# Hexagonal phase field lattice

Lucas Myers

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## 1 Hexagonal lattice phase-field and free energy

To begin, we create a scalar phase field $\psi$, which roughly corresponds to a time-average of the mass-density of atoms in the lattice. Hence, we would like to write down a form which has mass concentrated in a hexagonal lattice pattern. This looks like:

$$\psi(\mathbf{r}) = \psi_0 + \sum_n A_0 e^{i\,\mathbf{q}_n \cdot \mathbf{r}} \tag{1}$$

with $\psi_0$ some constant, $A_0$ an amplitude, and each $\mathbf{q}_n$ a lattice vector, given by:

$$\mathbf{q}_1 = \hat{\mathbf{y}}, \qquad \mathbf{q}_2 = \tfrac{\sqrt{3}}{2}\hat{\mathbf{x}} - \tfrac{1}{2}\hat{\mathbf{y}}, \qquad \mathbf{q}_3 = -\tfrac{\sqrt{3}}{2}\hat{\mathbf{x}} - \tfrac{1}{2}\hat{\mathbf{y}} \tag{2}$$

We will use this as an initial configuration to make sure that we can create a stable configuration and iterate it in time.

The free energy corresponding to a hexagonal lattice is given by:

$$\mathcal{F}[\psi] = \int_\Omega \left[ \frac{1}{2} \left[ \left( \nabla^2 + 1 \right) \psi \right]^2 + \frac{\epsilon}{2}\psi^2 + \frac{1}{4}\psi^4 \right] dV \tag{3}$$

where, if $\epsilon > 0$ the only stable solution is $\psi = \psi_0$, whereas $\epsilon < 0$ admits periodic solutions which we are interested in. Given this free energy, the corresponding time evolution is given by:

$$\frac{\partial \psi}{\partial t} = \nabla^2 \frac{\delta F}{\delta \psi} \tag{4}$$

Writing this out explicitly gives:

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \nabla^2 \left[ \left( \nabla^2 + 1 \right)^2 \psi + \epsilon \psi + \psi^3 \right] \\ &= \nabla^2 \left( \nabla^2 + 1 \right)^2 \psi + \epsilon \nabla^2 \psi + \nabla^2 \psi^3 \end{aligned} \tag{5}$$

## 2 Finite element method

To begin, we expand the equation as much as possible:

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \nabla^6 \psi + 2\nabla^4 \psi + (1 + \epsilon) \nabla^2 \psi + \nabla^2 \psi^3 \\ &= \nabla^6 \psi + 2\nabla^4 \psi + (1 + \epsilon) \nabla^2 \psi + 3\psi^2 \nabla^2 \psi + 6\psi \left( \nabla \psi \right)^2 \end{aligned} \tag{6}$$

For technical reasons associated with the use of piecewise polynomials for the finite element method, we choose to define the following auxiliary variables:

$$\chi \coloneqq \nabla^2 \psi, \quad \phi \coloneqq \nabla^2 \chi = \nabla^4 \psi \tag{7}$$

Substituting these auxiliary variables into our original equations yields:

$$\frac{\partial \psi}{\partial t} = \nabla^2 \phi + 2\phi + (1+\epsilon)\,\chi + 3\psi^2 \chi + 6\psi\,(\nabla\psi)^2 \tag{8}$$

Then we have three coupled second-order equations.

### 2.1 Time discretization

We may solve this equation numerically using the finite element method. To begin, we discretize in time. For this, we use a semi-implicit method parameterized by $\theta$ as in step 23 of the deal.II tutorials. This gives:

$$\begin{aligned}\frac{\psi_n - \psi_{n-1}}{\delta t} &= \theta\left[\nabla^2\phi_n + 2\phi_n + \left(1+\epsilon+3\psi_n^2\right)\chi_n + 6\psi_n\,(\nabla\psi_n)^2\right] \\ &\quad + (1-\theta)\left[\nabla^2\phi_{n-1} + 2\phi_{n-1} + \left(1+\epsilon+3\psi_{n-1}^2\right)\chi_{n-1} + 6\psi_n\,(\nabla\psi_{n-1})^2\right]\end{aligned} \tag{9}$$

Here $\delta t$ is the discrete timestep and $\theta$ is the discretization parameter: $\theta = 1$ corresponds to a fully-implicit method, $\theta = 0$ is a fully explicit method, and $\theta = 1/2$ is a Crank-Nicolson method. Of course, the definitions of the auxiliary variables still hold for timestep $n$ and $n-1$.

### 2.2 Linearizing the equation

Given that the equation is nonlinear, we must use Newton-Rhapson method to solve for each timestep. Because we have a series of three coupled equations, the residual is a three-component function defined at every point. The components are then given by:

$$\begin{aligned}R_1(\psi_n,\chi_n,\phi_n) &= \psi_n - \delta t\,\theta\left[\nabla^2\phi_n + 2\phi_n + \left(1+\epsilon+3\psi_n^2\right)\chi_n + 6\psi_n\,(\nabla\psi_n)^2\right] \\ &\quad - \psi_{n-1} - \delta t\;(1-\theta)\left[\nabla^2\phi_{n-1} + 2\phi_{n-1} + \left(1+\epsilon+3\psi_{n-1}^2\right)\chi_{n-1} + 6\psi_{n-1}\,(\nabla\psi_{n-1})^2\right] \\ R_2(\psi_n,\chi_n,\phi_n) &= \chi_n - \nabla^2\psi_n \\ R_3(\psi_n,\chi_n,\phi_n) &= \phi_n - \nabla^2\chi_n\end{aligned} \tag{10}$$

