

Landau-de Gennes free energy weak form

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1 Introduction

Here we will use an isotropic elasticity Landau-de Gennes free energy in order to come up with an Euler-Lagrange equation for a liquid crystal system.

2 Free energy and equation of motion

The free energy is given by:

$$f(Q_{ij}, \nabla Q_{ij}) = \frac{1}{2} A Q_{ij} Q_{ji} + \frac{1}{3} B Q_{ij} Q_{jk} Q_{ki} + \frac{1}{4} C (Q_{ij} Q_{ji})^2 + \frac{1}{2} L \partial_i Q_{jk} \partial_i Q_{jk} \quad (1)$$

Given the free energy, the Euler-Lagrange equations are given by:

$$\partial_t Q_{ij} = -\frac{\partial f}{\partial Q_{ij}} + \partial_k \frac{\partial f}{\partial (\partial_k Q_{ij})} \quad (2)$$

However, if we evolve the system according to this equation, Q will not necessarily remain symmetric and traceless. Hence, we have to use a Lagrange multiplier scheme which takes the form:

$$\partial_t Q_{ij} = -\frac{\partial f}{\partial Q_{ij}} + \partial_k \frac{\partial f}{\partial (\partial_k Q_{ij})} - \lambda \delta_{ij} - \lambda_k \epsilon_{kij} \quad (3)$$

for λ and λ_k appropriately chosen to make Q remain traceless and symmetric respectively. We do this one term at a time. Start with A :

$$\begin{aligned} -\frac{\partial}{\partial Q_{ij}} \frac{1}{2} A Q_{kl} Q_{lk} \\ &= -\frac{1}{2} A [\delta_{ik} \delta_{jl} Q_{lk} + Q_{lk} \delta_{ik} \delta_{jl}] \\ &= -A Q_{ij} \end{aligned} \quad (4)$$

Go to B :

$$\begin{aligned} -\frac{\partial}{\partial Q_{ij}} \frac{1}{3} B Q_{kl} Q_{lm} Q_{mk} &= -\frac{1}{3} B [\delta_{ik} \delta_{jl} Q_{lm} Q_{mk} + Q_{kl} \delta_{il} \delta_{jm} Q_{mk} + Q_{kl} Q_{lm} \delta_{im} \delta_{jk}] \\ &= -B Q_{im} Q_{mj} \end{aligned} \quad (5)$$

Now for C :

$$\begin{aligned} -\frac{\partial}{\partial Q_{ij}} \frac{1}{4} C (Q_{kl} Q_{lk})^2 &= -\frac{1}{2} C (Q_{kl} Q_{lk}) [\delta_{ik} \delta_{jl} Q_{lk} + Q_{kl} \delta_{il} \delta_{jk}] \\ &= -C Q_{ij} (Q_{kl} Q_{lk}) \end{aligned} \quad (6)$$

The elasticity (L) term:

$$\begin{aligned}\partial_k \frac{\partial}{\partial(\partial_k Q_{ij})} \frac{1}{2} L \partial_l Q_{mn} \partial_l Q_{mn} &= \frac{1}{2} L \partial_k [\delta_{kl} \delta_{im} \delta_{jn} \partial_l Q_{mn} + \partial_l Q_{mn} \delta_{kl} \delta_{im} \delta_{jn}] \\ &= L \partial_k^2 Q_{ij}\end{aligned}\quad (7)$$

Then the full equation of motion is given by:

$$\partial_t Q_{ij} = L \partial_k^2 Q_{ij} - A Q_{ij} - B Q_{im} Q_{mj} - C Q_{ij} (Q_{kl} Q_{lk}) - \lambda \delta_{ij} - \lambda_k \epsilon_{kij} \quad (8)$$

To find the Lagrange multipliers, first take the trace of $\partial_t Q_{ij}$:

$$\begin{aligned}\partial_t Q_{ii} &= L \partial_k^2 Q_{ii} - A Q_{ii} - B Q_{im} Q_{mi} - C Q_{ii} (Q_{kl} Q_{lk}) - \lambda \delta_{ii} - \lambda_k \epsilon_{kii} \\ &= -B Q_{im} Q_{mi} - 3\lambda \\ &= 0\end{aligned}\quad (9)$$

where we have used that $\epsilon_{kii} = 0$ is a property of the Levi-Civita tensor, and $\delta_{ii} = 3$ (one can work this out easily). From this we calculate:

$$\lambda = \frac{B}{3} Q_{nm} Q_{nm} \quad (10)$$

Additionally, one can work out that the right-hand side of the equation of motion is symmetric if $\lambda_k = 0$, so the final equation of motion is:

$$\partial_t Q_{ij} = L \partial_k^2 Q_{ij} - A Q_{ij} - B Q_{im} Q_{mj} - C Q_{ij} (Q_{kl} Q_{lk}) - \frac{B}{3} (Q_{kl} Q_{lk}) \delta_{ij} \quad (11)$$

