Non-dimensionalization

I will be using the following free energies here

$$f_{\text{bulk}} = A|\underline{\underline{E}}|^2 + \frac{C}{2}|\underline{\underline{E}}|^4 \tag{1}$$
$$f_{\text{comp}} = b_1|\nabla\underline{\underline{E}}|^2 \tag{2}$$
$$f_{\text{curv}} = b_2|\nabla^2\underline{\underline{E}}|^2 \tag{3}$$
$$\tag{4}$$

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 is that I omit the 2 extra factors of $\frac{1}{2}$ in the bulk contribution, deal with the $\|$ and $\perp$ parts slightly differently, and change μ to its inverse.

Here 3 dimensions come up – energy (E), length (L) and time (T) and the quantities above have units as follows:

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

This is all that is needed for 1c.a., and later on the projections operators can be introduced through $\underline{\nabla} \to b^{\|}\underline{\underline{\Pi}} \cdot \underline{\nabla} + b^{\perp}\underline{\underline{T}} \cdot \underline{\nabla}$ with both bs in there being dimensionless. Now there is currently more degrees of freedom here than needed, as both the $b_?$ and the $b^?$ affect the overall magnitudes of the terms in the free energy. I'm not too sure how to resolve that, maybe this picture isn't perfect, or maybe the $b^?$ should be constrained to remove a d.o.f.? One possible constraint would be to make them components of a unit vector.

Units for simulation

In the simulation we are free to choose the units we work with, so that leaves 3 quantities we can choose as we like.

Inspecting Jack's code I'm pretty sure he used C, b_1 (in 1c.a.) and μ, in the last version of his code I suspect he set C to 2 (maybe to test something) and μ and b_1 to 1.

Okay, so I'm kinda struggling to find the best way to do this, so let me just define a simple way to do it for the computations. Use units such that in them C, b_1 and μ each have the value 1 in their respective units, then

$$
\begin{aligned}
C =& \frac{E}{L^3} \\
b_1 =& \frac{E}{L} \\
\mu =& \frac{1}{ET}
\end{aligned} \tag{6}
$$

$$
\begin{aligned}
L &= \sqrt{\frac{b_1}{C}} \\
E &= b_1 L = \sqrt{\frac{b_1^3}{C}} \\
T &= \frac{1}{\mu E} = \frac{1}{\mu b_1 L} = \frac{1}{\mu}\sqrt{\frac{C}{b_1^3}}
\end{aligned} \tag{7}
$$

Resulting physical quantities

I also list the formulas for the quantities Jack discussed in section 3.5 of his thesis, here I'm a little unsure about the correctness however (say, I'm not sure if I should propagate the changes to the $\frac{1}{2}$ factors or not), one thing is that I'm not sure how the $\|$ and $\perp$ parts should be involved so what I quote is only for the 1c.a. case. Here the lowercase letters a and b represent the numeric values used in the code for A and b_2.

$$
\varepsilon = \sqrt{\frac{b_1}{|A|}} = \sqrt{\frac{1}{|a|}}L \tag{8}
$$

$$
\lambda = \sqrt{\frac{b_2}{b_1}} = \sqrt{b}L \tag{9}
$$

$$
\kappa = \frac{\lambda}{\varepsilon} = \sqrt{\frac{b}{|a|}} \tag{10}
$$

Implementation

This leaves 2 dimensionfull parameters, A which can be positive or negative and b_2 which can only be positive. A is specified directly as a which, as in the previous bit, is the numerical value in the units above. b_2 is specified through the square of the Ginzburg parameter κ^2 (dimensionless, see above).

Later on, when the projection operators are implemented, the two dimensionless $b^?$ will also be added.

Bit of a discussion that I'm not sure goes anywhere

Now for a uniaxial smectic we have $|\underline{\underline{E}}|^2 = \frac{d-1}{d}||\psi||^2$ Clearly for a fully isotropic phase $\underline{\underline{E}} = 0 \to \psi = 0$, if we want to "define" ψ such that it is 1 in a fully smectic phase.