Since our residual is vector-valued, the Gateaux derivative will be a matrix which acts on a vector-valued deviation $[\delta\psi, \delta\chi, \delta\phi]^T$. Taking the Gateaux derivative one row at a time yields:

$$\begin{aligned}dR_1(\psi,\chi,\phi;\;\delta\psi,\delta\chi,\delta\phi) &= \frac{d}{d\tau}R_1(\psi+\tau\delta\psi,\chi+\tau\delta\chi,\phi+\tau\delta\phi)\Big|_{\tau=0} \\ &= \frac{d}{d\tau}\Bigg[\psi_n + \tau\delta\psi_n - \delta t\,\theta\big[\nabla^2(\phi_n+\tau\delta\phi_n) + 2(\phi_n+\tau\delta\phi_n) \\ &\qquad + \left(1+\epsilon+3(\psi_n+\tau\delta\psi_n)^2\right)(\chi_n+\tau\delta\chi_n) \\ &\qquad + 6(\psi_n+\tau\delta\psi_n)\left(\nabla(\psi_n+\tau\delta\psi_n)\right)^2\big]\Bigg]_{\tau=0} \\ &= \delta\psi_n - \delta t\,\theta\big[\nabla^2\delta\phi_n + 2\delta\phi_n \\ &\qquad + \left(1+\epsilon+3\psi_n^2\right)\delta\chi_n + 6\psi_n\chi_n\,\delta\psi_n \\ &\qquad + 6(\nabla\psi_n)^2\,\delta\psi_n + 12\psi_n(\nabla\psi_n)\cdot\nabla\delta\psi_n\big] \\ dR_2(\psi,\chi,\phi;\;\delta\psi,\delta\chi,\delta\phi) &= \delta\chi_n - \nabla^2\delta\psi_n \\ dR_3(\psi,\chi,\phi;\;\delta\psi,\delta\chi,\delta\phi) &= \delta\phi_n - \nabla^2\delta\chi_n\end{aligned} \tag{11}$$

Given this derivative of the residual, then Newton-Rhapson method in functional space reads:

$$\begin{aligned} dR(\Psi_n)\delta\Psi_n &= -R(\Psi_n) \\ \Psi_{n+1} &= \Psi_n + \delta\Psi_n \end{aligned} \tag{12}$$

where we have defined:

$$\Psi = \begin{bmatrix} \psi \\ \chi \\ \phi \end{bmatrix} \tag{13}$$

$R$ is the vector residual, $\delta\Psi$ is the vector variation of $\Psi$ and:

$$dR(\Psi) = \begin{bmatrix} 1 - \delta t\theta \left[6\psi\chi + 6\left(\nabla\psi\right)^2 + 12\psi\left(\nabla\psi\right)\cdot\nabla\right] & -\delta t\theta\left(1+\epsilon+3\psi\right) & -\delta t\theta\left(\nabla^2+2\right) \\ -\nabla^2 & 1 & 0 \\ 0 & -\nabla^2 & 1 \end{bmatrix} \tag{14}$$

## 2.3 Space discretization

For this, we introduce a vector test function $A$:

$$A = \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} \tag{15}$$

Then our linear equation looks like:

$$A^T\, dR\, \delta\Psi = -A^T\, R \tag{16}$$

The left-hand side is given by:

$$\begin{aligned} A^T\, dR\, \delta\Psi = \; & \langle\alpha, \delta\psi_n\rangle - \delta t\theta\big[\left\langle\alpha, \nabla^2\delta\phi\right\rangle + 2\left\langle\alpha, \delta\phi_n\right\rangle \\ & + (1+\epsilon)\left\langle\alpha, \delta\chi_n\right\rangle + 3\left\langle\alpha, \psi_n^2\delta\chi_n\right\rangle + 6\left\langle\alpha, \psi_n\,\chi_n\,\delta\psi_n\right\rangle \\ & + 6\left\langle\alpha, \left(\nabla\psi_n\right)^2\delta\psi_n\right\rangle + 12\left\langle\alpha, \psi_n\left(\nabla\psi_n\right)\cdot\nabla\delta\psi_n\right\rangle\big] \\ & + \left\langle\beta, \delta\chi_n\right\rangle - \left\langle\beta, \nabla^2\delta\psi_n\right\rangle \\ & + \left\langle\gamma, \delta\phi_n\right\rangle - \left\langle\gamma, \nabla^2\delta\chi_n\right\rangle \\ = \; & \langle\alpha, \delta\psi_n\rangle - \delta t\theta\big[-\left\langle\nabla\alpha, \nabla\delta\phi\right\rangle + 2\left\langle\alpha, \delta\phi_n\right\rangle \\ & + (1+\epsilon)\left\langle\alpha, \delta\chi_n\right\rangle + 3\left\langle\alpha, \psi_n^2\delta\chi_n\right\rangle + 6\left\langle\alpha, \psi_n\,\chi_n\,\delta\psi_n\right\rangle \\ & + 6\left\langle\alpha, \left(\nabla\psi_n\right)^2\delta\psi_n\right\rangle + 12\left\langle\alpha, \psi_n\left(\nabla\psi_n\right)\cdot\nabla\delta\psi_n\right\rangle\big] \\ & + \left\langle\beta, \delta\chi_n\right\rangle + \left\langle\nabla\beta, \nabla\delta\psi_n\right\rangle \\ & + \left\langle\gamma, \delta\phi_n\right\rangle + \left\langle\nabla\gamma, \nabla\delta\chi_n\right\rangle \end{aligned} \tag{17}$$

and the right-hand side is given by:

