Therefore we introduce the ODF

$$f(\mathbf{n}, \mathbf{x}, t)\equiv f(\cdot), \quad (\cdot)\equiv(\mathbf{n}, \mathbf{x}, t)\in S^2\times\mathbb{R}^3\times\mathbb{R}^1, \tag{2}$$

which has a symmetry $f(-\mathbf{n}, \mathbf{x}, t)=f(\mathbf{n}, \mathbf{x}, t)$ according to the particle symmetry. In the case of total alignment, the ODF is given by

$$f(\cdot)=\tfrac{1}{2}[\delta(|\mathbf{n}+\mathbf{d}(\mathbf{x}, t)|)+\delta(|\mathbf{n}-\mathbf{d}(\mathbf{x}, t)|)], \tag{3}$$

and the microscopic director reduces to the macroscopic director $\mathbf{d}(\mathbf{x},t)$ introduced by Ericksen and Leslie [10] as we have shown in [4]. With this mesoscopic approach a new set of balance equations on this higher dimensional space $(\cdot)$ containing $\mathbf{n}$ as independent variable results [2]. Integrating over the additional variable $\mathbf{n}$ gives us the usual balance equations defined on $(\mathbf{x},t)$ and additional relations between the quantities for one orientational component and the quantities of the orientational mixture respectively [1]. For example, the relation for the spin density reads

$$\mathbf{s}(\mathbf{x},t)=\int_{S^2} f(\cdot)I\mathbf{n}\times\mathbf{u}(\cdot)\,d^2n. \tag{4}$$

This equation can only be satisfied by a macroscopic director $\mathbf{d}(\mathbf{x},t)$, as it is used in the classical 'director-theories' of Ericksen [6] and Leslie [10] (EL theory), if the mixture is composed of only one single component, i.e. if the mixture is totally aligned. This can also be shown by the following example [4]: presupposing we have a uniaxial orientation distribution function

$$f(\cdot)=f(|\mathbf{n}\cdot\mathbf{d}(\mathbf{x},t)|,\mathbf{x},t), \tag{5}$$

which is rotating around the axis $\mathbf{d}(\mathbf{x},t)$, then $\dot{\mathbf{d}}(\mathbf{x},t)$, of course is zero, and we get

$$\mathbf{s}(\mathbf{x},t)=I\mathbf{d}(\mathbf{x},t)\times\dot{\mathbf{d}}(\mathbf{x},t)=0 \text{ in EL theory,} \tag{6}$$

while

$$\mathbf{s}(\mathbf{x},t)=\int_{S^2} If(\cdot)\mathbf{n}\times\mathbf{u}(\cdot)d^2n\neq 0 \text{ in ODF theory,} \tag{7}$$

unless $f(\cdot)$ is the delta function (3).

2. Exploitation of the dissipation inequality

The dissipation inequality reads [11]

$$\frac{\partial}{\partial t}[\rho(\mathbf{x},t)\eta(\mathbf{x},t)]+\nabla\cdot[\rho(\mathbf{x},t)\eta(\mathbf{x},t)\mathbf{v}(\mathbf{x},t)-\boldsymbol{\phi}(\mathbf{x},t)]-\rho(\mathbf{x},t)\sigma(\mathbf{x},t)\geqslant 0. \tag{8}$$

With the usual ansatz $\sigma(\mathbf{x},t)=[r(\mathbf{x},t)]/[\theta(\mathbf{x},t)]$ (which can be considered as the definition of the temperature $\theta(\mathbf{x},t)$), and the definitions for the free energy density $F(\mathbf{x},t)$ and for the excess heat flux vector $\mathbf{Q}(\mathbf{x},t)$

$$F(\mathbf{x},t):=\varepsilon(\mathbf{x},t)-\theta(\mathbf{x},t)\eta(\mathbf{x},t),\quad \mathbf{Q}(\mathbf{x},t):=\mathbf{q}(\mathbf{x},t)-\theta(\mathbf{x},t)\boldsymbol{\phi}(\mathbf{x},t), \tag{9}$$

