Implementation details and non-dimensionalization

1 Full version with projection operators

This is the main version of the code and structs are designed for this, below is also a description of the one constant approximation version which uses some of the fields from below for its variables. Here I use:

$$
\begin{aligned}
f_{\text{bulk}} &= AE_{ij}E^*_{ij} + \frac{C}{2}(E_{ij}E^*_{ij})^2 && (1)\\
f_{\text{comp}} &= b_1^{\|}\Pi_{kl}E_{ij,k}E^*_{ij,l} + b_1^{\perp}T_{kl}E_{ij,k}E^*_{ij,l} && (2)\\
f_{\text{cdiv}} &= b_d|\underline{\nabla}\cdot\underline{\underline{E}}|^2 = b_dE_{ji,j}E^*_{ji,j} \quad \text{No } \underline{\underline{\Pi}} \text{ for now} && (3)\\
f_{\text{curv}} &= b_2^{\|}\Pi_{kl}E_{ij,lk}\Pi_{mn}E^*_{ij,nm} + b_2^{\perp}T_{kl}E_{ij,lk}T_{mn}E^*_{ij,nm} + b_2^{\|\perp}(\Pi_{kl}E_{ij,lk}T_{mn}E^*_{ij,nm} + T_{kl}E_{ij,lk}\Pi_{mn}E^*_{ij,nm}) && (4)
\end{aligned}
$$

where C, and all the bs are positive, but A can be negative. And a time evolution of form

$$\frac{\partial\underline{\underline{E}}}{\partial t} = -\mu\frac{\delta F}{\delta\underline{\underline{E}}^*} \tag{5}$$

Notable differences from Jack's are that I omit the 2 extra factors of $\frac{1}{2}$ in the bulk contribution, change μ to its inverse and add the divergence term (it can be set to 0).

Three dimensions come up – energy (E), length (L) and time (T) and the quantities above have units as follows:

quantity	$\underline{\underline{E}}$	A, C	$b_1^?$, b_d	$b_2^?$	μ
unit	1	$\frac{E}{L^3}$	$\frac{E}{L}$	EL	$\frac{1}{ET}$

1.1 Physical quantities

These are taken straight from Jack's, I do not account for the change of a $\frac{1}{2}$ factor in A and C as they are order of magnitude numbers anyway.

$$
\begin{aligned}
|\psi|_{eq} &= \sqrt{\frac{3}{2}*\frac{-A}{C}} \quad \text{The ideal smectic phase value} && (6)\\
\varepsilon &= \sqrt{\frac{b_1^{\|}}{|A|}} \quad \text{Lamellar in-plane coherence length} && (7)\\
\lambda &= \sqrt{\frac{b_2^{\perp}}{b_1^{\|}}} \quad \text{Penetration depth} && (8)\\
\kappa &= \frac{\lambda}{\varepsilon} = \sqrt{\frac{b_2^{\perp}|A|}{{b_1^{\|}}^2}} \quad \text{Ginzburg parameter} && (9)
\end{aligned}
$$

1.2 Non-dimensionalization

In the end I decided the simulation itself is best ran with all the constants above (they are all stored in the `lcParam` struct) so that things are easy to compare and the non-dimensionalization choices can be changed relatively easily.

The non-dimensionalization is however still implemented, just before the simulation itself. **Currently, the requirements are that $|\psi|_{eq} = 1$, $\varepsilon = 1$ and only allow A to be ± 1 (or 0).** For the $A \neq 0$ cases this implies $C = \frac{3}{2}$ and $b_1^{\|} = 1$. Out of the remaining parameters we can set $\mu = 1$ which will specify the time units and the rest needs to be set. This way $A, b_1^{\|}$ and μ are what sets the units as follows:

$$L = \sqrt{\frac{b_1^{\|}}{|A|}}, \qquad E = b_1 L = \sqrt{\frac{b_1^{\|3}}{|A|}}, \qquad T = \frac{1}{\mu E} = \frac{1}{\mu}\sqrt{\frac{|A|}{b_1^{\|3}}} \tag{10}$$

I haven't actually figured out the $A = 0$ case currently.

