A short introduction to the phase field approach

Benoît Appolaire

 $\mathsf{LEM}-\mathsf{Onera}/\mathsf{CNRS}$

2016, feb. 3rd



Karma et al.

Khatchaturyan et al.

Casademunt et al.

Du et al.

For all free boundary problems (potentially)

- Phase transformations (solidification, solid states, fluid ...)
- Fluid flow (free surfaces)
- Membranes (biology)
- Cracks . . .

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Identify the order parameter(s)

- Build the most relevant thermodynamic functional
- Our Derive the evolution equations
- Relate the parameters to physical quantities
- Solve (this afternoon)
- Post-process (this afternoon)

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- Pelated to choice of phase diagram to display the different states
 - Gas/liquid [Van der Waals, 1873!]: density
 - Ferromagnetic/paramagnetic [Weiss, 1907]: magnetization
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 - Crack (A. Karma, H. Levine, I. Aranson ...)
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Can be compared to level-set method: phase field can be considered as a physical regularization of the advective equation of the level-set In that case, must recover results from sharp interface descriptions

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1. What is an order parameter?

Co-existence of two different states: the order parameter is a field (heterogeneous)

Two visions of the problem

- Either interface are sharp (macroscopic), so discontinuities of the field
- Or diffuse, as proposed very early by van der Waals, 1893



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Same as usual macroscopic thermodynamics, with functionals rather than functions because variables are fields (depend on space ... and time)

- \bullet Isothermal condition and cst volume: Free energy ${\cal F}$
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Starting with the easiest model: Allen-Cahn

Oversimplified version (parameter free but unrealistic)

$$\mathcal{F}(\varphi(t,\underline{x})) = \int_{V} \left[\varphi^{4}(t,\underline{x}) - \varphi^{2}(t,\underline{x}) + |\nabla \varphi(t,\underline{x})|^{2} \right] \mathrm{d}V$$

Where does all these terms come from?

• Homogeneous system $\nabla \varphi = 0$: homogeneous free energy density I will consider two examples

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- What is this gradient term?

1.1. Homogeneous part: Van der Waals fluid

Equation of state for simple fluids: improvement wrt the ideal gas $pv_{\rm m} = RT$ by accounting for finite volume of atoms/molecules and interactions (liquid can sustain negative pressures)

$$(p - a/v_{\rm m}^2)(v_{\rm m} - b) = RT$$

Features a transition between liquid and gas below a critical point given by $\partial P/\partial v_{\rm m}=0$ and $\partial^2 P/\partial v_{\rm m}^2=0$

1.1. Homogeneous part: Van der Waals fluid

Critical point

$$p^{c} = \frac{a}{27b^{2}}$$
$$T^{c} = \frac{8a}{27bR}$$
$$v_{\rm m}^{c} = 3b$$

Reduced form

$$\pi = \frac{8\tau}{3v-1} - \frac{3}{v^2}$$

with $au = T/T^c$, $\pi = p/p^c$ and $v = v_{
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[J. Ericksen, Equilibrium of bars, 1975]

1.1. Homogeneous part: Van der Waals fluid

Free energy: integration of the law of state at constant temperature

$$\frac{1}{RT_c} \frac{\partial f_{\rm m}}{\partial v} \bigg|_{\tau} = -\pi$$

Below the critical point, $f_{\rm m}$ features a non-convex part: corresponds to states that cannot be observed

Liquid \leftrightarrow Gas transitions

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Free energy: integration of the law of state at constant temperature

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Liquid \leftrightarrow Gas transitions

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Free energy: integration of the law of state at constant temperature

$$\frac{f_{\rm m}}{RT_c} = K(\tau) - \frac{8}{3}\tau \ln(3v - 1) - \frac{3}{v}$$

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Equilibrium between liquid and gas: variational calculus

Minimum of ${\cal F}$ with constant total number of atoms (constraint) Miminize the Lagrangian ${\cal L}={\cal F}-\lambda\left(\int_V
ho{
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$$\delta \mathcal{L} = \int_{V} \left[\delta(\rho f_{\mathrm{m}}) - \lambda \delta \rho \right] \mathrm{d}V = 0$$