Given the discussion in the **maier-saupe-weak-form** document, we may index the degrees of freedom of Q by an index ρ in the following way:

$$Q_{ij} = \begin{bmatrix} Q_1 & Q_2 & Q_3 \\ Q_2 & Q_4 & Q_5 \\ Q_3 & Q_5 & -(Q_1 + Q_4) \end{bmatrix} \quad (12)$$

$$\partial_t Q_\rho = L \nabla^2 Q_\rho - A Q_\rho - B Q_{i(\rho)m} Q_{mj(\rho)} - C Q_\rho (Q_{kl} Q_{lk}) \quad (13)$$

3 Steady state solution and Newton's method

For a steady state system, the time derivative is zero. In this case, we can define the right side as a residual:

$$F_\rho(Q) = L \nabla^2 Q_\rho - A Q_\rho - B Q_{i(\rho)m} Q_{mj(\rho)} - C Q_\rho (Q_{kl} Q_{lk}) \quad (14)$$

We can take the Gateaux derivative of this residual to get the following:

$$\begin{aligned}F'_{\rho\sigma} \delta Q_\sigma &= L \nabla^2 \left(\frac{\partial Q_\rho}{\partial Q_\sigma} \delta Q_\sigma \right) - A \frac{\partial Q_\rho}{\partial Q_\sigma} \delta Q_\sigma \\ &\quad - B \frac{\partial Q_{i(\rho)m}}{\partial Q_\sigma} Q_{mj(\rho)} \delta Q_\sigma - B Q_{i(\rho)m} \frac{\partial Q_{mj(\rho)}}{\partial Q_\sigma} \delta Q_\sigma \\ &\quad - C \frac{\partial Q_\rho}{\partial Q_\sigma} (Q_{kl} Q_{lk}) \delta Q_\sigma - C Q_\rho \frac{\partial Q_{kl}}{\partial Q_\sigma} Q_{lk} \delta Q_\sigma - C Q_\rho Q_{kl} \frac{\partial Q_{lk}}{\partial Q_\sigma} \delta Q_\sigma \\ &= L \nabla^2 \delta Q_\rho - A \delta Q_\rho \\ &\quad - B (M_{i(\rho)m\sigma} Q_{mj(\rho)} + Q_{i(\rho)m} M_{mj(\rho)\sigma}) \delta Q_\sigma \\ &\quad - C Q_{kl} Q_{lk} \delta Q_\rho - 2C Q_\rho Q_{kl} M_{kl\sigma} \delta Q_\sigma\end{aligned}\quad (15)$$

where we have defined

$$M_{kl\sigma} = \frac{\partial Q_{kl}}{\partial Q_\sigma} \quad (16)$$

And then $i(\rho)$ and $j(\rho)$ are functions which return the column and row indices, respectively, corresponding to a degree of freedom indexed by ρ . Note that, for a fixed σ , M_{kl} just corresponds to the ρ th 3×3 basis vector in Q -tensor space. We can write this out as follows:

$$F'(Q)\delta Q = L\nabla^2\delta Q - A\delta Q - B\mathcal{B}\delta Q - CQ_{kl}Q_{lk}\delta Q - C\mathcal{C}\delta Q \quad (17)$$

where we have defined:

$$\mathcal{B} = \begin{bmatrix} 2Q_1 & 2Q_2 & 2Q_3 & 0 & 0 \\ Q_2 & Q_1 + Q_4 & Q_5 & Q_2 & Q_3 \\ 0 & Q_5 & -Q_4 & -Q_3 & Q_2 \\ 0 & 2Q_2 & 0 & 2Q_4 & 2Q_5 \\ -Q_5 & Q_3 & Q_2 & 0 & -Q_1 \end{bmatrix} \quad (18)$$

