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:

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

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

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

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:

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

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:

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

Go to B:

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

Now for C:

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

The elasticity (L) term:

$$\partial_k \frac{\partial}{\partial(\partial_k Q_{ij})} \tfrac{1}{2} L \partial_l Q_{mn} \partial_l Q_{mn} = \tfrac{1}{2} L \partial_k \left[\delta_{kl} \delta_{im} \delta_{jn} \partial_l Q_{mn} + \partial_l Q_{mn} \delta_{kl} \delta_{im} \delta_{jn} \right] \\ = L \partial_k^2 Q_{ij} \tag{7}$$

Then the full equation of motion is given by:

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

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

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

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:

$$\lambda = -\frac{B}{3} Q_{nm} Q_{nm} \tag{10}$$

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:

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

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:

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

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

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:

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

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

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

where we have defined

$$M_{kl\sigma} = \frac{\partial Q_{kl}}{\partial Q_\sigma} \tag{16}$$

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 ρth 3×3 basis vector in Q-tensor space. We can write this out as follows:

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

where we have defined:

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

and

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

Given this, Newton's method reads:

$$F'(Q^n)\delta Q^n = -F(Q^n) \tag{20}$$

$$Q^{n+1} = Q^n + \delta Q^n \tag{21}$$

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

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

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

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

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

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

We may rewrite this as a matrix equation given by:

$$A_{ij}\delta Q_j = b_i \tag{25}$$

where we have defined:

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

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