$$
\begin{aligned}
-A^T R = & -\langle \alpha, \psi_n \rangle + \delta t \theta \big[ \left\langle \alpha, \nabla^2 \phi_n \right\rangle + 2 \langle \alpha, \phi_n \rangle + (1+\epsilon) \langle \alpha, \chi_n \rangle \\
& \qquad + 3 \left\langle \alpha, \psi_n^2 \chi_n \right\rangle + 6 \left\langle \alpha, \psi_n \left(\nabla \psi_n\right)^2 \right\rangle \big] \\
& + \langle \alpha, \psi_{n-1} \rangle + \delta t \left(1-\theta\right) \left[ \left\langle \alpha, \nabla^2 \phi_{n-1} \right\rangle + 2 \langle \alpha, \phi_{n-1} \rangle + (1+\epsilon) \langle \alpha, \chi_{n-1} \rangle \right. \\
& \qquad \left. + 3 \left\langle \alpha, \psi_{n-1}^2 \chi_{n-1} \right\rangle + 6 \left\langle \alpha, \psi_{n-1} \left(\nabla \psi_{n-1}\right)^2 \right\rangle \right] \\
& \qquad - \langle \beta, \chi_n \rangle + \left\langle \beta, \nabla^2 \psi_n \right\rangle - \langle \gamma, \phi_n \rangle + \left\langle \gamma, \nabla^2 \chi_n \right\rangle \\
= & -\langle \alpha, \psi_n \rangle + \delta t \theta \big[ -\langle \nabla \alpha, \nabla \phi_n \rangle + 2 \langle \alpha, \phi_n \rangle + (1+\epsilon) \langle \alpha, \chi_n \rangle \\
& \qquad + 3 \left\langle \alpha, \psi_n^2 \chi_n \right\rangle + 6 \left\langle \alpha, \psi_n \left(\nabla \psi_n\right)^2 \right\rangle \big] \\
& + \langle \alpha, \psi_{n-1} \rangle + \delta t \left(1-\theta\right) \left[ -\langle \nabla \alpha, \nabla \phi_{n-1} \rangle + 2 \langle \alpha, \phi_{n-1} \rangle + (1+\epsilon) \langle \alpha, \chi_{n-1} \rangle \right. \\
& \qquad \left. + 3 \left\langle \alpha, \psi_{n-1}^2 \chi_{n-1} \right\rangle + 6 \left\langle \alpha, \psi_{n-1} \left(\nabla \psi_{n-1}\right)^2 \right\rangle \right] \\
& \qquad - \langle \beta, \chi_n \rangle - \langle \nabla \beta, \nabla \psi_n \rangle - \langle \gamma, \phi_n \rangle - \langle \nabla \gamma, \nabla \chi_n \rangle
\end{aligned}
\tag{18}
$$

Now our shape functions are vector-valued, composed like:

$$
\eta_i = \begin{bmatrix} \eta_{i,\psi} \\ \eta_{i,\chi} \\ \eta_{i,\phi} \end{bmatrix}
\tag{19}
$$

Note that, for primitive elements like we will use, only one component will be nonzero for any particular $i$. In any case, supposing we assume our solution vector can be written as a linear combinations of primitive test functions, and stipulating that the equation hold for any test function, we get the following left-hand side:

$$
\begin{aligned}
A^T \, dR \, \delta\Psi = \sum_j \Bigg[ & \langle \eta_{i,\psi}, \eta_{j,\psi} \rangle - \delta t \theta \big[ -\langle \nabla \eta_{i,\psi}, \nabla \eta_{j,\phi} \rangle + 2 \langle \eta_{i,\psi}, \eta_{j,\phi} \rangle \\
& + (1+\epsilon) \langle \eta_{i,\psi}, \eta_{j,\chi} \rangle + 3 \left\langle \eta_{i,\psi}, \psi_n^2 \eta_{j,\chi} \right\rangle + 6 \langle \eta_{i,\psi}, \psi_n \, \chi_n \, \eta_{j,\psi} \rangle \\
& + 6 \left\langle \eta_{i,\psi}, \left(\nabla \psi_n\right)^2 \eta_{j,\psi} \right\rangle + 12 \langle \eta_{i,\psi}, \psi_n \left(\nabla \psi_n\right) \cdot \nabla \eta_{j,\psi} \rangle \big] \\
& + \langle \eta_{i,\chi}, \eta_{j,\chi} \rangle + \langle \nabla \eta_{i,\chi}, \nabla \eta_{j,\psi} \rangle \\
& + \langle \eta_{i,\phi}, \eta_{j,\phi} \rangle + \langle \nabla \eta_{i,\phi}, \nabla \eta_{j,\chi} \rangle \Bigg] \delta\Psi_j
\end{aligned}
\tag{20}
$$

Finally, we may write our right-hand side as:

$$
\begin{aligned}
-A^T R = & -\langle \eta_{i,\psi}, \psi_n \rangle + \delta t \theta \big[ -\langle \nabla \eta_{i,\psi}, \nabla \phi_n \rangle + 2 \langle \eta_{i,\psi}, \phi_n \rangle + (1+\epsilon) \langle \eta_{i,\psi}, \chi_n \rangle \\
& \qquad + 3 \left\langle \eta_{i,\psi}, \psi_n^2 \chi_n \right\rangle + 6 \left\langle \eta_{i,\psi}, \psi_n \left(\nabla \psi_n\right)^2 \right\rangle \big] \\
& + \langle \eta_{i,\psi}, \psi_{n-1} \rangle + \delta t \left(1-\theta\right) \left[ -\langle \nabla \eta_{i,\psi}, \nabla \phi_{n-1} \rangle + 2 \langle \eta_{i,\psi}, \phi_{n-1} \rangle + (1+\epsilon) \langle \eta_{i,\psi}, \chi_{n-1} \rangle \right. \\
& \qquad \left. + 3 \left\langle \eta_{i,\psi}, \psi_{n-1}^2 \chi_{n-1} \right\rangle + 6 \left\langle \eta_{i,\psi}, \psi_{n-1} \left(\nabla \psi_{n-1}\right)^2 \right\rangle \right] \\
& \qquad - \langle \eta_{i,\chi}, \chi_n \rangle - \langle \nabla \eta_{i,\chi}, \nabla \psi_n \rangle - \langle \eta_{i,\phi}, \phi_n \rangle - \langle \nabla \eta_{i,\phi}, \nabla \chi_n \rangle
\end{aligned}
\tag{21}
$$

