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# Satisfaction of the eigenvalue constraints on the Q-tensor

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# The Q-tensor

Consider a nematic liquid crystal consisting of rod-like molecules, whose individual orientations can be described by a pair $\{p, -p\}$ of antipodal unit vectors $p$, or equivalently by matrices $p \otimes p$, $p \in S^2$.

The distribution of molecular orientations in a sufficiently small space-time neighbourhood of a fixed point $(x, t)$ can be described by a probability measure $\mu = \mu_{x,t}$ on the unit sphere $S^2$ satisfying $\mu(E) = \mu(-E)$ for any subset $E \subset S^2$.

The *de Gennes Q-tensor*

$$Q = \int_{S^2} (p \otimes p - \frac{1}{3} 1) \, d\mu(p)$$

measures the deviation of the second moment of $\mu$ from its isotropic value.

Note that $Q = Q^T$, $\operatorname{tr} Q = 0$, $Q \geq -\frac{1}{3}\mathbf{1}$,
so that the minimum eigenvalue of $Q$ satisfies

$$\lambda_{\mathrm{min}}(Q) \geq -\frac{1}{3}.$$

If $\lambda_{\mathrm{min}}(Q) = -\frac{1}{3}$ then for the corresponding eigenvector $e$ of $Q$ we have that

$$\int_{S^2} (p \cdot e)^2 d\mu(p) = 0,$$

so that $\mu$ is supported on the great circle perpendicular to $e$, for example

$$\mu = \frac{1}{2}(\delta_{\widehat{e}} + \delta_{-\widehat{e}}),$$

where $\widehat{e} \cdot e = 0$, corresponding to perfect alignment parallel to $\widehat{e}$.

If such perfect alignment is viewed as unphysical then we expect that

$$-\frac{1}{3} < \lambda_{\mathsf{min}}(Q) \leq \lambda_{\mathsf{max}}(Q) < \frac{2}{3}$$

Question: how are these inequalities to be preserved in the theory?

For statics we typically minimize the total free energy at temperature $T > 0$

$$I(Q,T) = \int_\Omega \psi(Q(x), \nabla Q(x), T)\, dx$$

subject to suitable boundary conditions. The free energy density is usually written as the sum of bulk and elastic terms

$$\psi(Q, \nabla Q, T) = \psi_B(Q,T) + \psi_E(Q, \nabla Q, T).$$

Often the forms

$$\psi_B(Q,T) = \frac{a(T)}{2}\mathrm{tr}\, Q^2 - \frac{b}{3}\mathrm{tr}\, Q^3 + \frac{c}{4}\mathrm{tr}\, Q^4,$$

$$\psi_E(Q, \nabla Q, T) = \sum_{i=1}^{4} L_i I_i$$

are used, where

$$I_1 = Q_{ij,j}Q_{ik,k}, \;\; I_2 = Q_{ik,j}\; Q_{ij,k}$$
$$I_3 = Q_{ij,k}Q_{ij,k}, \;\; I_4 = Q_{lk}Q_{ij,l}Q_{ij,k}$$

where $a(T) = \alpha(T - T^*)$, $T$ is the temperature and $\alpha, T^*, b, c, L_i = L_i(T)$ are constants.

For these forms of $\psi_B, \psi_E$ energy minimizers $Q$ do not in general satisfy the eigenvalue constraints, e.g. for MBBA with experimentally measured coefficients, the scalar order parameter of the nematic state exceeds 1 for temperatures only 7°C below the nematic initiation temperature.

Furthermore we have

**Theorem**

If $L_4 \neq 0$ then for any boundary conditions $I(Q)$ is unbounded below.

We propose that the eigenvalue constraints are satisfied because in a physically correct model

$$\psi_B(Q,T) \to \infty \text{ as } \lambda_{\mathrm{min}}(Q) \to -\frac{1}{3}+ .$$

Such a suggestion was made by Ericksen in the context of his model of nematic liquid crystals.

We show how such an $\psi_B$ can be constructed on the basis of a microscopic model, thus providing a rigorous analysis and development of work of Katriel, J., Kventsel, G. F., Luckhurst, G. R. and Sluckin, T. J.(1986).

# The Onsager model

In the Onsager model the probability measure $\mu$ is assumed to be continuous with density $\rho = \rho(p)$, and the bulk free-energy at temperature $T > 0$ has the form

$$A(\rho, T) = U(\rho) - k_B T \eta(\rho),$$

where the entropy is given by

$$\eta(\rho) = -\int_{S^2} \rho(p) \ln \rho(p) \, dp,$$

and $k_B$ is Boltzmann's constant.

With the Maier-Saupe molecular interaction, the internal energy is given by

$$U(\rho) \;=\; \kappa \int_{S^2} \int_{S^2} [\tfrac{1}{3} - (p \cdot q)^2] \rho(p)\rho(q)\, dp\, dq$$

where $\kappa > 0$ is a coupling constant.

