# KINETIC THEORY METHODS IN PHASE KINETICS


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# Particle dynamics

Let $\mathcal{T}_L$ be the $d$–dimensional square torus with side length $L$. Let $\Lambda_{L,\gamma}$ denote the part of the lattice $\gamma\mathbb{Z}^d$ contained in $\mathcal{T}_L$.

A *particle configuration*, is a function $s$ from $\Lambda_{L,\gamma}$ to $\{-1, 1\}$. The site $x(i) = \gamma\, i \in \Lambda_{L,\gamma} \subset \mathcal{T}_L$, $i \in \mathbb{Z}^d$ is *occupied* by a particle if $s(x(i)) = 1$, and is *unoccupied* if $s(x(i)) = -1$.
The Hamiltonian $H_{\gamma,L}$ for the system is

$$H_{\gamma,L}(s) = -\frac{\gamma^d}{2} \sum_{x(i),x(j)\in\Lambda_{L,\gamma}} J(|x(i) - x(j)|)s(x(i))s(x(j)) \ . \quad (1)$$

where $J$ is a a non negative smooth function $J$ on $\mathbb{R}_+$ supported by $[0, 1]$, and strictly monotone decreasing.

We assume the normalization

$$\int_{\mathbb{R}^d} J(|r|)\mathrm{d}r = 1 \ . \tag{2}$$

This function $J$ is the *interaction potential*. Since its range is of order $\gamma^{-1}$ in microscopic units, $H_{\gamma,L}$ is a *local mean field* Hamiltonian: A particle at site $x(i) = \gamma i \in \Lambda_{L,\gamma}$ interacts with a local mean field of neighboring particles:

$$\gamma^d \sum_{\gamma j \in \Lambda_{L,\gamma}} J(|x(i) - x(j)|)s(x(j)) \ . \tag{3}$$

Let $\Omega_{L,\gamma} = \{-1, 1\}^{\Lambda_{L,\gamma}}$ denote the set of all particle configurations. Also, for any $0 \leq N \leq |\Lambda|$, where $|\Lambda|$ denotes the number of sites in $\Lambda$, define

$$\Omega_{L,\gamma,N} := \{ \; s \in \Omega_{L,j} \; : \; \sum_{x \in \Lambda_{L,j}} (s(x)+1)/2 = N \; \} \; .$$

Then $\Omega_{L,\gamma,N}$ is the space of $N$-particle configurations. Given an inverse temperature $\beta$, the canonical Gibbs measure $P_{\mathrm{can}}$ on $\Omega_{L,\gamma,N}$ is defined by

$$P_{\mathrm{can},N}(\{s\}) = \frac{1}{Z_{\mathrm{can},N}} \exp[-\beta H(s)] \, , \qquad Z_{\mathrm{can},N} = \sum_{s \in \Omega_N} \exp[-\beta H(s)] \, ,$$

where we have dropped the subscripts from $H_{\gamma,L}$.

# Dynamics: detailed balance

Let $p(s, s')$ be a Markov transition function giving the probability of a transition from configuration $s$ to configuration $s'$
Then we have *detailed balance* or *reversibility* in case

$$P_{\text{can},N}(\{s\})p(s,s') = p(s,s')P_{\text{can},N}(\{s'\}) \ .$$

There are a number of ways to choose $p(s, s')$. If we only allow swaps at neighboring sites, we get a form of *Kawasaki dynamics*.

The Markov process will converge in the large time limit to equilibrium; i.e., the distribution will become the Gibbs distribution.

# Coarse graining

The probability measure on the spaces of coarse grained configurations $m$ is essentially of the form

$$\frac{1}{Z} e^{-\gamma^{-2}\beta[\mathcal{F}(m)-\mathcal{F}(m_\star)]} ,$$

where $\mathcal{F}$ is the GPL free energy functional, and $m_\star$ is a minimizing coarse-grained configuration, subject to the constraint on the average value:

$$\frac{1}{L^d}\int_{\mathcal{T}_L} m_\star(x)\mathrm{d}x = m , \quad \mathcal{F}(m_\star) = \inf\left\{\mathcal{F}(m) \ : \ \frac{1}{L^2}\int_{\mathcal{T}_L} m(x)\mathrm{d}x = m\right\}$$

$\varphi(m) := \lim_{L\to\infty} \frac{1}{L^2}\mathcal{F}(m_\star)$ is the *Helmholtz specific free energy*.

# The GPL free energy functional

$$\begin{aligned}\mathcal{F}(m) &= \frac{1}{\beta}\int_{\mathcal{T}_L} i(m(x))\mathrm{d}x - \frac{1}{2}\int_{\mathcal{T}_L}\int_{\mathcal{T}_L} J(|x-y|)m(x)m(y)\mathrm{d}x\mathrm{d}y \\ &= \int_{\mathcal{T}_L} f(m(x))\mathrm{d}x + \frac{1}{4}\int_{\mathcal{T}_L}\int_{\mathcal{T}_L} J(|x-y|)[m(x)-m(y)]^2\mathrm{d}x\mathrm{d}y\end{aligned}$$

where

$$f(m) := \frac{1}{\beta} i(m) - \frac{1}{2}m^2 \ ,$$

and

$$i(m) = \frac{1-m}{2}\log\frac{1-m}{2} + \frac{1+m}{2}\log\frac{1+m}{2} \ .$$

# The Cahn-Hilliard Equation

Let $\Omega$ be a bounded domain in $\mathbb{R}^2$.

