Kinetics of Phase Ordering, Domain Growth and Coarsening I:

Kinetic Ising Models and Phenomenological Models

by

Sanjay Puri

Overview

(a) Introduction

(b) Nonconserved Dynamics: Glauber Spin-Flip Ising Model

(c) Conserved Dynamics: Kawasaki Spin-Exchange Ising Model

(d) Phenomenological Models of Phase Ordering Systems

(e) Conclusion

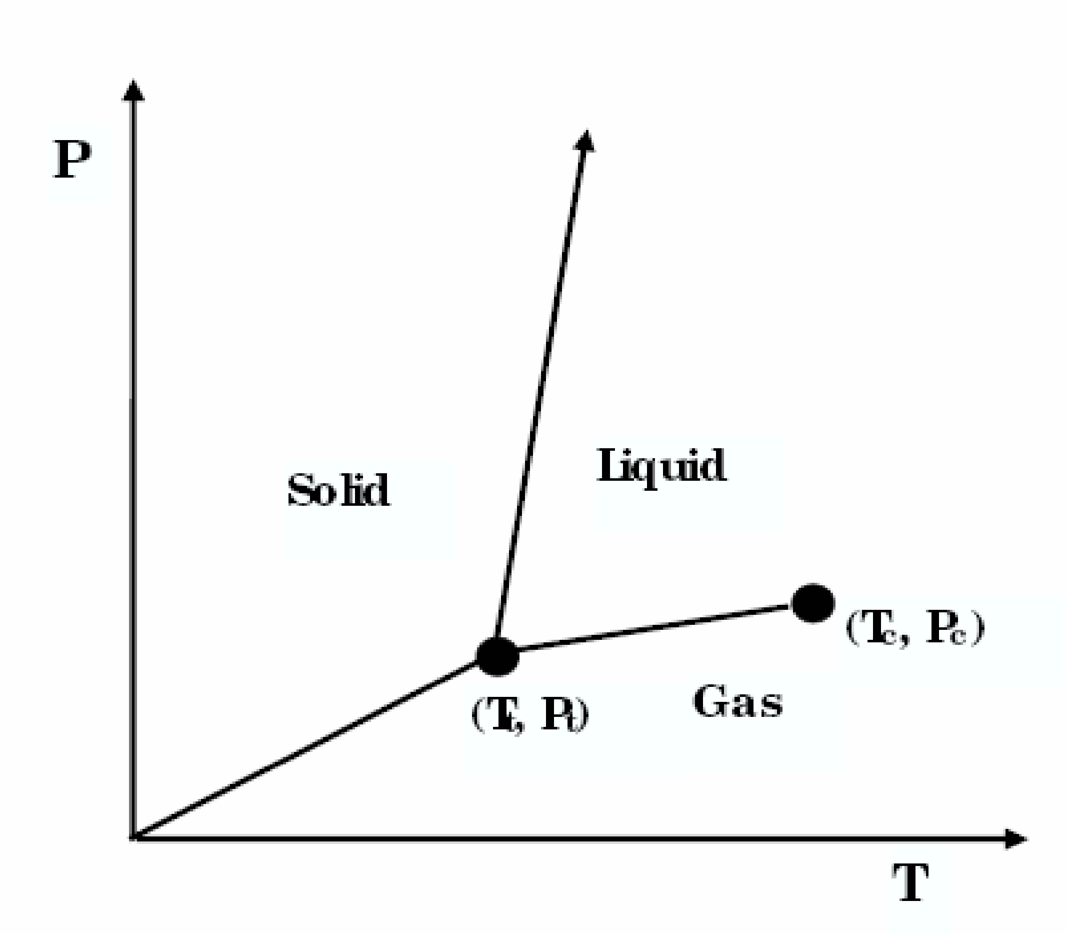
(a) Introduction

Evolution of a disordered system which has been made thermodynamically unstable by a rapid change of parameters, e.g., temperature, pressure, etc.

= Phase ordering kinetics, domain growth, coarsening.

