Geometry of Gradient Flows

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Abstract

• Seek evolution equations for aggregation of particles
• Show competition between length scales of forces
• History of the problem goes back to Debye and Hückel in 1923
• Use variational method based on the geometric analog of Darcy’s law
• Interested in the formation and interaction of singular solutions
• Treat lots of examples

“I shall speak of things . . . so singular in their oddity as in some manner to instruct, or at least entertain, without wearying.”
– Lorenzo da Ponte
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1 Lecture 1: Introduction

1.1 What these lectures will cover

1. Start with Cahn-Hilliard for phase separation and coarsening of patterns, discuss its coupling to Navier-Stokes


3. Discuss magnetic degrees of freedom

4. Discuss the part of KS that leads to chemotactic collapse in the parabolic-elliptic version, in preparation for singular solutions in GOP for porous media.

5. Treat lots of examples. Give several exercises and research problems.

6. Say something about combining Hamiltonian and dissipative structures using double brackets.

1.2 Collaborators

DDH, Vakhtang Putkaradze, Cesare Tronci and Lennon Ó Náraigh


3
2 Cahn-Hilliard equations

Introduce a scalar phase variable

\[ \phi(x, t) = \begin{cases} +1 & \text{if } x \text{ is in phase 1} \\ -1 & \text{if } x \text{ is in phase 2} \end{cases} \]

The Cahn-Hilliard equation is

\[ \partial_t \phi = \text{div} \left( M(\phi) \nabla \frac{\delta F}{\delta \phi} \right) = \text{div} \left( M(\phi) \nabla \left( \phi^3 - \phi - \gamma^2 \Delta \phi \right) \right) \]

when a double-well free energy is chosen, such as

\[ F[\phi] = \int \frac{1}{4} (\phi^2 - 1)^2 + \frac{\gamma^2}{2} |\nabla \phi|^2 \, d^nx \]

\( M(\phi) \geq 0 \) is the mobility (often a constant, or linear in \( \phi \)), \( \gamma \) is the interfacial thickness. The Cahn-Hilliard equation evolves \( \phi \) to minimize the free energy:

\[ \frac{dF}{dt} = -\int M(\phi) \left| \nabla \frac{\delta F}{\delta \phi} \right|^2 \, d^nx \leq 0 \]

2.1 Cahn–Hilliard solution behaviour in 1D

The most interesting evolutionary feature of solutions of the Cahn–Hilliard equation is that they model phase separation, or coarsening. Coarsening in 1D for \( M(c) = \text{const} \) looks like the following.

Figure 2.1: 1D solutions of Cahn-Hilliard: \( c = \pm 1 \) in domains with interfaces of thickness \( \gamma \). That is, in 1D Cahn-Hilliard solutions form STRIPES, which tend to merge in time. Figure by L O’Naraigh.
2.2 Cahn–Hilliard solution behaviour in 2D

Cahn–Hilliard “coarsening” in 2D at a given time looks like

Figure 2.2: In 2D, Cahn-Hilliard solutions form 2D stripe patterns, which tend to merge in time. Figure by L O’Naraigh. (How did the tiger/zebra/conch/etc. get stripes?)
2.3 Cahn–Hilliard solution behaviour in 3D

Figure 2.3: 3D Cahn-Hilliard evolution, courtesy L O’Naraigh.

Figure 2.4: Cahn-Hilliard solutions in 3D form regions $c = \pm 1$, which tend to merge in time. Figure by L O’Naraigh.

2.4 Connection of Cahn-Hilliard to Riemannian geometry

The Cahn-Hilliard equation,

$$\partial_t \phi = \text{div} \left( M(\phi) \nabla \frac{\delta F}{\delta \phi} \right)$$

implies, under the $L^2$ pairing $\langle f, h \rangle := \int_{\Omega} f h \, d^n x$,

$$\frac{dE[\phi]}{dt} = \left\langle \partial_t \phi, \frac{\delta E}{\delta \phi} \right\rangle = \left\langle \text{div} \left( M(\phi) \nabla \frac{\delta F}{\delta \phi} \right), \frac{\delta E}{\delta \phi} \right\rangle$$

$$= - \left\langle \left( M(\phi) \nabla \frac{\delta F}{\delta \phi} \right), \nabla \frac{\delta E}{\delta \phi} \right\rangle = \gamma \left( \frac{\delta F}{\delta \phi}, \frac{\delta E}{\delta \phi} \right)$$

in which the last line denotes a Riemannian metric based on $L^2$. Likewise, Cahn-Hilliard itself can be written in weak form as

$$\langle \partial_t \phi, \psi \rangle = \gamma \left( \frac{\delta F}{\delta \phi}, \psi \right)$$
2.5 Cahn–Hilliard coupled to Navier-Stokes

The Cahn–Hilliard formalism can be applied for interactions between a nonlinearly evolving scalar phase density and a fluid.

\[ \partial_t \phi + u \cdot \nabla \phi = \text{div} \left(M(\phi) \nabla \frac{\delta F}{\delta \phi} \right) \quad \text{div} u = 0 \]

\[ \rho_0 (\partial_t u + u \cdot \nabla u) = -\nabla p + \mu_0 \Delta u + \frac{\delta F}{\delta \phi} \nabla \phi \]

where \( \rho_0 \) and \( \mu_0 \) are constants.

This coupling introduces competition between the stirring mechanism \( u \cdot \nabla \phi \), and the demixing Cahn–Hilliard mechanism.