Let $m = m(x,t)$ be an integrable function on $\Omega$ which represents the value of a *conserved "order parameter"* at $x$ in $\Omega$ at time $t$. The order parameter is conserved in the sense that $\int_\Omega m(x,t)\mathrm{d}x$ is independent of $t$.

Therefore, the evolution equation for $m$ can be written in the form

$$\partial_t m(x,t) = \nabla \cdot \vec{J}(x,t),$$

where the *current* $\vec{J}$ is orthogonal to the outer normal of the boundary of $\Omega$.

We take

$$\vec{J}(x,t) = \sigma(m(x,t))\nabla\mu(x,t),$$

where $\sigma(m)$ is the *mobility* and $\mu(x,t)$ is the *chemical potential* of $x$ at time $t$. The mobility is positive and the chemical potential is defined as the $L^2(\Omega)$ Frechet derivative of a *free energy functional* $\mathcal{F}$:

$$\mu(x) = \frac{\delta \mathcal{F}}{\delta m}(x).$$

The simplest and most familiar example is the so called Cahn–Hilliard equation. It results by setting $\sigma(m) := 1$, i.e. constant mobility, and

$$\mathcal{F}(m) := \frac{1}{2}\int_\Omega |\nabla m(x)|^2 \mathrm{d}x + \frac{1}{4}\int_\Omega (m^2(x) - 1)^2 \mathrm{d}x.$$

This leads to the evolution equation

$$\partial_t m(x,t) = \Delta\left(-\Delta m(x,t) + f(m(x,t))\right),$$

where

$$f(m) = m^3 - m. \tag{4}$$

More generally, $f$ should be a derivative of a smooth double well potential with equal absolute minima.

If $m(x,t)$ solves this equation,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(m(\cdot,t)) = -\int_\Omega |\vec{J}(x,t)|^2 \mathrm{d}x,$$

and thus, evolution decreases the free energy. The minimizers of the free energy are the constant functions $m = \pm 1$. These minimizers represent the “pure phases” of the system. However, unless the initial condition $m_0$ happens to satisfy $\int_\Omega m_0(x)\mathrm{d}x = \pm|\Omega|$, these “pure phases” cannot be reached due to the mass conservation law. Instead, what will eventually be produced is a region in which $m \approx +1$ while $m \approx -1$ in its complement, with smooth transition across its boundary.

# Phase segregation

This phenomenon is referred to as *phase segregation*, where the boundary consists the *interface* between the two phases.

If we "stand far enough back" from $\Omega$, all we can observe is the interface's shape since the structure across the interface is placed on an invisibly small scale.

Once the phases have segregated, and the boundary across them is smooth, the motion becomes *very slow* in a large domain, and we must rescale space and time to see appreciable evolution on a unit time scale.

let $\varepsilon$ be a small parameter, and introduce $\tau$ and $\xi$ by

$$\tau := \varepsilon^3 t \qquad \text{and} \qquad \xi := \varepsilon x.$$

Then

$$\partial_t = \varepsilon^3 \partial_\tau \qquad \text{and} \qquad \partial_x = \varepsilon \partial_\xi \ .$$

Hence, if $m(x,t)$ is a solution of the Cahn–Hilliard equation and we define $m^\varepsilon(\xi,\tau) := m(x(\xi), t(\tau))$ then we obtain

$$\partial_\tau m^\varepsilon(\xi,\tau) = \Delta_\xi \left( -\varepsilon \Delta_\xi m^\varepsilon(\xi,\tau) + \frac{1}{\varepsilon} f(m^\varepsilon(\xi,\tau)) \right) .$$

If we think of $\varepsilon$ as representing the inverse of a large length scale, the variable $\xi$ will be dimensionless.

The dimensionless variables are “slow” and the original variables “fast” for small $\varepsilon$. In what follows, we keep the notation $\xi$ for the slow spatial variables, but we drop the use of $\tau$ and replace it by $t$ for convenience: we are looking at the evolution over a *very* long time scale when $\varepsilon$ is small.

For the reasons indicated above, it is natural to consider initial data $m_0(\xi)$ that is $-1$ in the region bounded by a smooth closed curve $\Gamma_0$ in $\Omega$, and $+1$ outside this region. At later times $t$ there will still be a fairly sharp interface between a region where $m(\xi, t) \approx +1$ and a region where $m(\xi, t) \approx -1$, centered on a smooth curve $\Gamma_t$.

# Evolution of curves

One might hope that for small values of $\varepsilon$, *all information about the evolution of* $m^\varepsilon(\xi, t)$ *is contained in the evolution of the interface* $\Gamma_t$. This is indeed the case.

To explain, let $\mathcal{M}$ denote the set of all smooth simple closed curves in $\Omega$. $\mathcal{M}$ can be viewed as a differentiable manifold. A vector field $V$ on $\mathcal{M}$ is a functional associating to each $\Gamma$ in $\mathcal{M}$ a function in $C^\infty(\Gamma)$. This function gives the normal velocity of a point on $\Gamma$, and thus describes a “flow” on $\mathcal{M}$. We may formally write

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_t = V(\Gamma_t). \tag{5}$$

Now, given a flow on $\mathcal{M}$, we can produce from it an evolution in $C^\infty(\Omega)$ through the following device: Let $m$ be any function from $\mathcal{M}$ to $C^\infty(\Omega)$. We write $m(\xi, \Gamma)$ to denote $m(\Gamma)$ evaluated at $\xi \in \Omega$. We can then define a time dependent function $m(\xi, t)$ on $\Omega$ by

$$m(\xi, t) := m(\xi, \Gamma_t). \tag{6}$$

Notice that time dependence in $m(\xi, t)$ enters *only* through the evolution of $\Gamma_t$.

