Dynamic Transition Theory and Equilibrium Phase Transitions

Shouhong Wang
Main Collaborator: Tian Ma
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http://www.indiana.edu/~fluid

I. Philosophy

For many problems in sciences, we need to understand

- the transitions from one state to another, and
- the stability/robustness of the new states

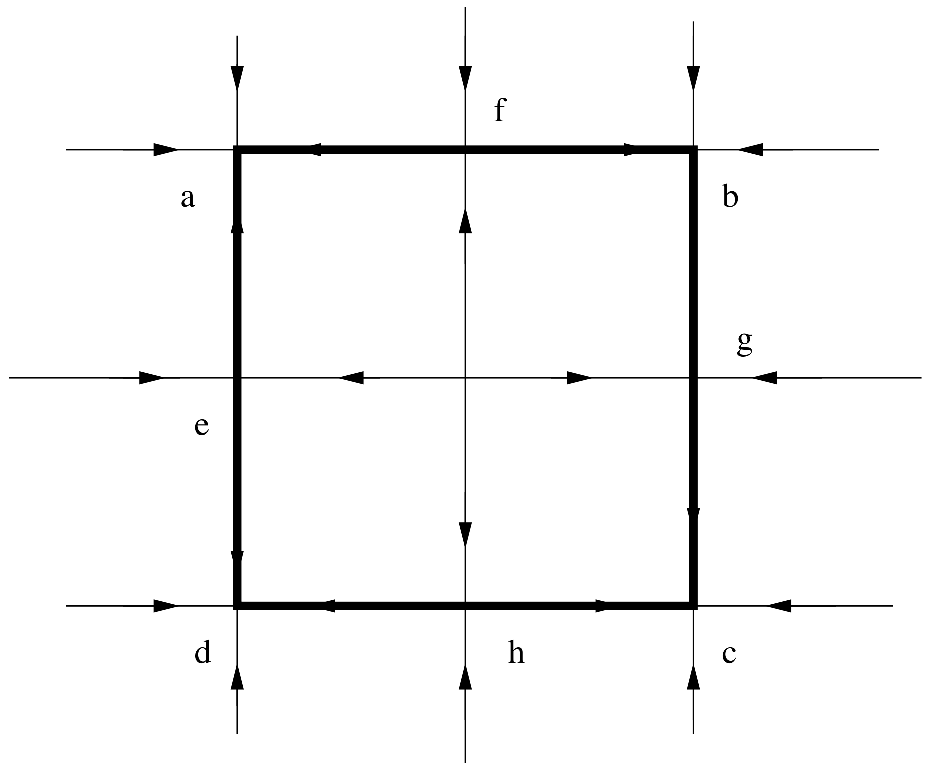
Our philosophy: to search for the complete set of transition states,

often represented by a local attractor.