This system dissipates the sum of the kinetic and potential energies

\[ E = \frac{\rho_0}{2} \| u \|_{L^2}^2 + F[\phi] \]

in the form

\[ \frac{dE}{dt} = - \int \mu_0 |\nabla u|^2 + M(\phi) \left| \nabla \frac{\delta F}{\delta \phi} \right|^2 \, dx \leq 0 \]

2.6 Stirred Cahn-Hilliard solutions in 2D

Figure 2.5: Two co-existing regimes may be identified for the stirred Cahn-Hilliard solution, depending on the strength \( \alpha \) of the stirring: these are bubbles and filaments. Courtesy L O’Naraigh.
2.7 Summary of stirred Cahn-Hilliard behaviour

- A steady state is always achieved, owing to the balance between the advection and Cahn-Hilliard terms.

- For small forcing ($\alpha$) the steady state comprises domains of constant size, while for larger forcing the mixed state is favoured.

- The domain growth always saturates – called “coarsening arrest”.

- Stirring vigorous enough may break up the domains and produce mixing.

  Research problem (hard): How vigorously? Is there such a thing as phase turbulence of Cahn–Hilliard coupled to Navier–Stokes?

  Research problem (easier): Compute the effect of the Cahn–Hilliard phase dynamics on the fluid using Cahn–Hilliard coupled to Navier–Stokes as an initial value problem. What are the boundary conditions?
3 Lecture 2: Chemotaxis


\[ n(t, x) = \text{number density of cells at time } t \text{ and position } x, \]
\[ c(t, x) = \text{concentration of chemo-attractant.} \]

In a collective motion, the chemo-attractant is emitted by the cells that react according to a biased random walk with six parameters \( D \) (diffusivity), \( \mu \) (mobility), \( \alpha \) (length) \& \( \beta, \gamma, \epsilon \), dimensionless

\[
\begin{align*}
\partial_t n(x, t) &= \text{div}(D \nabla n - \mu n \nabla c) \quad x \in \mathbb{R}^d \\
\epsilon \partial_t c(x, t) &= \alpha^2 \Delta c - \gamma c + \beta n
\end{align*}
\]

The parameter \( \mu \) measures the sensitivity of cells to the chemo-attractant. It is also called the mobility. Note: the equations change type from parabolic-parabolic to parabolic-elliptic when \( \epsilon \to 0_+ \).

PKS solution behaviour The PKS model, although very simple, is only understood well in 2D. It’s most interesting feature is chemotactic collapse, in which the density of the cells \( n \) becomes a delta function for certain values of the various constants in the PKS equations.

For other values of the PKS constants, the solution separates into domains, as for Cahn-Hilliard, but does not collapse.

Figure 3.1: Coupling the PKS model to a Navier-Stokes fluid flow would lead to interesting swirling patterns, too.

Research problem: Consider the self-consistent coupling, and investigate how the PKS dynamics stirs the fluid.
3.1 The set-up for chemotactic collapse

Consider the PKS equations with $\epsilon = 0$ and $\gamma = 1 = \beta$

$$\frac{\partial n(x, t)}{\partial t} = \text{div}(D \nabla n) - \text{div}(\mu n \nabla c)$$

$$0 = \alpha^2 \Delta c - c + n \iff c = (1 - \alpha^2 \Delta)^{-1} n =: \bar{n}$$

This represents a competition between diffusion ($D$) and a nonlocal attraction over a region size $\alpha$. The see how attraction could lead to chemotactic collapse, we now set $D = 0$ and $c = \bar{n}$, to find

$$\frac{\partial n(x, t)}{\partial t} = -\text{div}(n \mu \nabla \bar{n})$$

This equation is in Cahn–Hilliard form with mobility $M(n) = \mu n$,

$$\frac{\partial n(x, t)}{\partial t} = -\text{div}(\mu n \nabla \bar{n}) = -\text{div} \left(\mu n \nabla \frac{\delta F}{\delta n}\right) =: -\text{div} (n u[n])$$

where $F[n] = \frac{1}{2} \int n K_\alpha * n d^n x = \frac{1}{2} \int n \bar{n} d^n x$

3.2 Singular solutions of PKS for $\epsilon = 0 = D$ and $\gamma = 1 = \beta$

Consider an ansatz for $n(x, t)$ in 1D that is a sum over $\delta$-functions

$$n(x, t) = \sum_{a=1}^{N} w_a(t) \delta(x - q_a(t))$$

$$\bar{n}(x, t) = K_\alpha * n = \sum_{a=1}^{N} w_a(t) K_\alpha(x, q_a(t))$$

Substituting this into PKS for $\epsilon = 0 = D$ and $\gamma = 1 = \beta$ yields

$$\dot{w}_a(t) = 0 \quad \text{and} \quad \dot{q}_a(t) = \mu \nabla \bar{n}(q_a(t), t) =: u(q_a(t), t)$$

Thus, the weights $w_a$ are all preserved and the positions of the $\delta$-functions move with the Darcy velocity $u := \mu \nabla \bar{n}(q_a(t), t)$.

**Remark 3.1.** The formation of delta-function weak solutions is called blow up in PDE theory. But that is no cause for regret. Instead, it is an opportunity to investigate how the singularities interact with each other.