Finally, note that our matrix can be written in block form as:

$$
\begin{bmatrix} B & C & D \\ L_\psi & M_\chi & 0 \\ 0 & L_\chi & M_\phi \end{bmatrix}
\begin{bmatrix} \delta\psi \\ \delta\chi \\ \delta\phi \end{bmatrix}
=
\begin{bmatrix} F \\ G \\ H \end{bmatrix}
\tag{22}
$$

where $F$, $G$, $H$ are the different components of $-A^T R$:

$$
\begin{aligned}
F_i = \Big\langle \eta_{i,\psi}, -\psi_n + \psi_{n-1} \\
&+ \delta t \Big[ \theta \left( 2\phi_n + (1+\epsilon)\chi_n + 3\psi_n^2 \chi_n + 6\psi_n \left(\nabla \psi_n\right)^2 \right) \\
&+ (1-\theta) \left( 2\phi_{n-1} + (1+\epsilon)\chi_{n-1} + 3\psi_{n-1}^2 \chi_{n-1} + 6\psi_{n-1} \left(\nabla \psi_{n-1}\right)^2 \right) \Big] \Big\rangle \\
&- \delta t \left\langle \nabla \eta_{i,\psi}, \theta \nabla \phi_n + (1-\theta) \nabla \phi_{n-1} \right\rangle \\
G_i &= - \left\langle \eta_{i,\chi}, \chi_n \right\rangle - \left\langle \nabla \eta_{i,\chi}, \nabla \psi_n \right\rangle \\
H_i &= - \left\langle \eta_{i,\phi}, \phi_n \right\rangle - \left\langle \nabla \eta_{i,\phi}, \nabla \chi_n \right\rangle
\end{aligned}
\tag{23}
$$

$\delta\psi$, $\delta\chi$, $\delta\phi$ are the finite element vectors for each of the variations, and then:

$$
\begin{aligned}
B_{ij} &= \left\langle \eta_{i,\psi}, \eta_{j,\psi} \right\rangle - 6\delta t\, \theta \left[ \left\langle \eta_{i,\psi}, \psi_n\, \chi_n \eta_{j,\psi} \right\rangle + \left\langle \eta_{i,\psi}, \left(\nabla \psi_n\right)^2 \eta_{j,\psi} \right\rangle + 2 \left\langle \eta_{i,\psi}, \psi_n \left(\nabla \psi_n\right) \cdot \nabla \eta_{j,\psi} \right\rangle \right] \\
C_{ij} &= -\delta t\, \theta \left[ (1+\epsilon) \left\langle \eta_{i,\psi}, \eta_{j,\chi} \right\rangle + 3 \left\langle \eta_{i,\psi}, \psi_n^2 \eta_{j,\chi} \right\rangle \right] \\
D_{ij} &= -\delta t\, \theta \left[ - \left\langle \nabla \eta_{i,\psi}, \nabla \eta_{j,\phi} \right\rangle + 2 \left\langle \eta_{i,\psi}, \eta_{j,\phi} \right\rangle \right] \\
L_{ij} &= \left\langle \nabla \eta_i, \nabla \eta_j \right\rangle \\
M_{ij} &= \left\langle \eta_i, \eta_j \right\rangle
\end{aligned}
\tag{24}
$$

where $L$ is something like the Laplacian operator, and $M$ is the mass matrix.

## 2.4 Preconditioning

Given the block structure, we may try to get a nicer preconditioner as follows:

$$
\begin{aligned}
L_\chi \delta\chi + M_\phi \delta\phi = H \\
\implies \delta\phi = M_\phi^{-1} \left( H - L_\chi \delta\chi \right)
\end{aligned}
\tag{25}
$$

Additionally, we get:

$$
\begin{aligned}
L_\psi \delta\psi + M_\chi \delta\chi = G \\
\implies \delta\chi = M_\chi^{-1} \left( G - L_\psi \delta\psi \right)
\end{aligned}
\tag{26}
$$

Substituting this back into the first equation yields:

$$
\delta\phi = M_\phi^{-1} \left( H - L_\chi M_\chi^{-1} \left( G - L_\psi \delta\psi \right) \right) \tag{27}
$$

The first component of the matrix equation reads:

$$
B\delta\psi + C\delta\chi + D\delta\phi = F \tag{28}
$$

We may substitute eqs. (25) and (26) into eq. (28):

$$
B\delta\psi + C M_\chi^{-1} \left( G - L_\psi \delta\psi \right) + D M_\phi^{-1} \left( H - L_\chi M_\chi^{-1} \left( G - L_\psi \delta\psi \right) \right) = F \tag{29}
$$

Rewriting as a linear equation gives:

$$
\left( B + \left( D M_\phi^{-1} L_\chi - C \right) M_\chi^{-1} L_\psi \right) \delta\psi = F - C M_\chi^{-1} G + D M_\phi^{-1} \left( L_\chi M_\chi^{-1} G - H \right) \tag{30}
$$

Then the scheme is to solve eq. (30), then (26) and (25) are straightforward, in that one only has to invert the mass matrix which is generally well-conditioned and symmetric. We may try to come up with a more efficient preconditioner for eq. (30) at some point, but for now we will do a direct solve just to make sure everything is working correctly.