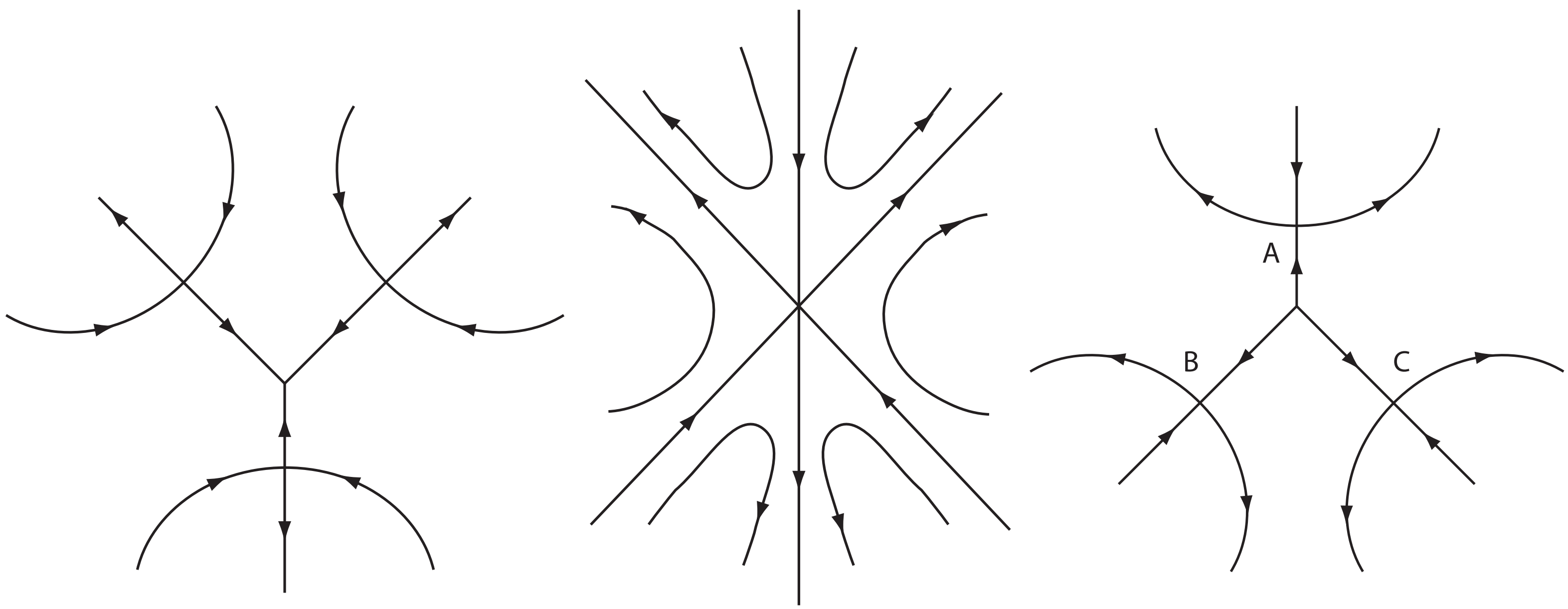
Examples:

$$\frac{dx_1}{dt} = \lambda x_1 - x_1^3 + o(|x|^3),$$
$$\frac{dx_2}{dt} = \lambda x_2 - x_2^3 + o(|x|^3)$$

The system undergoes a dynamic transition as $\lambda = 0$:



(1)
$$\dot{x}_1 = \lambda x_1 + x_1^2 + x_1 x_2 - 10x_1^3,$$
$$\dot{x}_2 = \lambda x_2 - 2x_1 x_2 - x_2^2 - 10x_2^3.$$



(a) (b) (c)

A new **dynamic transition theory** is developed recently:

- a new dynamic classification scheme of phase transitions, and
- methods to identify the types of transitions.

References:

- T. Ma & S. Wang, *Bifurcation Theory and Applications*, World Scientific Series on Nonlinear Science, Series A - Vol. 53, 2005.
- T. Ma & S. Wang, *Stability and Bifurcation of Nonlinear Evolution Equations*, Science Press, pp. 413, April, 2007.
- T. Ma & S. Wang, *Phase Transition Dynamics in Nonlinear Sciences*, about 700 pp., submitted.
- A few recent articles, downloadable from related journals listed on my web page or from Arxiv.

II. Dynamic Transition Theory

(2) $$\frac{du}{dt} = L_\lambda u + G(u, \lambda),$$
$$u(0) = u_0.$$

$u : [0, \infty) \to H,$

H, H_1 Hilbert spaces, $H_1 \hookrightarrow H$ dense and compact,

$-L_\lambda = A - B_\lambda$ a sectorial operator,

$A : H_1 \to H$ a linear homeomorphism,

$B_\lambda : H_1 \to H$ linear compact operators

$G(u, \lambda) = o(\|u\|_{H_\alpha}), \quad \forall\, \lambda \in \mathbb{R}^1, \quad \alpha < 1.$

Principle of Exchange of Stability (PES):