*Show that these delta-function solutions exist for PKS with $D = 0$ in any number of dimensions.*
3.3 Singular solution formation of PKS in 1D for density when $\mu \neq 0$

![Figure 3.2: Particle clumps emerge in 1D numerical simulations of PKS with $D = 0$. They merge when they collide. The vertical coordinate is $\tilde{n} = K \ast n$.](image)

3.4 Proof of finite-time blow-up of PKS

Consider 1D PKS without linear diffusion and screening $K_\alpha = e^{-|x|/\alpha}$, so that $\tilde{n} = K_\alpha \ast n$

$$\partial_t n(x, t) = -\partial_x (\mu n \partial_x \tilde{n}) =: -\partial_x (n \mathcal{U}[n]).$$

**Lemma 3.2.** $K_\alpha = \frac{1}{2} e^{-|x|/\alpha}$ satisfies $(1 - \partial_x^2) K_\alpha = \delta(x)$. That is, $K_\alpha$ is the Green’s function for the Helmholtz operator $(1 - \partial_x^2)$.

**Proof.** This is a standard result, which can be proved, for example by direct verification. □

**Theorem 3.3** (Anti-maximum theorem for PKS in 1D).

*If* $n$ *has a maximum $n_m(t)$ that exceeds the domain average of* $n$, *then the value of the maximum $n_m(t)$ must diverge in finite time.*

**Proof.** The following analysis of the evolution $n_m(t) = n(x_m(t), t)$ of a maximum in $n$ reveals that the clumping process results from the nonlinear instability of the gradient PKS flow above.

The idea of the proof is to show that for a high enough peak, the maximum value $n_m(t)$ blows up in finite time.

The motion of the maximum $n_m(t)$ is governed by $\partial_x (n \partial_x \tilde{n}) = n_x \tilde{n}_x + n \tilde{n}_{xx} = \alpha^{-2} n (\tilde{n} - n)$, where we have used that $\partial_x n|_{x_m(t)} = 0$ and $\tilde{n}_{xx} = (\tilde{n} - n)$. Hence,

$$\frac{dn_m}{dt} = \frac{\mu}{\alpha^2} \left(n_m - \tilde{n}(x_m)\right) \geq \frac{n_m}{\alpha^2} \left(n_m - \langle n \rangle\right)$$

(3.1)

where $\langle n \rangle$ is the (constant) domain average of $n$. The last inequality holds, because $K \leq 1$ is bounded and $n$ is everywhere positive.

From (3.1), the maximum value $n_m$ must diverge as $n_m \simeq \alpha^2/(t_0 - t)$. This divergence of $n_m$ in finite time produces $\delta$-functions in $n$. □
Figure 3.3: For PKS in 1D with $D = 0$, the inverse maximum amplitude goes to zero in finite time.

### 3.5 Jammed state solution for density when $\mu \to 0$

Exact steady equilibrium solutions exist for $\mu \approx (1 - n)$. These are called jammed states, because they achieve the maximum value, $n = 1$, then stop evolving.

Figure 3.4: Convergence to steady equilibrium solution for $\mu \approx (1 - n)$. In the figure $H \ast \rho$ would be $K \ast n$ in our notation.
Figure 3.5: Convergence to analytic equilibrium solution (circles) for different times (colored solid lines, see legend).

3.5.1 Exercise: Multiple species PKS models

Exercise: Write a multiple species version of the PKS equations, given by

\[
\begin{align*}
\partial_t n(x,t) &= \text{div}(D \nabla n - \mu n \nabla c) \quad x \in \mathbb{R}^d \\
\epsilon \partial_t c(x,t) &= \alpha^2 \Delta c - \gamma c - \beta n.
\end{align*}
\]

4 Magnetization models

The nonlocal Landau–Lifshitz–Gilbert equation is

\[
\frac{\partial m}{\partial \xi} = m \times \left( \mu_m \times \frac{\delta E}{\delta m} \right),
\]

where \( m \) is the magnetization density, \( \mu_m \) is the mobility, defined in 1D as

\[
\mu_m = \left(1 - \beta^2 \partial_x^2 \right)^{-1} m,
\]

and \( \delta E/\delta m \) is the variational derivative of the energy,

\[
\frac{\delta E}{\delta m} = \left(1 - \alpha^2 \partial_x^2 \right)^{-1} m,
\]

where \( \alpha \) and \( \beta \) are constants. The smoothened magnetization \( \mu_m \) and the force \( \delta E/\delta m \) can be computed using the theory of Green’s functions.

The energy functional

\[
E(t) = \frac{1}{2} \int_\Omega m \cdot \left(1 - \alpha^2 \partial_x^2 \right)^{-1} m \, d^3x,
\]
evolves in time according to the relation
\[
\frac{dE}{dt} = -\int_\Omega \left[ m \times (1 - \alpha^2 \partial_x^2)^{-1} m \right] \cdot \left[ \mu_m \times (1 - \alpha^2 \partial_x^2)^{-1} m \right] d^3 x.
\]
Additionally, the magnitude \(|m|\) of the vector \(m\) is constant.