# To the reduced dynamics and back

If, for small $\varepsilon$ and sharp interface initial data, all of the information about the evolution of solutions of the Cahn–Hilliard equation were contained in the motion of the interface, then one might hope to find a vector field $V$ on $\mathcal{M}$ governing the evolution of the interface, and a function $m$ from $\mathcal{M}$ to $C^\infty(\Omega)$ so that (6) defines the corresponding solution of the Cahn–Hilliard equation.
That is, one seeks a reduced dynamics, given in terms of a flow

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_t = V(\Gamma_t).$$

on the “manifold” of smooth interfaces such that around each integral curve of this ODE there is a solution of the original Cahn-Hilliard equation tracking it.

# The Mullins-Sekerka flow

Before going further with this question, we need to know what the vector field is in

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_t = V(\Gamma_t).$$

Let us fix a number $S > 0$ that will later be interpreted as a "surface tension', denote by $K(\xi) \equiv K(\xi, \Gamma)$ the curvature at $\xi \in \Gamma$ and by $\nu$ the unit outward normal either to $\partial\Omega$ or to $\Gamma$. Further, for each $\Gamma$ in $\mathcal{M}$, let $\mu$ be the solution of

$$\Delta\mu(\xi) = 0 \qquad \text{for} \qquad \xi \in \Omega \setminus \Gamma, \tag{7}$$

subject to the boundary conditions

$$\mu(\xi) = S\left(K(\xi) - \frac{2\pi}{|\Gamma|}\right) \quad \text{on} \quad \Gamma, \quad \partial_\nu \mu = 0 \quad \text{on} \quad \partial\Omega. \tag{8}$$

Now define $V_0(\Gamma)$ as the real valued function on $\Gamma$ given by

$$V_0(\xi, \Gamma) := \frac{1}{2} \left[\partial_\nu \mu\right]_\Gamma (\xi) \qquad \xi \in \Gamma, \tag{9}$$

where the brackets on the right-hand side denote the jump of the normal derivative across $\Gamma$.

This vector field on $\mathcal{M}$ generates a flow known as the Mullins–Sekerka flow.

For the local existence of a unique smooth solution of this free boundary problem see Chen and Escher and Simonetti.

As is well known, the Mullins–Sekerka flow conserves the area enclosed by $\Gamma_t$ and decreases the arc length of $\Gamma_t$.

Let $\Omega_\Gamma^\mp$ denote the interior and exterior of $\Gamma$ respectively. By Green's Theorem,

$$\int_{\Gamma_t} V_0(\eta)\mathrm{d}S_\eta = \int_{\Gamma_t} \frac{1}{2}\left[\partial_\nu \mu\right]_{\Gamma_t}(\eta)\mathrm{d}S_\eta = \int_{\Omega\backslash\Gamma_t} \Delta\mu = 0\ .$$

The left hand side is the rate of change of $|\Omega_{\Gamma_t}|$, and so the area enclosed by $\Gamma_t$ is constant.

Furthermore,

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Gamma_t| = \int_{\Gamma_t} K(\eta)V(\eta)\mathrm{d}S_\eta = \frac{1}{S}\int_{\Gamma_t} \mu\,[\partial_\nu \mu]_{\Gamma_t}\,\mathrm{d}S_\eta = -\frac{1}{S}\int_{\Omega} |\nabla\mu|^2 \mathrm{d}\xi\;.$$

Thus, under the Mullins-Sekerka flow, a region bounded by a smooth curve $\Gamma$ tends to relax towards some disk of the same area.

Notice the two or more disjoint circles *of the same radius* are stationary under the Mullins-Sekerka flow, however, no minimizers of the free energy $\mathcal{F}$ look like this.

The relation between the Chan-Hilliard equations and the Mullin-Sekerka flow was first worked out formally by Bob Pego. Later, Alikakos, Bates and Chen proved rigorously that near any smooth Mullins Sekerka flow, there is a solutions of the Cahn Hilliard equation that “looks the same”.

Before making this precise, it is natural to ask how one sees the connection between the Cahn-Hilliard equation and the Mullins-Sekerka flow. Perhaps even more interesting is the question: Given a phase segregation dynamics, how can one go about deriving equations for the sharp interface limit, and then justifying them?

# Hydrodynamics & Boltzmann

A similar, and conceptually simpler, problem of establishing a precise relation between a detailed dynamics and a reduced dynamics occurs in the study of dilute gasses, and concerns the relation between the Boltzmann equation and hydrodynamic equations, such as the Euler equation, and the compressible and incompressible Navier-Stokes equations.

It will be helpful to explain the connection between the “full” and reduced dynamics in this case first, as a paradigm.

