Energy driven systems from Liquid Crystals and Epitaxy

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A nice piece of technology...

- Lots of silicon
- Liquid Crystal Display

Epitaxy models:

- with elastic forces on vicinal surfaces: the $1+1$ dimensional case,
- with elastic forces on vicinal surfaces: the $2+1$ dimensional case,
- with wetting,
- attachment-detachment regime, and many, many others...

Nematic Liquid Crystals:

- Landau-De Gennes model.

Q: What do they have in common?
A1: All of these are governed by highly irregular PDEs...
A2: All these are **variational**.

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Gradient flows in non reflexive spaces

Burton-Cabrera-Frank (BCF) type models

$$\dot{x}_i = \frac{D}{ka^2}\left(\frac{\mu_{i+1}-\mu_i}{x_{i+1}-x_i+\frac{D}{k}} - \frac{\mu_i-\mu_{i-1}}{x_i-x_{i-1}+\frac{D}{k}}\right), \text{ for } 1 \le i \le N.$$

where

- D is the terrace diffusion constant,
- k is the hopping rate of an adatom to the upward or downward step,
- μ is the chemical potential

Attachment-detachment-limited (ADL) regime

the diffusion across the terraces is fast, i.e. $\frac{D}{k} \gg x_{i+1} - x_i$, so the dominated processes are the exchange of atoms at steps edges, i.e., attachment and detachment. The step-flow ODE in ADL regime becomes

$$\dot{x}_i = \frac{1}{a^2}\left(\mu_{i+1} - 2\mu_i + \mu_{i-1}\right), \text{ for } 1 \leq i \leq N.$$

- step slope as a new variable is a convenient way to derive the continuum PDE model (Al Hajj Shehadeh, Kohn and Weare, 2011)

Evolution equation

$$u_t = -u^2(u^3)_{hhhh}, \quad u(0) = u_0.$$

If we take $w_{hh} + c_0 = 1/u$:

$$w_t = (w_{hh} + c_0)^{-3}_{hh},$$

with proper, convex, lower semicontinuous energy

$$\phi(w) := \frac{1}{2}\int_0^1 (w_{hh} + c_0)^{-2} dh.$$

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- the "natural" functional space is $W^{2,1}(0,1)''$... not $H^2(0,1)$ (or any $W^{2,p}(0,1)$ with $p \geq 1$)... otherwise lack of coercivity means

$$J + \varepsilon\xi, \qquad \xi \in \partial\phi$$

  is **not** surjective...
- the "natural" convergence on w_{hh} is the weak-* convergence of Radon measures...

Also...

- Subdifferential of

$$\phi(w) = \frac{1}{2}\int_0^1 (w_{hh} + c_0)^{-2}\,dh\ldots$$

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So

$$\phi(w) = \frac{1}{2}\int_0^1 (w_{hh} + c_0)^{-2} dh$$

is more like

$$\phi(w) = \frac{1}{2}\int_0^1 (w_{hh_{||}} + c_0)^{-2} dh...$$

And

$$\partial\phi(w) = -(w_{hh_{||}} + c_0)^{-3} + \text{singular measures}$$

Set

$$E(w) := \frac{1}{2}\int_0^1 [(w_{hh}+c_0)^{-3}]_{hh}^2 dh = \int_0^1 w_t^2 dh$$

and note:

$$\begin{aligned}\frac{dE(w)}{dt} &= \int_0^1 [(w_{hh}+c_0)^{-3}]_{hh}[(w_{hh}+c_0)^{-3}]_{hht} dh \\ &= \int_0^1 -3\frac{[(w_{hh}+c_0)_t]^2}{(w_{hh}+c_0)^4} dh \leq 0,\end{aligned}$$

and

$$\frac{d}{dt}\int_0^1 (w_{hh}+c_0) dh = \int_0^1 [(w_{hh}+c_0)^{-3}]_{hhhh} dh = 0,$$

And note there is bound on

$$\int_0^1 [w_{hh} + c_0] dh$$

hence there is an invariant ball of the form $\{\|w_h\|_{BV} \leq C\}$...