By setting \(\beta = 0\) and replacing \((1 - \alpha^2 \partial_x^2)^{-1}\) with \(1 + \partial_x^2\), we recover the more familiar Landau–Lifshitz–Gilbert equation,
\[
\frac{\partial m}{\partial t} = m \times \left( m \times \frac{\partial^2 m}{\partial x^2} \right).
\]

4.1 Motion with both magnetization density and scalar density

Consider magnetization density \(m\), scalar density \(\psi\) and energy
\[
E(m, \psi) = \frac{1}{2} \int_\Omega m \cdot (1 - \alpha^2 m^2)^{-1} m - \psi(1 - \alpha^2 \psi^2)^{-1} \psi d^3 x,
\]
Darcy’s law for velocity is
\[
V = \mu_\psi \frac{\partial}{\partial x} \frac{\delta E}{\delta \psi} + \mu_m \cdot \frac{\partial}{\partial x} \frac{\delta E}{\delta m}
\]
Assume the following constitutive relations for mobilities:
\[
\mu_\psi = (1 - \beta_\psi^2 \Delta)^{-1} \psi \quad \text{and} \quad \mu_m = (1 - \beta_m^2 \Delta)^{-1} m
\]

Put it all together to find the motion equations,
\[
\partial_t \psi = \text{div}(\psi V)
\]
\[
\partial_t m = \text{div}(m V) + m \times \left( \mu_m \times \frac{\delta E}{\delta m} \right)
\]
\[
V = \mu_\psi \frac{\partial}{\partial x} \frac{\delta E}{\delta \psi} + \mu_m \cdot \frac{\partial}{\partial x} \frac{\delta E}{\delta m}
\]
Singular solutions (in which \(\psi\) and \(m\) are sums of delta functions) emerge spontaneously from smooth initial data, driven by the negative-definite component of the energy. (See figure, about which we will have more to say later.)

**Exercise:** What would the Darcy velocity be for the case of \(N\) scalar densities, \(\psi_a\) with \(a = 1, 2, \ldots, N\)?

**Exercise:** What would the motion equations have been for the case of \(N\) scalar densities, \(\psi_a\) with \(a = 1, 2, \ldots, N\)?
5 Lecture 3: Geometry of gradient flows

Gradient flows in weak form are written consistently with thermodynamics as,

$$\langle \partial_t \rho, \phi \rangle = \langle \text{div}(\rho v(\phi)), \frac{\delta E}{\delta \rho} \rangle = \langle \delta \rho, \frac{\delta E}{\delta \rho} \rangle$$

where $\rho$ is a concentration (number density), $\phi$ is a scalar function and the angle brackets denote $L^2$ pairing, $\langle f, g \rangle = \int f g d^nx$. At this point one summons Darcy’s law (velocity proportional to force, $v(\phi) = \mu(\rho) \nabla \phi$). Then

$$\langle \partial_t \rho, \phi \rangle = \langle \text{div} \left( \rho \mu(\rho) \nabla \frac{\delta E}{\delta \rho} \right), \phi \rangle$$

which is Cahn–Hilliard with $M(\rho) = \rho \mu(\rho)$. This approach leads to a geometry of gradient flows that applies to tensors, vectors, differential forms, etc.

The key idea is to notice that $\delta \rho = \text{div}(\rho v(\phi))$ is a Lie derivative wrt velocity $v(\phi)$ of the density regarded as a volume form $\rho d^nx$.

$$\text{div}(\rho v(\phi)) d^nx = \mathcal{L}_{v(\phi)}(\rho d^nx)$$

**Remark 5.1** (Lie derivatives).

Lie derivatives arise from the tangents to flows on manifolds

$$g_t : M \to M \quad \text{and} \quad g_t \circ g_s = g_{t+s} \quad \text{with} \quad g_0 = Id.$$
Definition 5.2 (Dynamic definition of Lie derivative).

Let \( \alpha \) be a \( k \)-form (or any tensor) defined on a manifold \( M \) and let \( v \) be a vector field with flow \( g_s \) on \( M \) whose action on a point \( x \in M \) is written as \( x(s) = g_s x \). The Lie derivative of the quantity \( \alpha \) along the vector field \( v \) is defined as

\[
\mathcal{L}_v \alpha = \left. \frac{d}{ds} \right|_{s=0} \lesssim \alpha(g_s) \alpha = \left. \frac{d}{ds} \right|_{s=0} \alpha(x(s)).
\] (5.1)

Think of Lie derivation as a time derivative along characteristics of a vector field.

For example, the Lie derivative on \( x(s) \in M \) along a vector field \( v \) is

\[
\mathcal{L}_v x = \left. \frac{d}{ds} \right|_{s=0} x(s) = v(x).
\]

- For a function \( f : M \to M \) it is
  \[
  \mathcal{L}_v f(x) = \left. \frac{d}{ds} \right|_{s=0} f(x(s)) = \nabla f \cdot v
  \]

  This Lie derivative is the geometric definition of gradient.

- For a density \( \rho d^3x \) on \( M \) we have
  \[
  \mathcal{L}_v (\rho(x) d^3x) = \left. \frac{d}{ds} \right|_{s=0} (\rho(x(s)) d^3x(s))) = \left. \frac{d}{ds} \right|_{s=0} (\rho(x(s)) d^3x(s))
  = \mathcal{L}_v (\rho) d^3x + \rho \mathcal{L}_v d^3x = v \cdot \nabla \rho d^3x + \rho \text{div} v d^3x = \text{div}(\rho v) d^3x
  \]

  This Lie derivative is the geometric definition of divergence.