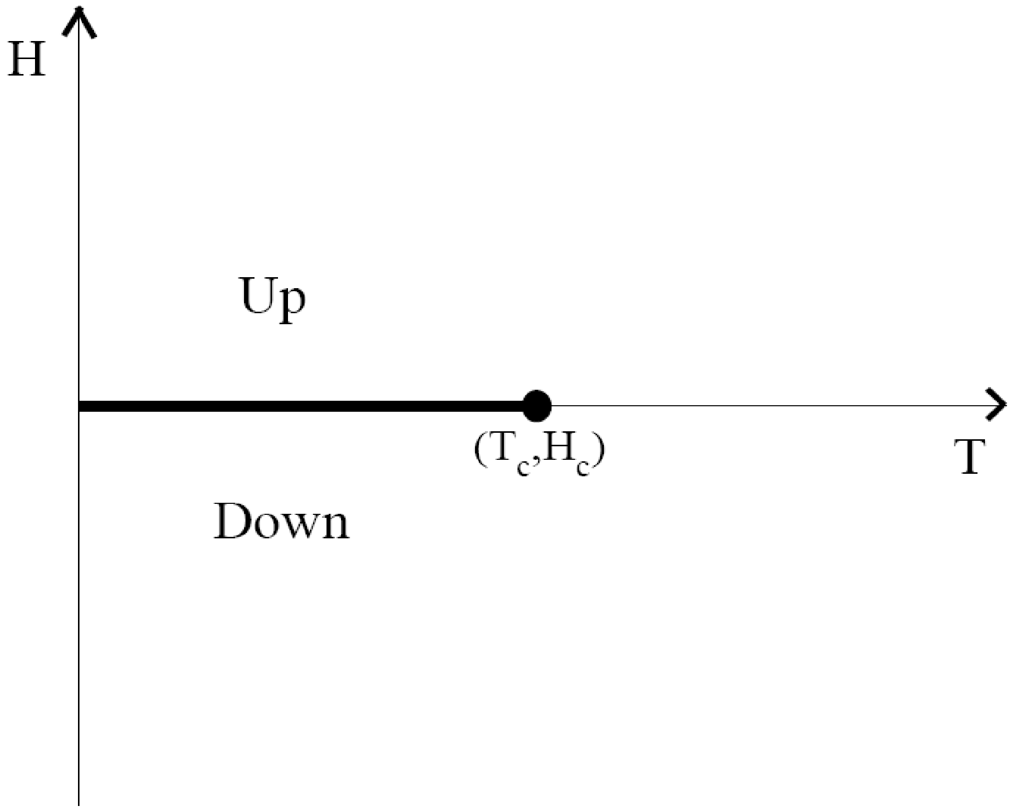
Problems in this area arise from diverse fields ranging from atmospheric physics to materials science and metallurgy to cosmology and astrophysics.