This is valid $\forall \delta \rho$

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1.1. Homogeneous part: Van der Waals fluid

Equilibrium between liquid and gas: variational calculus

$$f_{\rm m} + \rho \, \frac{\partial f_{\rm m}}{\partial \rho} = \lambda$$

Thus, if liquid L and gas G are coexisting, they must feature the same value for their respective Gibbs energies:

$$f^{\mathrm{L}}_{\mathrm{m}}(v^{\mathrm{L}}_{\mathrm{m}}) + p^{\mathrm{L}}v^{\mathrm{L}}_{\mathrm{m}} = f^{\mathrm{G}}_{\mathrm{m}}(v^{\mathrm{G}}_{\mathrm{m}}) + p^{\mathrm{G}}v^{\mathrm{G}}_{\mathrm{m}}$$

Moreover, more involved variational calculus considering two co-existing liquid and gas extending over volumes V^{L} and V^{G} respectively would prove that for a flat interface $p^{\text{L}} = p^{\text{G}}$.

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Equilibrium between liquid and gas: variational calculus

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Moreover, more involved variational calculus considering two co-existing liquid and gas extending over volumes V^{L} and V^{G} respectively would prove that for a flat interface $p^{\text{L}} = p^{\text{G}}$.

1.1. Homogeneous part: Van der Waals fluid

Equilibrium between liquid and gas: variational calculus

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Equilibrium between liquid and gas: variational calculus

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- Maxwell rule: both phases (Gibbs energies of both phases are equal)
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1.1. Homogeneous part: Van der Waals fluid

Most important feature: non-convexity of free energy Expansion with respect to the relevant order parameter $\phi = (v_m - v_m^c)/v_m^c$

$$\pi = \frac{8\tau}{3\phi + 2} - \frac{3}{(1+\phi)^2}$$
$$\pi \sim 4\tau - 3 + 6(1-\tau)\phi$$
$$+ 9(\tau - 1)\phi^2 + 3(4-9/2\tau)\phi^3$$

$f(\phi) = f_0 + A\phi + B\phi^2 + C\phi^3 + D\phi^4$

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1.2. Homogeneous part: Weiss molecular field for magnetism

A bit of statistical physics

In the canonical ensemble ${\mathcal F}$

At equilibrium, the configurations follow the Boltzmann distribution

$$\mathcal{P}_{i} = \frac{1}{\mathcal{Z}} \exp\left(-\beta E_{i}\right)$$
$$\mathcal{Z} = \sum_{i} \exp\left(-\beta E_{i}\right) \qquad \text{with } \beta = 1/(k_{\mathrm{B}}T)$$
$$\mathcal{F} = -k_{\mathrm{B}}T \ln \mathcal{Z}$$

Most simple model for magnetism: Ising N atoms with nearest neighbors

$$\mathcal{H} = -J \sum_{l \in \mathcal{S}} s_l s_j - h \sum_i s_i$$
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Most simple model for magnetism: Ising N atoms with spins $s_i=\pm 1$ interacting with nearest neighbors

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$$

1.2. Homogeneous part: Weiss molecular field for magnetism

A bit of statistical physics

Let's consider a single atom: can display only two states with probabilities

$$\mathcal{P}_{+} = \frac{1}{\mathcal{Z}} \exp(+\beta h)$$
 $\mathcal{P}_{-} = \frac{1}{\mathcal{Z}} \exp(-\beta h)$

Partition function

 $\mathcal{Z} = \exp(+\beta h) + \exp(-\beta h)$

Magnetization: average spin

 $m = \langle s \rangle = (+1)\mathcal{P}_{+} + (-1)\mathcal{P}_{-}$ $= \tanh(\beta h)$

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10

5

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Now, let's consider N atoms: there are 2^N different configurations Hard to calculate $\mathcal Z$ and so the probability of a given configuration (aka microstate)

- Brute force: Monte Carlo with Metropolis algorithm
- Mean field approximation
 - Reducing the N bodies problem into a problem involving a single body in an effective field
 - Neglect correlations between fluctuations

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Bolztmann has related entropy to combinatorics:

$$S = k. \log W$$

Simple when there is no correlation.

