Chap. 2. Reaction - Diffusion system.

1、BVP、IVP、IBVP、Equilibrium

BVP: boundary value problem.

IVP: initial value problem.

1. no general qualitative thereom for PDE: a property holds only for certain situations
2. IV、BV are important.

derivation of reaction-diffusion equation.

Balance law:

$$\frac{d}{dt}\int_B \rho(x,t)\,dx = -\int_B \nabla\cdot\vec{F}\,dx + \int_B R(x,t)\,dx$$

(Smooth) $\Rightarrow$ $$\frac{\partial \rho(x,t)}{\partial t} = -\nabla\cdot\vec{F}(x,t) + R(x,t)$$

constitutive equation 本构方程

equation of state 状态方程

Fick's law: $F(x,t) = -D\nabla\rho$

$$\Rightarrow \rho_t = D\rho_{xx} + R$$

for reaction: $A + B \rightarrow 2B + \text{others}$

$$\begin{cases} \frac{\partial}{\partial t}\rho_A = D_A\partial_{xx}\rho_A - \rho_A\rho_B \\ \frac{\partial}{\partial t}\rho_B = D_B\partial_{xx}\rho_B + \rho_A\rho_B \end{cases}$$

(D_A、D_B: diffusivity 扩散系数)

stationary solution, steady state: $\frac{\partial}{\partial t} = 0$

$$\begin{cases} D_A\rho_{A,xx} - \rho_A\rho_B = 0 \\ D_B\rho_{B,xx} + \rho_A\rho_B = 0 \end{cases}$$

2、Dispersion relation, linearity & non-linearity.

fisher equation:

$$u_t = u_{xx} + u(1-u)$$

steady state equ. $u_{xx} + u(1-u) = 0$

① first integral

$$2u_x u_{xx} + (u^2 - u^2)\cdot 2u_x = 0$$

$$u_x^2 + u - \frac{2}{3}u^3 = \text{Constant}$$

② Critical points

$$(u^*, u_x^*) = (0,0),\ (1,0)$$

$u(x,t) \sim (u^*, u^*_x)_{(u^*=0)}$ Ground state

$u(x,t) = u^* + \tilde{u}(x,t)_{(\leq 1)}$

linearized equation. $\tilde{u}_t = \tilde{u}_{xx} + \tilde{u}$

for solution $\tilde{u}(x,t) = \tilde{U} e^{\lambda t + i w x}$, we get $\lambda = -w^2 + 1$ (dispersion relation 色散关系)

let $\tilde{u}(x,0) = \sum_w \tilde{U}_w e^{iwx} \Rightarrow \tilde{u}(x,t) = \sum_w \tilde{U}_w e^{(1-w^2)t} e^{iwx}$

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define $p = \rho_A$, $q = \rho_B$, for Ground state $\begin{cases} p^* = P^*, & p^*_x = 0 \\ q^* = 0 & q^*_x = 0 \end{cases}$

for solution $\begin{cases} p = p^* + \tilde{p} \\ q = 0 + \tilde{q} \end{cases}$, $(\tilde{p}, \tilde{q} \ll 1)$

linearized equation $\begin{cases} \tilde{p}_t = D_1 \tilde{p}_{xx} - p^* \tilde{q} \\ \tilde{q}_t = D_2 \tilde{q}_{xx} + p^* \tilde{q} \end{cases}$

for $\tilde{p} = P e^{\lambda t + iwx}$, $\tilde{q} = Q e^{\lambda t + iwx}$.

$$\begin{cases} \lambda P = D_1(-w^2) P - p^* Q \\ \lambda Q = D_2(-w^2) Q + p^* Q. \end{cases}$$

when $\begin{vmatrix} \lambda + D_1 w^2 & p^* \\ 0 & \lambda + D_2 w^2 - p^* \end{vmatrix} = 0$

$$\begin{cases} \lambda_1 = -D_1 w^2 \\ \lambda_2 = -D_2 w^2 + p^*. \end{cases}$$

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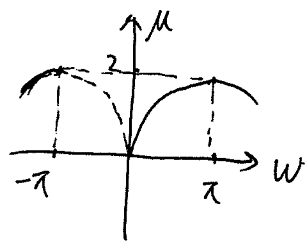
phase velocity : $\frac{\mu}{w}$, group velocity : $\frac{d\mu}{dw}$.