UPDATE

So I changed the above now so that I can better explore different params. I now allow A to be set to any value and set C relatively to it to make the bulk energy minimum at $|\psi_1| = 1$ (if negative A). I allow both $b_1^?$ values to be set to any non-negative numbers directly. For the $b_2^?$ values I still have a Ginzburg parameter input, but then I also have one input for each $b_2^?$ and they are scaled by $\sqrt{K}$.

1.3 Implementation

So $A, C, b_1^{\|}$ and μ are set already from units, then we can still use the Ginzburg parameter to set $b_2^{\perp}$ and set b_d directly as it is an extra for now. Finally then I set the other b_1 value via $b_1^{\|}$ and respectively with $b_2^{\perp}$.

2 One constant approximation version

Here I use the simplified free energies:

$$\begin{aligned} f_{\text{bulk}} &= A|\underline{\underline{E}}|^2 + \frac{C}{2}|\underline{\underline{E}}|^4 && (11)\\ f_{\text{comp}} &= b_1|\nabla\underline{\underline{E}}|^2 && (12)\\ f_{\text{cdiv}} &= b_d|\nabla\cdot\underline{\underline{E}}|^2 && (13)\\ f_{\text{curv}} &= b_2|\nabla^2\underline{\underline{E}}|^2 && (14)\\ & && (15) \end{aligned}$$

where C, and all the bs are positive, but A can be negative. And a time evolution of form

$$\frac{\partial\underline{\underline{E}}}{\partial t} = -\mu\frac{\delta F}{\delta\underline{\underline{E}}^*} \tag{16}$$

Still holds that notable differences from Jack's are that I omit the 2 extra factors of $\frac{1}{2}$ in the bulk contribution, change μ to its inverse and add the divergence term (it can be set to 0).

quantity	$\underline{\underline{E}}$	A	C	b_1	b_d	b_2	μ
unit	1	$\frac{E}{L^3}$	$\frac{E}{L^3}$	$\frac{E}{L}$	$\frac{E}{L}$	EL	$\frac{1}{ET}$

2.1 Physical quantities

Here I adopt the quantities from above as

$$|\psi|_{eq} = \sqrt{\frac{3}{2} * \frac{-A}{C}} \quad \text{The ideal smectic phase value} \tag{17}$$

$$\varepsilon = \sqrt{\frac{b_1}{|A|}} \quad \text{Lamellar in-plane coherence length} \tag{18}$$

$$\lambda = \sqrt{\frac{b_2}{b_1}} \quad \text{Penetration depth} \tag{19}$$

$$\kappa = \frac{\lambda}{\varepsilon} = \sqrt{\frac{b_2|A|}{b_1^2}} \quad \text{Ginzburg parameter} \tag{20}$$

2.2 Units and non-dimensionalization for simulation

Exactly as above, the requirements are that $|\psi|_{eq} = 1$, $\varepsilon = 1$ and only allow A to be ± 1 or 0. For the $A \neq 0$ cases this implies $C = \frac{3}{2}$ and $b_1 = 1$. Out of the remaining parameters we can set $\mu = 1$ which will specify the time units, set b_2 via the Ginzburg parameter and b_d directly. This way A, b_1 and μ are what sets the units as follows:

$$L = \sqrt{\frac{b_1}{|A|}}, \qquad E = b_1 L = \sqrt{\frac{b_1^3}{|A|}}, \qquad T = \frac{1}{\mu E} = \frac{1}{\mu}\sqrt{\frac{|A|}{b_1^3}} \tag{21}$$

I haven't actually figured out the $A = 0$ case as of now.

2.3 Summary

So A, b_1 and μ are used to set the units, $|\psi|$ is in the 0 to 1 range and coherence length is $1L$ which sets C to $\frac{3}{2}$. Then the user specifies K to set b_2 and possibly a non-zero b_d.