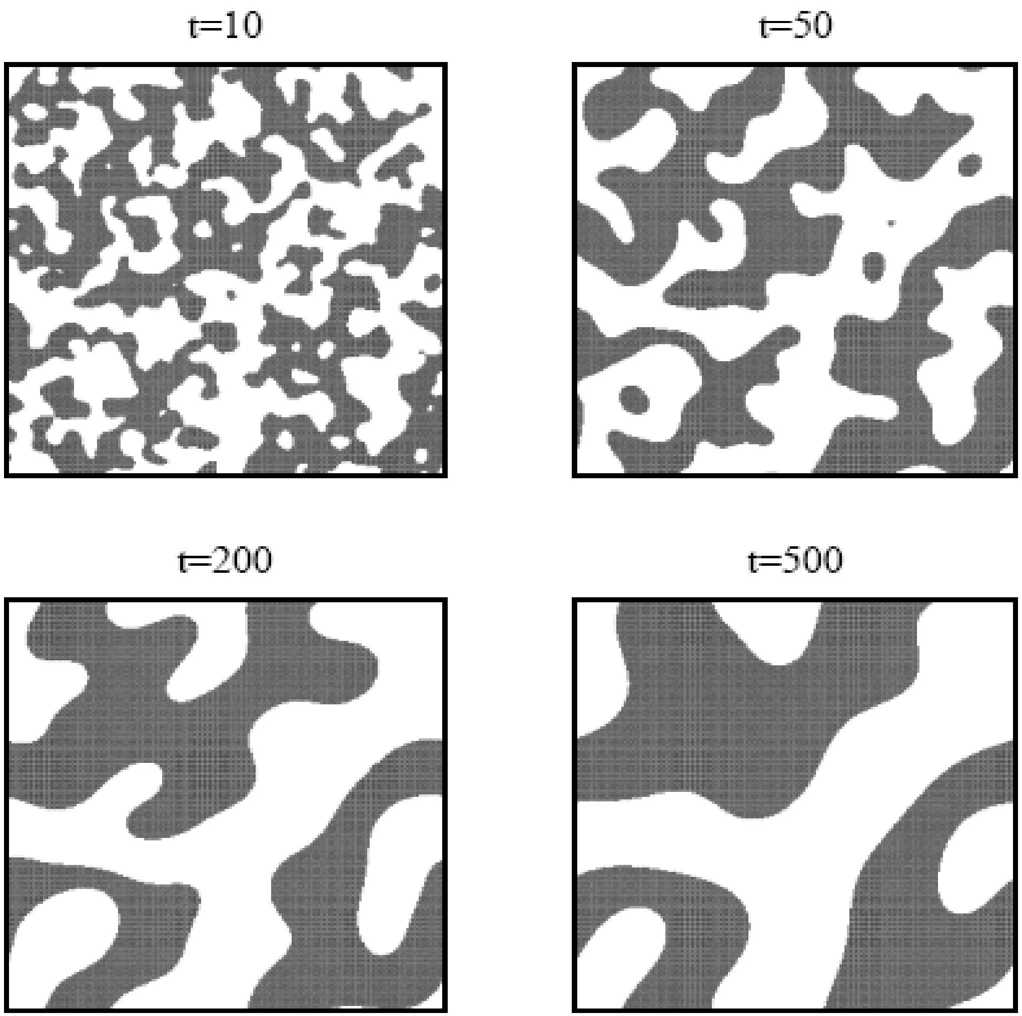
Phase diagram of a fluid



- Example 1: Ordering of a magnet

Rapid cooling at time t=0 from T>T_c to T<T_c produces far-from-equilibrium system.





1) Domain growth is driven by interfaces or domain boundaries (defects).

2) $$v(\vec{a}) = -\nabla \cdot \hat{n} = -K(\vec{a})$$

Allen-Cahn equation

$$\frac{dL}{dt} = \frac{1}{L} \Rightarrow L(t) \sim t^{1/2}$$

3) System shows dynamical scaling

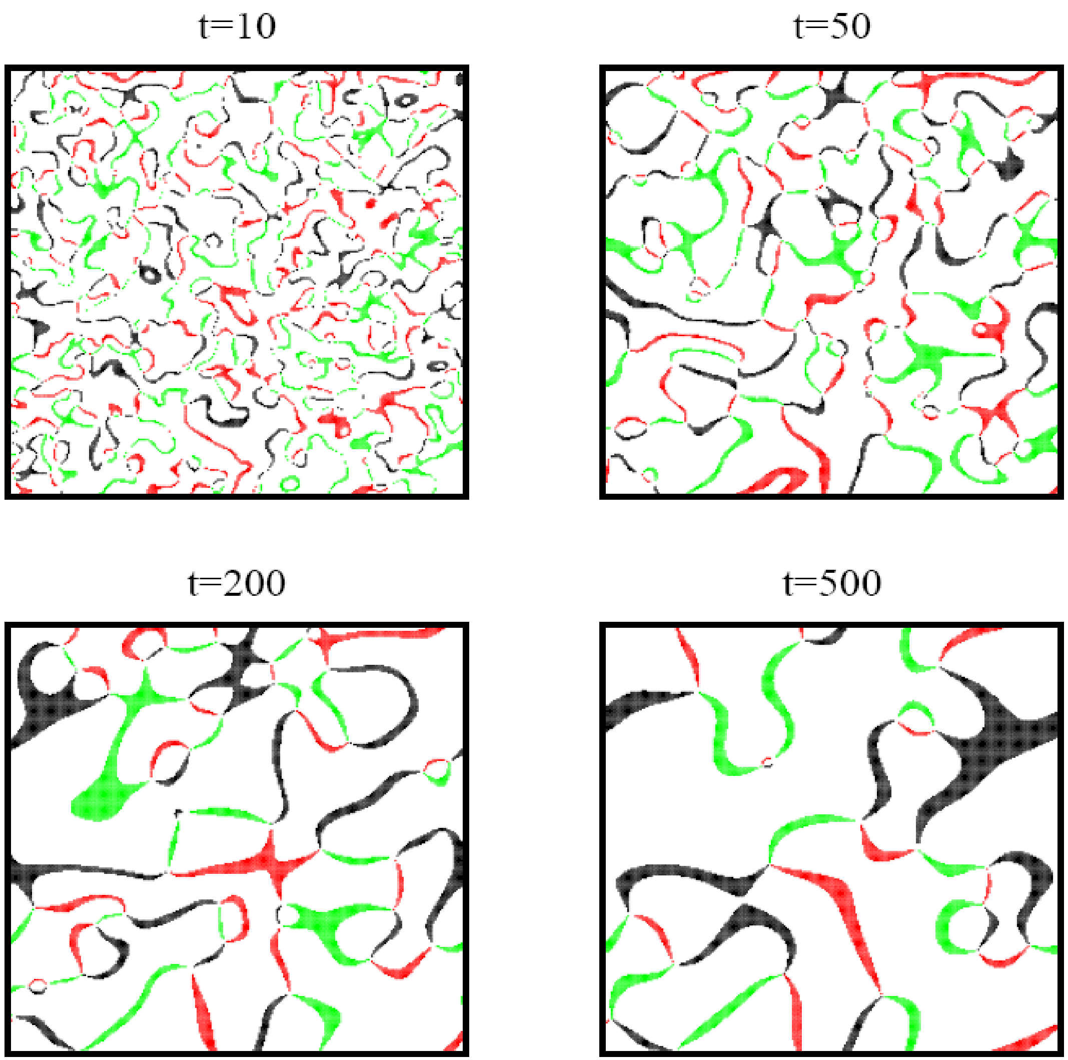
$$C(r,t) = g(r/L)$$

$$g(r) = \frac{2}{\pi} \sin^{-1}\left[\exp\left(-\frac{r^2}{L^2}\right)\right]$$

Ohta-Jasnow-Kawasaki function (with Porod tail)

- Example 2: Ordering of a super-conductor or super-fluid from normal state

Rapid cooling at time $t=0$ from $T>T_c$ to $T<T_c$, where the system prefers to be in its super-state.