- For a 1-form \( A_i(x) dx^i \) it is
  \[
  \mathcal{L}_v (A_i(x) dx^i) = \left. \frac{d}{ds} \right|_{s=0} (A_i(x(s)) dx^i(s)) \quad \text{along} \quad \frac{dx}{ds} = v(x(s))
  = \left. \frac{\partial A_i}{\partial x^j} v^j \right| dx^i + A_j dv^j = (A_i_j^dv^j + A_j^v^j) dx^i = (\mathbf{v} \times \text{curl} \mathbf{A} + \nabla \cdot (v \cdot A)) \cdot \mathbf{d}x
  \]

Each geometric object (e.g., tensor) has its own corresponding definition of Lie derivative. This is the key idea for generalizing Darcy’s Law, and thereby define the gradient flow of a geometric object. Namely, for any quantity \( \alpha \), which may be a scalar, density, vector field, \( k \)-form, tensor, etc., we set

\[
\delta \alpha = - \mathcal{L}_{u,\alpha} \alpha
\]

Exercise: Use the dynamic definition of the Lie derivative in (5.1) to show that

\[
\mathcal{L}_v d^3x = \text{div} v d^3x.
\]
5.1 Variational derivations of gradient flow equations

We take a thermodynamic viewpoint and define a gradient flow as one that decreases the energy until it reaches a critical point:

\[ \langle \frac{\partial \rho}{\partial t}, \phi \rangle = \langle \delta \rho, \frac{\delta E}{\delta \rho} \rangle = -\langle -L_{u(\phi)} \rho, \frac{\delta E}{\delta \rho} \rangle \]

set \( \delta \rho = -L_{u(\phi)} \rho \)

\[ = \langle -\text{div} \rho u(\phi), \frac{\delta E}{\delta \rho} \rangle \]

\[ = \langle u(\phi), \rho \text{grad} \frac{\delta E}{\delta \rho} \rangle \]

\[ = \langle \left( \mu[\rho] \text{grad} \phi \right)^\sharp, \rho \text{grad} \frac{\delta E}{\delta \rho} \rangle \] (Darcy’s Law, \( \sharp \) raises vector indices)

\[ = \langle -\text{div} \left( \mu[\rho] \left( \rho \text{grad} \frac{\delta E}{\delta \rho} \right)^\sharp \right), \phi \rangle \]

\[ \langle \frac{\partial \rho}{\partial t}, \phi \rangle = \langle -L_{\left( \mu[\rho] \nabla \frac{\delta E}{\delta \rho} \right)^\sharp} \rho, \phi \rangle \] (GOP equation for densities)

where \( \sharp \) raises vector indices in the pairing. That is, superscript sharp \( \sharp \) converts a (covariant) 1-form density to a (contravariant) vector field. The inverse of \( \sharp \) is \( \flat = \sharp^{-1} \), which lowers indices in the same sense, by taking a vector field into its dual 1-form density.

**Exercise:** Write Cahn-Hilliard and PKS as GOP equations for densities.

5.2 Geometric equation for density

If the generalized Darcy velocity \( (\mu[\rho] \nabla \frac{\delta E}{\delta \rho})^\sharp \) depends only on the smoothed density \( \bar{\rho} = H * \rho \) then

\[ \frac{\partial \rho}{\partial t} = -L_{(\mu[\rho] \nabla \frac{\delta E}{\delta \rho})^\sharp} \rho = -\text{div} \left( \rho \left( \mu[\rho] \nabla \frac{\delta E}{\delta \rho} \right)^\sharp \right) \]

admits solutions \( \rho(x,t) \) that are sums of delta functions,

\[ \rho(x,t) = \sum_a \int_s p_a(t,s) \delta(x - q_a(t,s)) \, ds, \]

\[ \bar{\rho}(x,t) = H * \rho = \int H(x',x') \rho(x') \, d^3 x' \]

\[ = \sum_a \int_s p_a(t,s) H(x, q_a(t,s)) \, ds. \]
5.3 Divergence, Gradient, Lie derivative, Diamond ($\diamond$)

The diamond operation ($\diamond$) is defined by

$$\langle b \diamond a , \eta \rangle_X := \langle a , - \mathcal{L}_\eta b \rangle_V$$

For vector fields in the Lie algebra $\mathfrak{X}$ acting on $k$-forms, or other tensor fields in the vector space $V$, both of these pairings are $L^2$ pairings.

Recall Darcy’s law for densities:

$$u(\phi) = - (\mu[\kappa] \nabla \phi)^\sharp$$

Propose the following geometric Darcy law for arbitrary tensors, 1-forms, vector fields, etc.:  

$$u(\phi) = - (\mu[\kappa] \circ \phi)^\sharp$$

5.4 Properties of diamond ($\diamond$) are inherited from the Lie derivative

Consider the following computation based on the properties of the Lie derivative $\mathcal{L}_\eta$ with respect to a vector field $\eta \in \mathfrak{X}$ and the $L^2$ pairing,

$$\langle \mathcal{L}_\eta a , b \rangle =: - \langle \eta , b \diamond a \rangle = \langle a , \mathcal{L}_\eta^T b \rangle := - \langle a , \mathcal{L}_\eta b \rangle = \langle \eta , a \circ b \rangle$$

provided $\mathcal{L}_\eta^T = - \mathcal{L}_\eta$, which holds for $L^2$ pairing. Hence,

Diamond ($\diamond$) is antisymmetric for $L^2$ pairing

$$\langle b \diamond a + a \circ b , \eta \rangle = 0$$

Diamond ($\diamond$) satisfies the chain rule for Lie derivative

$$\langle \mathcal{L}_\xi (b \diamond a) , \eta \rangle = \langle (\mathcal{L}_\xi b) \circ a + b \circ (\mathcal{L}_\xi a) , \eta \rangle$$