The Boltzmann equation for hard-sphere collisions is

$$\frac{\partial}{\partial t} f(x,v,t) + \mathrm{div}(v f(x,v,t)) = Q(f,f)(v,t) \ ,$$

$$(x,v,t) \in \Omega \times \mathbb{R}^3 \times (0,\infty)$$

where

$$Q(f,f)(v,t) = \int_{\mathbb{R}^3 \times S^2} |(v - v_*) \cdot \sigma| (f' f'_* - f f_*) \mathrm{d}\sigma \mathrm{d}v_*,$$

$f = f(v,t), f' = f(v',t), f_* = f(v_*,t), f'_* = f(v'_*,t),$

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|\sigma}{2}, \qquad v'_* = \frac{v + v_*}{2} - \frac{|v - v_*|\sigma}{2}, \qquad \sigma \in S^2 \ .$$

The *equilibrium*; i.e, steady state solutions of the Boltzmann equation are the *Maxwellians:*

$$M(v) = \rho \left( \frac{1}{2\pi\Theta} \right)^{3/2} e^{-|v-u|^2/2\Theta}$$

where $\rho$ and $\Theta$ are positive numbers, and $u \in \mathbb{R}^3$. To see that these are steady states, note that

$$M(v)M(v_*) = M(v')M(v'_*)$$

for all $v$, $v_*$ and $\sigma$.

Now let us consider some fixed probability density $f_0(x, v)$ on $\Omega \times \mathbb{R}^3$, and let $f(x, v, t)$ denote the solution of the Boltzmann equation starting from this initial data.
Now scale: Pick a small $\epsilon > 0$ and define

$$f^\epsilon(\xi, v, \tau) = f(\xi/\epsilon, v, \tau/\epsilon)$$

and note that

$$\frac{\partial}{\partial \tau} f^\epsilon(\xi, v, \tau) + \operatorname{div}(v f(\xi, v, \tau)) = \frac{1}{\epsilon} Q(f^\epsilon, f^\epsilon)(\xi, v, \tau) \ ,$$

$$(x, v, t) \in \Omega_\epsilon \times \mathbb{R}^3 \times (0, \infty)$$

Think of $\Omega$ as large, and $1/\epsilon$ the diameter, say, of $\Omega$.

If the initial data is such that $|\nabla_x f(x,v,0)| = \mathcal{O}(1)$ in $\Omega$, the diameter of $\Omega$ is large and set equal to $1/\epsilon$, the $|\nabla_\xi f^\epsilon(\xi,v,\tau)| = \mathcal{O}(\epsilon)$ in the domain $\Omega_\epsilon$ which has unit diameter: It is slowly varying in $x$. The evolution is dominated by the collision kernel and effectively reduces to

$$\frac{\partial}{\partial\tau} f^\epsilon(\xi,v,\tau) = \frac{1}{\epsilon} Q(f^\epsilon, f^\epsilon)(\xi,v,\tau) \ ,$$

in which $\xi$ is simply a parameter. It then relaxes toward the "local equilibrium"

$$M(\xi,v) = \rho(\xi)\left(\frac{1}{2\pi\Theta(\xi)}\right)^{3/2} e^{-|v-u(\xi)|^2/2\Theta(\xi)}$$

Once this initial layer passes and $f^\epsilon(\xi, v, \tau)$ is sufficiently close to $M(\xi, v)$, the collision term ceases to dominate, and a balance is struck: The hydrodynamic moments begin to evolve, but because of the dissipative effects of the collisions, the solutions always stays close to a local Maxwellian, and we have

$$f^\epsilon(\xi, v, \tau) \approx \rho(\xi, \tau)\left(\frac{1}{2\pi\Theta(\xi, \tau)}\right)^{3/2} e^{-|v-u(\xi,\tau)|^2/2\Theta(\xi,\tau)}$$

To specify the density function $f^\epsilon$, it suffices to specify the evolution of the *hydrodynamical moments*

$$\rho(\xi, \tau) \qquad u(\xi, \tau) \quad \text{and} \quad \Theta(\xi, \tau)\ .$$

If a function of the form

$$\rho(\xi,\tau)\left(\frac{1}{2\pi\Theta(\xi,\tau)}\right)^{3/2} e^{-|v-u(\xi,\tau)|^2/2\Theta(\xi,\tau)}$$

did exactly satisfy the Boltzmann equation, it is easy to see what equations $\rho$, $u$ and $\Theta$ must solve – the compressible Euler equations.

For example, integrating

$$\frac{\partial}{\partial\tau}f^{\epsilon}(\xi,v,\tau)+\mathrm{div}(vf(\xi,v,\tau))=0$$

in $v$, we find the *continuity equation*:

$$\frac{\partial}{\partial\tau}\rho(\xi,\tau)+\mathrm{div}(u(\xi,\tau)\rho f(\xi,v,\tau))=0\ .$$

# Euler Equations

Computing other moments, the rest of the Euler system is found.

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho u) = 0$$

$$\frac{\partial}{\partial t}u_i + u \cdot \nabla u_i + \frac{1}{\rho}\frac{\partial}{\partial \xi_i}(\rho\Theta) = 0$$

$$\frac{\partial}{\partial t}\Theta + u \cdot \nabla\Theta + \frac{2}{3}\Theta\nabla \cdot u = 0$$

# From Euler back to Boltzmann

Now suppose that one has a smooth solution of the the Euler equations. We ask if there is a corresponding solution $f(\xi, v, \tau)$ of the Boltzmann equation such that

$$f^{\epsilon}(\xi, v, \tau) \approx \rho(\xi, \tau) \left( \frac{1}{2\pi\Theta(\xi, \tau)} \right)^{3/2} e^{-|v-u(\xi,\tau)|^2/2\Theta(\xi,\tau)}$$

How can one construct such a solution? We have obtained a reduced dynamics by making several reasonable approximations, but in what sense do solutions of our reduced equations describe motion of matter that “looks like” a solution of the full dynamics.