we insert the balance of internal energy into the dissipation inequality and get

$$-\rho(\mathbf{x},t)\left[\frac{d}{dt}F(\mathbf{x},t+\eta(\mathbf{x},t)\frac{d}{dt}\theta(\mathbf{x},t)\right]+\nabla\cdot\mathbf{Q}(\mathbf{x},t)+\boldsymbol{\phi}(\mathbf{x},t)\cdot\nabla\theta(\mathbf{x},t)+E(\mathbf{x},t)\geqslant 0, \tag{10}$$

$$E(\mathbf{x},t):=[\nabla\mathbf{v}(\mathbf{x},t)]:\mathbf{t}(\mathbf{x},t)+\frac{1}{I}[\nabla\mathbf{s}(\mathbf{x},t)]:\mathbf{m}(\mathbf{x},t)-\frac{1}{I}\mathbf{s}(\mathbf{x},t)\cdot\varepsilon:\mathbf{t}(\mathbf{x},t). \tag{11}$$

We now transform (11) using the expressions for $\mathbf{s}(\mathbf{x},t)$, $\mathbf{t}(\mathbf{x},t)$ and $\mathbf{m}(\mathbf{x},t)$ we have obtained from the orientational balances [4], under the assumption that there is no coupling between orientation and diffusion, i.e. $\delta\mathbf{v}(\cdot)=\mathbf{0}$. Introducing $D_{ij}(\mathbf{x},t)$ and $\omega_{ij}(\mathbf{x},t)$ for the symmetric and skew-symmetric part of the velocity gradient, and

$N_i(\cdot):=D_t^{(1)}n_i=u_i(\cdot)-n_j\omega_{ji}(\mathbf{x},t)$ for the co-rotational time derivative of $\mathbf{n}$, we get from (11) by a straightforward calculation

$$E(\mathbf{x},t)=D_{ij}(\mathbf{x},t)t_{ji}(\mathbf{x},t)+\omega_{ij}(\mathbf{x},t)t_{ji}(\mathbf{x},t)+2B_{ilk}(\mathbf{x},t)M_{lki}(\mathbf{x},t)+2C_{lik}(\mathbf{x},t)M_{lki}(\mathbf{x},t)$$
$$+2(\nabla_i A_{lo}(\mathbf{x},t))\omega_{ok}(\mathbf{x},t)M_{lki}(\mathbf{x},t)-2\Gamma_{ml}(\mathbf{x},t)t_{ml}(\mathbf{x},t)-2A_{kn}(\mathbf{x},t)\omega_{nj}(\mathbf{x},t)t_{[kj]}(\mathbf{x},t), \qquad (12)$$

where we introduced the following abbreviations

$$B_{ilk}(\mathbf{x},t):=\int_{S^2}(\nabla_i f(\cdot))n_l N_k(\cdot)\,d^2n; \quad C_{lik}(\mathbf{x},t):=\int_{S^2} f(\cdot)n_l\nabla_i u_k(\cdot)d^2n, \qquad (13)$$

$$M_{lki}(\mathbf{x},t):=\int_{S^2} n_{[l}h_{k]i}(\cdot)\,d^2n\equiv-\tfrac{1}{2}\varepsilon_{lkj}m_{ji}(\mathbf{x},t), \qquad (14)$$

$$\Gamma_{ml}(\mathbf{x},t):=\int_{S^2} f(\cdot))n_{[m}N_{l]}(\cdot)\,d^2n; \quad A_{kn}(\mathbf{x},t):=\int_{S^2} f(\cdot)n_k n_n\,d^2n. \qquad (15)$$