Diamond ($\diamond$) is antisymmetric under integration by parts

$$\langle db \diamond a + b \circ da , \eta \rangle = 0.$$ 

5.5 Generalizing beyond densities, $\kappa \in V, \Lambda^n, g$, etc.

$$\langle \frac{\partial \kappa}{\partial t} , \phi \rangle = \langle \delta \kappa , \frac{\delta E}{\delta \kappa} \rangle = \langle \frac{\delta E}{\delta \kappa} , \delta \kappa \rangle \quad (L^2 \text{ pairing is symmetric})$$

$$= \langle \frac{\delta E}{\delta \kappa} , - \mathcal{L}_{u(\phi)} \mu[\kappa] \rangle \quad (\text{variations } \delta \kappa \text{ are defined by a Lie derivative})$$

$$= - \langle \mu[\kappa] \circ \frac{\delta E}{\delta \kappa} , u(\phi) \rangle \quad (\text{one uses the definition of } \circ)$$

$$= \langle \left( \mu[\kappa] \circ \frac{\delta E}{\delta \kappa} \right) , (\phi \circ \kappa)^\sharp \rangle \quad (\text{insert the geometric Darcy Law})$$

$$= \langle (\phi \circ \kappa) , \left( \mu[\kappa] \circ \frac{\delta E}{\delta \kappa} \right)^\sharp \rangle \quad (\text{rearrange using symmetry of the pairing})$$

Hence,  

$$\langle \frac{\partial \kappa}{\partial t} , \phi \rangle = \langle - \mathcal{L}_{(\mu[\kappa] \circ \frac{\delta E}{\delta \kappa})}, \kappa , \phi \rangle \quad (\text{Obtain the GOP equation from the definition of } \circ)$$

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6 Lecture 4: Properties of the GOP equation

Note: GOP is an acronym for “Geometric Order Parameter”.

6.1 Leibniz bracket

The GOP equation defines a (symmetric, Leibniz) bracket \(\{\{E, F\}\}[\kappa]\)

\[
\frac{dF[\kappa]}{dt} = \left< \frac{\partial \kappa}{\partial t}, \frac{\delta F}{\delta \kappa} \right> = -\left< -\mathcal{L}_{(\mu[\kappa] \delta E \delta \kappa)^{\gamma \kappa}} \left( \frac{\delta F}{\delta \kappa} \right) \right>
\]

Thus, the GOP equation may be written in bracket form as

\[
\frac{\partial \kappa}{\partial t} = -\mathcal{L}_{(\mu[\kappa] \delta E \delta \kappa)^{\gamma \kappa}} = \{\{E, \kappa\}\}
\]

For \(\mu[\kappa] \geq 0\) the energy decays \(\frac{dE}{dt} \leq 0\) (by \(F \rightarrow E\) above)

**Proof of Leibnitz property of the symmetric bracket** The Leibnitz property for the functional derivative and for the Lie derivative together imply

\[
\left< \kappa \diamond \left( \frac{\delta (EF)}{\delta \kappa} \right), \eta \right> = \left< \kappa \diamond \left( E \frac{\delta F}{\delta \kappa} + F \frac{\delta E}{\delta \kappa} \right), \eta \right>
\]

\[
= \left< \kappa, -\mathcal{L}_{\eta} \left( E \frac{\delta F}{\delta \kappa} + F \frac{\delta E}{\delta \kappa} \right) \right>
\]

\[
= E \left< \kappa, -\mathcal{L}_{\eta} \frac{\delta F}{\delta \kappa} \right> + F \left< \kappa, -\mathcal{L}_{\eta} \frac{\delta E}{\delta \kappa} \right>
\]

for arbitrary scalar functionals \(E\) and \(F\) of \(\kappa\) and any smooth vector field \(\eta\).

Choosing \(\eta = \left( \mu[\kappa] \diamond \frac{\delta \kappa}{\delta \kappa} \right)^{\gamma \kappa}\) then proves the Leibnitz relation, \(\{\{EF, G\}\} = F\{\{E, G\}\} + E\{\{F, G\}\}\)

**Exercise:** write the GOP equation for \(T = \frac{1}{2} \epsilon_{ijk} n^i dn^j \wedge dn^k\), the 2-form for liquid crystal texture. Show that GOP dissipates an arbitrary energy functional \(E[T]\) when \(\mu(T) = \mu_0 T\) with constant \(\mu_0 > 0\).

**Research problem:** Propose an energy functional \(E[T]\) and derive the formula for evolution of solutions of the GOP equation for the liquid crystal texture. Does this model how liquid crystal defects interact with each other when they collide?

