Diffuse Interface Models

M. Ceriotti - MSE304

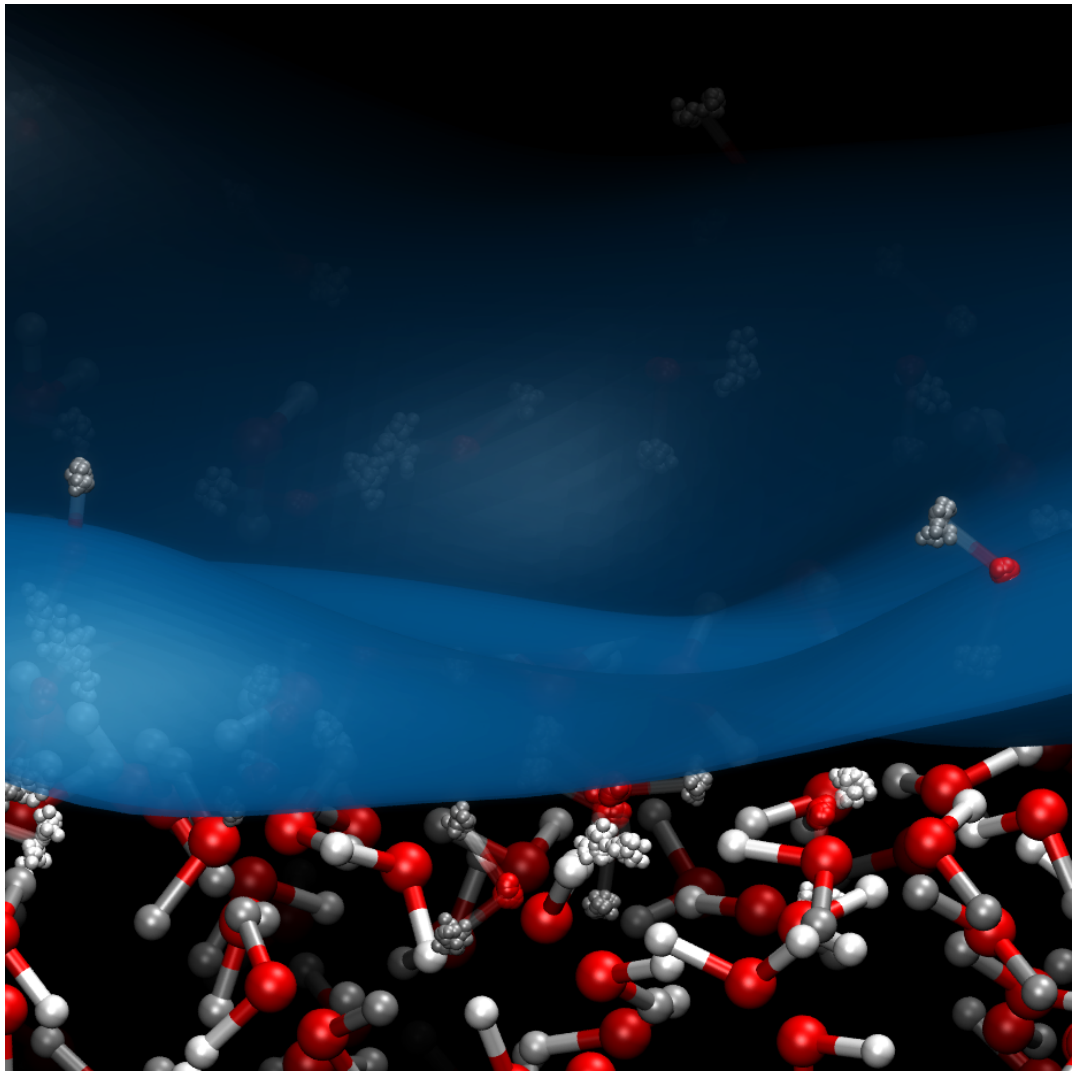
EPFL

Outline

- Surface of liquids
- The Gibbs isotherm
- A reminder on regular solutions
- Cahn-Hillard model of phase segregation
- Diffusion and the dynamical behavior of the Cahn-Hillard model

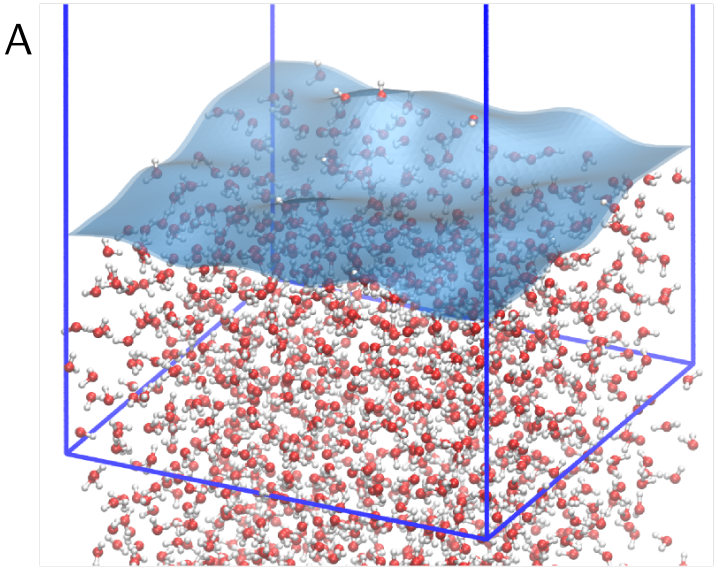
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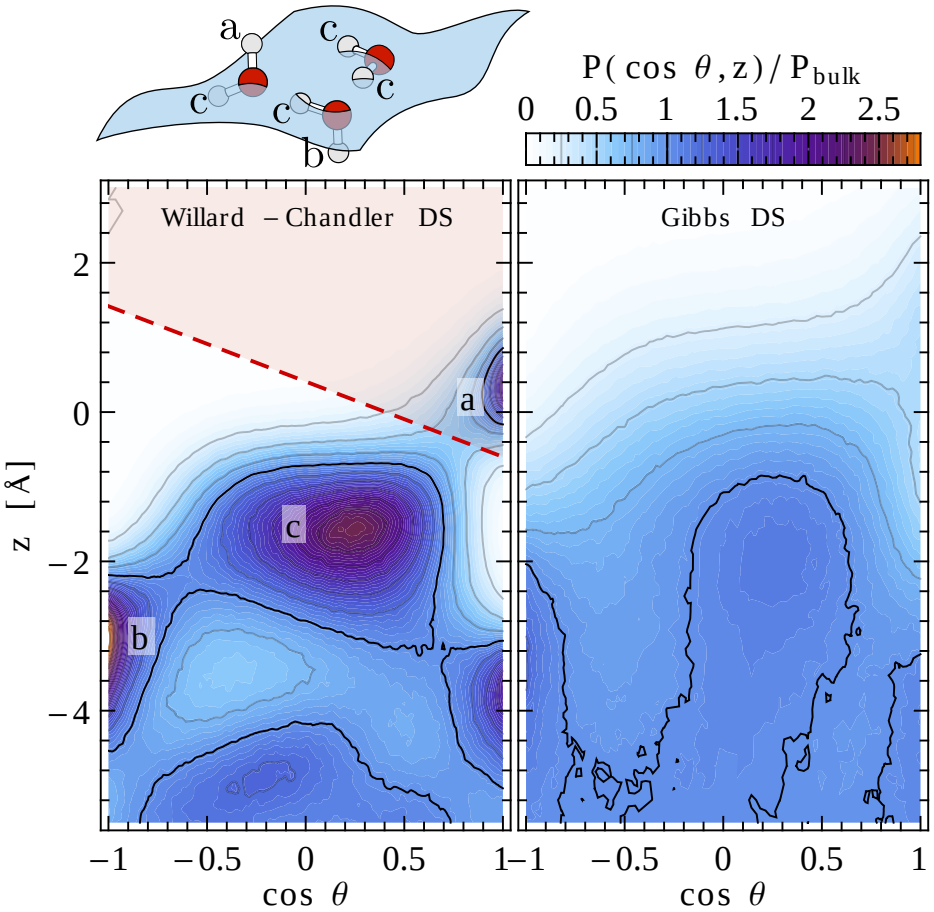
- How does a liquid surface look like at the atomic scale?



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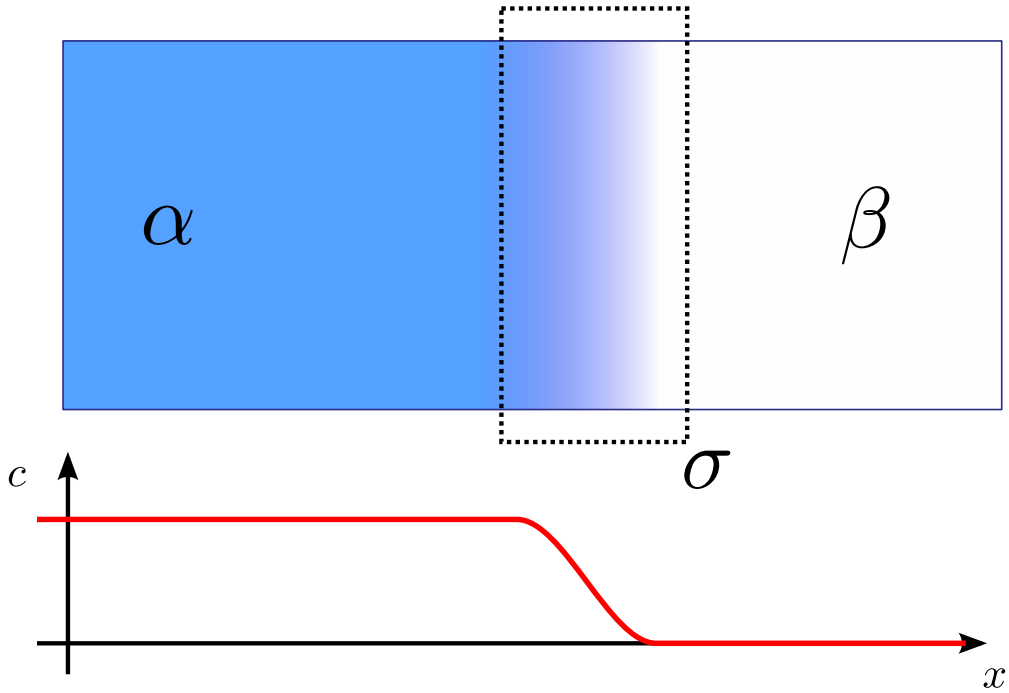
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Gibbs Dividing Surface