Indeed reduces to count how many configurations with $N_{\!+}$ indistinguishable positive spins over the N atoms

$$W = \binom{N}{N_+} = \frac{N!}{N_+!N_-!}$$

with $N_{\!+}=N(1+m)/2$ and $N_{\!-}=N(1-m)/2$

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Stirling formula: $n! \sim \sqrt{2\pi} n^{n+1/2} \exp(-n)$ or $\ln n! \sim n \ln n - n$ (very good for n > 10)

 $\ln W = N \ln N - N - (N_{+} \ln N_{+} - N_{+} + N_{-} \ln N_{-} - N_{-})$

Of course $N_+ + N_- = N$, then

 $\ln W = -(N_{+} \ln(N_{+}/N) + N_{-} \ln(N_{-}/N))$

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Find a polynomial expansion!

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Expanding not far from the critical point, i.e. $m\sim 0$:

$$\ln W \sim -N \left[-\ln 2 + \frac{1+m}{2} \left(m - \frac{m^2}{2} + \frac{m^3}{3} \right) + \frac{1-m}{2} \left(-m - \frac{m^2}{2} - \frac{m^3}{3} \right) \right]$$

$$\ln W \sim -N\Big(-\ln 2 + \frac{1}{2}m^2 + \frac{1}{12}m^4\Big)$$

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$$S \sim -k_{\rm B}N \Big(-\ln 2 + \frac{1}{2}m^2 + \frac{1}{12}m^4 \Big)$$



1.2. Homogeneous part: Weiss molecular field

• Mean field approximation

End up with some $-\phi^2 + \phi^4$ potential Indeed the free energy now reads:

 $nf_{\rm m} = \mathcal{F} = \mathcal{E} - T\mathcal{S}$

 $\frac{f_{\rm m}}{N_a} = -\frac{zJ}{2}m^2 - hm + k_{\rm B}T\left(-\ln 2 + \frac{1}{2}m^2 + \frac{1}{12}m^4\right)$

At the critical temperature $rac{\partial^2 f_{
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$$\frac{f_{\rm m}}{N_a} + \text{cste} = -hm + \frac{k_{\rm B}}{2}(T - T_c) m^2 + \frac{k_{\rm B}T}{12}m^4$$

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2.1. Gradient: spinodal decomposition [Hillert 1956]

Equivalent to the mean field approximation of Ising model



• Mean field neglects fluctuations

$$G(\underline{r},\underline{r}') = \left\langle \delta\psi(\underline{r})\,\delta\psi(\underline{r}')\right\rangle = 0$$
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2.1. Gradient: spinodal decomposition [Hillert 1956]

Mean field

• Energies of first nearest neighbors ij

$$\mathcal{E}_{ij} = -c_i(1 - c_j) V + (1 - c_j) V^{AA} + c_i V^{BB} + (c_j - c_i) V^{AB}$$

with $V=V^{\rm AA}+V^{\rm BB}-2V^{\rm AB}$

Proove it (better to know what to get)

Internal energy becomes

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Proove it (better to know what to get)

• Internal energy becomes

$$\mathcal{E} = N V^{AA} + (V^{BB} - V^{AA}) \sum_{i} c_{i} - \frac{1}{2} \sum_{ij} c_{i} (1 - c_{j}) V$$

- 2. Build the relevant thermodynamic functional
- 2.1. Gradient: spinodal decomposition [Hillert 1956]

• Entropy of a random assembly (ideal solution)

$$S = -k_{\rm B} \sum_{i} \left[c_i \, \ln c_i + (1 - c_i) \, \ln(1 - c_i) \right]$$