# The Hilbert expansion

To answer this question we must go more deeply into the relation between the full and reduced dynamics. In doing so we will be led to several other reduced dynamics for the hydrodynamic moments, each relevant in different kinds of scaling limits, or otherwise put, for different classes of initial data.

A key idea for this goes back to David Hilbert. He begins with the following *ansatz*: Write the solution of the Boltzmann equation

$$\frac{\partial}{\partial \tau} f^{\epsilon}(\xi, v, \tau) + \mathrm{div}(v f(\xi, v, \tau)) = \frac{1}{\epsilon} Q(f^{\epsilon}, f^{\epsilon})(\xi, v, \tau)$$

as a formal power series in $\epsilon$:

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \ldots \ .$$

Now, plug this into the Boltzmann equation, and collect like powers of $\epsilon$. Demand that the equations be satisfied term by term in the formal power series.

The leading term, for $\epsilon^{-1}$, gives us the equation

$$Q(f_0, f_0) = 0 \ .$$

This forces $f_0$ to be some local Maxwellian.

It will be helpful to rewrite our expansion as

$$f = f_0(1 + \epsilon h_1 + \epsilon^2 h_2 + \dots) .$$

Next, let us look at the $\epsilon^0$ term. This is

$$\begin{aligned} \frac{\partial}{\partial \tau} f_0(\xi, v, \tau) + \mathrm{div}(v f_0) &= Q(f_0, f_1) + Q(f_1, f_0) \\ &= f_0 \mathcal{L}_{f_0} h_1 \ . \end{aligned}$$

The operator $\mathcal{L}_{f_0}$ is self adjoint in $L^2(f_0)$ with a 5 dimensional nullspace corresponding to the 5 hydrodynamic moments. The Fredholm Alternative requires that the left hand side be orthogonal to the nullspace. This gives us the Euler equations, and then we can solve for the part of $f_1$ orthogonal to the nullspace of $\mathcal{L}_{f_0}$.

The 5 dimensional piece that still must be specified is determined by imposing the Fredholm Alternative at the next order. This gives corrections to the evolution of the hydrodynamic moments, and the moments obtained at this order satisfy the *Navier-Stokes equations*.

# Navier-Stokes

$$\frac{\partial}{\partial t}\rho + \nabla \cdot (\rho u) = 0$$

$$\frac{\partial}{\partial t}u_i + u \cdot \nabla u_i + \frac{1}{\rho}\frac{\partial}{\partial \xi_i}(\rho\Theta) = \frac{2\nu}{\rho}\sum_{j=1}^{3}\frac{\partial}{\partial \xi_j}D_{ij}$$

$$\frac{\partial}{\partial t}\Theta + u \cdot \nabla\Theta + \frac{2}{3}\Theta\nabla \cdot u = \frac{2}{3\rho}[\nabla \cdot (\lambda\nabla\Theta) + 2\nu\sum_{i,j=1}^{3} D_{ij}D_{ij}]$$

where

$$D_{ij} = \frac{1}{2}\Big(\frac{\partial}{\partial \xi_j}u_i + \frac{\partial}{\partial \xi_i}u_j\Big) - \frac{1}{3}(\nabla \cdot u)\delta_{ij} \ .$$

Now, suppose that one goes through this procedure, and produces

$$f = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \dots \ .$$

Is this a good approximate solution of the Boltzmann equation, and then can we find a actual solution nearby? Such a result was proved in the 1980's by Russ Caflisch starting from a smooth solution of the Boltzmann equation. This has been done more recently past the time of the first shock in certain settings by Hsieh-shien Yu.

# Back to Cahn-Hilliard

We shall now explain how to do something similar to understand the relations between the Chan-Hilliard equation and its sharp interface limit, as well as to understand the sharp interface limit for other phase kinetics equations. We would like to go from a solution of

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_t = V(\Gamma_t)$$

for appropriate $V(\Gamma)$ to a solution of the Cahn-Hilliard equation:

$$\partial_\tau m^\varepsilon(\xi,\tau) = \Delta_\xi \left( -\varepsilon \Delta_\xi m^\varepsilon(\xi,\tau) + \frac{1}{\varepsilon} f(m^\varepsilon(\xi,\tau)) \right) .$$

We will construct $V$ as a series

$$V = V_0 + \lambda V_1 + \lambda^2 V_2 + \dots$$

and define

$$V^{(N)} = \sum_{j=0}^{N} \lambda^j V_j \ .$$

once $V_0, \dots, V_N$ are determined. We then then let $\Gamma_t^{(N)}$ denote the solution to

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_t = V^{(N)}(\Gamma_t)$$

starting from a given smooth curve $\Gamma_0$. Let $T$ be the lifetime of this solution.

We shall then construct a sequence of functionals $m^{(N)}$ from $\mathcal{M}$ to $C^\infty(\Omega)$ so that

$$(\xi, t) \mapsto m^{(N)}(\xi, \Gamma_t^{(N)})$$

is an $(N-1)$th order approximate solution of the Cahn-Hilliard equation. More precisely, if we call this function $m(\xi, t)$ for short, then

$$\partial_\tau m^\varepsilon(\xi, \tau) = \Delta_\xi \left( -\varepsilon \Delta_\xi m^\varepsilon(\xi, \tau) + \frac{1}{\varepsilon} f(m^\varepsilon(\xi, \tau)) \right) + \Delta R^{(N)}(x, t)$$

where

$$\sup_{(\xi,t)\in\Omega\times[0,T]} |R^{(N)}(\xi, t)| \leq C_N \lambda^{N-1} \ .$$

We shall see that the vector fields are uniquely determined: $V_k$ is determined of to a term of $\mathcal{O}(\lambda^{k+1})$.