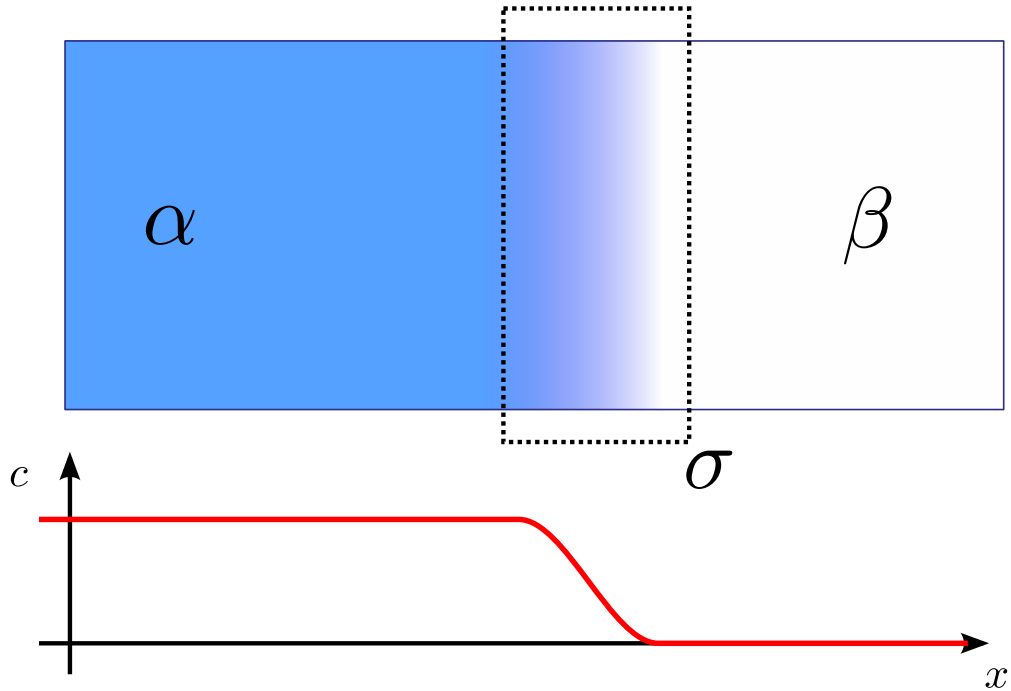
- One can see the surface as a smooth transition between two bulk phases α and β
  - It is arbitrary to define a surface volume.
  - We can as well just assume $V^\alpha + V^\beta = V$, and introduce a surface excess $N^\sigma = \Gamma A$, which is still arbitrary
  - *Define* σ as the surface corresponding to $\Gamma = 0$



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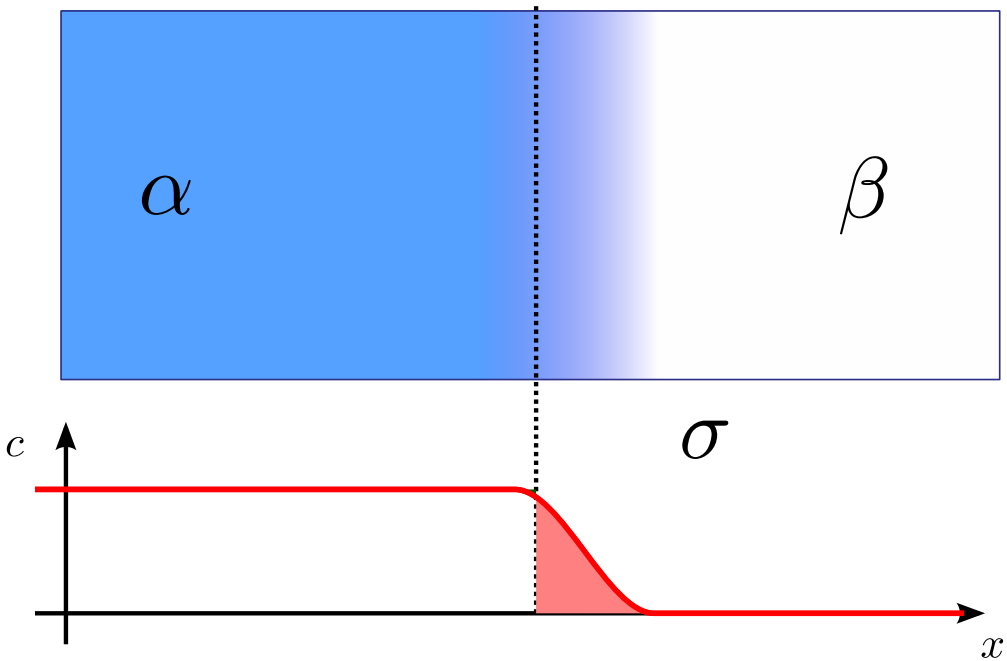
$$N = c^\alpha V^\alpha + c^\beta V^\beta + V^\sigma \langle c \rangle_\sigma$$



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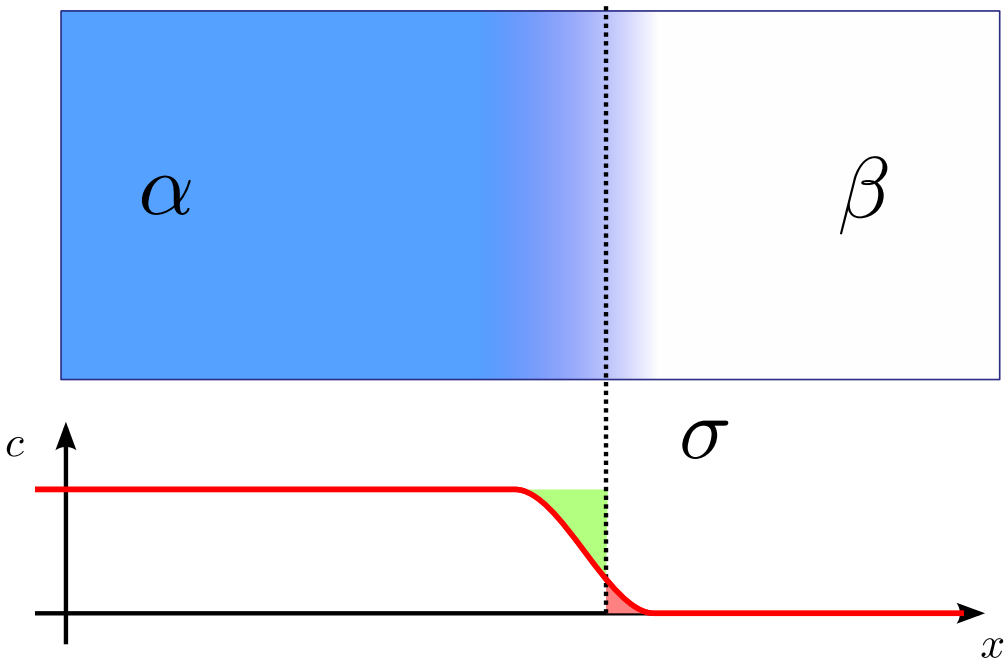
$$N^\sigma = V^\sigma \langle c \rangle_\sigma = \Gamma A = N - c^\alpha V^\alpha - c^\beta V^\beta$$



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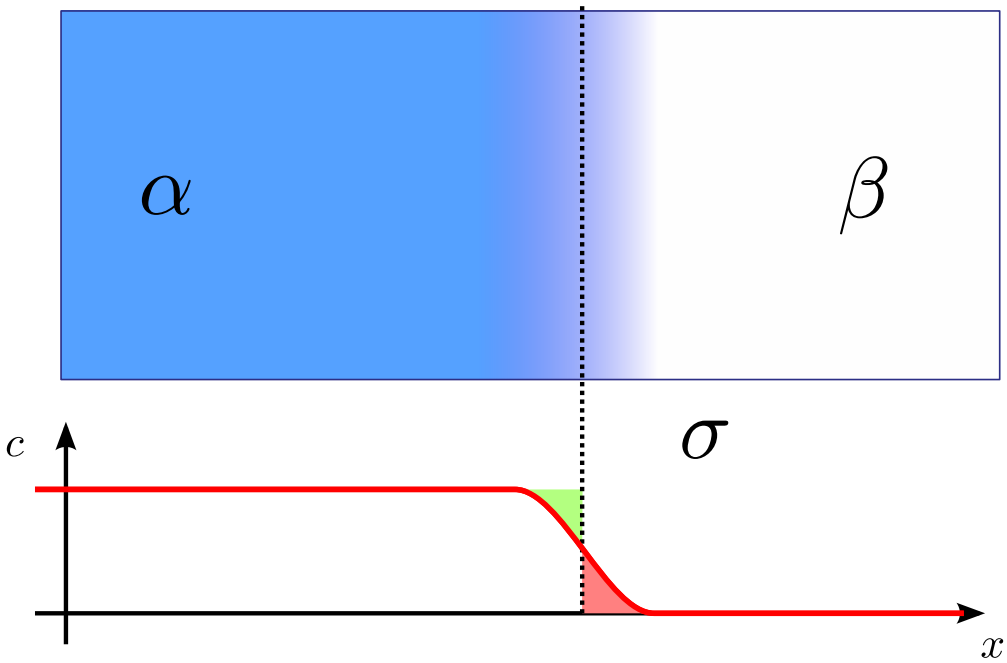
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$$N = c^\alpha \left(V - V^\beta\right) + c^\beta V^\beta$$



Multi-component Systems

- Consider multiple substances, each with a total number of molecules N_i. The surface excess of each component has still an arbitrary dependence on V^β

$$A\Gamma_i = N_i - c_i^\alpha V^\alpha - c_i^\beta V^\beta = N_i - c_i^\alpha V + \left(c_i^\alpha - c_i^\beta\right) V^\beta$$

- How can we define a quantity that does not depend on the choice of dividing surface? **Relative excess**

$$A\Gamma_i^{(1)} = A\Gamma_i - A\Gamma_1 \frac{c_i^\alpha - c_i^\beta}{c_1^\alpha - c_1^\beta} = N_i - c_i^\alpha V - (N_1 - c_1^\alpha V) \frac{c_i^\alpha - c_i^\beta}{c_1^\alpha - c_1^\beta}$$

- $\Gamma_i^{(1)}$ is the surface excess corresponding to the dividing surface that sets $\Gamma_1 = 0$