We will assume that $\kappa$ is independent of $T$. If $\kappa$ depends on $T$ (due to steric effects) then the analysis is similar.

Denoting by

$$Q(\rho) = \int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1})\rho(p)\, dp$$

the corresponding $Q$-tensor, we have that

$$\begin{aligned} |Q(\rho)|^2 &= \int_{S^2}\int_{S^2} (p \otimes p - \frac{1}{3}\mathbf{1}) \cdot (q \otimes q - \frac{1}{3}\mathbf{1})\rho(p)\rho(q) dp\, dq \\ &= \int_{S^2}\int_{S^2} [(p \cdot q)^2 - \frac{1}{3}]\rho(p)\rho(q)\, dp\, dq. \end{aligned}$$

Hence $U(\rho) = -\kappa|Q(\rho)|^2$ and

$$A(\rho, T) = k_B T \int_{S^2} \rho(p) \ln \rho(p)\, dp - \kappa|Q(\rho)|^2.$$

Given $Q$ we define

$$\begin{aligned}\psi_B(Q,T) &= \inf_{\{\rho:Q(\rho)=Q\}} A(\rho,T) \\ &= k_B T \inf_{\{\rho:Q(\rho)=Q\}} \int_{S^2} \rho \ln \rho \, dp - \kappa |Q|^2.\end{aligned}$$

Thus we just need to understand how to minimize

$$I(\rho) = \int_{S^2} \rho(p) \ln \rho(p) \, dp$$

subject to $Q(\rho) = Q$.

Given $Q$ with $Q = Q^T, \operatorname{tr} Q = 0$ and satisfying $\lambda_i(Q) > -1/3$ we seek to minimize $I(\rho) = \int_{S^2} \rho(p) \ln \rho(p)\, dp$ on

$$\mathcal{A}_Q = \{\rho \in L^1(S^2) : \rho \geq 0, Q(\rho) = Q\}.$$

Remarks: Note that for $\rho \in \mathcal{A}_Q$ the constraint

$$\int_{S^2} \rho(p)\, dp = 1$$

follows from $\operatorname{tr} Q(\rho) = 0$. Also we do not impose the condition $\rho(p) = \rho(-p)$, since it turns out that the minimizer in $\mathcal{A}_Q$ satisfies this condition automatically.

**Lemma.** $\mathcal{A}_Q$ is nonempty.

*Sketch of proof.* We can suppose that $Q = \text{diag}\,(\lambda_1, \lambda_2, \lambda_3)$. The singular measure

$$\mu(p) = \frac{1}{2}\sum_{i=1}^{3}\left(\lambda_i - \frac{1}{3}\right)(\delta_{e_i} + \delta_{-e_i})$$

satisfies $\int_{S^2}\left(p \otimes p - \frac{1}{3}\mathbf{1}\right)\, d\mu(p) = Q$ and can be approximated by an $L^1$ function $\rho$ satisfying $Q(\rho) = Q$.

*Theorem.* $I$ attains a minimum at a unique $\rho_Q \in \mathcal{A}_Q$.

# The Euler-Lagrange equation for I

*Theorem.* Let $Q = \text{diag}\,(\lambda_1, \lambda_2, \lambda_3)$. Then

$$\rho_Q(p) = \frac{\exp(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2)}{Z(\mu_1, \mu_2, \mu_3)},$$

where

$$Z(\mu_1, \mu_2, \mu_3) = \int_{S^2} \exp(\mu_1 p_1^2 + \mu_2 p_2^2 + \mu_3 p_3^2)\, dp.$$

The $\mu_i$ (unique up to adding a constant to each) solve the equations

$$\frac{\partial \ln Z}{\partial \mu_i} = \lambda_i + \frac{1}{3}, \quad i = 1, 2, 3.$$

The existence can be proved via the direct method of the calculus of variations, and then it can be shown that the unique minimizer satisfies the corresponding Euler-Lagrange equation, the $\mu_i$ appearing as Lagrange multipliers. However, this is a bit tricky because of the possibility that the minimizer $\rho$ is not bounded away from zero. A quicker proof is to use a 'dual' variational principle for $\mu = (\mu_1, \mu_2, \mu_3)$ (cf Mead & Papanicolaou 1984).