1) Super-state is described by a macroscopic quantum-mechanical wave-function.

$$\Psi = |\Psi| \exp(i\theta)$$

2) Domain growth is driven by annihilation of vortices and anti-vortices (defects).

3) $$L(t) \sim t^{1/2}$$

4) System shows dynamical scaling

$$C(r,t) = g(r/L)$$

$$g(r/L) = \frac{n\gamma}{2\pi} F\left(\frac{1}{2}, \frac{1}{2}; \frac{n+2}{2}; \gamma^2\right)$$

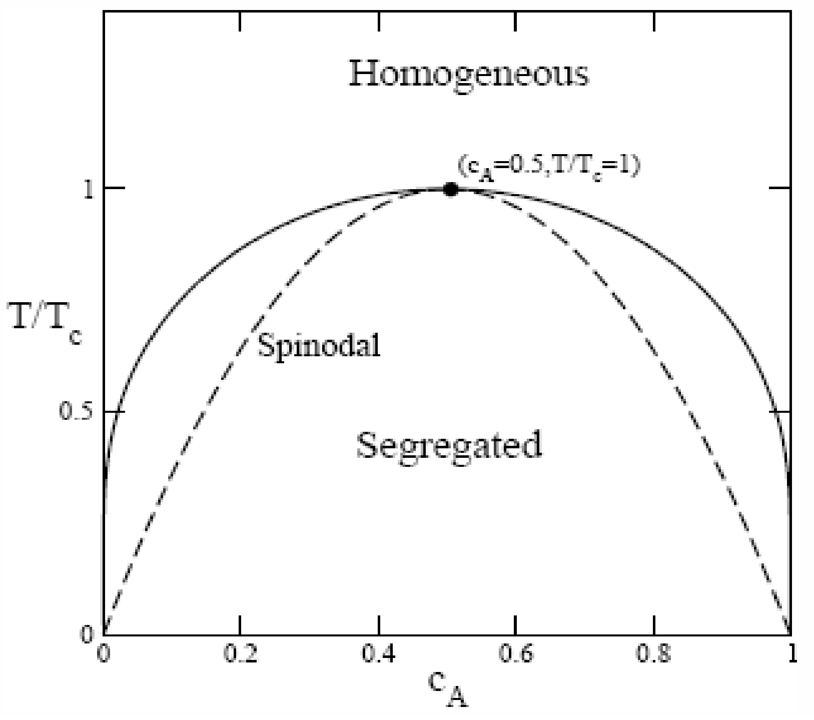
$$\gamma = \exp\left(-\frac{r^2}{L^2}\right)$$

Bray-Puri function (with generalized Porod tail)