By this calculation the fields $\mathbf{s}(\mathbf{x},t)$ and $\mathbf{m}(\mathbf{x},t)$ in (11) are replaced by the new macroscopic fields $\mathbf{B}(\mathbf{x},t)$, $\mathbf{C}(\mathbf{x},t)$, $\mathbf{M}(\mathbf{x},t)$, $\mathbf{\Gamma}(\mathbf{x},t)$, and $\mathbf{A}(\mathbf{x},t)$ which are mesoscopically defined by (13) to (15). The quantity $\mathbf{A}(\mathbf{x},t)$ in (15) is a second order alignment tensor, for which we can derive a relaxation equation of the form

$$D_t^{(2)}A_{jk}(\mathbf{x},t)=G_{jk}(\mathbf{x},t):=\int_{S^2} f(\cdot)n_{(j}N_{k)}(\cdot)\,d^2n, \qquad (16)$$

with $D_t^{(2)}\,\mathbf{A}(\mathbf{x},t)$ being the co-rotational time derivative of $\mathbf{A}$. Thus we introduce the stats space as

$$Z:=\{\rho,\theta,\nabla_{\mathbf{x}}\theta,\mathbf{D},\boldsymbol{\omega},\mathbf{A},\nabla_{\mathbf{x}}\mathbf{A},\nabla_{\mathbf{x}}\nabla_{\mathbf{x}}\mathbf{A},\mathbf{D}_t^{(2)}\mathbf{A},\mathbf{\Gamma}\}(\mathbf{x},t). \qquad (17)$$

The Coleman–Noll evaluation of the transformed dissipation inequality with the state space (17) leads to a set of algebraic differential equations coupling the derivatives of F and $\mathbf{Q}$ and the constitutive equations, which results for example in

$$\rho F(\rho,\theta,\mathbf{A},\nabla\mathbf{A})=F_0(\rho,\theta,\mathbf{A})+W(\theta,\mathbf{A},\nabla\mathbf{A}). \qquad (18)$$

In equilibrium, a Taylor expansion of the rest dissipation equation around equilibrium, under the presupposition $\mathbf{H}(\mathbf{X})\cdot\mathbf{X}\geqslant 0\rightarrow\mathbf{H}(\mathbf{0})=\mathbf{0}$ [11], leads to further restrictions to the constitutive equations; for example in the case of homogeneous alignment

$$\left(\frac{\partial F_0}{\partial A_{ij}}\right)^{\mathrm{eq}}=0 \qquad (19)$$

results, which is fundamental in the Landau theory of homogeneous alignment [3].

3. Constitutive equations

With the ansatz of W and $\mathbf{Q}$ being maximal second order in $(\nabla\theta,\nabla\mathbf{A},\nabla\nabla\mathbf{A},\mathbf{D}_t^{(2)}\mathbf{A},\mathbf{D},\boldsymbol{\omega},\mathbf{\Gamma})$, and maximal linear in the traceless alignment tensor $\mathbf{a}:=\mathbf{A}-\frac{1}{3}\boldsymbol{\delta}$ [12] we get for the elastic free energy

$$W=[\beta_1+\tfrac{1}{3}(\beta_5+\beta_6)]\nabla_i a_{ij}\nabla_k a_{kj}+[\beta_2+\tfrac{1}{3}(\beta_7+\beta_8)]\nabla_i a_{jk}\nabla_i a_{kj}$$
$$+[\beta_3+\tfrac{1}{3}(\beta_9+\beta_{10})]\nabla_i a_{jk}\nabla_k a_{ji}+\beta_4\nabla_i a_{ij}\nabla_j a_{kl}a_{lk}+\beta_5 a_{ji}\nabla_i a_{jk}\nabla_l a_{lk}$$
$$+\beta_6\nabla_i a_{ij}a_{jk}\nabla_l a_{lk}+\beta_7\nabla_i a_{jk}a_{il}\nabla_l a_{kj}+\beta_8\nabla_i a_{jk}\nabla_i a_{jl}a_{lk}+\beta_9\nabla_i a_{jk}\nabla_k a_{il}a_{lj}$$
$$+\beta_{10}\nabla_i a_{jk}\nabla_k a_{jl}a_{li}, \qquad (20)$$