## 3 Initializing hexagonal lattice

For this, we need to initialize $\psi$, $\chi$, and $\phi$. $\psi$ is given in eq. (1). However, $\psi$ is real so that we must only take the real part of the equation to get:

$$\psi\left(\mathbf{r}\right) = \psi_0 + \sum_n A_0 \cos\left(\mathbf{q}_n \cdot \mathbf{r}\right) \tag{31}$$

The other fields are then given as:

$$\chi(\mathbf{r}) = \nabla^2\psi(\mathbf{r}) = -A_0 \sum_n q_n^2 \cos\left(\mathbf{q}_n \cdot \mathbf{r}\right) = -A_0 \sum_n \cos\left(\mathbf{q}_n \cdot \mathbf{r}\right) \tag{32}$$

and

$$\phi(\mathbf{r}) = \nabla^2\chi(\mathbf{r}) = A_0 \sum_n q_n^4 \cos\left(\mathbf{q}_n \cdot \mathbf{r}\right) = A_0 \sum_n \cos\left(\mathbf{q}_n \cdot \mathbf{r}\right) \tag{33}$$

because each $\mathbf{q}_n$ is a unit vector.

## 4 Configurations wtih dislocations

According to Fei's report, the way to make a dislocation at point $\mathbf{u}_j$ with Burgers vector $\mathbf{b}_j$ is to first define the quantity:

$$s_{n,j} = \frac{1}{2\pi}\left(\mathbf{q}_n \cdot \mathbf{b}_j\right) \tag{34}$$

Given this, we can define a phase distortion given by:

$$\varphi_{n,j}\left(\mathbf{r}\right) = s_{n,j}\,\theta_j\left(\mathbf{r} - \mathbf{u}_j\right) = s_{n,j}\,\mathrm{atan2}\left(r_y - u_{j,y}, r_x - u_{j,x}\right) \tag{35}$$

where $\theta_j$ is the polar angle centered at $\mathbf{u}_j$. The phase field then becomes:

$$\psi(\mathbf{r}) = \psi_0 + A_0 \sum_n e^{i(\mathbf{q}_n\cdot\mathbf{r} + \varphi_{n,j}(\mathbf{r}))} \tag{36}$$

For an arbitrary number of defects, this becomes:

$$\psi(\mathbf{r}) = \psi_0 + A_0 \sum_n e^{i\left(\mathbf{q}_n\cdot\mathbf{r} + \sum_j \varphi_{n,j}(\mathbf{r})\right)} \tag{37}$$

Given this, we calculate the auxiliary fields:

$$\begin{aligned}\chi(\mathbf{r}) &= \nabla^2\psi(\mathbf{r}) \\ &= A_0 \sum_n e^{i\left(\mathbf{q}_n\cdot\mathbf{r} + \sum_j \varphi_{n,j}(\mathbf{r})\right)} \left(-q_n^2 + \sum_j \nabla^2 i\varphi_{n,j}\right) \\ &= -A_0 \sum_n q_n^2 e^{i\left(\mathbf{q}_n\cdot\mathbf{r} + \sum_j \varphi_{n,j}(\mathbf{r})\right)}\end{aligned} \tag{38}$$

Here, note that $\varphi_{n,j}$ is proportional to a polar angle centered at $\mathbf{u}_j$. Additionally, in two dimensions in polar coordinates the Laplacian operator is given by:

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} \tag{39}$$

Since this is independent of basis, we can change basis to be centered around $\mathbf{u}_j$ in which case $\nabla^2\varphi_{n,j} = 0$ is easily calculated. Similarly:

$$\phi(\mathbf{r}) = A_0 \sum_n q_n^4 e^{i\left(\mathbf{q}_n\cdot\mathbf{r} + \sum_j \varphi_{n,j}(\mathbf{r})\right)} \tag{40}$$

# 5 Calculating configurational stress

The energy due to an infinitesimal distortion of the phase field is given by:

$$\mathcal{E} = \left[ -\frac{\partial f}{\partial(\partial_{ik}\psi)} \partial_{jk}\psi + \left( \partial_k \frac{\partial f}{\partial(\partial_{ik}\psi)} \right) \partial_j \psi + \delta_{ij} f \right] \partial_i u_j \tag{41}$$

The configurational stress is the derivative of this with respect to the displacement gradient:

$$\begin{aligned} \sigma_{ij} &= \frac{\partial \mathcal{E}}{\partial(\partial_i u_j)} \\ &= -\frac{\partial f}{\partial(\partial_{ik}\psi)} \partial_{jk}\psi + \left( \partial_k \frac{\partial f}{\partial(\partial_{ik}\psi)} \right) \partial_j \psi + \delta_{ij} f \end{aligned} \tag{42}$$

Which, given the specific free energy density $f$ gives:

$$\sigma_{ij} = [\partial_i \mathcal{L}\psi] \, \partial_j \psi - [\mathcal{L}\psi] \, \partial_{ij}\psi + f\delta_{ij} \tag{43}$$

where $\mathcal{L} = 1 + \nabla^2$. Written out in its entirety we get:

$$\sigma_{ij} = (\partial_i\psi)(\partial_j\psi) + (\partial_i\nabla^2\psi)(\partial_j\psi) - \psi\partial_{ij}\psi - (\nabla^2\psi)(\partial_{ij}\psi) + \left(\nabla^6\psi + 2\nabla^4\psi + (1+\epsilon)\nabla^2\psi + \nabla^2\psi^3\right)\delta_{ij} \tag{44}$$

Finally, written in terms of our auxiliary variables:

$$\sigma_{ij} = (\partial_i\psi)(\partial_j\psi) + (\partial_i\chi)(\partial_j\psi) - \psi\partial_{ij}\psi - \chi(\partial_{ij}\psi) + \left(\nabla^2\phi + 2\phi + (1+\epsilon)\chi + 3\psi^2\chi + 6\psi\left(\nabla\psi\right)^2\right)\delta_{ij} \tag{45}$$

Written in terms of general vector operators, we get the following:

$$\sigma = \nabla\left(\psi + \chi\right) \otimes \nabla\psi - (\psi+\chi)\nabla(\nabla\psi) + \left(\nabla^2\phi + 2\phi + (1+\epsilon)\chi + 3\psi^2\chi + 6\psi\left(\nabla\psi\right)^2\right) I \tag{46}$$

Now note that we will not actually be able to calculate this at each of the quadrature points because we are only using linear elements.