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Gibbs Adsorption Isotherm

- The differential form for the surface internal energy can be written as

$$\mathrm{d}U^\sigma = \sum_i \mu_i \mathrm{d}N_i^\sigma + T\mathrm{d}S^\sigma - p\mathrm{d}V^\sigma$$

  - These are all extensive variables, so one can integrate to a finite system size to obtain

$$U^\sigma = \sum_i \mu_i^\sigma N_i^\sigma + \gamma A + TS$$

- Comparison with the total differential form reads at constant T

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$$0 = \sum_i N_i^{\sigma} \mathrm{d}\mu_i + S^{\sigma} \mathrm{d}T + A\mathrm{d}\gamma$$

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$$-\sum_i N_i^{\sigma} \mathrm{d}\mu_i = A\mathrm{d}\gamma$$

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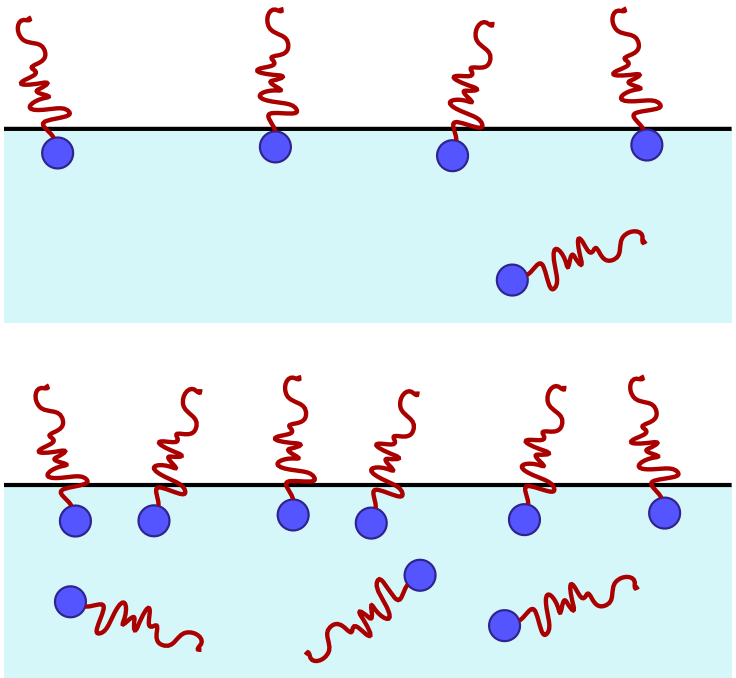
$$\boxed{\mathrm{d}\gamma = -\sum_i \Gamma_i \mathrm{d}\mu_i = -\sum_i \Gamma_i RT \frac{\mathrm{d}c_i}{c_i}}$$ Gibbs's Adsorption Isotherm

Implications of the Gibbs Isotherm

- Adding substances with a surface affinity ($\Gamma > 0$) *decreases* the surface tension of a liquid.

$$\mathrm{d}\gamma = -RT\frac{\Gamma}{c}\mathrm{d}c$$

- This is because to increase the surface one has to sequester more molecules from the bulk, which is made easier by increasing the bulk concentration



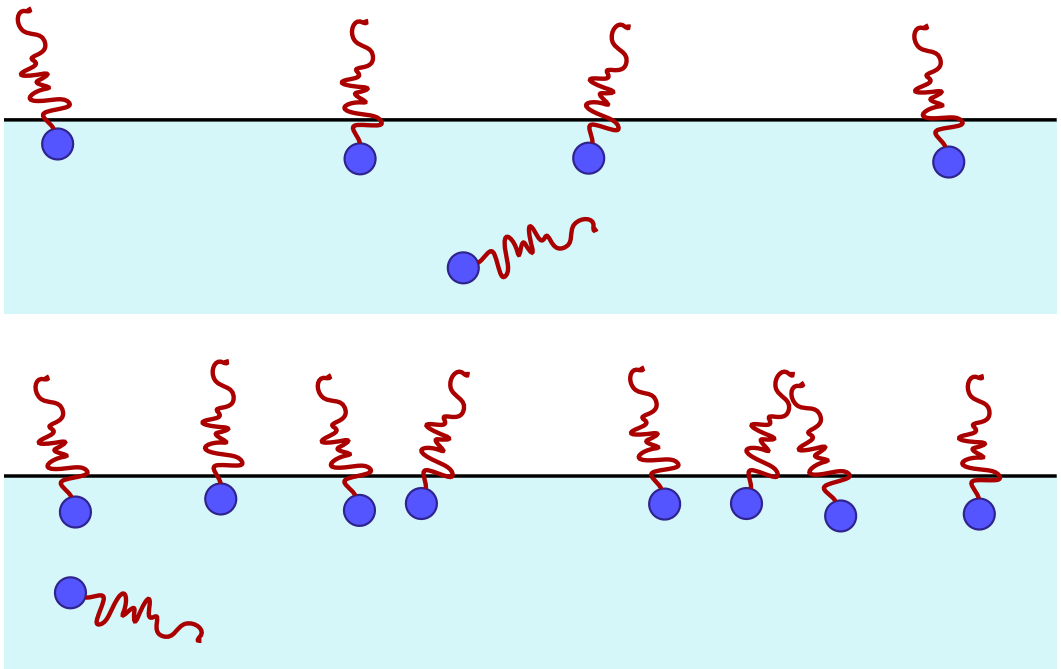
$$\Gamma > 0 \Rightarrow \frac{\partial \gamma}{\partial c} < 0$$

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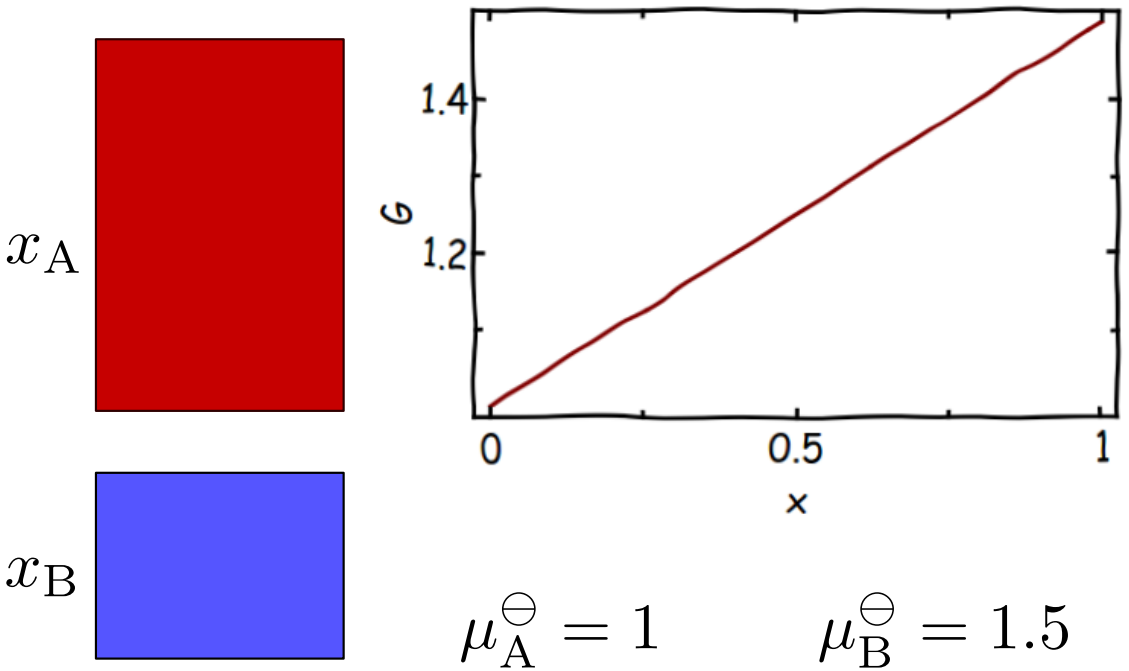


Regular Solution Model - A Reminder

- Take x_A moles of compound A, and $x_B = 1 - x_A$ moles of compound B, and **physically** mix them
- Assume only the entropy of solution matters (**ideal solution**)

$$\mu_{A,B} = \mu^{\ominus}_{A,B} + RT \ln x_{A,B}$$

- Add an enthalpy of mixing term $\Omega x_A x_B$ (**regular solution**)



$$\mu^{\ominus}_{A} = 1 \qquad \mu^{\ominus}_{B} = 1.5$$

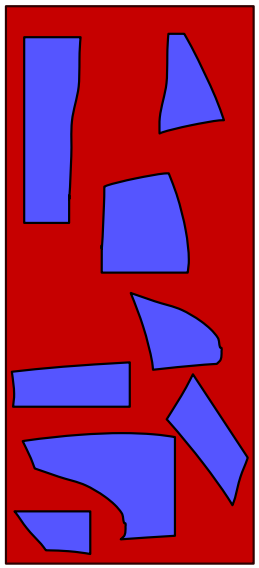
$$G = x_A \mu^{\ominus}_{A} + (1 - x_A)\, \mu^{\ominus}_{B}$$