and for the couple stress tensor

$$
\begin{aligned}
M_{lki} = {} & \tfrac{1}{4}[\gamma_1 + \tfrac{1}{3}(\gamma_6+\gamma_7+\gamma_8)](\nabla_j a_{jk}\delta_{il} - \nabla_j a_{jl}\delta_{ki}) \\
& + \tfrac{1}{4}[\gamma_2 + \tfrac{1}{3}(\gamma_{10}-\gamma_{11}-\gamma_{12})](\nabla_l a_{ki} - \nabla_k a_{li}) + \tfrac{1}{4}\gamma_5(\nabla_k a_{jm}\delta_{il}a_{jm} - \nabla_l a_{jm}\delta_{ik}a_{jm}) \\
& + \tfrac{1}{4}\gamma_6(\nabla_j a_{km}\delta_{il}a_{mj} - \nabla_j a_{lm}\delta_{ik}a_{mj}) + \tfrac{1}{4}\gamma_7(\nabla_j a_{jk}a_{li} - \nabla_j a_{jl}a_{ki}) \\
& + \tfrac{1}{4}\gamma_8(\nabla_j a_{jm}\delta_{il}a_{km} - \nabla_j a_{jm}\delta_{ik}a_{lm}) + \tfrac{1}{4}\gamma_9(\nabla_i a_{lj}a_{kj} - \nabla_i a_{kj}a_{lj}) \\
& + \tfrac{1}{4}\gamma_{10}(\nabla_l a_{ji}a_{jk} - \nabla_k a_{ji}a_{jl}) + \tfrac{1}{4}\gamma_{11}(\nabla_j a_{li}a_{kj} - \nabla_j a_{ki}a_{lj}) + \tfrac{1}{4}\gamma_{12}(\nabla_k a_{lj}a_{ij} - \nabla_l a_{kj}a_{ij}) \\
& + \tfrac{1}{4}[\bar\gamma_1 + \tfrac{2}{3}\bar\gamma_3](\nabla_k\theta\delta_{il} - \nabla_l\theta\delta_{ki}) + \tfrac{1}{4}\bar\gamma_3(\nabla_j\theta a_{jk}\delta_{il} - \nabla_j\theta a_{jl}\delta_{ik} + \nabla_k\theta a_{li} - \nabla_l a_{ki}). \qquad (21)
\end{aligned}
$$

In equilibrium we get additional constitutive equations; for example the skew-symmetric part of the stress tensor then reads

$$
\begin{aligned}
t^{\mathrm{eq}}_{[jk]} = {} & -\tfrac{1}{4}[\gamma_1+\gamma_2+\tfrac{1}{3}(\gamma_6+\gamma_7+\gamma_8+\gamma_{10}-\gamma_{11}-\gamma_{12})][(\nabla_j\nabla_p a_{pk})^{\mathrm{eq}} - (\nabla_k\nabla_p a_{pj})^{\mathrm{eq}}] \\
& -\tfrac{1}{4}(\gamma_6-\gamma_{12})[a^{\mathrm{eq}}_{oq}(\nabla_j\nabla_q a_{ko})^{\mathrm{eq}} - a^{\mathrm{eq}}_{oq}(\nabla_k\nabla_q a_{jo})^{\mathrm{eq}}] - \tfrac{1}{4}(\gamma_7-\gamma_{11})[a^{\mathrm{eq}}_{jp}(\nabla_p\nabla_q a_{qk})^{\mathrm{eq}} \\
& - a^{\mathrm{eq}}_{kp}(\nabla_p\nabla_q a_{qj})^{\mathrm{eq}}] - \tfrac{1}{4}(\gamma_8+\gamma_{10})[a^{\mathrm{eq}}_{ko}(\nabla_j\nabla_p a_{po})^{\mathrm{eq}} - a^{\mathrm{eq}}_{jo}(\nabla_k\nabla_p a_{po})^{\mathrm{eq}}] \\
& -\tfrac{1}{4}(\gamma_6+\gamma_{10})[\nabla_p a_{ko}\nabla_j a_{op} - \nabla_p a_{jo}\nabla_k a_{op}]^{\mathrm{eq}} \\
& -\tfrac{1}{4}(\gamma_8-\gamma_{12})[\nabla_p a_{po}\nabla_j a_{ko} - \nabla_p a_{po}\nabla_k a_{jo}]^{\mathrm{eq}}. \qquad (22)
\end{aligned}
$$