Write $\gamma_i = \lambda_i + \frac{1}{3}$, so that $\gamma_i > 0, \sum_{j=1}^{3} \gamma_j = 1$, and $\gamma = (\gamma_1, \gamma_2, \gamma_3)$. For $\nu \in \mathbb{R}^3$ let

$$J(\nu) = \gamma \cdot \nu - \ln Z(\nu).$$

Note that if $m = (1, 1, 1)$ then for any $\tau \in \mathbb{R}$

$$\begin{aligned} J(\nu + \tau m) &= \gamma \cdot \nu + \tau - \ln \int_{S^2} \exp\left( \sum_{i=1}^{3} \nu_i p_i^2 + \tau \right) d \\ &= \gamma \cdot \nu - \ln Z(\nu) = J(\nu), \end{aligned}$$

so that it is sufficient to consider $J(\nu)$ for $\nu$ with $\nu \cdot m = 0$.

Consider the problem

$$\max_{\mu\in\mathbb{R}^3} J(\mu),$$

or equivalently

$$\max_{\nu\in m^\perp} J(\nu),$$

where $m^\perp = \{\nu \in \mathbb{R}^3 : \nu \cdot m = 0\}$.

**Lemma.** $J(\nu)$ is a strictly concave function on $m^\perp$ with $J(\nu) \to -\infty$ as $|\nu| \to \infty$, and hence attains a unique maximum on $m^\perp$.

*Proof.* If $a \cdot m = 0$ then a calculation shows that

$$\frac{\partial^2 \ln Z(\mu)}{\partial \mu_i \partial \mu_j} a_i a_j = \frac{1}{2Z(\mu)^2} \int_{S^2} \int_{S^2} \left( \sum_{i=1}^{3} a_i (p_i^2 - q_i^2) \right)^2 \exp\left( \sum_{k=1}^{3} \mu_k (p_k^2 + q_k^2) \right) dp\, dq.$$

To prove that $J(\nu) \to -\infty$ as $|\nu| \to \infty$ it suffices to prove that $\exp(-J(\nu)) \to \infty$. But

$$\exp(-J(\nu)) = \int_{S^2} \exp\left(\sum_{i=1}^{3} \nu_i (p_i^2 - \gamma_i)\right) dp$$

and

$$\begin{aligned}\sum_{i=1}^{3} \nu_i (p_i^2 - \gamma_i) &= \nu_1 (2p_1^2 + p_2^2 - 2\gamma_1 - \gamma_2) \\ &\quad + \nu_2 (2p_2^2 + p_1^2 - 2\gamma_2 - \gamma_1).\end{aligned}$$

The result follows by examining the sets of $p \in S^2$ where the two quantities in brackets are positive and negative.

Given a maximizer $\mu$ of $J$ we have that $\nabla_\mu J(\mu) = 0$, that is

$$\frac{\nabla_\mu Z(\mu)}{Z(\mu)} = \gamma,$$

expressing the fact that

$$\rho_Q(p) = \frac{\exp\left(\sum_{i=1}^{3} \mu_i p_i^2\right)}{Z(\mu)}$$

satisfies $Q(\rho) = Q$.

Now let $\rho \in \mathcal{A}_Q$, $\rho \neq \rho_Q$. Then by the strict convexity of $\rho \ln \rho$ we have that

$$\begin{aligned} I(\rho) &= \int_{S^2} \rho \ln \rho \, dp \\ &> \int_{S^2} [\rho_Q \ln \rho_Q + \\ &\qquad (\rho - \rho_Q)(1 + \sum_{i=1}^{3} \mu_i p_i^2 - \ln Z(\mu))] \, dp \\ &= I(\rho_Q), \end{aligned}$$

so that $\rho_Q$ is the unique global minimizer.

Note that we have the dual extremum result

$$\min_{\rho \in \mathcal{A}_Q} I(\rho) = \max_{\mathbb{R}^3} J(\mu),$$

whereas the usual Lagrange duality principle (cf Borwein & Lewis 1991) is

$$\min_{\rho \in \mathcal{A}_Q} I(\rho) = \max_{\mathbb{R}^3} \hat{J}(\mu),$$

where

$$\hat{J}(\mu) = \gamma \cdot \mu - \int_{S^2} \exp\Big(\sum_{i=1}^{3} \mu_i p_i^2 - 1\Big)\, dp \leq J(\mu).$$

Let $f(Q) = I(\rho_Q) = \inf_{\rho \in \mathcal{A}_Q} I(\rho)$, so that

$$\psi_B(Q,T) = Tf(Q) - \kappa |Q|^2.$$

Hence the bulk free energy has the form

$$\psi_B(Q,T) = k_B T \left( \sum_{i=1}^{3} \mu_i (\lambda_i + \frac{1}{3}) - \ln Z(\mu) \right) - \kappa \sum_{i=1}^{3} \lambda_i^2.$$

## Theorem

$f$ is strictly convex in $Q$ and

$$\lim_{\lambda_{\min}(Q)\to -\frac{1}{3}+} f(Q) = \infty.$$

*Proof*

The strict convexity of $f$ follows from that of $\rho \ln \rho$. Suppose that $\lambda_{\min}(Q^{(j)}) \to -\frac{1}{3}$ but $f(Q^{(j)})$ remains bounded. Then

$$Q^{(j)}e^{(j)}\cdot e^{(j)} + \frac{1}{3}|e^{(j)}|^2 = \int_{S^2} \rho_{Q^{(j)}}(p)(p\cdot e^{(j)})^2 dp \to 0,$$

where $e^{(j)}$ is the eigenvector of $Q^{(j)}$ corresponding to $\lambda_{\min}(Q^{(j)})$.