The functionals $m_k$ from $\mathcal{M}$ to $C^\infty(\Omega)$ are a ll built in the following way: Let $\Gamma$ be a smooth, simple closed curve; i.e., $\Gamma \in \mathcal{M}$. Let $d(\xi, \Gamma)$ denote the *signed distance function* from $\xi$ to $\Gamma$. That is,

$$|d(\xi, \Gamma)| = \int_{\eta \in \Gamma} |\xi - \eta| \ ,$$

and let $d(\xi, \Gamma)$ be positive if $\xi$ is exterior to $\Gamma$ and negative if $\xi$ is interior to $\Gamma$.

Within a tubular neighborhood of $\Gamma$ whose width is $1/K$, the maximum curvature on $\Gamma$, the signed distance function is smooth. Moreover, for $\xi$ in this tubular neighborhood, there is a unique point $s(\xi, \Gamma)$ on $\Gamma$ that is closest to $\xi$.
Now, if $h$ is an $C^\infty$ function on $\mathbb{R} \times \Gamma$ such that $h(z, \cdot) = 0$ for $|z| \geq 1/(\lambda K)$, then

$$\xi \mapsto h\left(\frac{d(\xi, \Gamma)}{\lambda}, s(\xi, \Gamma)\right)$$

is in $C^\infty(\Omega)$.

Our functional $m^{(N)}$ will be of the form

$$m^{(N)} = \sum_{j=0}^{N} \lambda^j m_j$$

where each $m_j$ has the from given above, or is a potential of such a function.
In fact, $m_0$ will have the form

$$\overline{m}\left(\frac{d(\xi, \Gamma)}{\lambda}\right)$$

where $\overline{m}$ is a small modification of the optimal front $\tanh(z/\sqrt{2})$.

# Finding $V_0$

Before explaining the full construction, we explain how to find $V_0$, which is the Mullins-Sekerka vector field.

The first step, following Pego, is to write the Cahn-Hilliard equation as a system

$$\partial_t m = \Delta \mu$$

$$\mu = \lambda \Delta m + \frac{1}{\lambda} f(m) \ .$$

To first order, we seek

$$m_1(\xi,t) = \overline{m}\left(\frac{d(\xi,\Gamma_t)}{\lambda}\right) + \lambda h_1\left(\frac{d(\xi,\Gamma_t)}{\lambda}, s(\xi,\Gamma_t)\right) + \lambda\phi_1(\xi,\Gamma_t)$$

together with a chemical potential $\mu_0$ such that

$$\partial_t m_1 = \Delta\mu_0 + \mathcal{O}(\lambda)$$

$$\mu_0 = \lambda\Delta m_1 + \frac{1}{\lambda}f(m_1) + \mathcal{O}(\lambda) \ ,$$

with $h_1$ vanishing at a distance $\mathcal{O}(\lambda)$ from $\Gamma_t$.

To leading order,

$$\partial_t m_1 \approx \frac{1}{\lambda}\overline{m}'\left(\frac{d(\xi,\Gamma_t)}{\lambda}\right) V_0(s(\xi,\Gamma_t)) \ .$$

Integrating over $\Omega$,

$$0 = \int_\Omega \overline{m}'\left(\frac{d(\xi,\Gamma_t)}{\lambda}\right) V_0(s(\xi,\Gamma_t))\mathrm{d}\xi.$$

Since $\mathrm{d}\xi = \lambda(1-\lambda z K(s))\mathrm{d}z\mathrm{d}s$, and since $\overline{m}'$ is even, this holds if and only if $\int_{\Gamma_t} V_0 \mathrm{d}s = 0$.

$$0 = \int_{\Omega} \overline{m}' \left( \frac{d(\xi, \Gamma_t)}{\lambda} \right) V_0(s(\xi, \Gamma_t)) \mathrm{d}\xi$$

is the solvability condition for

$$\Delta \mu_0 = \frac{1}{\lambda} \overline{m}' \left( \frac{d(\xi, \Gamma_t)}{\lambda} \right) V_0(s(\xi, \Gamma_t)) \ .$$

and we take this to define $\mu_0$, in terms of the still unknown $V_0$.

Then $\mu_0$ is very nearly equal to the *single layer potential*

$$\mu_{00}(\xi, \Gamma_t) := 2 \int_{\Gamma_t} G(\xi, \eta) V_0(\eta, \Gamma_t) \delta s_\eta + c_0(t) \ .$$

Now let us go back to

$$\mu_0 = \lambda \Delta m_1 + \frac{1}{\lambda} f(m_1) + \mathcal{O}(\lambda) \ .$$

Suppose $h_1$ vanishes far from $\Gamma_t$. Note that far from $\Gamma_t$, $\overline{m}(d(\xi, \Gamma_t)/\lambda) \approx \pm 1$. Hence, away from $\Gamma_t$,

$$m_1 \approx \pm 1 + \lambda \phi_1 \ , \qquad \Delta m_1 \approx \lambda \Delta \phi_1 \ .$$

To leading order,

$$\mu_0 \approx \frac{1}{\lambda} f(\pm 1 + \lambda \phi_1) \approx \lambda f'(1) \phi_1 \ .$$

So we must have

$$\phi_1 = \frac{1}{f'(1)} \mu_0$$

for $\xi$ outside the tubular neighborhood of $\Gamma_t$. It will be convenient to use this to define $\phi_1$ *everywhere* in $\Omega$. It will be the role of $h_1$ to provide any necessary corrections close to $\Gamma_t$.