$y = e^{i(\mu t + wx)}$

Harmonic lattice : $\ddot{u}_n = u_{n-1} - 2u_n + u_{n+1}$
谐振子



Nonlinearity.

$$\begin{cases} u_t = u_{xx} - u + u^2 & x \in [0,\pi] \\ u(x,0) = u_0(x), & u(0,t) = u(1,t) = 0. \end{cases}$$

estimation:

$$f(t) = \int_0^\pi u(x,t) \cdot \sin x \, dx$$

$$\frac{d f(t)}{dt} = -2f + \int_0^\pi u^2 \sin x \, dx$$

$$f = \int_0^\pi u \sin x \, dx = \int_0^\pi (u^2 \sin x)^{\frac{1}{2}} (\sin x)^{\frac{1}{2}} dx$$

$$\le \left(\int_0^\pi u^2 \sin x \, dx\right)^{\frac{1}{2}} \left(\int_0^\pi \sin x \, dx\right)^{\frac{1}{2}}$$

$\Rightarrow f^2 \le 2 \int_0^\pi u^2 \sin x \, dx. \Rightarrow \frac{df}{dt} \ge -2f + \frac{1}{2} f^2$

$\Rightarrow$ if $f(0) > 4$, then $f(t) \nearrow$ exponentially

~~$\int_0^\pi u_0(x) \sin x \, dx$~~

$\therefore$ $f^2 \le \int_0^\pi u^2 dx \int_0^\pi \sin^2 x \, dx = \frac{\pi}{2} \int_0^\pi u^2 dx$

$\therefore$ $\int_0^\pi u^2(x,t) dx \nearrow$ (go to infinity at finite time).

3、invariant domain. 不变区域.

Comparison principle

$u, v \overset{(u_0 > v_0)}{\Rightarrow} u \ge v$

(S_u) (S_v)

Maximum principle

$W = u - v$ $\quad W_0 > 0 \Rightarrow w(t) \ge 0$

S_W

equ. $\begin{cases} u_t = \Delta u + f(u,x,t), & (x \in \Omega, t > 0) \\ \alpha u + \beta \nabla u \cdot \vec{n} = g(x,t), & (x \in \partial\Omega) \end{cases}$

$(\alpha \beta \ge 0)$

if $\begin{cases} \bar{u}_t \ge \Delta \bar{u} + f(\bar{u}, x, t), & (x \in \Omega, t > 0) \\ \bar{u}(x,0) \ge u(x,0) & (x \in \Omega) \\ \alpha \bar{u} + \beta \nabla \bar{u} \cdot \vec{n} \ge g(x,t) & (x \in \partial\Omega) \end{cases}$

then $\bar{u}(x,t)$ is a super-solution to $u(x,t)$. ie.

$$\bar{u} \ge u, \quad (x \in \Omega, t > 0)$$

$$Lu = \frac{\partial u}{\partial t} - \sum_{i,j=1}^n a_{ij}(x,t) \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^n b_i(x,t) \frac{\partial u}{\partial x_i}$$

$Bu = \alpha u + \beta \nabla u \cdot \vec{n}$ $\quad (x \in \partial\Omega \times (0,T])$

$h(x,t)$ is bounded in $Q_T \equiv \Omega \times (0,T]$

1° if $\begin{cases} Lu + h(x,t) \ge 0 & \text{in } Q_T \\ Bu \ge 0 & \text{on } \partial\Omega \times (0,T] \\ u(x,0) \ge 0, \text{ and is smooth enough} \\ \partial\Omega \text{ is good enough} \end{cases}$

then $u(x,t) \ge 0$ on Q_T

2° if further $u(x,0) > 0$

then $u(x,t) > 0$ on Q_T.

invariant domain:

for reaction-diffusion system:

$$u_t = D \Delta u + f(u)$$

define $B = \prod_{i=1}^m [\underline{u_i}, \overline{u_i}]$ is a rectangular area in state space, and $\vec{N}$ is the outer normal of B,

if 1° $u(x,0) \in B$, $u(x,t)|_{x \in \partial\Omega} \in B$

or 2° $u(x,0) \in B$, boundary conditions that guarantees $\begin{cases} \nabla u_i \cdot \vec{n} \le 0 & \text{when } u_i = \overline{u_i} \\ \nabla u_i \cdot \vec{n} \ge 0 & \text{when } u_i = \underline{u_i} \end{cases}$ $(x \in \partial\Omega)$

then the solution will remain in B.