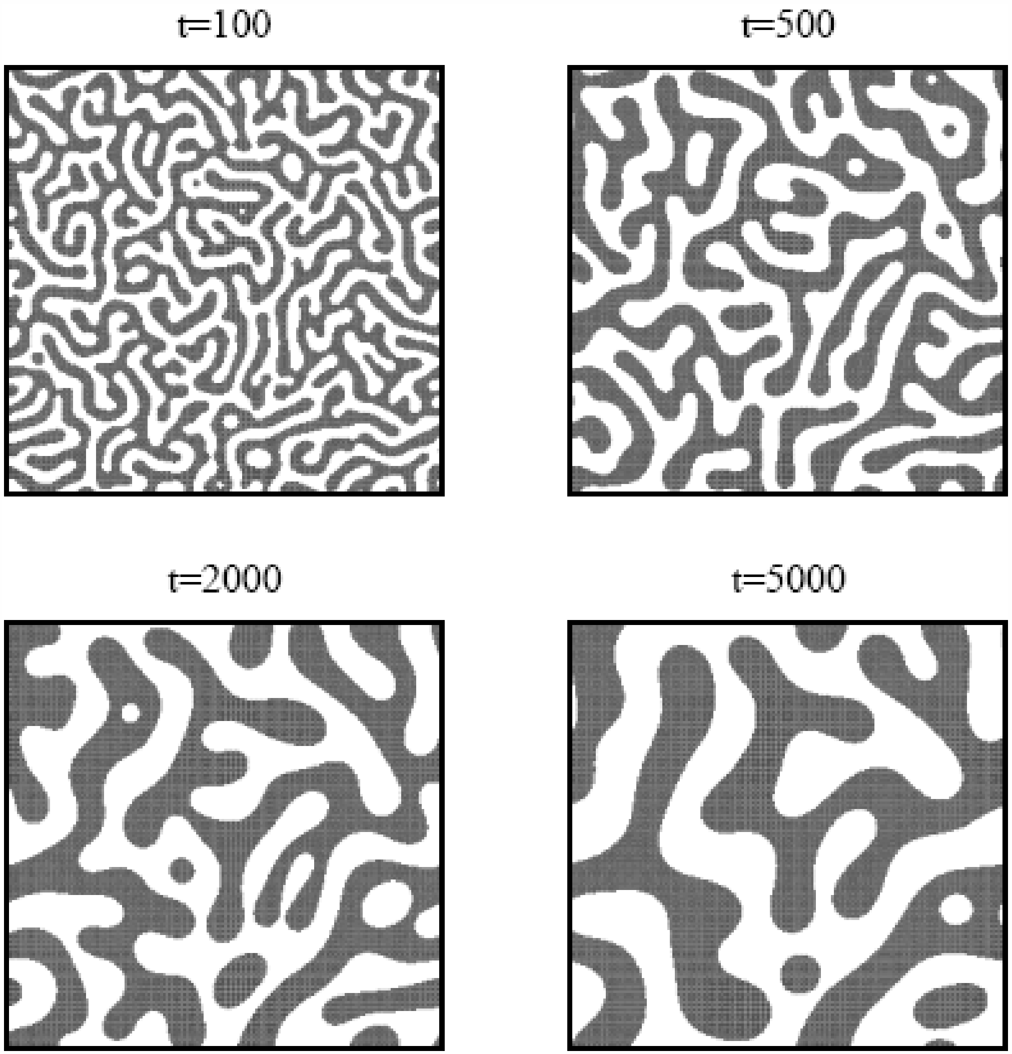
- Example 3: Phase separation of a binary mixture after a quench below the miscibility gap

- Bulk binary mixture, e.g., oil-water, polymer blends, binary alloys, etc.

- Rapid quench from homogeneous region to segregated region results in far-from-equilibrium evolution.



Critical Mixture (50% A and 50% B)



1) Phase separation is driven by interfaces (defects).

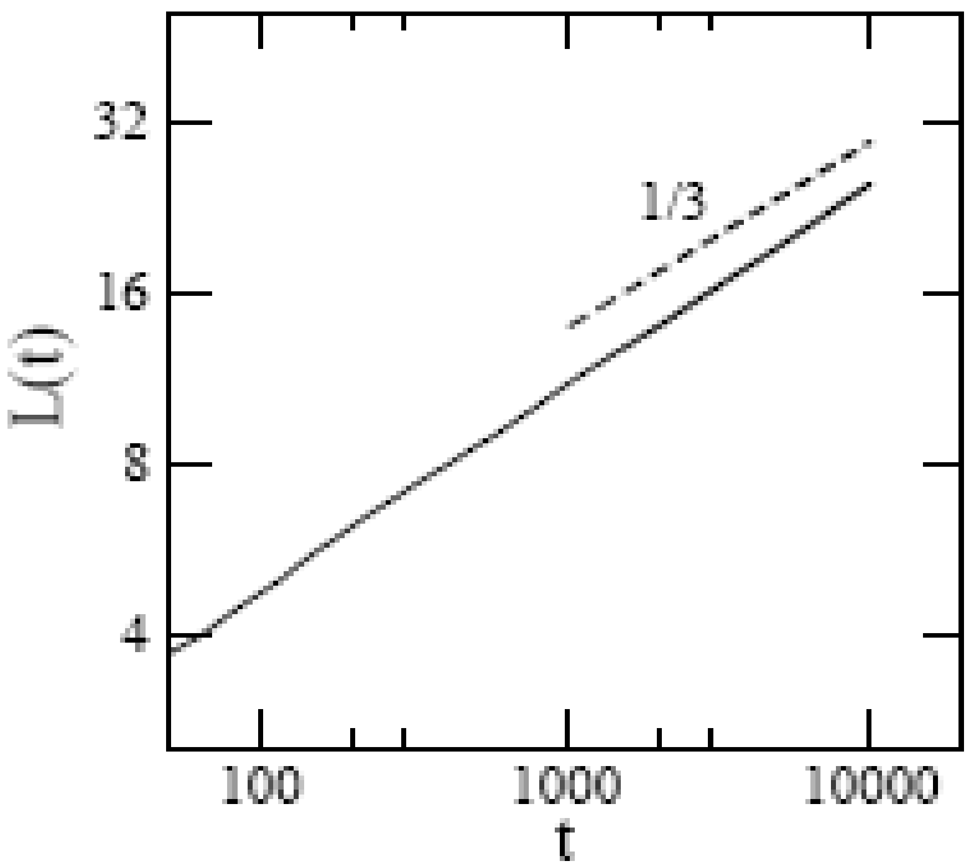
2) Composition must be conserved during evolution.