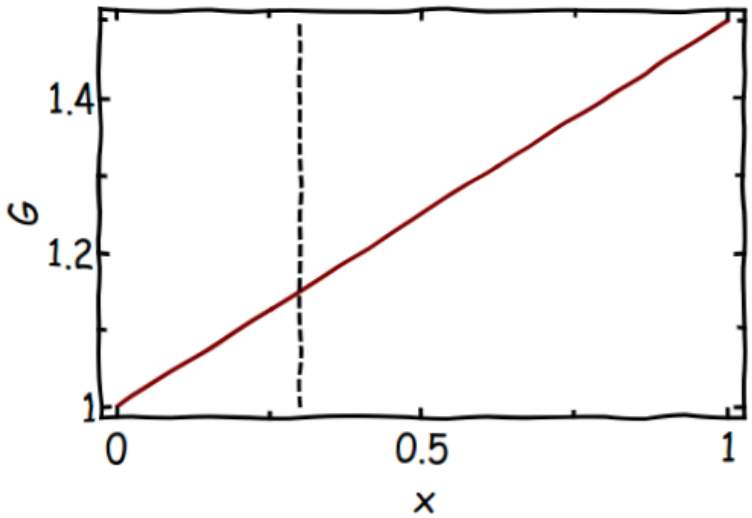
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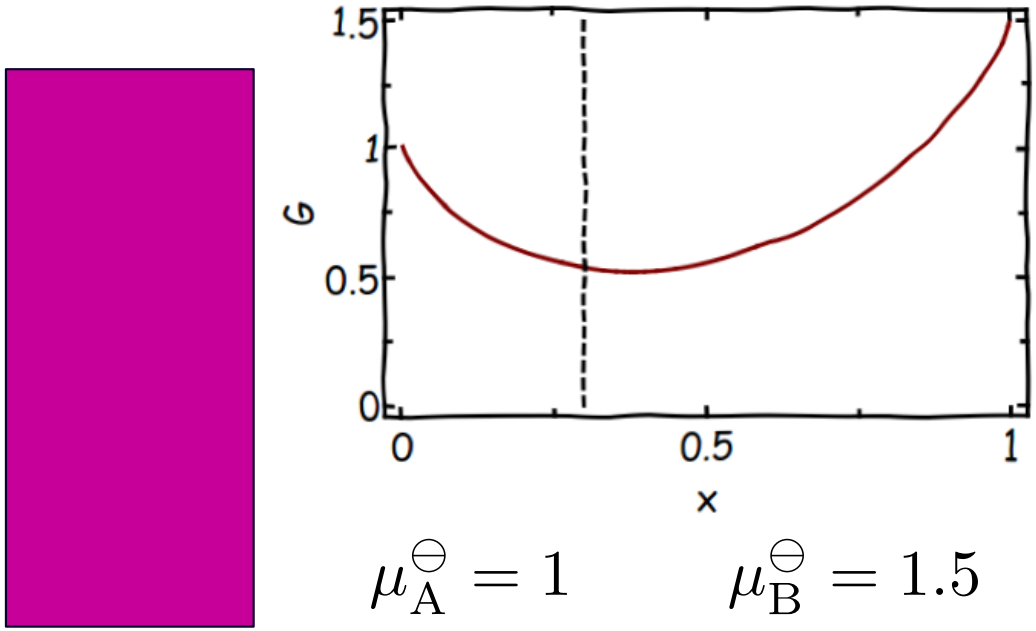
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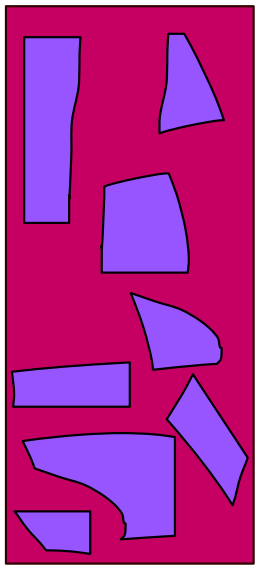
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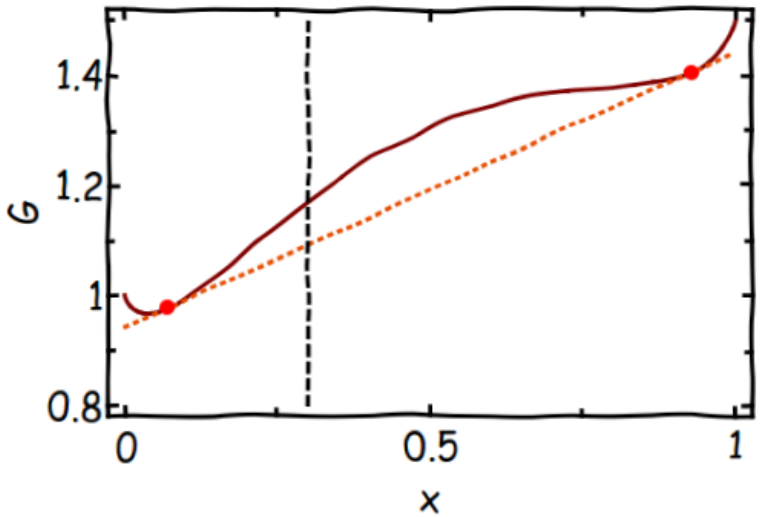
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$$\mu^{\ominus}_{A} = 1 \qquad \mu^{\ominus}_{B} = 1.5$$
$$RT = 1 \qquad \Omega = 2.5$$

$$G = x_A \left(\mu^{\ominus}_{A} + RT \ln x_A\right) + (1 - x_A)\left(\mu^{\ominus}_{B} + RT \ln (1 - x_A)\right) + \Omega x_A (1 - x_A)$$

A Thermodynamic Model of Interfaces

- We define a *local* molar free energy g, that depends on the local concentration, its gradient,etc. Then one can expand it in a Taylor series. . . and consider the symmetries that would arise in an isotropic system
- Let's apply the divergence theorem using a region for which the boundary term vanishes

$$G = \rho \int_V g\left(c, \nabla c, \nabla^2 c, \ldots\right) \mathrm{d}V$$

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$$g_0(c) + \frac{\partial g}{\partial \nabla_i c}\nabla_i c + \frac{\partial g}{\partial \nabla^2 c}\nabla^2 c + \frac{1}{2}\nabla_i c \frac{\partial^2 g}{\partial \nabla_i c \partial \nabla_j c}\nabla_j c + \dots$$

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$$\int_V \nabla \cdot \mathbf{f} \mathrm{d}V = \int_{\delta V} \mathbf{f} \cdot \hat{\mathbf{n}} \mathrm{d}S$$

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$$\kappa_1 \nabla \cdot (\nabla c) = \nabla \cdot (\kappa_1 \nabla c) - \nabla \kappa_1 \cdot (\nabla c) = \nabla \cdot (\kappa_1 \nabla c) - \frac{\partial \kappa_1}{\partial c} \nabla c \cdot \nabla c$$

$$g_0(c) + \underbrace{\left.\frac{\partial g}{\partial \nabla^2 c}\right|_0}_{\kappa_1} \nabla^2 c + \underbrace{\left.\frac{\partial^2 g}{\partial |\nabla c|^2}\right|_0}_{\kappa_2} |\nabla c|^2 + \dots$$

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$$\int_V \kappa_1 \nabla^2 c \, \mathrm{d}V = \cancel{\int_{\partial V} \nabla \cdot (\kappa_1 \nabla c) \, \mathrm{d}V} - \int_V \frac{\partial \kappa_1}{\partial c} \left|\nabla c\right|^2 \mathrm{d}V$$

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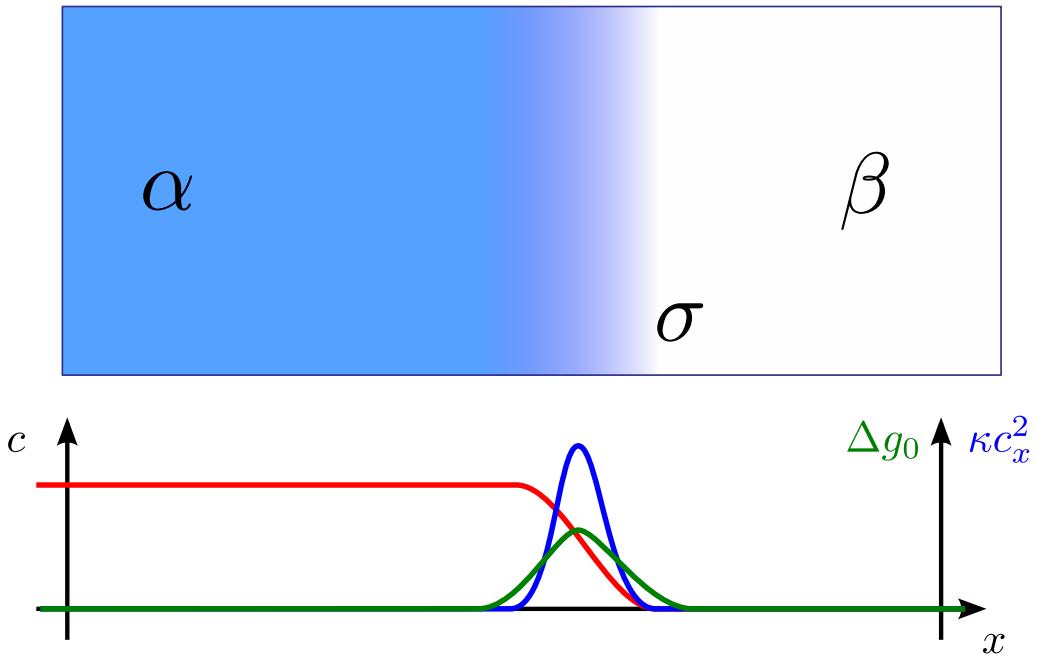
$$\boxed{G = \rho \int_V g_0(c) + \kappa |\nabla c|^2 \, \mathrm{d}V}$$ Cahn-Hilliard Equation

$$\kappa = \left. \frac{\partial^2 g}{\partial |\nabla c|^2} \right|_0 - \left. \frac{\partial^2 g}{\partial c \partial \nabla^2 c} \right|_0$$

Excess Free Energy of an Interface

- Now consider a 1D interface between two phases α and β. If the system was homogeneous the free energy would be

$$G_0 = \int_V c(x)\,\mu_A + (1 - c(x))\,\mu_B dx$$

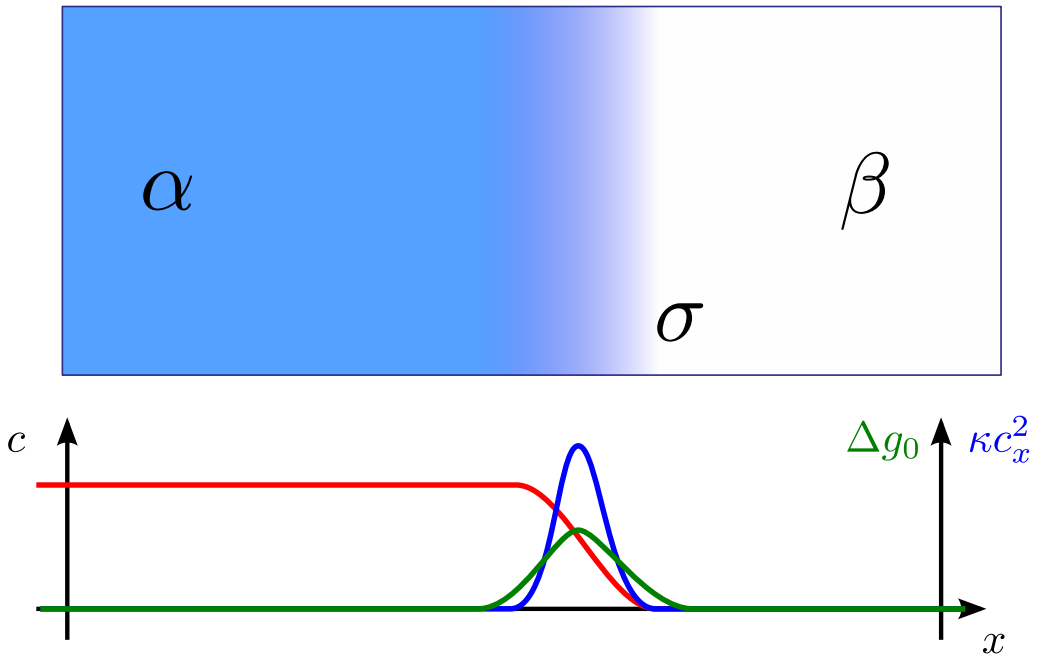


Excess Free Energy of an Interface

- We can define an excess free energy associated with the interface

$$\Delta G = \rho \int \Delta g_0 (c) + \kappa |c'|^2 \, \mathrm{d}x, \qquad \Delta g_0 = g_0 (c) - c\mu_A - (1 - c)\, \mu_B$$