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• Free energy

$$\begin{aligned} \mathcal{F} &= N V^{AA} + (V^{BB} - V^{AA}) \sum_{i} c_{i} \\ &+ k_{B} T \sum_{i} \left[c_{i} \ln c_{i} + (1 - c_{i}) \ln(1 - c_{i}) \right] - \frac{1}{2} \sum_{ij} c_{i} \left(1 - c_{j} \right) V \end{aligned}$$

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 \bullet Free energy with respect to pure A & B

$$\Delta \mathcal{F} = k_{\rm B} T \sum_{i} \left[c_i \, \ln c_i + (1 - c_i) \, \ln(1 - c_i) \right] - \frac{1}{2} \sum_{ij} c_i \, (1 - c_j) \, V$$

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• Then the density for an homogeneous solution (i.e. $c_i = c \quad \forall i$)

$$\Delta f_0 = k_{\rm B} T \left[c \, \ln c + (1-c) \, \ln(1-c) \right] - \frac{1}{2} c \left(1-c\right) V$$

• Demixing possible for V < 0 such as $rac{\partial}{\partial c^2} \Delta f_0 < 0$

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Mean field

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2.1. Gradient: spinodal decomposition [Hillert 1956]

Mean field

• At equilibrium

$$\frac{\partial}{\partial c_i} \mathcal{F} = \mu \quad \forall \, i$$

Using the homogeneous free energy density (do it!)

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$$\frac{\partial}{\partial c_i} \Delta \mathcal{F} = \mu' \quad \forall i$$

Using the homogeneous free energy density (do it!)

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$$\frac{\partial}{\partial c_i} \Delta \mathcal{F} = k_{\rm B} T \, \ln\left(\frac{c_i}{1-c_i}\right) + \sum_j c_j \, V - \frac{V}{2} = 0$$

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2.1. Gradient: spinodal decomposition [Hillert 1956]

Mean field

 \bullet At equilibrium ~~ (symetrical case $V^{\rm AA}=V^{\rm BB}$ and $\mu=0)$

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 $\sum_{j} (c_j - c_i)$ is the Laplacian discretized at the scale of the first neighbors spacing: may have something to do with the gradient term

- 2. Build the relevant thermodynamic functional
- 2.2. Gradient: spinodal decomposition by Cahn-Hilliard
 - Lowest order expansion (continuum limit of a mean field model with first neighbor approximation [Hillert, 1956, 1961])

$$f(c, \nabla c, \nabla^2 c \dots) \approx f_0(c) + \sum_i \frac{\partial f}{\partial(\partial_{x_i}c)} \bigg|_c \frac{\partial_{x_i}c}{\partial_x_i} + \sum_{ij} \frac{\partial f}{\partial(\partial_{x_i}^2 c_i)} \bigg|_c \frac{\partial^2_{x_ix_j}c}{\partial(\partial_x_i c_i)} + \frac{1}{2} \sum_{ij} \frac{\partial^2 f}{\partial(\partial_x_i c_i)\partial(\partial_x_j c_i)} \bigg|_c (\partial_{x_i}c) (\partial_{x_j}c) + \dots$$

• In an isotropic medium, f is invariant wrt $x_i o -x_i$ and $x_i o x_j$ $f(c,
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The gradient terms can be gathered

$$\int_{V} \left[\kappa_{1} \nabla^{2} c + \kappa_{2} |\nabla c|^{2} \right] \mathrm{d}V = \int_{V} \left[\nabla \cdot (\kappa_{1} \nabla c) - d\kappa_{1} / dc |\nabla c|^{2} + \kappa_{2} |\nabla c|^{2} \right] \mathrm{d}V$$
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Generally, no prescription at the boundaries for different reasons:

Periodic boundary conditions

• Surfaces can be described by diffuse interfaces

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Benoît Appolaire (LEM)



Following usual non-equilibrium thermodynamics

• Considering some "Allen-Cahn" free energy functional

$$\mathcal{F} = \int_{V} \psi \, \mathrm{d}V = \int_{V} \left[f_0(\varphi) + \frac{\alpha}{2} |\nabla \varphi|^2 \right] \mathrm{d}V$$

where φ is not conserved (e.g. order, magnetization...) and where f_0 displays two minima separated by a non convex part