3) $$\frac{dL}{dt} = \frac{\sigma}{L} \times \frac{1}{L} \Rightarrow L(t) \sim (\sigma t)^{1/3}$$

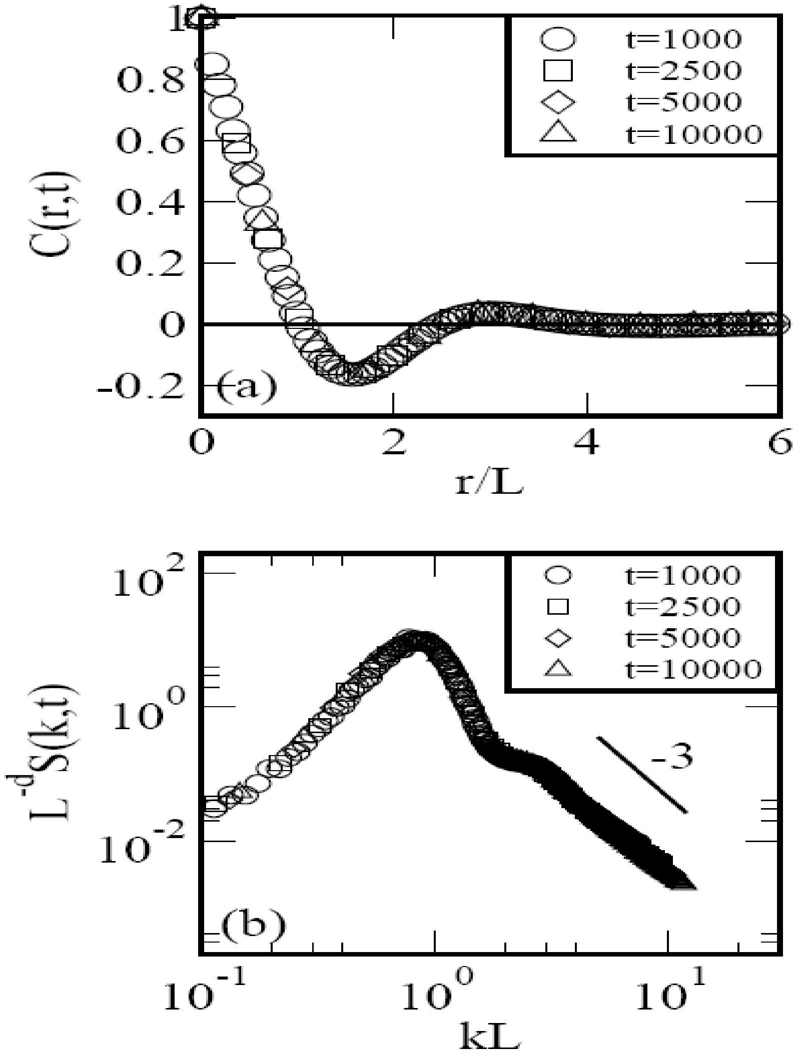
Lifshitz-Slyozov growth law

4) System shows dynamical scaling. However, there is still no complete understanding of the correlation function or structure factor.