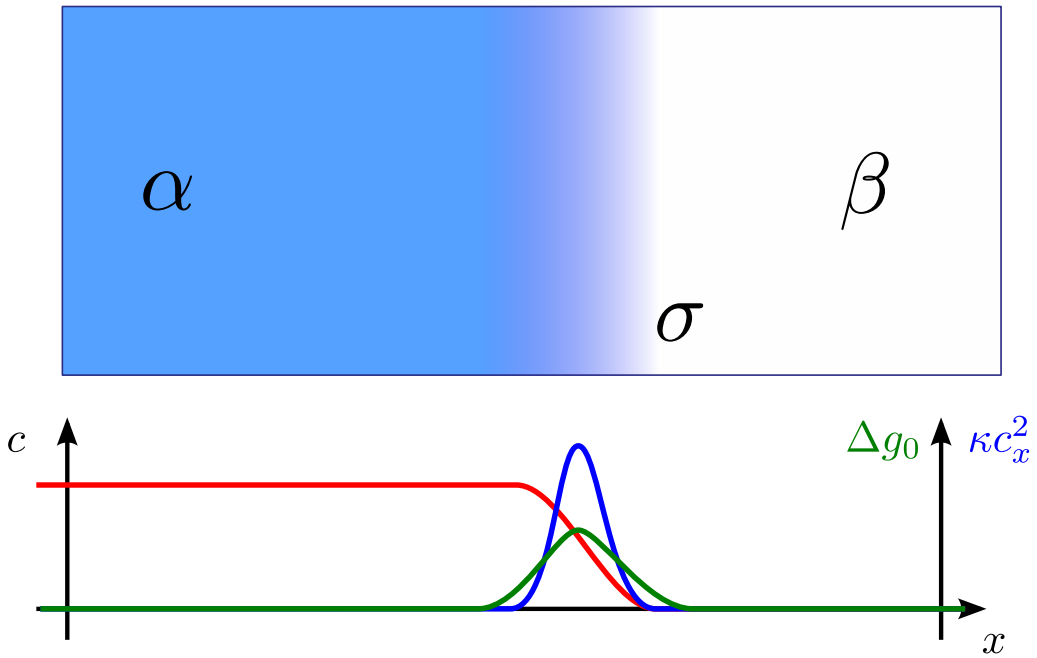
- A more diffuse interface (small $|c'|$) reduces the free energy, but has a larger region with non-equilibrium concentrations.



Excess Free Energy of an Interface

- One can obtain the equilibrium interface shape by *calculus of variations*:

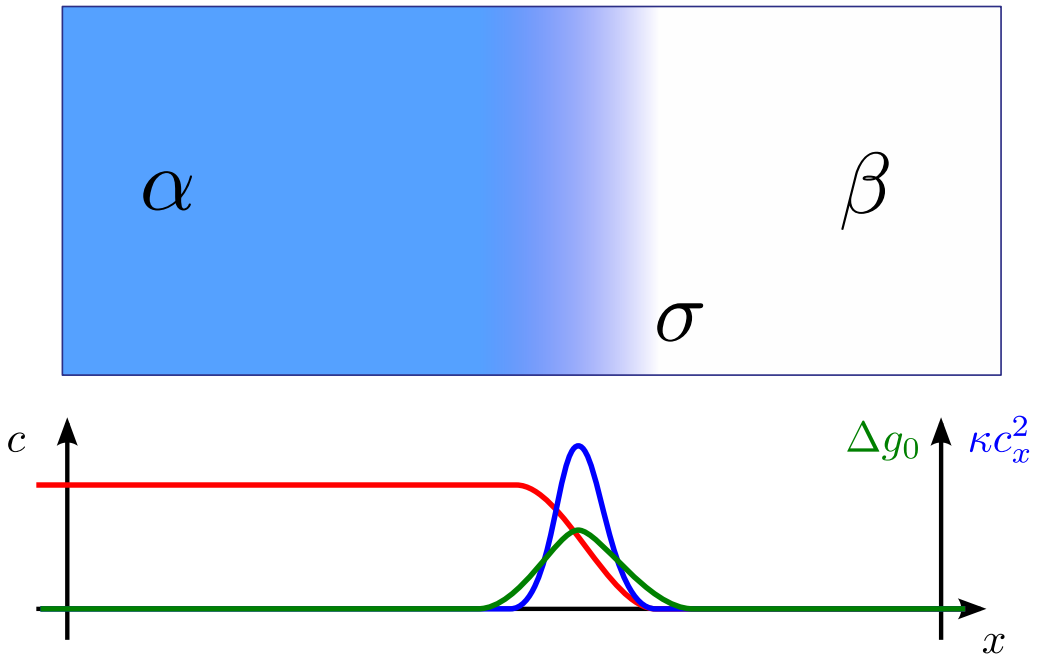
$$J = \int I(c, c')\,\mathrm{d}x, \qquad \frac{\delta J}{\delta c} = \frac{\partial I}{\partial c} - \nabla \cdot \frac{\partial I}{\partial \nabla c}$$



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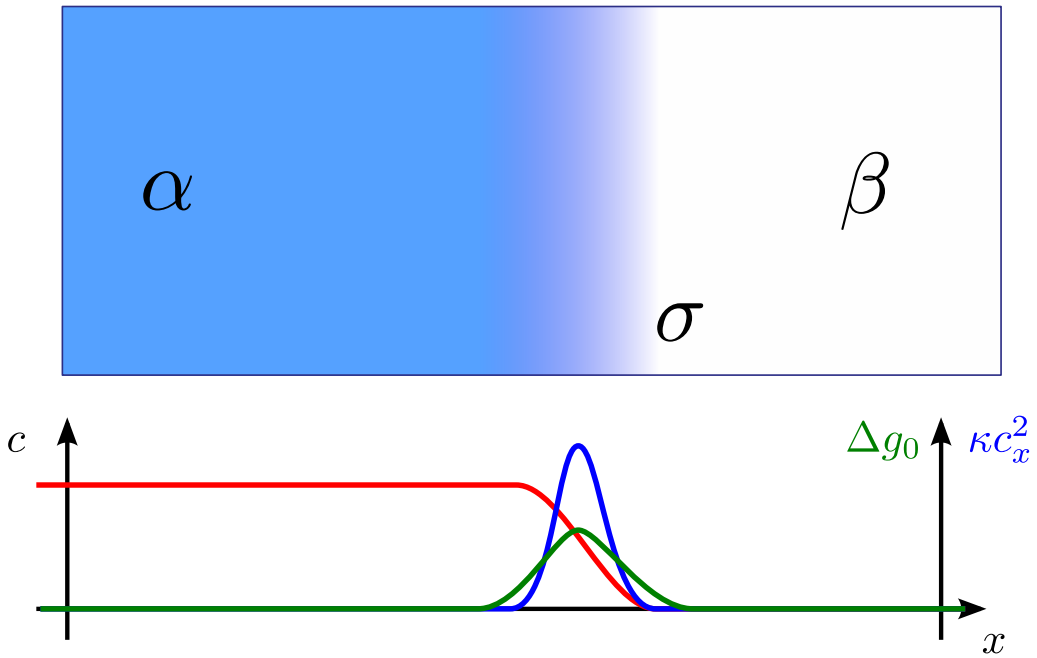
$$\frac{\delta J}{\delta c} = 0 \quad \rightarrow \quad I - c' \frac{\partial I}{\partial c'} = K$$



Excess Free Energy of an Interface

- One can obtain the equilibrium interface shape by *calculus of variations*:

$$\frac{\delta \Delta G}{\delta c} = 0 \rightarrow K = \Delta g_0(c) + \kappa c'^2 - c'(2\kappa c') \rightarrow \Delta g_0(c) - K = \kappa c'^2$$

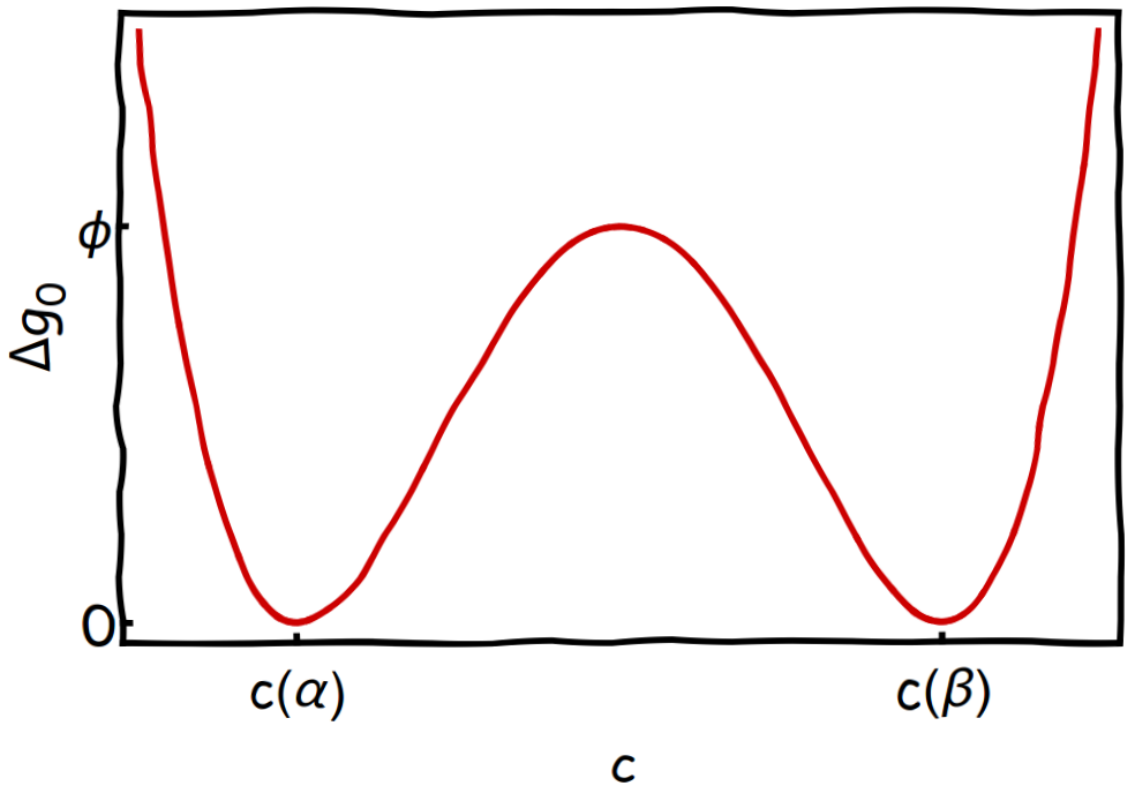


A Simplified Solution for the Interface

- Let's try a simple model for the excess free energy, $\Delta g_0(c) = \phi\left(c^2-1\right)^2$

$$\kappa c_x^2 = \phi\left(c^2-1\right)^2 \rightarrow \sqrt{\frac{\kappa}{\phi}}\frac{\partial c}{\partial x} = \pm\left(c^2-1\right)$$