## 5.1 Weak form of the configurational stress

Because we are using piecewise linear elements, we need to write down a weak form if we are to accurately calculate the higher order derivatives. Taking the inner product with a tensor test function $\tau$ yields:

$$\begin{aligned} \langle\tau,\sigma\rangle &= \langle\tau, \nabla\left(\psi+\chi\right)\otimes(\nabla\psi)\rangle - \langle\tau, (\psi+\chi)\nabla(\nabla\psi)\rangle + \left\langle\tau, \left(\nabla^2\phi + 2\phi + (1+\epsilon)\chi + 3\psi^2\chi + 6\psi\left(\nabla\psi\right)^2\right) I\right\rangle \\ &= \langle\tau, \nabla\left(\psi+\chi\right)\otimes(\nabla\psi)\rangle + \langle\nabla\cdot\left((\psi+\chi)\tau\right), \nabla\psi\rangle - \langle(\psi+\chi)\mathbf{n}\cdot\tau, \nabla\psi\rangle_{\partial\Omega} \\ &\qquad + \left\langle \mathrm{tr}(\tau), \left(\nabla^2\phi + 2\phi + (1+\epsilon)\chi + 3\psi^2\chi + 6\psi\left(\nabla\psi\right)^2\right)\right\rangle \\ &= \langle\tau, \nabla\left(\psi+\chi\right)\otimes(\nabla\psi)\rangle + \langle(\nabla\psi+\nabla\chi)\cdot\tau, \nabla\psi\rangle + \langle(\psi+\chi)\nabla\cdot\tau, \nabla\psi\rangle - \langle(\psi+\chi)\mathbf{n}\cdot\tau, \nabla\psi\rangle_{\partial\Omega} \\ &\qquad - \langle\mathrm{tr}(\nabla\tau), \nabla\phi\rangle + \langle\mathbf{n}\mathrm{tr}(\tau), \nabla\phi\rangle_{\partial\Omega} + \left\langle \mathrm{tr}(\tau), \left(2\phi + (1+\epsilon)\chi + 3\psi^2\chi + 6\psi\left(\nabla\psi\right)^2\right)\right\rangle \end{aligned} \tag{47}$$

Given that we're working with periodic boundary conditions, there is no boundary so the equation reduces to:

$$\begin{aligned} \langle\tau,\sigma\rangle = \; &\langle\tau, \nabla\left(\psi+\chi\right)\otimes(\nabla\psi)\rangle + \langle(\nabla\psi+\nabla\chi)\cdot\tau, \nabla\psi\rangle + \langle(\psi+\chi)\nabla\cdot\tau, \nabla\psi\rangle \\ &- \langle\mathrm{tr}(\nabla\tau), \nabla\phi\rangle + \left\langle \mathrm{tr}(\tau), \left(2\phi + (1+\epsilon)\chi + 3\psi^2\chi + 6\psi\left(\nabla\psi\right)^2\right)\right\rangle \end{aligned} \tag{48}$$

To actually project this onto a finite element space, we consider an approximation of $\sigma$:

$$\sigma_h = \sum_i \sigma_i \tau_i \tag{49}$$

where each $\sigma_i$ is a scalar. Then the problem becomes:

$$M_{ij}\sigma_j = b_i \tag{50}$$

where

$$M_{ij} = \langle \tau_i, \tau_j \rangle \tag{51}$$

is the mass matrix and

$$\begin{aligned} b_i = \; & \langle \tau_i, \nabla (\psi + \chi) \otimes (\nabla\psi) \rangle + \langle (\nabla\psi + \nabla\chi) \cdot \tau_i, \nabla\psi \rangle + \langle (\psi + \chi) \nabla \cdot \tau_i, \nabla\psi \rangle \\ & - \langle \mathrm{tr}(\nabla \tau_i), \nabla\phi \rangle + \left\langle \mathrm{tr}(\tau_i), \left( 2\phi + (1+\epsilon)\chi + 3\psi^2\chi + 6\psi \left(\nabla\psi\right)^2 \right) \right\rangle \end{aligned} \tag{52}$$

# 6 Deriving the time evolution

In general, we would like to impose that the free energy only decrease over time due to dissipative effects:

$$\frac{\partial \mathcal{F}}{\partial t} \leq 0 \tag{53}$$

Additionally, we would like to impose conservation of momentum, which takes the form:

$$\frac{\partial \psi}{\partial t} + \nabla \cdot \mathbf{J} = 0 \tag{54}$$

where $\mathbf{J}$ is the mass current. Given this constraint, we may write this as a Lagrange multiplier problem:

$$\mathcal{L}[\psi] = \mathcal{F}[\psi] - \int_\Omega \lambda(x) \left( \frac{\partial \psi}{\partial t} + \nabla \cdot \mathbf{J} \right) dV \tag{55}$$

for some scalar $\lambda$. Now we try to minimize $\mathcal{L}$:

$$\frac{\partial \mathcal{L}}{\partial t} = \frac{\delta \mathcal{L}}{\delta \psi} \frac{\partial \psi}{\partial t} \tag{56}$$

First let's explicitly calculate the functional derivative of the Lagrange multiplier part:

$$\frac{d}{d\tau} \left[ \int_\Omega \lambda(x) \left( \frac{\partial(\psi + \tau\delta\psi)}{\partial t} + \nabla \cdot \mathbf{J} \right) dV \right]_{\tau=0} = \int_\Omega \lambda(x) \frac{\partial \delta\psi}{\partial t} dV \tag{57}$$