**Research problem:** Write and analyze the GOP equation for liquid crystals in the Erickson-Leslie setting.
6.2 Connection to Riemannian geometry

Following Otto (2001), we use the symmetric bracket to introduce a metric tensor $\gamma_\kappa(\cdot, \cdot)$ defined on vectors from the dual space as

$$\{E, F\} = \gamma_\kappa \left( \frac{\delta E}{\delta \kappa}, \frac{\delta F}{\delta \kappa} \right) = -\left\langle \mu[\kappa] \odot \frac{\delta E}{\delta \kappa}, \left( \kappa \odot \frac{\delta F}{\delta \kappa} \right)^z \right\rangle$$

and recover the GOP evolution equation in the weak Riemannian form as

$$\left\langle \frac{\partial \kappa}{\partial t}, \psi \right\rangle = \gamma_\kappa \left( \frac{\delta \kappa}{\delta \kappa}, \psi \right) = -\left\langle \mu[\kappa] \odot \frac{\delta \kappa}{\delta \kappa}, (\kappa \odot \psi)^z \right\rangle = -\left\langle \mathcal{L}_{(\mu[\kappa] \odot \frac{\delta \kappa}{\delta \kappa})^z} \psi, \kappa \right\rangle$$

for an arbitrary element $\psi$ of the space dual to the $\kappa$ space.

By definition (note minus sign)

$$\gamma_\kappa(\phi, \psi) = -\left\langle \mu[\kappa] \odot \phi, (\kappa \odot \psi)^z \right\rangle$$

For any two elements $\phi, \psi$ of the space dual to $\kappa \in V$

- $\gamma(\phi, \phi) \leq 0$ implies energy decay.
- $\gamma(\phi, \psi)$ is a symmetric negative functional on the dual space of $\kappa \in V$

6.3 Singular solutions for functions

For scalar functions $f : \mathbb{R}^n \to \mathbb{R}$, the properties of diamond give,

$$\left\langle \mu[f] \odot \frac{\delta E}{\delta f}, (\phi \circ f)^z \right\rangle = -\left\langle \left( \frac{\delta E}{\delta f} \nabla \mu[f] \right), (\phi \nabla f)^z \right\rangle$$

(6.1)

The Leibnitz bracket (6.1) for functionals of a scalar function $f$ is

$$\{\{ E, F \}\}[f] = -\int \frac{\delta E}{\delta f} \frac{\delta F}{\delta f} \nabla f : \nabla \mu[f] \, d^3x$$

The GOP equation for scalar functions is a nonlocal wave equation

$$\frac{\partial f}{\partial t} = -\mathcal{L}_{(\mu[f] \odot \frac{\delta \kappa}{\delta \kappa})^z} f$$

$$= -\mathcal{L}_{\left( \frac{\delta \kappa}{\delta f} \nabla \mu[f] \right)^z} f$$

$$= -\left( \frac{\delta E}{\delta f} \nabla \mu[f] \right)^z \cdot \nabla f$$

(6.2)

Hence,

$$f(x, t) = \text{constant along } \frac{dx}{dt} = \left( \frac{\delta E}{\delta f} \nabla \mu[f] \right)^z \text{ Signal speed}$$
If the characteristic signal speed \( \left( \frac{\delta E}{\delta f} \nabla_\mu[f] \right)^2 \) depends only on smoothed \( \bar{f} = H * f \), then singular solutions emerge. That is, the GOP equation for scalar functions admits solutions of the form,

\[
f(x, t) = \sum_{a=1}^{N} w_a(t) \delta(x - q_a(t)), \quad \bar{f}(x, t) = \sum_{a=1}^{N} w_a(t) H(x - q_a(t))
\]

### 6.4 Nonlocal wave evolution of initial delta functions

![Waterfall plot showing numerical simulation results of initial delta functions in f. The vertical coordinate represents \( \bar{f} = H * f \).](image)

**Figure 6.1:** This is a waterfall plot showing the results of a numerical simulation with an initial set of \( \delta \)-functions in \( f \). The vertical coordinate represents \( \bar{f} = H * f \).

### 6.5 2-clumpon interaction for nonlocal wave eqn

![Solution of (6.2) with two \( \delta \)-functions, collapsing in finite time.](image)

**Figure 6.2:** A solution of (6.2) whose initial condition comprises two \( \delta \)-functions with equal and opposite strength, collapses in finite time. Solid lines: exact solution. Dashed lines: numerics.
More examples: Aggregation of magnetic particles

We are now ready to write out explicit equations for the motion of magnets in 1D, 2D, or 3D. As before in section 4.1, $M(x) \in \mathbb{R}^3$ is the average magnetization density. The equations for mass density and magnetization density ($\rho, M$) are written as follows:

$$\partial_t \rho = \text{div}(\rho V)$$
$$\partial_t M = \text{div}(M \otimes V) + M \times \left( \mu_m \times \frac{\delta E}{\delta M} \right)$$
$$V = \mu_p \frac{\partial}{\partial x} \frac{\delta E}{\delta \rho} + \mu_m \cdot \frac{\partial}{\partial x} \frac{\delta E}{\delta M}$$

This is a generalization of the Landau-Lifshitz-Gilbert and Debye-Hückel, or Cahn-Hilliard equations. When the velocity $V$ is smooth, these equations allow single particle solutions of the form

$$\rho(x, t) = w_\rho(t) \, \delta(x - Q(t)),
M(x, t) = w_M(t) \, \delta(x - Q(t)),$$

where $w_\rho$, $w_M$ and $Q$ undergo the following dynamics

$$\dot{w}_\rho = 0,
\dot{w}_M = \left( w_M \times \mu_M \times \frac{\delta E}{\delta M} \right)_{x=Q}
\dot{Q} = \left( \mu_\rho \nabla \frac{\delta E}{\delta \rho} + \mu_M \cdot \nabla \frac{\delta E}{\delta M} \right)_{x=Q}$$

These solutions have an important physical meaning, since they represent particles that aggregate and align. This phenomenon is of fundamental importance in the theory of anisotropic self-assembly.
6.7 Simulations of aggregation of magnetic particles

A typical result of simulations is presented in the figure below.