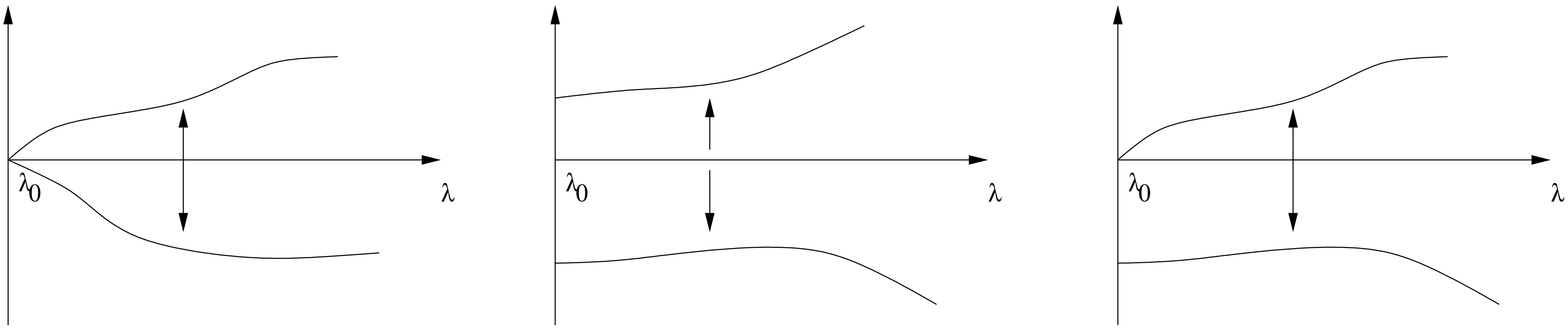
$\beta_1(\lambda), \beta_2(\lambda), \cdots \in \mathbb{C}$ eigenvalues of L_λ:

(3) $$\mathrm{Re}\beta_i(\lambda) \begin{cases} < 0 & \text{if } \lambda < \lambda_0, \\ = 0 & \text{if } \lambda = \lambda_0, \\ > 0 & \text{if } \lambda > \lambda_0 \end{cases} \qquad 1 \leq i \leq m,$$

(4) $$\mathrm{Re}\beta_j(\lambda_0) < 0 \qquad m + 1 \leq j.$$

$$E_0 = \bigcup_{1 \leq i \leq m} \bigcup_{k \in \mathbb{N}} ker(L_{\lambda_0} - \beta_j(\lambda_0))^k$$

Theorem [MA & W., 07] *Under the conditions, the system (1) undergoes a dynamic transition from* $(u, \lambda) = (0, \lambda_0)$ *to one of the following three types:*



Type-I Type-II Type-III

The transitions states are **local attractors**.

Features of Dynamic Classification

- With the above theorem, we can classify all dynamic transitions into three categories: Type-I, Type-II, and Type-III, for both equilibrium and non-equilibrium transitions.

- The classical classification scheme in equilibrium phase transitions is labeled by the lowest derivative of the free energy that is discontinuous at the transition.

- For a specific equilibrium transition problem, once the dynamic classification type is determined, the transition type in the classical sense will become transparent.

- Dynamic properties of the system are explicitly given.

An important aspect of the dynamic transition theory is to determine which of the three types of transitions occurs in a specific problem. The theory we have developed is good enough for all applications we have encountered.

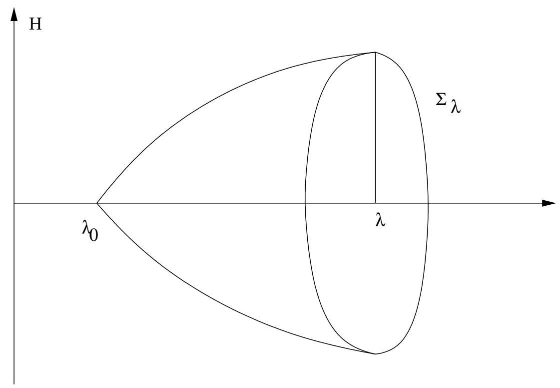
One crucial ingredient for applications is the reduction of (2) to the center manifold:

$$\frac{dx}{dt} = J_\lambda x + g(x,\lambda) \qquad \text{for } x \in \mathbb{R}^m \text{ and near } \lambda = \lambda_0, \tag{5}$$

where

$g(x,\lambda) = (g_1(x,\lambda), \cdots, g_m(x,\lambda))$	
$g_j(x,\lambda) = (G(x+\Phi(x,\lambda),\lambda), e_j^*)$	$\forall 1 \leq j \leq m$
e_j and e_j^*	eigenvectors of L_λ and L_λ^* respectively
J_λ	$m \times m$ Jordan matrix
$\Phi(x,\lambda)$	the center manifold function