# 7 Time evolution of this configuration

For debugging purposes, let's calculate the right-hand side of the time evolution equation given this configuration:

$$
\begin{aligned}
\nabla^2\phi &= -A_0 \sum_n q_n^6 \cos(\mathbf{q}_n \cdot \mathbf{r}) \\
2\phi &= 2A_0 \sum_n q_n^4 \cos(\mathbf{q}_n \cdot \mathbf{r}) \\
(1+\epsilon)\chi &= -(1+\epsilon)A_0 \sum_n q_n^2 \cos(\mathbf{q}_n \cdot \mathbf{r}) \\
3\psi^2\chi &= 3\left(\psi_0 + A_0 \sum_l \cos(\mathbf{q}_l \cdot \mathbf{r})\right)\left(\psi_0 + A_0 \sum_m \cos(\mathbf{q}_m \cdot \mathbf{r})\right)\left(-A_0 \sum_n q_n^2 \cos(\mathbf{q}_n \cdot \mathbf{r})\right) \\
&= 3\left(\psi_0^2 + 2\psi_0 A_0 \sum_l \cos(\mathbf{q}_l \cdot \mathbf{r}) + A_0^2 \sum_{l,m} \cos(\mathbf{q}_l \cdot \mathbf{r})\cos(\mathbf{q}_m \cdot \mathbf{r})\right)\left(-A_0 \sum_n q_n^2 \cos(\mathbf{q}_n \cdot \mathbf{r})\right) \\
&= -3\left(\psi_0 A_0 \sum_n q_n^2 \cos(\mathbf{q}_n \cdot \mathbf{r}) + 2\psi_0 A_0^2 \sum_{n,l} \cos(\mathbf{q}_l \cdot \mathbf{r})\cos(\mathbf{q}_n \cdot \mathbf{r}) + A_0^3 \sum_{l,m,n} \cos(\mathbf{q}_l \cdot \mathbf{r})\cos(\mathbf{q}_m \cdot \mathbf{r})\cos(\mathbf{q}_n \cdot \mathbf{r})\right) \\
&= -3\Bigg(\psi_0 A_0 \sum_n q_n^2 \cos(\mathbf{q}_n \cdot \mathbf{r}) \\
&\qquad + \psi_0 A_0^2 \sum_{n,l} \left[\cos((\mathbf{q}_n - \mathbf{q}_l)\cdot \mathbf{r}) + \cos((\mathbf{q}_n + \mathbf{q}_l)\cdot \mathbf{r})\right] \\
&\quad + \frac{1}{2}A_0^3 \sum_{l,m,n} \cos(\mathbf{q}_m \cdot \mathbf{r})\left[\cos((\mathbf{q}_n - \mathbf{q}_l)\cdot \mathbf{r}) + \cos((\mathbf{q}_n + \mathbf{q}_l)\cdot \mathbf{r})\right]\Bigg) \\
6\psi\left(\nabla\psi\right)^2 &= 6\left(\psi_0 + A_0 \sum_l \cos(\mathbf{q}_l \cdot \mathbf{r})\right)\left(A_0^2 \sum_{n,m} \mathbf{q}_n \cdot \mathbf{q}_m \sin(\mathbf{q}_n \cdot \mathbf{r})\sin(\mathbf{q}_m \cdot \mathbf{r})\right) \\
&= 3\Bigg(\psi_0 A_0^2 \sum_{n,m}\left(\frac{3}{2}\delta_{m,n} - \frac{1}{2}\right)\left[\cos((\mathbf{q}_m - \mathbf{q}_n)\cdot \mathbf{r}) - \cos((\mathbf{q}_m + \mathbf{q}_n)\cdot \mathbf{r})\right] \\
&\quad + A_0^3 \sum_{l,m,n}\left(\frac{3}{2}\delta_{m,n} - \frac{1}{2}\right)\cos(\mathbf{q}_l \cdot \mathbf{r})\left[\cos((\mathbf{q}_m - \mathbf{q}_n)\cdot \mathbf{r}) - \cos((\mathbf{q}_m + \mathbf{q}_n)\cdot \mathbf{r})\right)\Bigg)
\end{aligned}
$$

First we note that, because $q_n^2 = 1$ we get:

$$\nabla^2\phi + 2\phi + (1+\epsilon)\chi = \epsilon A_0 \sum_n \cos(\mathbf{q}_n \cdot \mathbf{r})$$

Then, taking $\psi_0 = 0$ for ease of calculation we get:

$$3\psi^2\chi + 6\psi\left(\nabla\psi\right)^2 = \frac{9}{2}A_0^3 \sum_l \cos(\mathbf{q}_l \cdot \mathbf{r}) \tag{58}$$

For debugging purposes, let's calculate the right-hand side of the time evolution equation given this configuration. For ease of calculation, we take the complex exponential with the understanding that at the end we take the real part of the entire expression:

$$\nabla^2\phi = -A_0 \sum_n q_n^6 e^{i\mathbf{q}_n \cdot \mathbf{r}}$$

$$2\phi = 2A_0 \sum_n q_n^4 e^{i\mathbf{q}_n \cdot \mathbf{r}}$$

$$(1+\epsilon)\chi = -(1+\epsilon)A_0 \sum_n q_n^2 e^{i\mathbf{q}_n\cdot\mathbf{r}}$$

Thus:

$$\nabla^2\phi + 2\phi + (1+\epsilon)\chi = -\epsilon A_0 \sum_n q_n^2 e^{i\mathbf{q}_n\cdot\mathbf{r}} \tag{59}$$