4. Constitutive equations assuming special ODF

Several simplifications of the constitutive equations may be derived by assuming a special form for the orientation distribution function:

(i) If $f(\cdot)$ is uniaxial (5), we get $a_{ij} = S(d_i d_j = S(d_i d_j - \frac{1}{3}\delta_{ij})$ [8] with S the Maier–Saupe order parameter, yielding

$$
\begin{aligned}
W = {} & ([\beta_1 + \tfrac{1}{3}(\beta_5+\beta_6)] + S[-\tfrac{1}{3}\beta_5 + \tfrac{2}{3}\beta_6])S^2(\nabla_k d_k)(\nabla_j d_j) \\
& + ([\beta_1 + \tfrac{1}{3}(\beta_5+\beta_6) + \beta_3 + \tfrac{1}{3}(\beta_9+\beta_{10})] \\
& + S[\tfrac{2}{3}\beta_5 - \tfrac{1}{3}\beta_6 + 2\beta_7 - \tfrac{1}{3}\beta_9 + \tfrac{2}{3}\beta_{10}])S^2(d_i\nabla_i d_k)(d_j\nabla_j d_k) \\
& + (2[\beta_2 + \tfrac{1}{3}(\beta_7+\beta_8)] + S[-\tfrac{2}{3}\beta_7 + \tfrac{1}{3}\beta_8])S^2(\nabla_j d_k)(\nabla_j d_k) \\
& + ([\beta_3 + \tfrac{1}{3}(\beta_9+\beta_{10})] + S[\tfrac{2}{3}\beta_9 - \tfrac{1}{3}\beta_{10}])S^2(\nabla_j d_k)(\nabla_k d_j) \\
& + (\tfrac{1}{3}[\beta_1 + \tfrac{1}{3}(\beta_5+\beta_6)] + \tfrac{1}{3}[\beta_3 + \tfrac{1}{3}(\beta_9+\beta_{10})] \\
& + S[\tfrac{2}{3}\beta_4 + \tfrac{1}{3}\beta_5 + \tfrac{1}{3}\beta_6 + \tfrac{2}{3}\beta_7 + \tfrac{1}{3}\beta_9 + \tfrac{1}{3}\beta_{10}])(d_i\nabla_i S)(d_j\nabla_j S) \\
& + (\tfrac{4}{3}[\beta_1 + \tfrac{1}{3}(\beta_5+\beta_6)] - \tfrac{2}{3}[\beta_3 + \tfrac{1}{3}(\beta_9+\beta_{10})] \\
& + S[\tfrac{2}{3}\beta_4 + \tfrac{2}{9}\beta_5 + \tfrac{8}{9}\beta_6 + \tfrac{2}{9}\beta_9 - \tfrac{1}{9}\beta_{10}])S(d_i\nabla_i S)(\nabla_j d_j) \\
& + (-\tfrac{2}{3}[\beta_1 + \tfrac{1}{3}(\beta_5+\beta_6)] + \tfrac{4}{3}[\beta_3 + \tfrac{1}{3}(\beta_9+\beta_{10})] \\
& + S[\tfrac{2}{3}\beta_4 - \tfrac{1}{9}\beta_5 + \tfrac{2}{9}\beta_6 + \tfrac{8}{9}\beta_9 + \tfrac{2}{9}\beta_{10}])S(d_i\nabla_i d_j)(\nabla_j S) \\
& + (\tfrac{1}{9}[\beta_1 + \tfrac{1}{3}(\beta_5+\beta_6)] + \tfrac{2}{3}[\beta_2 + \tfrac{1}{3}(\beta_7+\beta_8)] + \tfrac{1}{9}[\beta_3 + \tfrac{1}{3}(\beta_9+\beta_{10})] \\
& + S[-\tfrac{2}{9}\beta_4 - \tfrac{1}{27}\beta_5 - \tfrac{1}{27}\beta_6 - \tfrac{2}{9}\beta_7 + \tfrac{2}{9}\beta_8 - \tfrac{1}{27}\beta_9 - \tfrac{1}{27}\beta_{10}])(\nabla_i S)(\nabla_i S) \qquad (23)
\end{aligned}
$$