Type-I Transition is ”essentially characterized” by **attractor bifurcation** as shown (Ma & Wang, 04):



Theorem (Ma & W., 04, 05). Assume (3)-(4), and $u = 0$ is locally asymptotically stable for (2) at $\lambda = \lambda_0$. Then there exists a bifurcated attractor Σ_λ, homologic to S^{m-1}, for $\lambda > \lambda_0$ and near λ_0.

III. Binary System Modeled by Cahn-Hilliard Equation

Consider a binary system, and let u_A and u_B be the concentrations of components A and B respectively, then $u_B = 1 - u_A$. The Cahn-Hilliard free energy is given by

$$F(u) = F_0 + \int_\Omega \Big[\frac{\mu}{2}|\nabla u_B|^2 + f(u_B)\Big]dx, \tag{6}$$

where the molar Gibbs free energy takes the following form

$$\begin{aligned} f =& \mu_A(1-u_B) + \mu_B u_B + RT(1-u_B)\ln(1-u_B) \\ & + RTu_B \ln u_B + a u_B(1-u_B), \end{aligned} \tag{7}$$

where μ_A, μ_B are the chemical potentials of A and B respectively, R the molar gas constant, $a > 0$ the measure of repel action between A and B.

In a homogeneous state, $u_B = u_0$ is a constant, and let $u = u_B - u_0$.

Cahn-Hilliard equation:

(8)
$$\frac{\partial u}{\partial t} = -k\Delta^2 u + \Delta[b_1 u + b_2 u^2 + b_3 u^3]$$

$$k = \mu D,$$
$$b_1 = \frac{D}{2}\frac{d^2 f(u_0)}{du^2} = \left[\frac{RT}{u_0(1-u_0)} - 2a\right]\frac{D}{2}$$
$$b_2 = \frac{D}{3!}\frac{d^3 f(u_0)}{du^3} = \frac{2u_0 - 1}{6u_0^2(1-u_0)^2} DRT,$$
$$b_3 = \frac{D}{4!}\frac{d^4 f(u_0)}{du^4} = \frac{1 - 3u_0 + 3u_0^2}{12u_0^3(1-u_0)^3} DRT,$$

where D is the diffusion coefficient.

Nondimensional CH equation:

(9)
$$
\begin{aligned}
&\frac{\partial u}{\partial t} = -\Delta^2 u - \lambda \Delta u + \Delta(\gamma_2 u^2 + \gamma_3 u^3),\\
&\frac{\partial u}{\partial n} = 0, \qquad \frac{\partial \Delta u}{\partial n} = 0 \qquad \text{on } \partial\Omega,\\
&\int_\Omega u(x,t)dx = 0,\\
&u(x,0) = \varphi.
\end{aligned}
$$

Let $\gamma_3 > 0$, and $\rho_1 > 0$ be the first eigenvalue of $-\triangle$ with the Neumann boundary condition with $\int_\Omega u = 0$.

With the dynamic transition theory, we can prove (Ma-Wang, 08) that at $\lambda = \rho_1$, CH undergoes a Type-I transition for $\gamma_2 = 0$, and a Type-II or Type-III transition for $\gamma_2 \neq 0$. Detailed structure of the transition can be derived as well.