Second principle implies at cst temperature:

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = -T\,\dot{S}_i + \mathcal{P}_{\mathrm{ext}} \quad \text{with } \dot{S}_i \ge 0$$

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• Dissipation $T \dot{S}_i$

$$\int_{V} \left[-\frac{\partial f_{0}}{\partial \varphi} \frac{\partial \varphi}{\partial t} + \alpha \frac{\partial \varphi}{\partial t} \Delta \varphi \right] \mathrm{d} V \geq 0$$

Local dissipation T s_i

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Usual argument (linear regime) [I. Prigogine, E. Guggenheim]

$$\begin{split} \dot{s}_i &= J F \ge 0 \quad \longrightarrow \quad J \propto F \\ \dot{\varphi} &= M \left(\alpha \Delta \varphi - \frac{\partial f_0}{\partial \varphi} \right) \qquad \text{ with } M > 0 \end{split}$$

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$$\frac{\partial c}{\partial t} = -\nabla \cdot J$$

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Benoît Appolaire (LEM)

Following usual non-equilibrium thermodynamics

Integration by parts identifies S_i and S_{ext}
 Same as before, so I go directly to the result

$$T \, \dot{\mathcal{S}}_i + T \, \dot{\mathcal{S}}_{\text{ext}} = \int_V \left[-\frac{\partial f_0}{\partial c} + \alpha \, \Delta c \right] \frac{\partial c}{\partial t} \mathrm{d}V + \alpha \int_S \frac{\partial c}{\partial t} \, \nabla c \cdot \underline{n} \, \mathrm{d}S$$

The solute balance must be accounted for

 $T\dot{S}_{i} + T\dot{S}_{\text{ext}} = \int_{V} \mu \nabla \cdot J \, \mathrm{d}V - \alpha \int_{S} \nabla \cdot J \, \nabla c \cdot \underline{n} \, \mathrm{d}S$

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Following usual non-equilibrium thermodynamics

• So we proceed to a second integration by parts

$$\mu \nabla \cdot J = \nabla \cdot \left(\mu J\right) - J \cdot \nabla \mu$$

Then

$$T \, \dot{S}_i + T \, \dot{S}_{\text{ext}} = \int_S \mu J \cdot \underline{n} \, \mathrm{d}S - \int_V J \cdot \nabla \mu \, \mathrm{d}V - \alpha \int_S \nabla \cdot J \, \nabla c \cdot \underline{n} \, \mathrm{d}S$$

and we identify

$$T \dot{S}_{i} = -\int_{V} J \cdot \nabla \mu \, \mathrm{d}V \ge 0$$
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$$T\dot{\mathcal{S}}_i = -\int_V J \cdot \nabla \mu \, \mathrm{d}V \ge 0$$

In the linear regime

$$J = -L \nabla \mu = -L \nabla \left(\frac{\partial f_0}{\partial c} - \alpha \Delta c \right) \quad \text{with } L > 0$$

Inserting the full expression of J into the solute balance gives the famous Cahn-Hilliard equation

$$\frac{\partial c}{\partial t} = \nabla \cdot \left[L \, \nabla \left(\frac{\partial f_0}{\partial c} - \alpha \Delta c \right) \right]$$

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4. Parameters

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Benoît Appolaire (LEM)

Master DMS B3: Phase field

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4. Parameters

Equilibrium profile of φ in a simple Allen-Cahn

1D system with a flat interface perpendicular to \boldsymbol{x} and

The equilibrium condition reads

$$\delta \mathcal{F} = \delta \int_{V} \left[f_{0}(\varphi) + \frac{\alpha}{2} |\nabla \varphi|^{2} \right] \mathrm{d}V = 0 \quad \Leftrightarrow \quad \alpha \frac{d^{2}\varphi}{dx^{2}} = \frac{df_{0}}{d\varphi}$$