But we can assume that $\rho_{Q(j)} \rightharpoonup \rho$ in $L^1(S^2)$, where $\int_{S^2} \rho(p)\,dp = 1$ and that $e^{(j)} \to e$, $|e| = 1$. Passing to the limit we deduce that

$$\int_{S^2} \rho(p)(p \cdot e)^2 dp = 0.$$

But this means that $\rho(p) = 0$ except when $p \cdot e = 0$, contradicting $\int_{S^2} \rho(p)\,dp = 1$. $\square$

# Asymptotics

**Theorem**

$$C_1 - \frac{1}{2}\ln(\lambda_{\min}(Q) + \frac{1}{3}) \le f(Q) \le C_2 - \ln(\lambda_{\min}(Q) + \frac{1}{3})$$

for constants $C_1, C_2$.

The proof uses our initial construction of a function $\rho \in \mathcal{A}_Q$ to get the upper bound, and the dual variational principle to get the lower bound.

# Other predictions

1. All stationary points uniaxial and phase transition predicted from isotropic to uniaxial nematic phase just as in the quartic model.

2. Minimizers $\rho^*$ of $A(\rho, T)$ correspond to minimizers over $Q$ of $\psi_B(Q, T)$. These $\rho^*$ were calculated and shown to be uniaxial by Fatkullin and Slastikov (2005), and by Liu, Zhang & Zhang (2005).

3. Existence when $L_4 \neq 0$ under suitable inequalities on the $L_i$, because $I_4 = Q_{lk}Q_{ij,l}Q_{ij,k} \geq -\frac{1}{3}|\nabla Q|^2$.

4. Near $Q = 0$ we have (see also Katriel *et al*) the expansion

$$\frac{1}{Tk_B}\psi_B(Q,T) = \ln 4\pi + \left(\frac{15}{4} - \frac{\kappa}{2Tk_B}\right)\mathrm{tr}\, Q^2 - \frac{225}{42}\mathrm{tr}\, Q^3 + \frac{225}{112}(\mathrm{tr}\, Q^2)^2 + \dots$$

The ratio of the coefficients of the last two terms gives $\frac{b}{c} = 2$, while experimental values reported in the literature are for MBBA 1.19, and for 5CB 0.82.

Given appropriate boundary conditions, do minimizers of

$$I(Q) = \int_\Omega [\psi_B(Q) + \psi_E(Q, \nabla Q)]\, dx$$

have eigenvalues which are *bounded away from* $-\frac{1}{3}$, i.e. for some $\varepsilon > 0$

$$-\frac{1}{3} + \varepsilon \leq \lambda_{\text{min}}(Q(x)) < \frac{2}{3} - \varepsilon \text{ for a.e. } x \in \Omega?$$

If not, this would mean that a minimizer of $I$ would have an unbounded integrand. Surely this is inconsistent with being a minimizer ....

## Theorem

Let $Q$ minimize

$$I(Q) = \int_{\Omega} [\psi_B(Q) + K|\nabla Q|^2] \, dx,$$

subject to $Q(x) = Q_0(x)$ for $x \in \partial\Omega$, where $K > 0$ and $Q_0(\cdot)$ is sufficiently smooth with $\lambda_{\mathrm{min}}(Q_0(x)) > -\frac{1}{3}$. Then

$$\lambda_{\mathrm{min}}(Q(x)) > -\frac{1}{3} + \varepsilon,$$

for some $\varepsilon > 0$ and $Q$ satisfies the Euler-Lagrange equation.

Proof: Project onto the convex set

$$K = \{Q : f(Q) \leq M\}$$

for large $M$. It can be shown that this reduces *both* terms in the integral.

**Open problem.** Prove this for the case of three or more elastic constants. The above method does not work. In the three elastic constant case Evans & Tran prove partial regularity, but not $\lambda_{\text{min}}(Q(x)) > -\frac{1}{3} + \varepsilon$.

# Dynamics

Using our bulk energy $\psi_B(Q)$

M. Wilkinson, *Strict Physicality of Global Weak Solutions of a Navier-Stokes Q-tensor System with Singular Potential* (2012)

shows that for the corresponding Beris & Edwards equation (one elastic constant) the eigenvalue bounds are satisfied instantaneously in time.