Consider $\Omega = (0, L_1) \times (0, L_2) \times (0, L_3)$ and $L = L_1$.

$$\text{Case I:} \quad L = L_1 > L_j \qquad \forall j = 2, 3,$$
$$\text{Case II:} \quad L = L_1 = L_2 > L_3 \text{ or } L_1 = L_2 = L_3.$$

Let

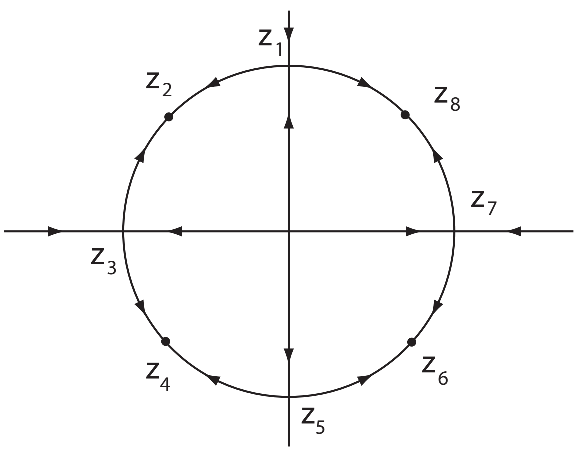
$$K = \begin{cases} \dfrac{2L^2}{9\pi^2}\gamma_2^2 - \gamma_3 & \text{for Case I,} \\ \dfrac{26L^2}{27\pi^2}\gamma_2^2 - \gamma_3 & \text{for Case II.} \end{cases}$$

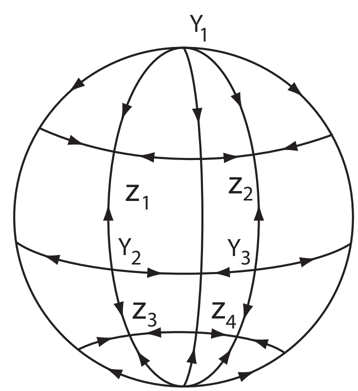
$$K_d = \begin{cases} \dfrac{2L_d^2}{9\pi^2}\dfrac{b_2^2}{k} - b_3 & \text{for Case I,} \\ \dfrac{26L_d^2}{27\pi^2}\dfrac{b_2^2}{k} - b_3 & \text{for Case II.} \end{cases}$$

where $L_d = L \cdot l$ is the dimensional length scale.

Main Results (Ma & W., 08)

- If $K < 0$, then CH equation undergoes Type-I transition at $\lambda_0 = \pi^2/L^2$:
  - Case I: CH equation bifurcates on $\lambda > \pi^2/L^2$ to two attractors u_1^T and u_2^T.
  - Case II: The problem bifurcates on $\lambda > \pi^2/L^2$ to an attractor $\Sigma_\lambda = S^{m-1}$, containing exactly $3^m - 1$ non-degenerate singular points with 4 being minimal attractors if $m = 2$, and with with either 8 minimal attractors for $\gamma_3 < \frac{22L^2}{9\pi^2}\gamma_2^2$, or 6 minimal attractors for $\gamma_3 > \frac{22L^2}{9\pi^2}\gamma_2^2$, if $m = 3$.



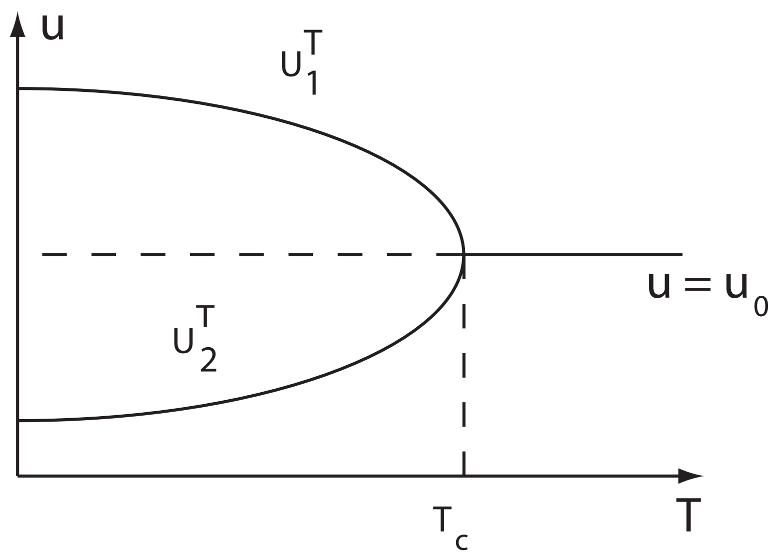


(a)