Integration of this ODE is elementary calculus. Recognize that darphi/dx is an integrating factor, the previous ODE become

$$lpha rac{d arphi}{d x} rac{d^2 arphi}{d x^2} = rac{d f_0}{d arphi} rac{d arphi}{d x}$$
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Equilibrium profile of φ in a simple Allen-Cahn

Then we integrate from $x = -\infty$ to some x:

$$\frac{\alpha}{2} \int_{-\infty} \frac{d}{dx} \left(\frac{d\varphi}{dx}\right)^2 \mathrm{d}x = \int_{-\infty} \frac{df_0}{dx} \mathrm{d}x$$

Complying with the boundary conditions (sign)

$$\sqrt{\frac{\alpha}{2}}\frac{d\varphi}{dx} = -\sqrt{f_0(\varphi(x)) - f_0(\varphi(-\infty))}$$

In the general case (f_0 non-convex but cumbersome function), integrate numerically: the profile features a sigmoidal shape (smooth step function)

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When

 $f_0(\varphi) = W g(\varphi) = W \varphi^2 (1 - \varphi)^2$, the sigmoidal shape can be computed analytically and displays nice features

$$\frac{d\varphi}{dx} = -\sqrt{2W/\alpha}\,\varphi(1-\varphi)$$



Just basic calculus



Just do it!

Hint: substitute $\psi = arphi/(1-arphi)$ and use symmetry

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Master DMS B3: Phase field

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$$\frac{d\varphi}{\varphi(1-\varphi)} = -4 \frac{dx}{\delta}$$
 with $\delta = 4\sqrt{\alpha/(2W)}$

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$$\frac{d\psi}{\psi} = -4\frac{dx}{\delta}$$

$$\ln\left(\frac{\psi}{\psi}\right) = -4\frac{\pi}{\delta}$$

$$\frac{\varphi}{\psi} = \exp\left(-4\pi/\delta\right)$$

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$$\exp\left(-2\pi/\delta\right)$$

$$\frac{d\psi}{\psi} = -4\frac{dx}{\delta}$$
$$\ln\left(\frac{\psi}{\psi(x=0)}\right) = -4\frac{x}{\delta}$$
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$$\ln\left(\frac{\psi}{\psi(x=0)}\right) = -4\frac{x}{\delta}$$
$$\frac{\varphi}{1-\varphi} = \exp\left(-4x/\delta\right)$$
$$\varphi(x) = \frac{\exp(-4x/\delta)}{1+\exp(-4x/\delta)}$$

$$\begin{aligned} \frac{d\psi}{\psi} &= -4\frac{dx}{\delta} \\ &\ln\left(\frac{\psi}{\psi(x=0)}\right) = -4\frac{x}{\delta} \\ &\frac{\varphi}{1-\varphi} = \exp\left(-4x/\delta\right) \\ &\varphi(x) = \frac{\exp(-4x/\delta)}{1+\exp(-4x/\delta)} \\ &\varphi(x) = \frac{\exp(-2x/\delta)}{\exp(-2x/\delta) + \exp(-2x/\delta)} \end{aligned}$$



Interface energy in a simple Allen-Cahn

The interface energy is the excess of the relevant potential: free energy in Allen-Cahn $(f_0(\varphi_{(-\infty)}) = f_0(\varphi_{(+\infty)}))$

$$\gamma = \int_{-\infty}^{+\infty} \left[\Delta f_0 + \frac{\alpha}{2} \left| \frac{d\varphi}{dx} \right|^2 \right] \mathrm{d}x$$

with $\Delta f_0 = f_0 ig(arphi(x) ig) - f_0 ig(arphi(-\infty) ig)$

Let's recall that at equilibrium (cf. Eq.(1)):

$$\frac{\alpha}{2} \left(\frac{d\varphi}{dx}\right)^2 = \Delta f_0$$

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Thus

$$\gamma = \int_{-\infty}^{+\infty} 2\,\Delta f_0ig(arphi^{(x)}ig)\,\mathrm{d}x = \int_{-\infty}^{+\infty} lpha \Big|rac{darphi}{dx}\Big|^2\mathrm{d}x$$