So consider the evolution equation

$$w_t \in -\partial\phi(w) - \partial\psi(w), \qquad \psi(w) := \chi_{\{\|w_h\|_{BV} \leq C\}}$$

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Gao, Liu, L., Xu, 2018

Given $T > 0$, initial data $w^0 \in D(B)$, there exists a strong solution w of

$$w_t = (\eta_{hh} + c_0)^{-3}_{hh},$$

for a.e. $(t,h) \in [0,T] \times [0,1]$. Besides, we have $((\eta_{hh} + c_0)^{-3})_{hh} \in L^\infty([0,T]; L^2(0,1))$ and the dissipation inequality

$$E(t) := \frac{1}{2}\int_0^1 \left[((\eta_{hh} + c_0)^{-3})_{hh}\right]^2 dh \le E(0),$$

where η_{hh} is the absolutely continuous part of w_{hh}.

However, w_{hh} might have singular parts... (Liu and Xu, Ji and Witelski)

Similarly, the multidimensional model

$$u_t = \Delta e^{-\Delta u}$$

can be treated with the same techniques:

Gao, Liu, L., 2017

Given $T > 0$, initial data u^0, there exists a strong solution w of

$$u_t = \Delta e^{-\Delta u},$$

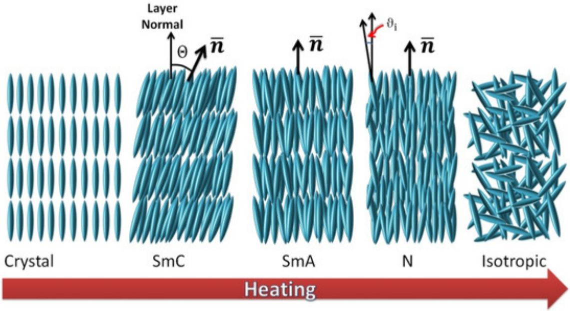
for a.e. $(t, h) \in [0, T] \times \Omega$. Moreover,

$$(\Delta e^{-\Delta u})_{\|} \in L^2(0, T; L^2(\Omega)).$$

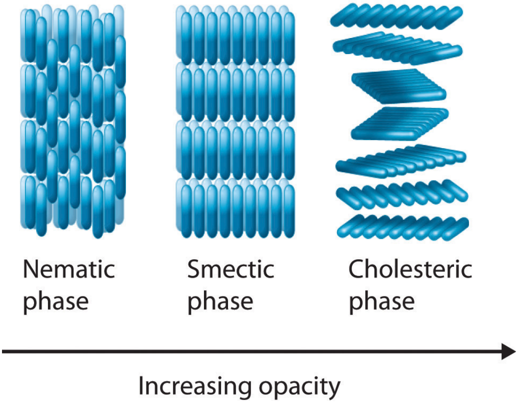
However, Δu might have singular parts... (Ji and Witelski)

Nematic Liquid Crystals

Liquid crystals (LC): a state of the matter between crystalline and liquid...



Different states of LC:



Landau-De Gennes theory for nematic liquid crystals: the evolution is driven by the energy of the form

$$E[Q] := \int F(\nabla Q(x), Q(x))dx - \kappa \|Q\|^2_{L^2(\Omega)},, \qquad \kappa > 0$$

Q varies in the Q-tensor space

$$S^{(d)} := \{\text{symmetric, trace free matrices of } \mathbb{R}^{d \times d}\}.$$

Interesting case $d = 3$.

Energy

$$F = F_{el} + F_{BM},$$

where

$$F_{el}(\nabla Q) := \sum_{i,j,k=1}^{d} \left[L_1 |Q^{ij}_{x_k}|^2 + L_2 Q^{ik}_{x_j} Q^{ij}_{x_k} + L_3 Q^{ij}_{x_j} Q^{ik}_{x_k} \right], \; L_1 \gg L_2, L_3$$

$$F_{BM}(Q) := \inf_{\rho \in A_Q} \int_{S^2} \rho(p) \log \rho(p) dp \qquad \text{(Ball \& Majumdar, 2009)}$$

$$A_Q := \left\{ \rho : S^2 \longrightarrow \mathbb{R} : \rho \geq 0, \int_{S^2} \rho dx = 1, \int_{S^2} \rho(x) \left[x \otimes x - id/3 \right] dx = Q \right\}.$$