Appendix: proof of Invariant Domain:

Condition 1°: $u(x,0) \in B$, $u(x,t)|_{x\in\partial\Omega} \in B$

If (x',t') satisfies $u(x',t') \in \partial B$, say $u_i(x',t') = \bar{u}_i$ for instance, then $\Delta u_i(x',t')$ ~~$= \sum_i u_{x_i x_i}(x',t') \le 0$~~

$$= \sum_j \frac{\partial^2 u_i}{\partial x_j^2}(x',t') \le 0,$$

because $u_i(x,t') \le \bar{u}_i$, for any x near x'.

Then $\frac{\partial}{\partial t} u_i(x',t') = D\Delta u_i(x',t') + f_i(u(x',t')) \le 0$,

since $f \cdot \vec{N} \overset{= f_i \le 0}{}$ now.

Then $u_t \vec{N} = \frac{\partial}{\partial t} u_i \le 0$, which show any point reached at the boundary of B will move inward.

Condition 2°: $u(x,0) \in B$, $\begin{cases} \nabla u_i|_{x\in\partial\Omega} \cdot \vec{n} < 0, & \text{when } u_i|_{x\in\partial\Omega} = \bar{u}_i \\ \nabla u_i|_{x\in\partial\Omega} \cdot \vec{n} > 0, & \text{when } u_i|_{x\in\partial\Omega} = \underline{u}_i \end{cases}$ $(\vec{n} \times \partial\Omega = 0)$

if when t evolves, there exist a point (x',t') that satisfies $u(x',t') \in \partial B$, and $x' \in \partial\Omega$ for the first time, say $u_i(x',t') = \bar{u}_i$,

then from the condition, $\nabla u_i(x',t') \cdot \vec{n} < 0$, which implies that inside domain Ω, there is a point (x'',t') which satisfies $u_i(x'',t') > \bar{u}_i$, and this contradicts with out supposition of (x',t').

Hence, $u(x,t)|_{x\in\partial\Omega}$ with always be in B.

Discussion: From the proof, we can see that "$u(x,0) \in B$" alone restricts possible solutions in B, but we made discussions on boundary conditions. The reason that we ~~consider~~ add boundary conditions is that they are necessary for definite solution. And the reason why we put restrictions on boundary conditions is that some boundary conditions will leave no possible solutions.

4. perturbation method

$P(u, x, t; \varepsilon) = 0$ $\qquad$ (0) − system.

Fisher's equation: (steady state)

$$\begin{cases} V_{yy} + L^2 V (1-V) = 0 \\ V|_{y=0,1} = 0 \end{cases}$$

solution: $\begin{cases} V(y) = V_0 + \varepsilon V_1 + \varepsilon^2 V_2 + \cdots \\ L = \pi + \varepsilon \end{cases}$

by substituting and since ε is a small parameter, we have

$$\begin{cases} V_0'' + \pi^2 V_0 - \pi^2 V_0^2 = 0 \\ \varepsilon\left[V_1'' + (\pi^2 V_1 + 2\pi V_0) - (2\pi^2 V_0 V_1 + 2\pi V_0^2)\right] = 0 \\ \varepsilon^2\left[V_2'' + (\pi^2 V_2 + 2\pi V_1 + V_0) - (\pi^2(V_1^2 + 2V_0V_2) + 4\pi V_0 V_1 + V_0^2)\right] = 0 \\ \cdots \end{cases}$$

① $V_0 = 0$ (we choose it to be so, the trivial equilibrium).