Interface energy in a simple Allen-Cahn

Rather than integrating wrt x, better to integrate wrt φ

$$\gamma = \int_{-\infty}^{+\infty} \alpha \left| \frac{d\varphi}{dx} \right|^2 dx = \int_{-\infty}^{+\infty} \alpha \left| \frac{d\varphi}{dx} \right|^2 \frac{dx}{d\varphi} d\varphi = \int_{0}^{1} \alpha \left| \frac{d\varphi}{dx} \right| d\varphi$$

is again Eq.(1)

$$\gamma = \int_{0}^{1} \sqrt{2\alpha \Delta f_0} d\varphi$$

$$\gamma = \int_{0}^{1} \sqrt{2\alpha W} \varphi(1 - \varphi) d\varphi$$

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Using again Eq.(1)

Try!

For $f_0(\varphi) = W g(\varphi) = W \varphi^2 (1 - \varphi)^2$

 $\gamma = \int_0^1 \sqrt{2 lpha W} \, arphi(1-arphi) \, \mathrm{d}arphi \, .$

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$$\gamma = \int_0^1 \sqrt{2\alpha \Delta f_0} \,\mathrm{d}\varphi$$

$$\gamma = \int_0^1 \sqrt{2\alpha W} \,\varphi(1-\varphi) \,\mathrm{d}\varphi = \sqrt{2\alpha W} \Big[\frac{\varphi^2}{2} - \frac{\varphi^3}{3}\Big]_0^1 = \frac{\sqrt{\alpha W}}{3\sqrt{2}}$$

Allen-Cahn: equilibrium

$\varphi_0 = \frac{1}{2} \left[1 - \tanh\left(\frac{r}{2\delta}\right) \right]$







Allen-Cahn: equilibrium

$$\varphi_{0} = \frac{1}{2} \left[1 - \tanh\left(\frac{r}{2\delta}\right) \right] \qquad \qquad \delta \propto$$
$$\gamma = \int e^{2} \left[\nabla \varphi_{0} \right]^{2} d\Omega \qquad \qquad \gamma \propto$$

 $\frac{\varepsilon}{\sqrt{W}}$

Allen-Cahn: equilibrium

$$\varphi_0 = \frac{1}{2} \left[1 - \tanh\left(\frac{r}{2\delta}\right) \right]$$

$$\gamma = \int \varepsilon^2 \left| \nabla \varphi_0 \right|^2 \mathrm{d}\Omega$$



$$\gamma \propto \varepsilon \sqrt{W}$$



A few words on the spectral method used this afternoon

Use Fourier transforms for periodic microstructures

- Spatial differential operators become algebraic operations
- Very fast algorithms for performing the transforms back and forth: FFT [Cooley, Tukey]
- \bullet Scale as $N\log N$ rather than N^2
- Small memory footprints: 3D!!

Hi, Dr. Elizabeth? Yeah, uh... I accidentally took the Fourier transform of my cat... Meow

I will not give any rigorous definitions and proofs

More like a quick and (very) dirty recipes

$$\begin{split} \hat{\varphi}(\underline{k}) &= \int_{V} \varphi(\underline{x}) \exp\left(-\,\mathrm{i}\underline{k} \cdot \underline{x}\right) \mathrm{d}^{3}x \\ \varphi(\underline{x}) &= \frac{1}{(2\pi)^{3}} \int_{K} \hat{\varphi}(\underline{k}) \exp\left(+\,\mathrm{i}\underline{k} \cdot \underline{x}\right) \mathrm{d}^{3}k \end{split}$$

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Derivative

$$\frac{\widehat{\partial \varphi}}{\partial x_i} = \mathrm{i} k_i \,\hat{\varphi}$$

(proof: integration by parts, considering that the functions are well behaved such that the integrals are convergent)

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Apply to Allen-Cahn equation