- One can also evaluate the free energy associated with the interface
  - With this simplified model, $\Delta G = \frac{\rho}{6}\left(c(\beta)-c(\alpha)\right)^3\sqrt{\phi\kappa}$

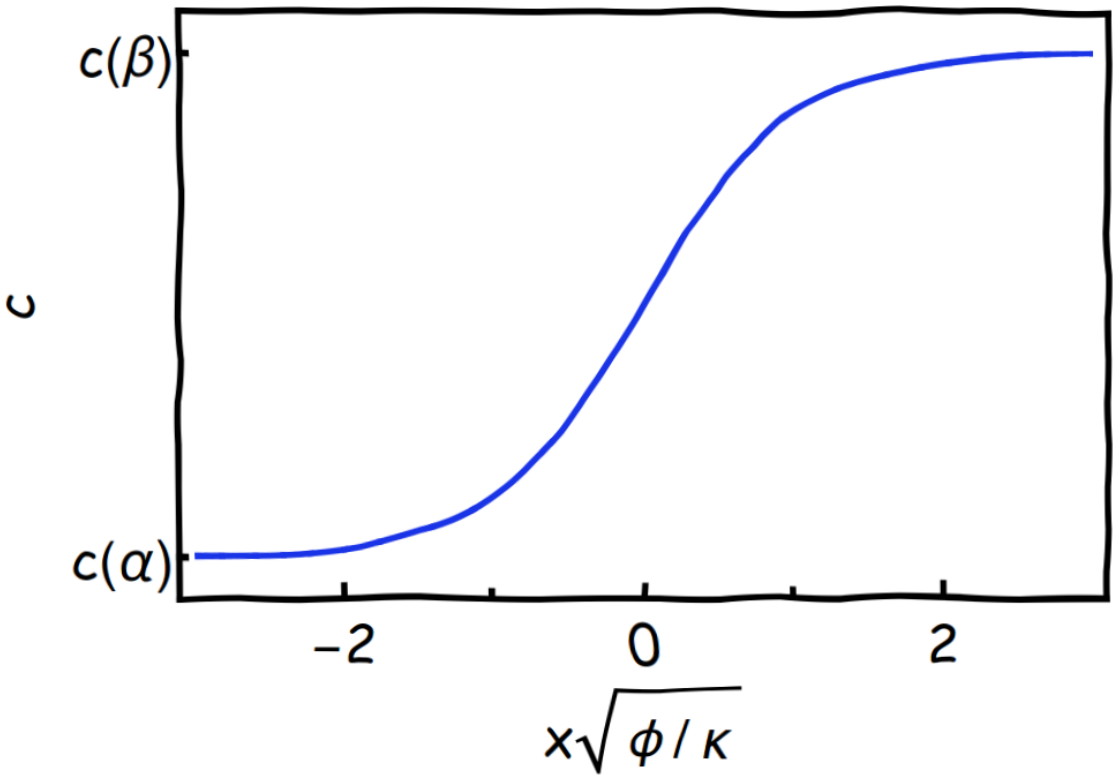


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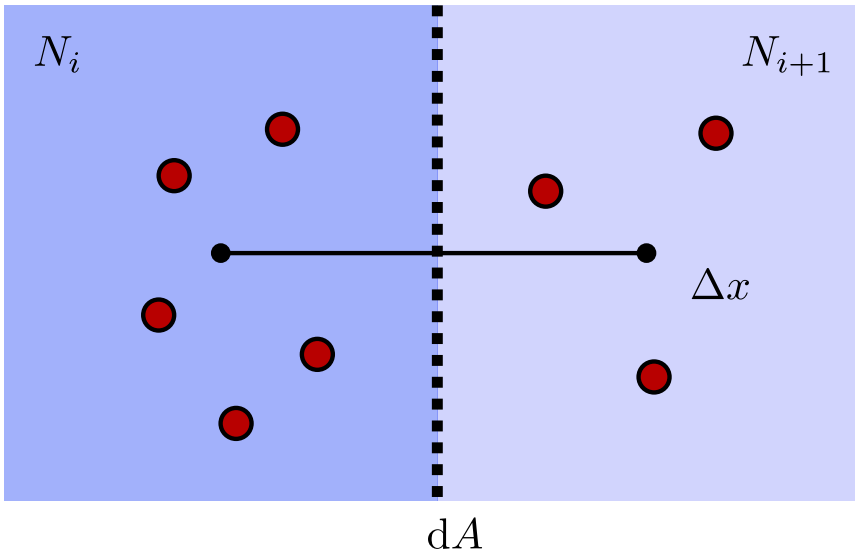
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$$\Delta G = 2\rho\int \Delta g_0(c)\,\mathrm{d}x = 2\rho\kappa\int \frac{\partial c}{\partial x}\frac{\partial c}{\partial x}\mathrm{d}x = 2\rho\sqrt{\kappa}\int_{c(\alpha)}^{c(\beta)}\sqrt{\Delta g_0(c)}\mathrm{d}c$$

Fick's Law - A Reminder

- Discretized flux across the interface is proportional to the number of particles in each volume
- Can be generalized to many dimensions and a non-ideal solutions
- Continuity equation imposes balance between concentration and flux

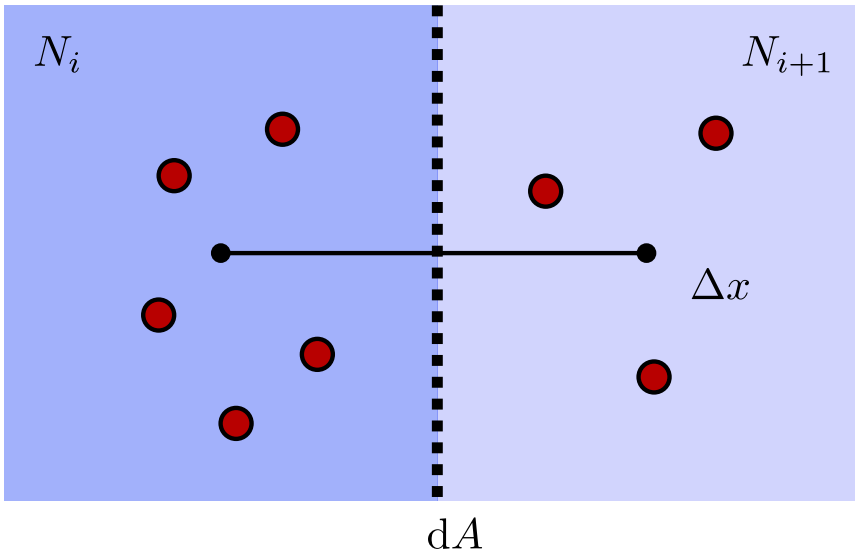
$$j\mathrm{d}A = \frac{k}{2}\left[N_i - N_{i+1}\right] = \frac{k}{2}\mathrm{d}A\Delta x\left[c\left(-\Delta x/2\right) - c\left(\Delta x/2\right)\right]$$



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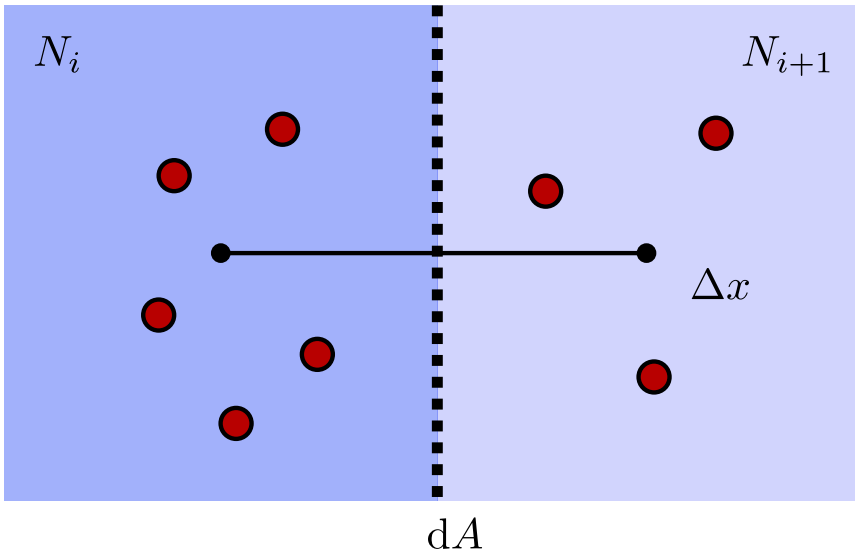
$$j = \frac{k}{2}\Delta x \left[\left[c\left(0\right) - c'\left(0\right)\Delta x/2\right] - \left[c\left(0\right) + c'\left(0\right)\Delta x/2\right]\right]$$