Figure 6.3: Left: Aggregation of magnetization density in 1D. Right: The corresponding waterfall plot for evolution of averaged density $\bar{\rho} = H * \rho$. Horizontal coordinate is space. Sharp peaks correspond to the formation of $\delta$-function singularities in the density variable $\rho$.

Magnetic filaments  Assume that the solution is concentrated on a set of curves in space defined by $\mathbf{x} = \mathbf{Q}(s, t)$, where $s$ is the arclength. For simplicity of notation, we work at first with a single curve. We are interested in singular solutions of the form

$$\rho(\mathbf{x}, t) = \int w_\rho(s, t) \delta(\mathbf{x} - \mathbf{Q}(s, t)) \, ds$$

$$\mathbf{M}(\mathbf{x}, t) = \int \mathbf{w}_\mathbf{M}(s, t) \delta(\mathbf{x} - \mathbf{Q}(s, t)) \, ds.$$  

Multiplying the LLG equations by a test function and integrating produces its equations of motion:

$$\frac{\partial}{\partial t} w_\rho(s, t) = 0,$$

$$\frac{\partial}{\partial t} \mathbf{w}_\mathbf{M}(s, t) = \mathbf{w}_\mathbf{M} \times \mu_\mathbf{M}(\mathbf{Q}(s, t)) \times \frac{\delta E}{\delta \mathbf{M}}(\mathbf{Q}(s, t)),$$

$$\frac{\partial}{\partial t} \mathbf{Q}(s, t) = \mu_\rho(s, t) \nabla \frac{\delta E}{\delta \rho}(\mathbf{Q}(s, t)) + \mu_\mathbf{M}(s, t) \nabla \frac{\delta E}{\delta \mathbf{M}}(\mathbf{Q}(s, t)).$$

Now one may restore indices so that the interactions of a number of magnetic filaments may be investigated.
6.8 Numerical solution of curve evolution

Two oriented curves interact through a potential. Initially, the curves are far apart and their magnetization distributions $M$ are unrelated. Eventually, the curves collapse to two parallel lines and the $M$ vectors on both curves align.

Figure 6.4: An example of two oriented curves (red and green) attracting each other and unwinding at the same time. The blue vectors illustrate the vector $M \in \mathfrak{so}(3)$ at each point on the curve.

6.9 Theory of clumping of oriented particles

Denote the density at a point $x$ as $\rho(x)$ and orientation as $\sigma(x)$. Assume the total energy is additive,

$$E[\kappa] = E_\rho + E_\sigma,$$

Take the energy of compressibility to be

$$E_\rho = \frac{1}{2} \int \rho(x)\rho(x')G(|x - x'|)dxdx'$$

For $k$-fold symmetry, we must take into account that $\sigma(x)$ and $\sigma(x')$ can differ by $2\pi/k$ without affecting the interaction energy. Thus, the following form of the interaction energy is proposed:

$$E_\sigma = \frac{1}{2} \int \rho(x)\rho(x')K(|x - x'|) \cos[k(\sigma(x) - \sigma(x'))] dxdx'$$
6.10 Another example: Numerical clumping of oriented particles

We take a Gaussian distribution of initial density, possessing random initial orientations.

Figure 6.5: Numerical simulation shows the emergence of particle clumps when the interaction energy for orientation has 5-fold symmetry. The smoothed density starts as a Gaussian, while the smoothed orientation starts randomly.
6.11 Experiments by Patrick Weidmann on clumping with anisotropy

Self-assembly of 4 mm stars

Figure 6.6: Stars (4mm across) floating on water clump into branching trees.
7 Adding inertia

Let’s imagine what happens if we include both inertia and damping in these equations.

For the motion \( x(t) \in \mathbb{R}^3 \), a model set of ordinary differential equations with both even and odd parts, corresponding to inertia and dissipation, respectively, may be written in terms of functions \( C, H : \mathbb{R}^3 \to \mathbb{R} \) as

\[
\frac{dx}{dt} = \nabla C \times \nabla H + \nabla C \times (\nabla C \times \nabla H) \\
= \nabla C \times (\nabla H + \nabla C \times \nabla H)
\]

Thus,

\[
\frac{dH}{dt} = \frac{dx}{dt} \cdot \nabla H = -|\nabla C \times \nabla H|^2 \quad \text{and} \quad \frac{dC}{dt} = \frac{dx}{dt} \cdot \nabla C = 0
\]

\[
\frac{dF}{dt} = \nabla F \cdot \nabla C \times \nabla H + \nabla F \cdot (\nabla C \times (\nabla C \times \nabla H)) \\
= -\nabla C \cdot \nabla F \times \nabla H - (\nabla C \times \nabla F) \cdot (\nabla C \times \nabla H) \\
= \{ F, H \} + \{ \{ F, H \} \}
\]

Conserv Dissip

The conservative bracket is Poisson and Leibniz, while the dissipative bracket is only Leibniz. (It is even under exchanging \( E \leftrightarrow F \) and does not satisfy the Jacobi identity). The motion takes place on a level surface of \( C \) determined by the initial conditions.

**Exercise:** Draw a picture explaining how dissipation of energy works with gradient vectors in \( \mathbb{R}^3 \).