We now examine

$$\mu_0 = \lambda \Delta m_1 + \frac{1}{\lambda} f(m_1) + \mathcal{O}(\lambda)$$

within the tubular neighborhood of $\Gamma_t$ in which we have the $(z, s)$ coordinates, and have for any smooth function $g$ in this neighborhood,

$$\lambda^2 \Delta g = (g_{zz} + \lambda^2 g_{ss}) - \lambda K(s) g_z - \lambda^2 K^2(s) z g_z + \mathcal{O}(\lambda^3) \ .$$

Then

$$\lambda^2 \Delta h_1(z, s) = \partial^2_{zz} h_1(z, s) + \mathcal{O}(\lambda) \ .$$

Likewise,

$$\lambda\overline{m}(z,s) = \left[\frac{1}{\lambda}\partial^2_{zz} - K(s)\partial_z\right]\overline{m}(z,s) + \mathcal{O}(\lambda) \ .$$

Putting everything together into

$$\mu_0 = \lambda\Delta m_1 + \frac{1}{\lambda}f(m_1) + \mathcal{O}(\lambda) \ ,$$

$$\begin{aligned}\mu_0(\lambda z, s) &= \frac{1}{\lambda}\left[-\overline{m}'' + f(\overline{m})\right] \\ &+ \left[\partial^2_{zz}h_1(z,s) + K(s)\overline{m}'(z) + f'(\overline{m})(\phi_1 + h_1)\right] + \mathcal{O}(\lambda)\end{aligned}$$

The term proportional to $1/\lambda$ must vanish (to $\mathcal{O}(\lambda)$), so we must have that $\overline{m}$ is (approximately) the minimal transition profile.

Defining $\mathcal{L}$ by

$$\mathcal{L}g(z) = -g''(z) + f'(\overline{m}(z))g(z) \ ,$$

we have

$$\mathcal{L}h_1(z,s) = \left(1 - \frac{f'(\overline{m})}{f'(1)}\right)\mu_0 - K(s)\overline{m}'(z) + \mathcal{O}(\lambda) \ .$$

Now for $\overline{m}(z) = \tanh(z/\sqrt{2})$,

$$\left(1 - \frac{f'(\overline{m})}{f'(1)}\right) = \frac{3}{\sqrt{2}}\overline{m}' \ .$$

Hence our equation reduces to

$$\mathcal{L}h_1(z,s) = \left(\frac{3}{\sqrt{2}}\mu_{0)} - K(s)\right)\overline{m}' + \mathcal{O}(\lambda) \ ,$$

where we have used $\mu_0 = \mu_{00} + \mathcal{O}(\lambda)$.

The operator $\mathcal{L}$ is self-adjoint on $L^2(\mathbb{R})$, and the nullspace is spanned by $\overline{m}'$.

Therefore, the solvability condition for $\mathcal{L}h_1 = g$ is

$$\int g(z)\overline{m}'(z)\mathrm{d}z = 0 \ .$$

In our case we therefore have

$$\mu_{00}(0,s) = SK(s) \ , \qquad S = \frac{\sqrt{2}}{3} = \int_{\mathbb{R}} |\overline{m}'|^2 \mathrm{d}z \ .$$

Now go back to

$$\mu_{00}(\xi,\Gamma_t) := 2\int_{\Gamma_t} G(\xi,\eta)V_0(\eta,\Gamma_t)\mathrm{d}s_\eta + c_0(t) \ .$$

# Dirichlet-Neumann operator

Let $\Gamma$ be a fixed smooth simple closed curve in . Let $h$ be any continuous function on $\Gamma$ such that

$$\int_\Gamma h \mathrm{d}s = 0 \ .$$

Define

$$\varphi_h(\xi) = \int_\Gamma G(\xi, \eta) h(\eta) \mathrm{d}s_\eta \ .$$

Then $\varphi_h$ is harmonic in $\Omega \backslash \Gamma$ and

$$\left[ \frac{\partial}{\partial n} \varphi_h \right] \Big|_\Gamma = h \ .$$

This is a standard result of potential theory.

On the other hand, let $\varphi$ be any continuous function that is harmonic in $\Omega\backslash\Gamma$, and define

$$h := \left[\frac{\partial}{\partial n}\varphi\right]\Big|_{\Gamma} \ .$$

Then

$$\left[\frac{\partial}{\partial n}(\varphi - \varphi_h)\right]\Big|_{\Gamma} = 0 \ ,$$

and so $\varphi = \varphi_h$ is constant, and hence $0$.
Thus, there is a one-to-one correspondence between single layer potentials of functions $h$ integrating to $0$ on $\Gamma$, and harmonic functions on $\Omega\backslash\Gamma$ that are continuous on $\Omega$ and integrate to $0$ on $\Omega$.