and

$$\mathcal{C} = \begin{bmatrix} Q_1(2Q_1 + Q_4) & 2Q_1Q_2 & 2Q_1Q_3 & Q_1(Q_1 + 2Q_4) & 2Q_1Q_5 \\ Q_2(2Q_1 + Q_4) & 2Q_2^2 & 2Q_2Q_3 & Q_2(Q_1 + 2Q_4) & 2Q_2Q_5 \\ Q_3(2Q_1 + Q_4) & 2Q_2Q_3 & 2Q_3^2 & Q_3(Q_1 + 2Q_4) & 2Q_3Q_5 \\ Q_4(2Q_1 + Q_4) & 2Q_2Q_4 & 2Q_3Q_4 & Q_4(Q_1 + 2Q_4) & 2Q_4Q_5 \\ Q_5(2Q_1 + Q_4) & 2Q_2Q_5 & 2Q_3Q_5 & Q_5(Q_1 + 2Q_4) & 2Q_5^2 \end{bmatrix} \quad (19)$$

Given this, Newton's method reads:

$$F'(Q^n)\delta Q^n = -F(Q^n) \quad (20)$$

$$Q^{n+1} = Q^n + \delta Q^n \quad (21)$$

Now we must find the weak form of this equation. Integrating against a test function ϕ gives:

$$\begin{aligned} L\langle\phi, \nabla^2\delta Q\rangle - A\langle\phi, \delta Q\rangle - B\langle\phi, \mathcal{B}\delta Q\rangle \\ - CQ_{kl}Q_{lk}\langle\phi, \delta Q\rangle - C\langle\phi, \mathcal{C}\delta Q\rangle = -L\langle\phi, \nabla^2Q\rangle + A\langle\phi, Q\rangle \\ + B\langle\phi, Q_{i(\rho)m}Q_{mj(\rho)}\rangle + C\langle\phi, Q(Q_{kl}Q_{lk})\rangle \end{aligned} \quad (22)$$

Integrating by parts and setting the test functions to be zero at the boundary (since we are assuming Dirichlet boundary conditions) we get:

$$\begin{aligned} -L\langle\nabla\phi, \nabla\delta Q\rangle - A\langle\phi, \delta Q\rangle - B\langle\phi, \mathcal{B}\delta Q\rangle \\ - CQ_{kl}Q_{lk}\langle\phi, \delta Q\rangle - C\langle\phi, \mathcal{C}\delta Q\rangle = L\langle\nabla\phi, \nabla Q\rangle + A\langle\phi, Q\rangle \\ + B\langle\phi, Q_{i(\rho)m}Q_{mj(\rho)}\rangle + C\langle\phi, Q(Q_{kl}Q_{lk})\rangle \end{aligned} \quad (23)$$

Indexing the test functions by i and then rewriting the variation as a sum of solution functions, we get:

$$\begin{aligned} \sum_j [-L\langle\nabla\phi_i, \nabla\phi_j\rangle - A\langle\phi_i, \phi_j\rangle \\ - B\langle\phi_i, \mathcal{B}\phi_j\rangle - CQ_{kl}Q_{lk}\langle\phi_i, \phi_j\rangle - C\langle\phi_i, \mathcal{C}\phi_j\rangle]\delta Q_j = L\langle\nabla\phi_i, \nabla Q\rangle + A\langle\phi_i, Q\rangle \\ + B\langle\phi_i, Q_{i(\text{comp}(i))m}Q_{mj(\text{comp}(i))}\rangle \\ + C\langle\phi_i, Q(Q_{kl}Q_{lk})\rangle \end{aligned} \quad (24)$$

We may rewrite this as a matrix equation given by:

$$A_{ij}\delta Q_j = b_i \quad (25)$$

where we have defined:

$$A_{ij} = -[L\langle\nabla\phi_i, \nabla\phi_j\rangle + (A + CQ_{lk}Q_{lk})\langle\phi_i, \phi_j\rangle + \langle\phi_i, (B\mathcal{B} + C\mathcal{C})\phi_j\rangle] \quad (26)$$

$$b_i = L\langle\nabla\phi_i, \nabla Q\rangle + A\langle\phi_i, Q\rangle + B\langle\phi_i, Q_{i(\text{comp}(i))m}Q_{mj(\text{comp}(i))}\rangle + C\langle\phi_i, Q(Q_{kl}Q_{lk})\rangle \quad (27)$$