Now for the nonlinear terms:

$$\begin{aligned}
3\psi^2\chi &= 3\left(\psi_0 + A_0\sum_n e^{i\mathbf{q}_n\cdot\mathbf{r}}\right)\left(\psi_0 + A_0\sum_m e^{i\mathbf{q}_m\cdot\mathbf{r}}\right)\left(-A_0\sum_l e^{i\mathbf{q}_l\cdot\mathbf{r}}\right)\\
&= 3\left(\psi_0^2 + 2\psi_0 A_0\sum_n e^{i\mathbf{q}_n\cdot\mathbf{r}} + A_0^2\sum_{n,m} e^{i(\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}}\right)\left(-A_0\sum_l e^{i\mathbf{q}_l\cdot\mathbf{r}}\right)\\
&= -3\psi_0^2 A_0\sum_l e^{\mathbf{q}_l\cdot\mathbf{r}} - 6\psi_0 A_0^2\sum_{n,m} e^{i(\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}} - 3A_0^3\sum_{n,m,l} e^{i(\mathbf{q}_n+\mathbf{q}_m+\mathbf{q}_l)\cdot\mathbf{r}}
\end{aligned}$$

$$\begin{aligned}
6\psi\left(\nabla\psi\right)^2 &= 6\left(\psi_0 + A_0\sum_n e^{i\mathbf{q}_n\cdot\mathbf{r}}\right)\left(A_0\sum_m i\mathbf{q}_m e^{i\mathbf{q}_m\cdot\mathbf{r}}\right)\cdot\left(A_0\sum_l i\mathbf{q}_l e^{i\mathbf{q}_l\cdot\mathbf{r}}\right)\\
&= -6\psi_0 A_0^2\sum_{n,m}\mathbf{q}_n\cdot\mathbf{q}_m e^{i(\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}} - 6A_0^3\sum_{n,m,l}\mathbf{q}_n\cdot\mathbf{q}_m e^{i(\mathbf{q}_n+\mathbf{q}_m+\mathbf{q}_l)\cdot\mathbf{r}}
\end{aligned}$$

Now we have to establish some identities of the lattice vectors for this configuration. Note that:

$$\begin{aligned}
\mathbf{q}_m\cdot\mathbf{q}_n &= \begin{cases} 1 & m=n \\ -\frac{1}{2} & m\neq n \end{cases}\\
&= \left(\frac{3}{2}\delta_{mn} - \frac{1}{2}\right)
\end{aligned} \tag{60}$$

Additionally,

$$\mathbf{q}_m + \mathbf{q}_n = \begin{cases} 2\mathbf{q}_m & m=n \\ -\mathbf{q}_l & m\neq n, \text{ (where } m\neq l\neq n) \end{cases} \tag{61}$$

Given these, we may make some progress:

$$\begin{aligned}
\sum_{n,m}\mathbf{q}_n\cdot\mathbf{q}_n e^{i(\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}} &= \sum_n e^{2\mathbf{q}_n\cdot\mathbf{r}} - \frac{1}{2}\sum_{m\neq n} e^{i(\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}}\\
&= \sum_n\left(e^{2i\mathbf{q_n}\cdot\mathbf{r}} - e^{-i\mathbf{q_n}\cdot\mathbf{r}}\right)
\end{aligned} \tag{62}$$

Additionally,

$$\begin{aligned}
\sum_{n,m,l}\mathbf{q}_n\cdot\mathbf{q}_m e^{i(\mathbf{q}_n+\mathbf{q}_m+\mathbf{q}_l)\cdot\mathbf{r}} &= \sum_{n,m}\left(e^{2i\mathbf{q}_n\cdot\mathbf{r}} - e^{-i\mathbf{q}_n\cdot r}\right)e^{i\mathbf{q}_m\cdot\mathbf{r}}\\
&= \sum_{n,m} e^{i(2\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}} - \sum_{n,m} e^{i(\mathbf{q}_n-\mathbf{q}_m)\cdot\mathbf{r}}
\end{aligned} \tag{63}$$

Also:

$$\sum_{n,m} e^{i(\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}} = \sum_n e^{i2\mathbf{q}_n\cdot\mathbf{r}} + 2\sum_n e^{-i\mathbf{q}_n\cdot\mathbf{r}} \tag{64}$$

and finally:

$$\begin{aligned}
\sum_{n,m,l} e^{i(\mathbf{q}_n+\mathbf{q}_m+\mathbf{q}_l)\cdot\mathbf{r}} &= \sum_{n,m}\left(e^{i2\mathbf{q}_n\cdot\mathbf{r}} + 2e^{-i\mathbf{q}_n\cdot\mathbf{r}}\right)e^{i\mathbf{q}_m\cdot\mathbf{r}}\\
&= \sum_{n,m} e^{i(2\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}} + 2\sum_{n,m} e^{i(\mathbf{q}_n-\mathbf{q}_m)\cdot\mathbf{r}}
\end{aligned} \tag{65}$$

Substituting we get:

$$6\psi\left(\nabla\psi\right)^2=-6\psi_0A_0^2\sum_n e^{2i\mathbf{q}_n\cdot\mathbf{r}}+6\psi_0A_0^2\sum_n e^{-i\mathbf{q_n}\cdot\mathbf{r}}-6A_0^3\sum_{n,m}e^{i(2\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}}+6A_0^3\sum_{n,m}e^{i(\mathbf{q}_n-\mathbf{q}_m)\cdot\mathbf{r}} \quad (66)$$

and

$$3\psi^2\chi=-3\psi_0^2A_0\sum_n e^{i\mathbf{q}_n\cdot\mathbf{r}}-6\psi_0A_0^2\sum_n e^{i2\mathbf{q}_n\cdot\mathbf{r}}-12\psi_0A_0^2\sum_n e^{-i\mathbf{q}_n\cdot\mathbf{r}}-3A_0^3\sum_{n,m}e^{i(2\mathbf{q}_n+\mathbf{q}_m)\cdot\mathbf{r}}-6A_0^3\sum_{n,m}e^{i(\mathbf{q}_n-\mathbf{q}_m)\cdot\mathbf{r}} \quad (67)$$