Next, consider any continuous function $\phi$ on $\Omega$ that is harmonic in $\Omega \backslash \Gamma$. Define

$$g := \phi\Big|_{\Gamma} .$$

We refer to $g$ as the *Dirichlet data* for $\phi$. The *Neumann data* is

$$\left[\frac{\partial}{\partial n}\phi\right]\Bigg|_{\Gamma} .$$

The *Dirichlet to Neumann operator* $\mathcal{T}_{\Gamma}$ is denied by

$$\mathcal{T}_{\Gamma} g = \left[\frac{\partial}{\partial n}\phi\right]\Bigg|_{\Gamma} .$$

$\mathcal{T}_\Gamma$ is self adjoint and positive on $^2(\Gamma, \mathrm{d}s)$. Indeed, given $h, g$, let $\varphi$ and $\psi$ be harmonic in $\Omega\backslash\Gamma$ with Dirichlet data $h, g$ respectively. Then

$$\begin{aligned} \int_\Gamma f\mathcal{T}_\Gamma g \mathrm{d}s &= \int_\Gamma \psi \left[\frac{\partial}{\partial n}\psi\right] \mathrm{d}s \\ &= \int_\Omega \nabla\varphi \cdot \nabla\psi \mathrm{d}\xi \end{aligned}$$

It is easy to see that the nullspace consists exactly of the constants, and so $\mathcal{T}_\Gamma$ is invertible on the orthogonal complement of the constants.

Since

$$\mathcal{S}_\Gamma v(\xi) := \int_\Gamma G(\xi,\eta)v(\eta)\mathrm{d}s_\eta - \int_\Gamma\int_\Gamma G(\xi,\eta)v(\eta)\mathrm{d}s_\xi\mathrm{d}s_\eta \ ,$$

restricted to $\Gamma$, is Dirichelt data for a harmonic function with Neumann data $v$, provided $v$ integrates to zero on $\Gamma$, we see that $\mathcal{S}_\Gamma$ is the inverse of $\mathcal{T}_\Gamma$.

# Back to $V_0$

Now go back to

$$\mu_{00}(\xi, \Gamma_t) := 2 \int_{\Gamma_t} G(\xi, \eta) V_0(\eta, \Gamma_t) \delta s_\eta + c_0(t) \ .$$

This says $\mu_{00}$ has Neumann data $2V_0$. What we have just derived above says that $\mu_{00}$ has Dirichlet data $SK$, up to a constant. Hence

$$V_0 = \frac{1}{2} \mathcal{T}_\Gamma \left( K - \frac{2\pi}{|\Gamma|} \right) \ ,$$

which gives the Mullins-Sekerka flow.
Now that $V_0$ is determined, so is $\mu_0$ and $\phi_1$, and we have $h_1 = 0$.

# Higher order

The method we have dust described can be iterated to find $m_2 = h_2 + \phi_2$. It is not the case that $h_2 = 0$. For $V_1$ we have

$$V_1 = V_1^{(0)} + \langle V_1 \rangle_\Gamma \ ,$$

where

$$\langle V_1 \rangle_G = \frac{1}{4|\Gamma|} \int_\Omega D_{V_0 \mu))} \mathrm{d}\xi$$

$$\begin{aligned} V_1^{(0)} &= \frac{1}{4}(2S + C)\mathcal{T}_\Gamma V_0 - \frac{1}{2}\mathcal{T}_\Gamma p \\ &- \langle V_1 \rangle_G \mathcal{T}_\Gamma \left[ \int_\Gamma G(\cdot, \eta) \mathrm{d}s_\eta - \frac{1}{|\Gamma|} \int_\Gamma \int_\Gamma G(\xi, \eta) \mathrm{d}s_\eta \mathrm{d}s_\xi \right] \end{aligned}$$

where

$$p(\xi, \Gamma) = \frac{1}{2} \int_{\Omega} G(\xi, \eta) D_{V_0} \mu_{00} \mathrm{d}\eta \ .$$

# The GPL variant of Cahn-Hilliard

The same method works to prove an analog of this result for the non-local GPL functional. The result involves Dircihlet-Neumann operators for a modified Laplacian involving the mobility.

Other variants can be treated. Antonopoulou, Karali and Orlandi have very recently treated a modified Cahn-Hilliard equation

$$\partial_\tau m^\varepsilon(\xi,\tau) = \Delta_\xi \left( -\varepsilon \Delta_\xi m^\varepsilon(\xi,\tau) + \frac{1}{\varepsilon} f(m^\varepsilon(\xi,\tau)) - G_2 \right) + G_1 .$$

# Mullins Sekerka revisited

The sharp interface limit of the Cahn-Hilliard free energy functional in the sharp interface limit is simply

$$\mathcal{F}(\Gamma) = S|\Gamma| \ .$$

If $\Gamma_t$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}\Gamma_t = V(\Gamma_t) \ ,$$

Then

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\Gamma_t) &= \int_{\Gamma_t} K(\eta)V(\eta)\mathrm{d}s_\eta \\ &= \int_{\Gamma_t} \mathcal{T}_{\Gamma_t}K(\eta)\mathcal{S}_{\Gamma_t}V(\eta)\mathrm{d}s_\eta \end{aligned}$$

We can write the right hand side as the the inner produce

$$\langle \mathcal{T}_{\Gamma_t} K, V \rangle_{\Gamma_t}$$

where

$$\langle W, V \rangle_\Gamma := \int_\Gamma W(\eta) \mathcal{S}_\Gamma V(\eta) \mathrm{d}s_\eta$$

defines a Riemannian metric on $\mathcal{M}$. (Recall the $\mathcal{S}_\Gamma$ on area preserving vector fields).

The Mullins-Sekerka flow is gradient flow for the arc length (surface area) under for this metric.