for the elastic free energy. Clearly the coefficients in (23) are in their first approximation with respect to S the coefficients $K_1 \ldots K_4$ and $L_1 \ldots L_4$ Ericksen [8] has introduced. This sum of eight terms, each having a factor being linear in S, is determined by 16 coefficients which are not independent of each other because they are composed of the 10 numbers $\beta_1 \ldots \beta_{10}$.

(ii) In the case of total alignment ($S=1$) the elastic free energy reduces to

$$W=(\beta_1+\beta_6)(\nabla_k d_k)(\nabla_j d_j)+(\beta_1+\beta_3+\beta_5+2\beta_7+\beta_{10})(d_i\nabla_i d_k)(d_j\nabla_j d_k)$$
$$+2(\beta_2-\tfrac{1}{3}\beta_7+\tfrac{2}{3}\beta_8)(\nabla_j d_k)(\nabla_j d_k)+(\beta_3+\beta_9)(\nabla_j d_k)(\nabla_k d_j), \qquad (24)$$

which compared to the Frank notation [9]

$$2W=k_{22}(\nabla_j d_i)(\nabla_j d_i)+(k_{11}-k_{22}-k_{24})(\nabla_i d_i)(\nabla_j d_j)$$
$$+(k_{33}-k_{22})(d_i\nabla_i d_k)(d_j\nabla_j d_k)+k_{24}(\nabla_j d_i)(\nabla_i d_j), \qquad (25)$$

leads to

$$\left.\begin{aligned} &k_{11}=2(\beta_1+2\beta_2+\beta_3+\beta_6-\tfrac{2}{3}\beta_7+\tfrac{4}{3}\beta_8+\beta_9), \qquad k_{22}=4(\beta_2-\tfrac{1}{3}\beta_7+\tfrac{2}{3}\beta_8),\\ &k_{24}=2(\beta_3+\beta_9), \qquad k_{33}=2(\beta_1+2\beta_2+\beta_3+\beta_5+\tfrac{4}{3}\beta_7+\tfrac{4}{3}\beta_8+\beta_{10}). \end{aligned}\right\} \qquad (26)$$

(iii) Finally in the one constant approximation we get

$$K_{11}=K_{22}=K_{33}=4\beta_2+\tfrac{8}{3}\beta_8. \qquad (27)$$

5. Conclusions

The main results of the theory presented here may be stated as:

a fully mesoscopic founded theory is presented, introducing quite naturally a second rank alignment tensor [12],

the Ericksen–Leslie theory, as well as the Erickson '91 theory (introducing the Maier–Saupe order parameter) are shown to be special cases (i.e. the case of total alignment and the uniaxial case) of this approach,

the coefficients of the free energy are determined in comparison with the Frank theory,

the Landau condition for equilibrium in liquid crystals can be derived and extended to inhomogeneous alignment,

the couple stress tensor and the stress tensor in equilibrium can be calculated explicitly.

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