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About $F_{BM}(Q)$:

- well defined
- convex and isotropic
- log speed asymptote if any eigenvalue of Q approaches $-1/3, 2/3$
- smooth in its effective domain

Energy

$$E[Q] = \int F_{el}(\nabla Q) + F_{BM}(Q)dx - \kappa \|Q\|^2_{L^2(\Omega)}, \qquad \kappa > 0$$

satisfies

- Boundedness from below: $\inf E > -\infty$ since convex functions are bounded from below, and $\|Q\|^2_{L^2(\Omega)}$ is also bounded due to requirement that all eigenvalues of Q are in $(-1/3, 2/3)$.
- Lower semicontinuity: consider a sequence $Q_n \to Q$ strongly: we have then

$$\liminf_{n \to +\infty} E(Q_n) \geq E(Q).$$

- λ-convexity along segments, with $\lambda = -2\kappa$: we have indeed

$$E((1-t)Q + tP) \leq (1-t)E(Q) + tE(P) + \kappa t(1-t)\|Q - P\|^2_{L^2(\Omega)}.$$

Existence and regularity

For any initial datum $Q_0 \in \overline{D(E)}$ there exists a unique function Q such that:

- Regularizing effect: Q is locally Lipschitz regular, and $Q(t) \in D(|\partial E|) \subseteq D(E)$ for all $t > 0$. In particular, all eigenvalues of Q stay in $(-1/3, 2/3)$ for a.e. x and all $t > 0$.
- Variational inequality: Q is the unique solution of the evolution variational inequality

$$\frac{1}{2}\frac{d}{dt}\|Q(t) - P\|^2_{L^2(\Omega)} - \kappa\|Q(t) - P\|^2_{L^2(\Omega)} + E(Q(t)) \leq E(P)$$

among all the locally absolutely continuous curves such that $Q(t) \to Q_0$ as $t \downarrow 0^+$.

More properties:

- Exponential semigroup formula: $Q(t) = \lim_{n\to+\infty} J^n_{t/n}(Q_0)$, with J denoting the resolvent

$$X \in J_\tau(Y) \iff X \in \operatorname{argmin}\left(E(\cdot) + \frac{1}{2\tau}\|Y - \cdot\|^2_{L^2(\Omega)}\right).$$

- Contraction semigroup: for initial data $Q_0, P_0 \in \overline{D(E)}$, the corresponding solutions Q, P satisfy

$$\|Q(t) - P(t)\|_{L^2(\Omega)} \leq e^{2\kappa t}\|Q_0 - P_0\|_{L^2(\Omega)}.$$

This is not enough... Physicality fails if eigenvalues reach $-1/3, 2/3$ **anywhere**...

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Main result (Liu, L. and Xu, 2018)

There exists some time $T_0 > 0$ such that all eigenvalues of $Q(t)$ are uniformly bounded away from $-1/3, 2/3$ for all $t > T_0$.

AGS gives more or less

$$-\Delta Q(t) + F'_{BM}(Q(t)) + \xi(Q(t)) \in L^2(0, T; L^2(\Omega)).$$

Issues:

- $\Delta Q(t) + F'_{BM}(Q(t)) \in L^2(\Omega)$ does not give $\Delta Q(t) \in L^2(\Omega)$... (Not enough regularity)
- $\xi(Q(t))$ perturbation of Laplacian destroys any comparison/maximum principle... (So no way to follow $L^1 \to L^\infty$ arguments from [Constantin, Kiselev, Ryzhik, Zlatoš, 2008])

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Main arguments:

1. Approximate F_{BM} with F_n, and analyze the gradient flow of $E_n := F_{el} + F_n$.
2. Use the Γ-convergence to infer convergence of gradient flows.
3. Achieve $\Delta Q(t) \in L^2(0, T; L^2(\Omega))$.
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Thank you for your attention!