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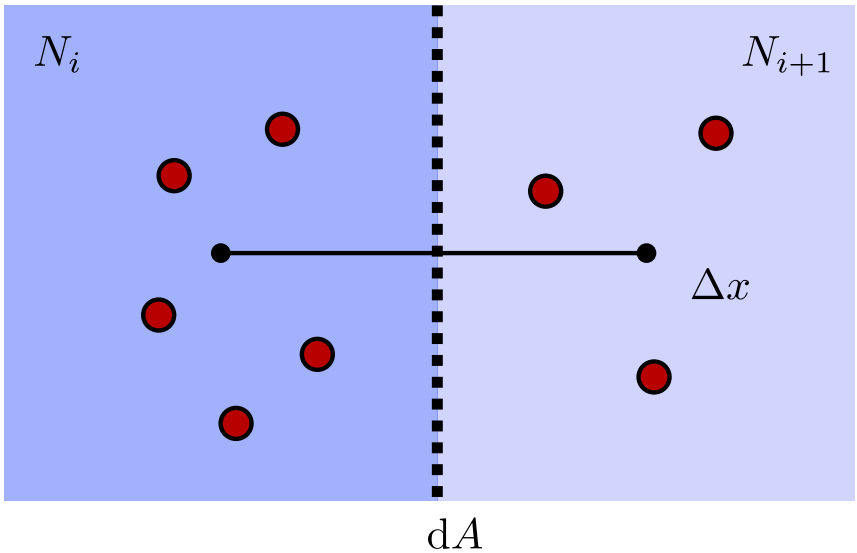
$$j = -k\Delta x^2 c'(0)$$



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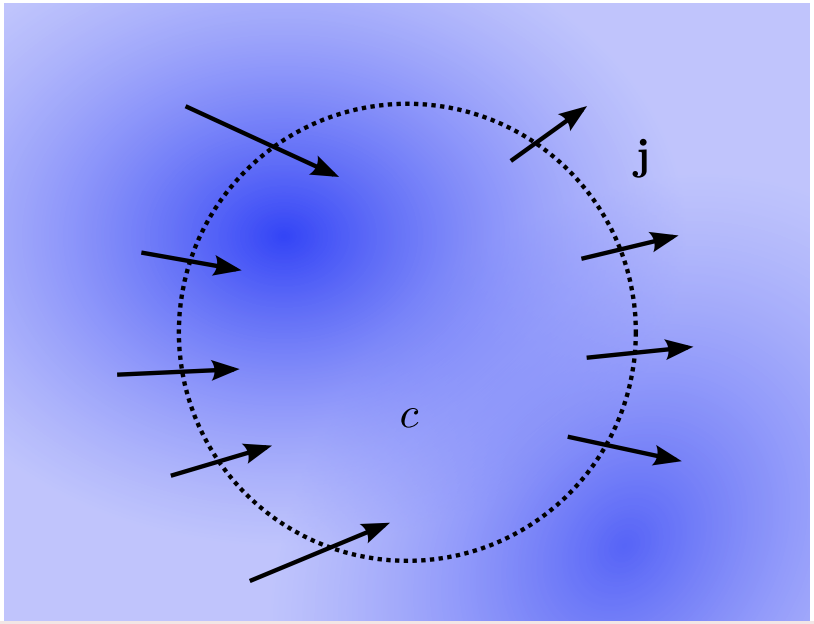
$$\boxed{\mathbf{j} = -D\nabla\mu} \qquad 1^{st}\text{Fick's law}$$



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$$\frac{\partial}{\partial t}\int_V c\,\mathrm{d}V = -\int_{\delta V}\mathbf{j}\cdot\hat{\mathbf{n}}\,\mathrm{d}A = -\int_V \nabla\cdot\mathbf{j}\,\mathrm{d}V$$

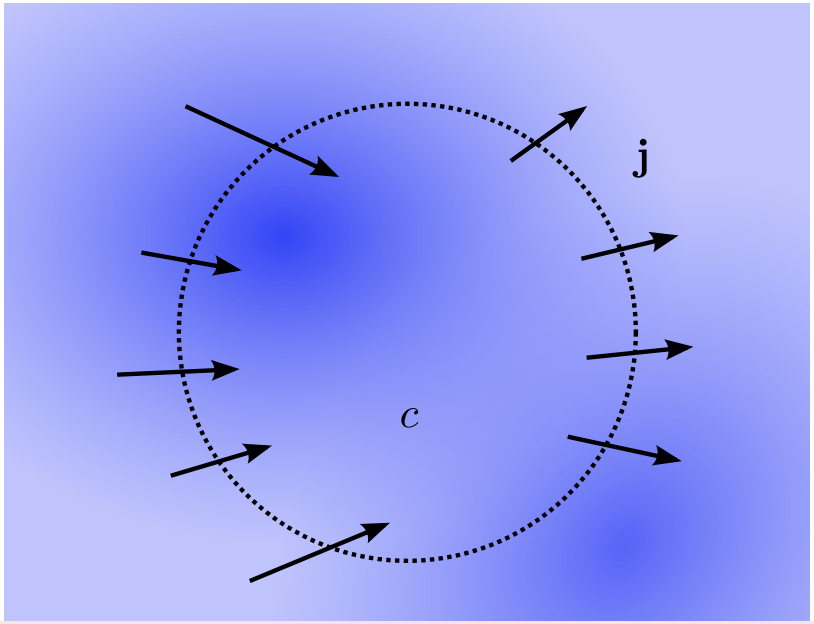


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$$\boxed{\frac{\partial c}{\partial t} = -\nabla \cdot \mathbf{j} = D\nabla^2 \mu}$$

2^{nd} Fick's law



Dynamics of the C-H Model

- Get the chemical potential as a functional derivative of the free energy of the Cahn-Hilliard model

$$G = \rho \int_V \Delta g_0(c) + \kappa |\nabla c|^2 \, \mathrm{d}V, \qquad J = \int_V I(c, \nabla c) \, \mathrm{d}V, \frac{\delta J}{\delta c} = \frac{\partial I}{\partial c} - \nabla \cdot \frac{\partial I}{\partial \nabla c}$$

- Dynamical C-H equation is a model of *spinodal decomposition*

Dynamics of the C-H Model

- Get the chemical potential as a functional derivative of the free energy of the Cahn-Hilliard model

$$\frac{\delta G}{\delta c} = \frac{\partial}{\partial c}\Delta g_0\left(c\right) - 2\nabla\cdot\left(\kappa\nabla c\right)$$

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Dynamics of the C-H Model

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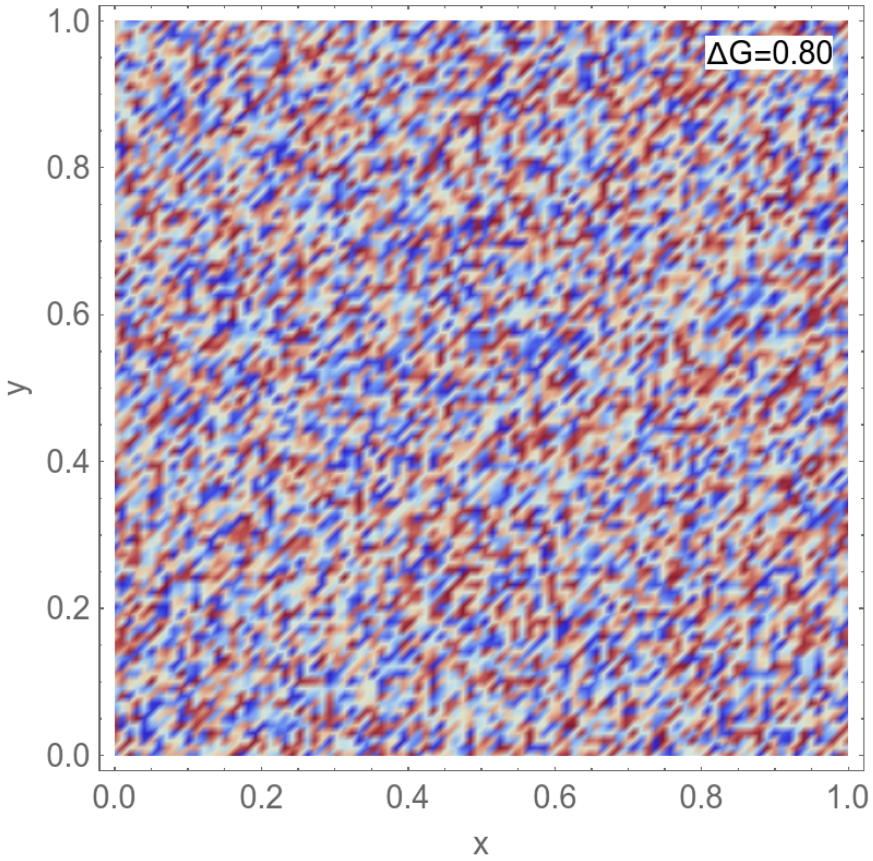
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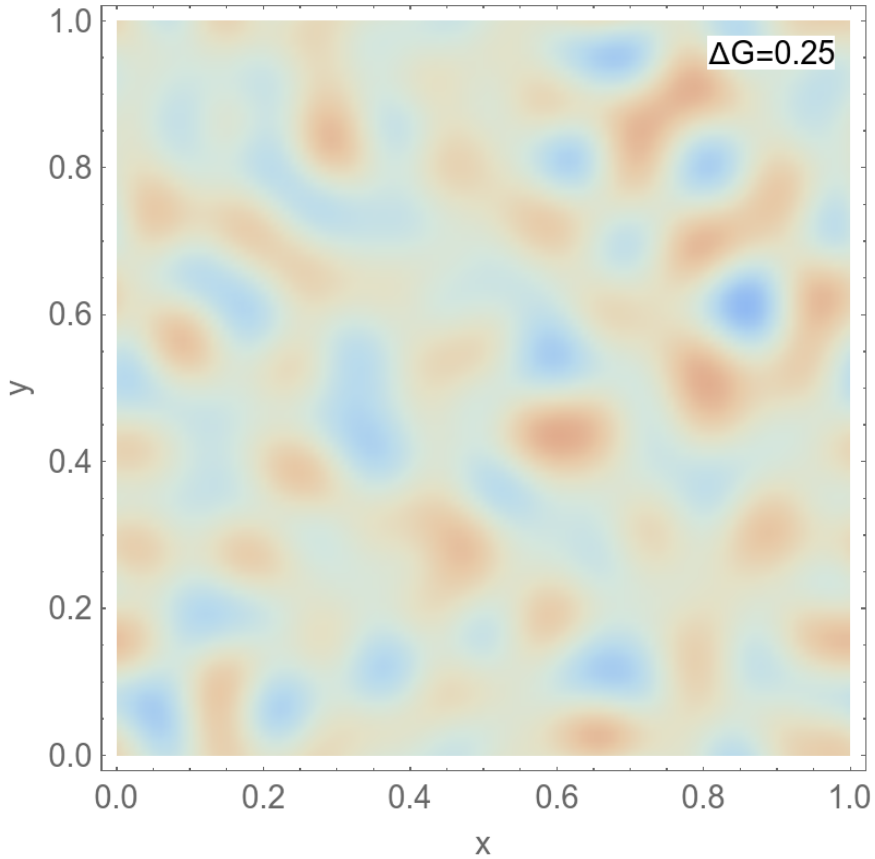