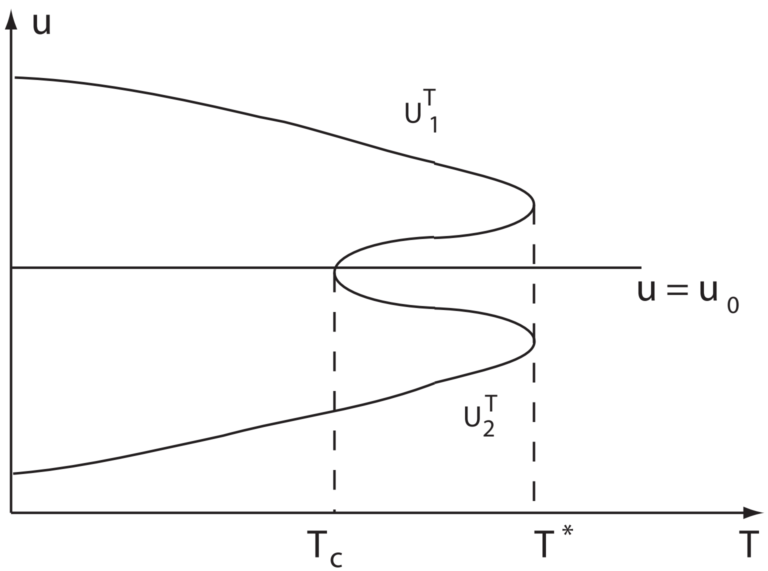
- If $K > 0$, then the problem undergoes Type-II transition at $\lambda_0 = \pi^2/L^2$, and has a saddle-node bifurcation on $\lambda^* < \pi^2/L^2$.

Physical Conclusions

$$\lambda = -\frac{l^2 D}{2k}\left(\frac{RT}{u_0(1-u_0)} - 2a\right).$$



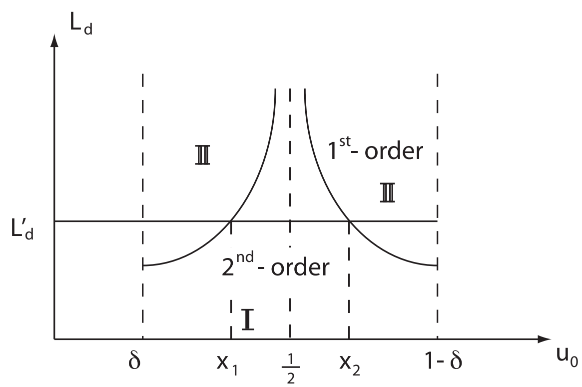
$K_d < 0$: The state $u_0 = \bar{u}_B$ is stable if $T_c < T$, and the state u_0 is unstable, U_1^T and U_2^T are stable if $T < T_c$.

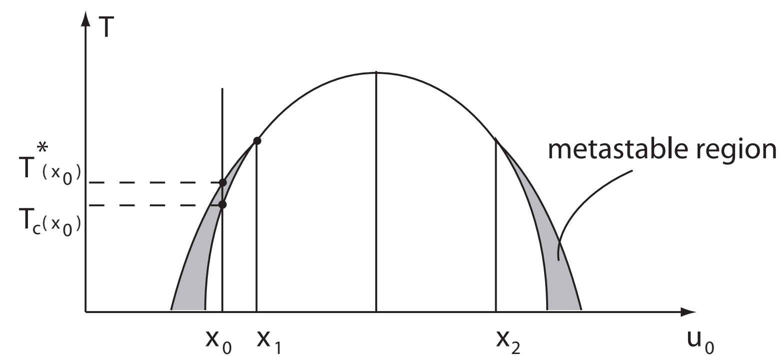


For fixed u_0 and L, the transition for the case where $K_d > 0$ is first order separation with latent heat and with hysteresis: U_1^T and U_2^T represent separation states, and u_0 is the homogeneous state. In this case, for $T_c < T < T^*$, all states u_0, U_1^T, u_2^T are metastable states. For $T < T_c$, u_0 is unstable, and U_1^T and U_2^T are stable states.