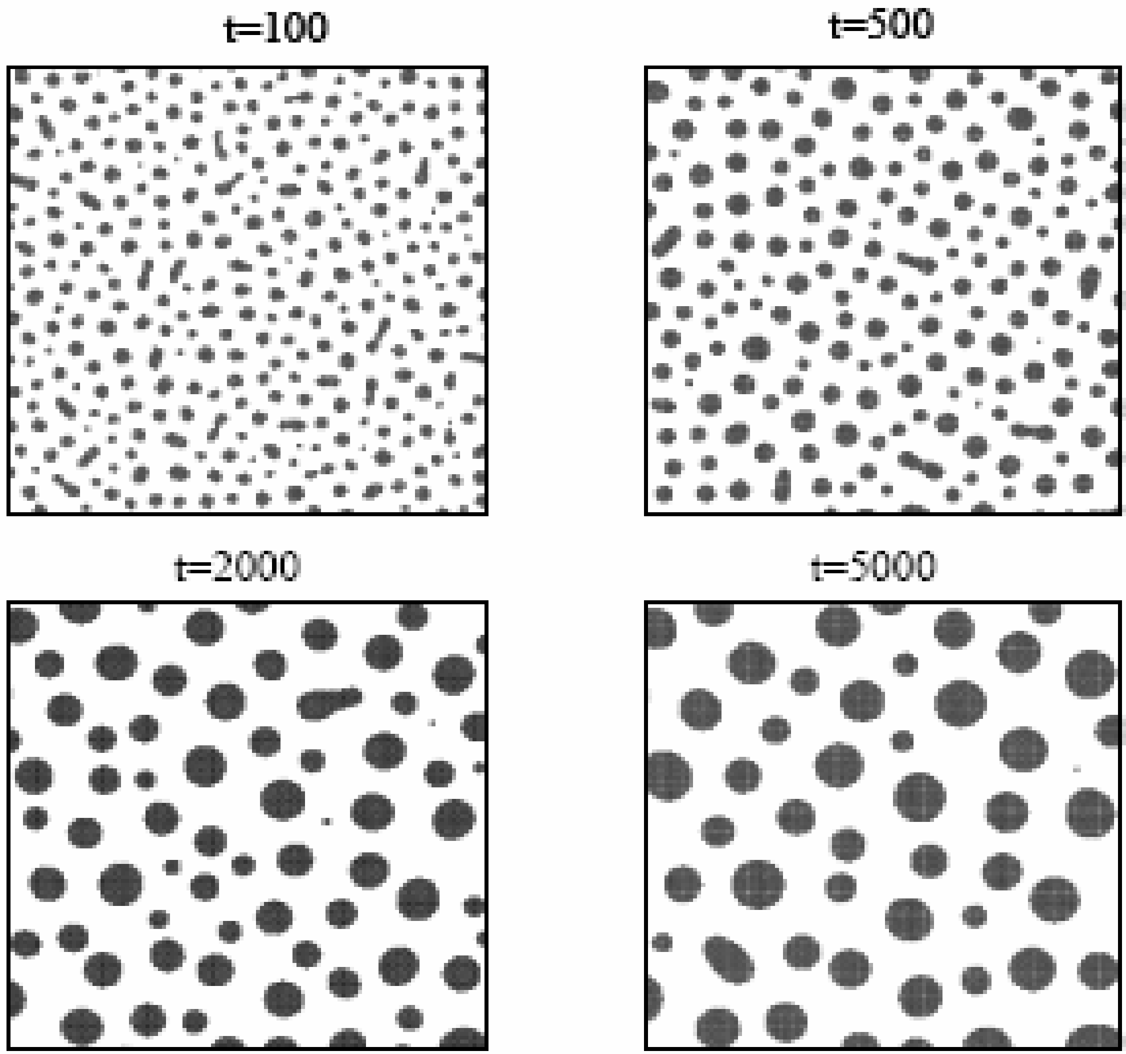
Critical Mixture (50% A and 50% B)
Domain Growth Law



Critical Mixture (50% A and 50% B) Dynamical Scaling



Off-critical Mixture (30% A and 70% B)



(b) Nonconserved Dynamics: Glauber Spin-Flip Ising Model

- Ising model gives the phase diagrams of ferromagnets and binary mixtures.

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j, \quad S_i = \pm 1$$

- The Ising model has no intrinsic kinetics. We associate stochastic kinetics by placing the system in contact with a heat bath.

Glauber spin-flip kinetics corresponds to flipping a randomly-chosen spin ($S_i = -S_i$).

- We can use a master-equation approach to derive the equivalent coarse-grained model, the time-dependent Ginzburg-Landau (TDGL) equation or Model A.

$$\lambda^{-1}\frac{\partial}{\partial t}\psi(\vec{r},t) = \left(\frac{T_c}{T}-1\right)\psi - \frac{1}{3}\left(\frac{T_c}{T}\right)^3\psi^3 + \frac{T_c}{qT}a^2\nabla^2\psi$$

$\psi(\vec{r},t)$	Order parameter (magnetization)
$T_c = qJ$	Mean-field critical temperature
a	Lattice spacing

(c) Conserved Dynamics: Kawasaki Spin-Exchange Ising Model

- For conserved dynamics, we use the Ising model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j, \quad S_i = \pm 1$$

+ Kawasaki spin-exchange kinetics ($S_i \leftrightarrow S_j$), where i and j are usually nearest-neighbors.

- We can use the master-equation approach to obtain the analogous coarse-grained model, the Cahn-Hilliard-Cook (CHC) equation or Model B.

$$2\lambda^{-1}\frac{\partial}{\partial t}\psi(\vec{r},t) = -a^2\nabla^2\left[\left(\frac{T_c}{T}-1\right)\psi - \frac{1}{3}\left(\frac{T_c}{T}\right)^3\psi^3 + \frac{T_c}{qT}a^2\nabla^2\psi\right]$$

$\psi(\vec{r},t)$ Order parameter (density difference of A and B)

- In this case, the integral of the order parameter is conserved.