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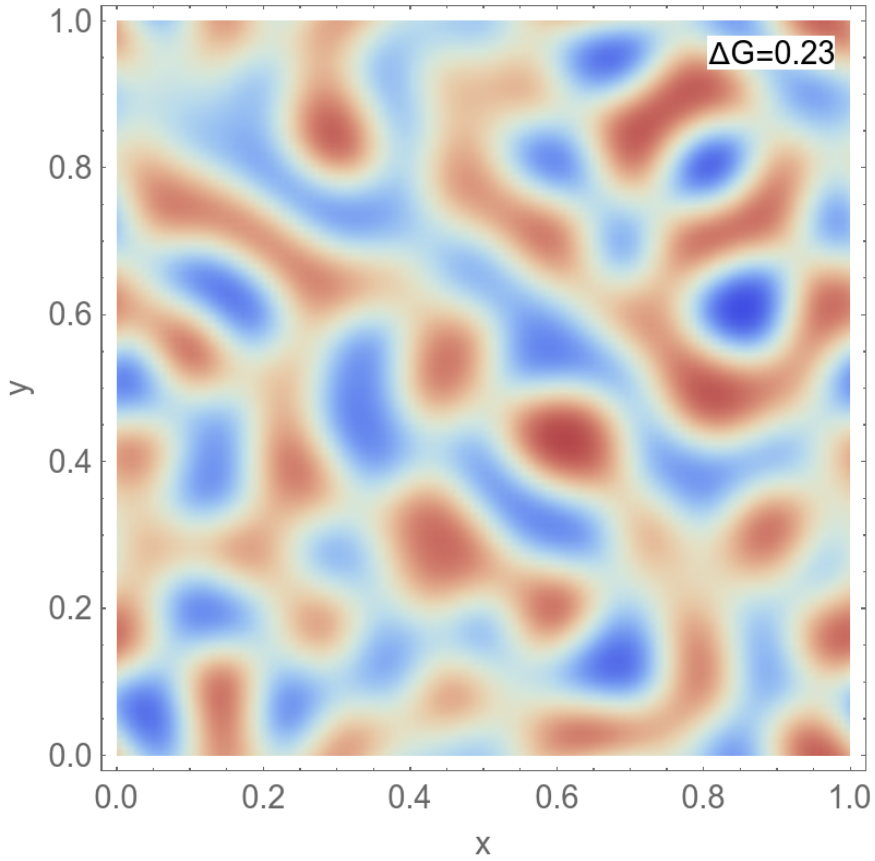


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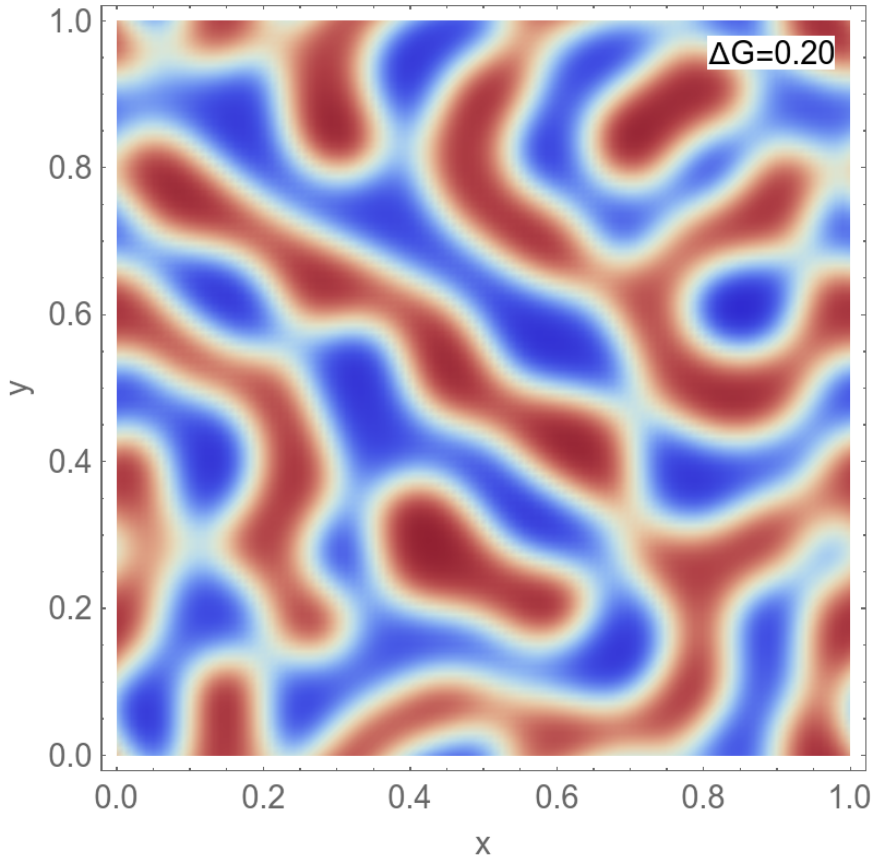


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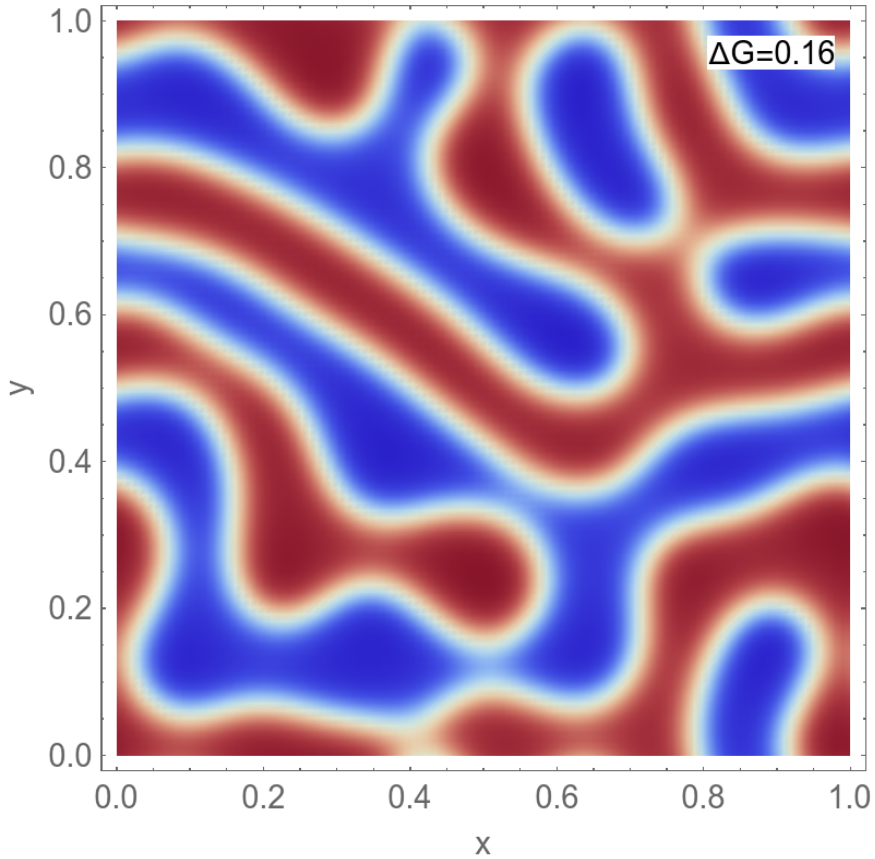


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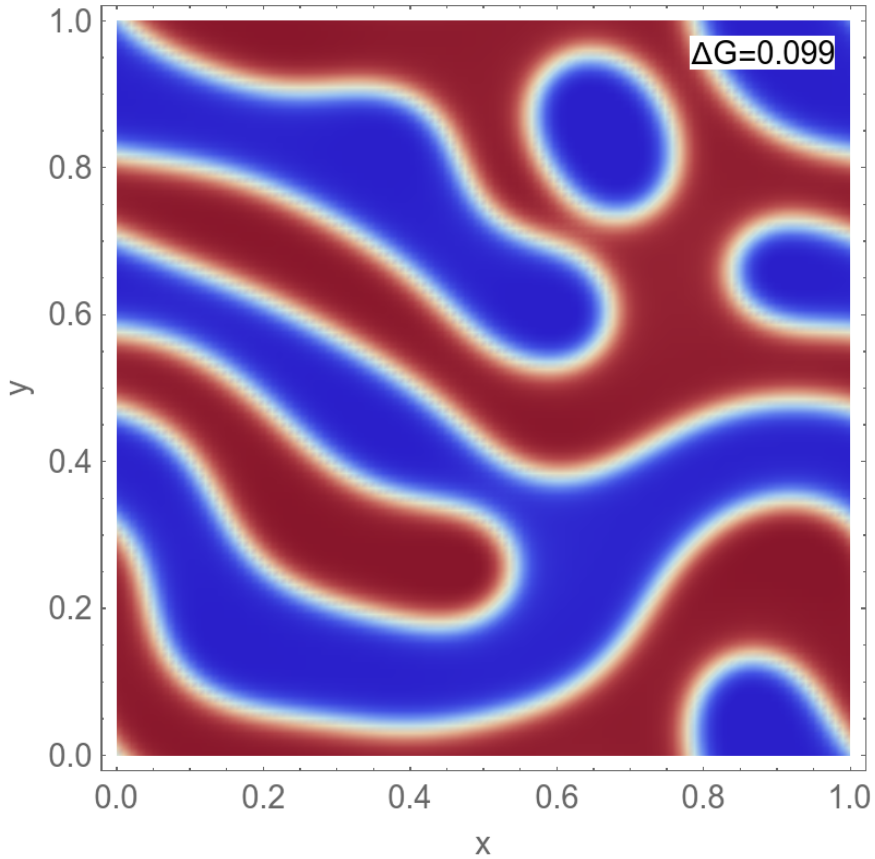


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