Solving $K_d = 0$ gives a critical (dimensional) length scale L_d:

$$L_d = \begin{cases} \dfrac{3\sqrt{3k}\pi}{8\sqrt{2DRT_c}|u_0 - \frac{1}{2}|} + O(1) & \text{for Case I,} \\ \dfrac{9\sqrt{k}\pi}{8\sqrt{26DRT_c}|u_0 - \frac{1}{2}|} + O(1) & \text{for Case II,} \end{cases} \tag{10}$$

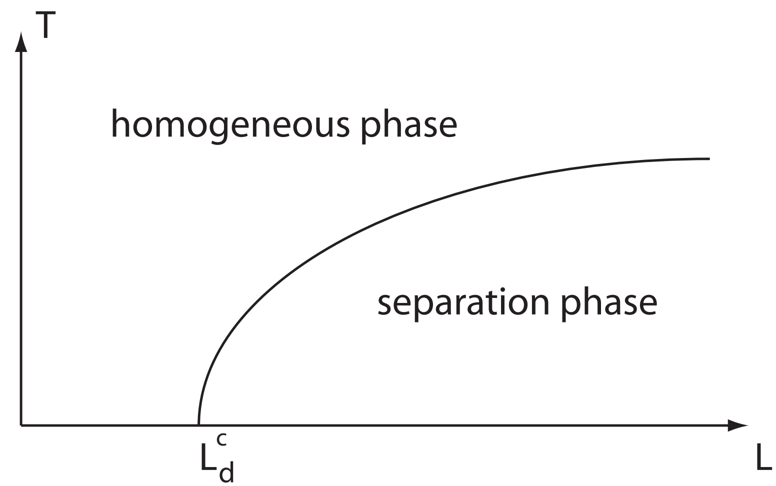




The shadowed region is metastable region

Critical temperature:

$$T_c = \frac{u_0(1-u_0)}{RD}\left(a - \frac{k\pi^2}{2L_d^2}\right).$$



IV. Ideas of the Proof

- Reduction to the center manifold:

$$(11) \qquad \frac{dy_i}{dt} = \beta_1(\lambda) y_i - \frac{\pi^2}{2L^2}\left[\sigma_1 y_i^3 + \sigma_2 y_i \sum_{j\neq i} y_j^2\right] + o(|y|^3) \quad \forall 1 \le i \le m$$

$$\sigma_1 = \frac{3\gamma_3}{2} + \frac{\gamma_2^2}{\lambda - \frac{4\pi^2}{L^2}}, \qquad \sigma_2 = 3\gamma_3 + \frac{4\gamma_2^2}{\lambda - \frac{2\pi^2}{L^2}}.$$

- Careful examination of (11) using the dynamic transition theory.

Equations (11) are derived using the following formula for the center manifold function: If J_λ is diagonal near $\lambda = \lambda_0$, then

$$-\mathcal{L}_\lambda \Phi(x,\lambda) = P_2 G_k(x,\lambda) + o(\|x\|^k) + O(|\beta|\|x\|^k), \tag{12}$$

where $\beta(\lambda) = (\beta_1(\lambda), \cdots, \beta_m(\lambda))$ are the eigenvalues of J_λ.

V. Remarks

The theory has been applied to **a wide range of problems in nonlinear sciences,** leading to a number of **new physical predictions**.

- **equilibrium phase transitions**: PVT system, ferromagnetism, Cahn-Hilliard model for binary systems, superconductivity, and superfluidity (He-3, He-4, and their mixture).

- **Classical Fluid Dynamics:** Bénard convection, Taylor problem, and Taylor-Couette-Poiseuille flows

- **Geophysical Fluid Dynamics and Climate Dynamics:** rotating Boussinesq equations (joint with C. Hsia), double-diffusive models (joint with J. Bona & C. Hsia), thermohaline circulation, Arctic ocean circulations, atmospheric meridional circulations, and ENSO.