(d) Phenomenological Models of Phase Ordering Systems

- The TDGL equation models the dissipative (over-damped) relaxation of a ferromagnetic system to its free-energy minimum.

$$\frac{\partial}{\partial t}\psi(\vec{r},t) = -\Gamma \frac{\delta G[\psi]}{\delta \psi} + \theta(\vec{r},t)$$

$$G[\psi] = \int d\vec{r} \left[g(\psi) + \frac{1}{2} K \left(\vec{\nabla}\psi \right)^2 \right]$$

$$\beta G_{Glauber}(\psi) = \int d\vec{r} \left[-\frac{1}{2}\left(\frac{T_c}{T} - 1\right)\psi^2 + \frac{1}{12}\left(\frac{T_c}{T}\right)^3 \psi^4 + \frac{T_c}{2qT} a^2 \left(\vec{\nabla}\psi\right)^2 \right]$$

- Dimensionless form of TDGL equation for T<T_c

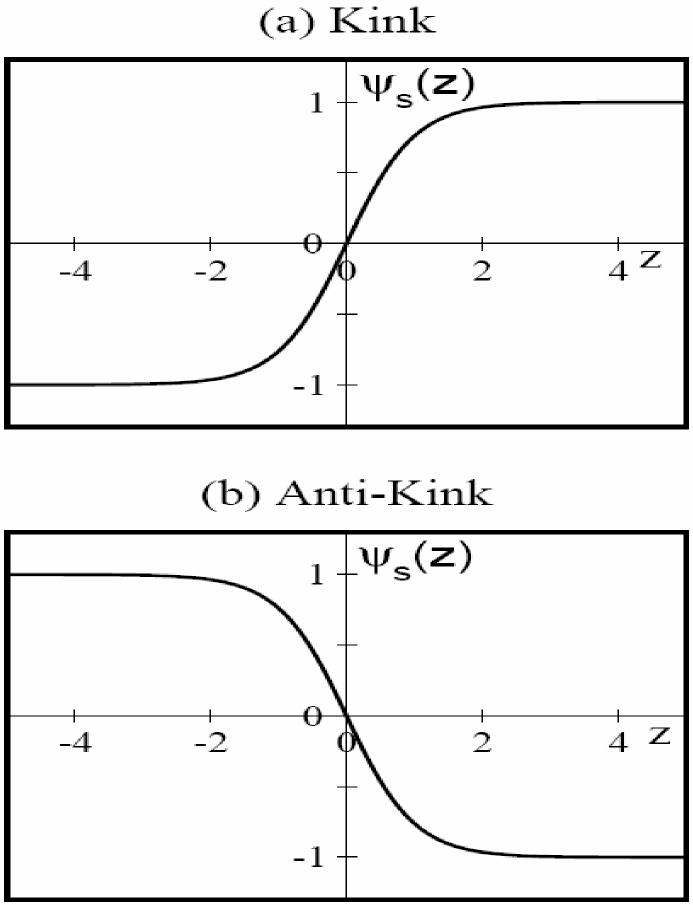
$$\frac{\partial}{\partial t}\psi(\vec{r},t) = \psi - \psi^3 + \nabla^2\psi + \theta(\vec{r},t)$$

- Static kink or defect solutions

$$0 = \psi_s - \psi_s^3 + \frac{d^2\psi_s}{dz^2}$$

$$\psi_s(z) = \tanh\left[\pm\frac{(z - z_0)}{\sqrt{2}}\right]$$

The ordering dynamics is understood via the motion of these defects.



- The CHC equation is obtained from the continuity equation.

$$\frac{\partial}{\partial t}\psi(\vec{r},t) = -\vec{\nabla}\bullet\left[\vec{J}(\vec{r},t)+\vec{\theta}(\vec{r},t)\right]$$

$$\vec{J}(\vec{r},t) = -D\vec{\nabla}\mu(\vec{r},t)$$

$$\mu(\vec{r},t) = \frac{\delta F[\psi]}{\delta\psi}$$

$$\frac{\partial}{\partial t}\psi(\vec{r},t) = -\vec{\nabla}\bullet\left[-D\vec{\nabla}\left(\frac{\delta F[\psi]}{\delta\psi}\right)+\vec{\theta}(\vec{r},t)\right]$$

- Dimensionless version has the same kink solutions as the TDGL equation. In this case, the motion of the defects is strongly correlated.

(e) Conclusion

- We have focused on two examples of the kinetics of phase transitions:

  dynamics of ordering

  dynamics of phase separation

- Our analytic understanding of pattern formation relies on the dynamics of "defects" in the system, e.g., interfaces, vortices, monopoles, etc. They may be thought of as "elementary particles" in this context.