② $\begin{cases} V_1'' + \pi^2 V_1 = 0 \\ V_1(0) = V_0(1) = 0 \end{cases}$ $\qquad V_1(y) = A \sin \pi y$

③ $\begin{cases} V_2'' + \pi^2 V_2 = -2\pi V_1 + \pi^2 V_1^2 \\ V_2(0) = V_2(1) = 0 \end{cases}$

$\Rightarrow V_2'' + \pi^2 V_2 = -2\pi A \sin \pi y + \pi^2 A^2 \sin^2 \pi y$

(integration by parts) $\quad 0 = -2\pi A \int_0^1 \sin^2 \pi y \, dy + A^2 \int_0^1 \sin^3 \pi y \, dy$

$\therefore A = 0$ or $\frac{3}{4}$, $\quad V_1(y) = \frac{3}{4} \sin \pi y$.

A is an operator on function space : $X \to X$, $X = \{w \mid (w,w) < +\infty, w(0) = w(1) = 0\}$

$$Af \equiv f'' + \pi^2 f \quad , \text{ and } \quad (w,v) \equiv \int_0^1 w(y)\,v(y)\,dy$$

Fredholm's alternative:

$Af = b$ is solvabe, iff b is perpendicular to the nullspace of the adjoint operator of A.

Adjoint operator (伴随算子): $(W, \cancel{A}^{B} Y) = (AW, Y)$, where $(*,*)$ is inner product (内积). then ~~A~~ B is the adjoint operator.

(for linear algebra, $(W, A^T Y) = W^T A^T Y = (W^T A^T Y)^T = Y^T A W = (Y, AW) = (AW, Y)$)

proof: $\forall y \in (A^T)^{-1}\{0\}$, $(y, b) = (y A x) = (A^T y, x) = (0, x) \underset{(\text{scalar})}{=} 0$. $\square$.

$A = f'' + \pi^2$ is self-adjoint:

$$(w, Dv) = \int_0^1 w(v'' + \pi^2 v)\,dy$$
$$= \int_0^1 w'' v + \pi^2 w v\,dy + (-w'v + w v')\big|_0^1$$
$$= \int_0^1 v(w'' + \pi^2 w)\,dy$$
$$= (Dw, v)$$

6. Burger's equation and Cole-Hopf transform

equ: $u_t + u u_x = \nu u_{xx}$

$$\Rightarrow u_t + \left(\frac{u^2}{2} - \nu u_x\right)_x = 0$$

$$\Rightarrow \begin{cases} u = \psi_x \\ \frac{u^2}{2} - \nu u_x = -\psi_t \end{cases}$$

$$\Rightarrow \begin{cases} \psi = \int u\,dx \\ \psi_t = \nu \psi_{xx} - \frac{\psi_x^2}{2} \end{cases}$$

transform: $u = -2\nu \frac{\varphi_x}{\varphi} = -2\nu (\ln \varphi)_x$

$$\Rightarrow \varphi_t = \nu \varphi_{xx}$$

5. travelling wave

for reaction-diffusion equation $u_t = D u_{xx} + f(u)$.

we guess a travelling wave solution $u(x,t) = U(\xi) = U(x - ct)$

then $\frac{\partial}{\partial t} U = -c U_\xi$, $\frac{\partial}{\partial x} U = U_\xi$.

denot U_ξ as U', now the equation is

$$-c U' = D U'' + f(u)$$

For Allen-Cahn equation: $f(u) = u + u^2 - u^3$, and $D = 1$

we get $-cu' = u'' + u + u^2 - u^3$

rewrite it

$$\begin{cases} u' = v \\ v' = -cv - (u + u^2 - u^3) \end{cases}$$

for $u' = v' = 0$, the critical points we get

$$u_1 = \frac{1-\sqrt{5}}{2}, \quad u_2 = 0, \quad u_3 = \frac{1+\sqrt{5}}{2} \quad ; \quad v = 0$$

check the Jacobian

$$\begin{bmatrix} 0 & 1 \\ -1-2u+3u^2 & -c \end{bmatrix}$$

for $(0,0)$, $\quad J = \begin{bmatrix} 0 & 1 \\ -1 & -c \end{bmatrix}$, $\quad \lambda = -\frac{c}{2} \pm \frac{\sqrt{c^2-4}}{2}$

for $\left(\frac{1 \pm \sqrt{5}}{2}, 0\right)$, $J = \begin{bmatrix} 0 & 1 \\ \frac{5 \pm \sqrt{5}}{2} & -c \end{bmatrix}$