III. Population Dynamics in Spatially extended Systems

A. Spatial range expansion

1. Diffusion equation

if individuals perform random walk then the local density $\rho(\vec{r},t)$ evolves according to the diffusion equation

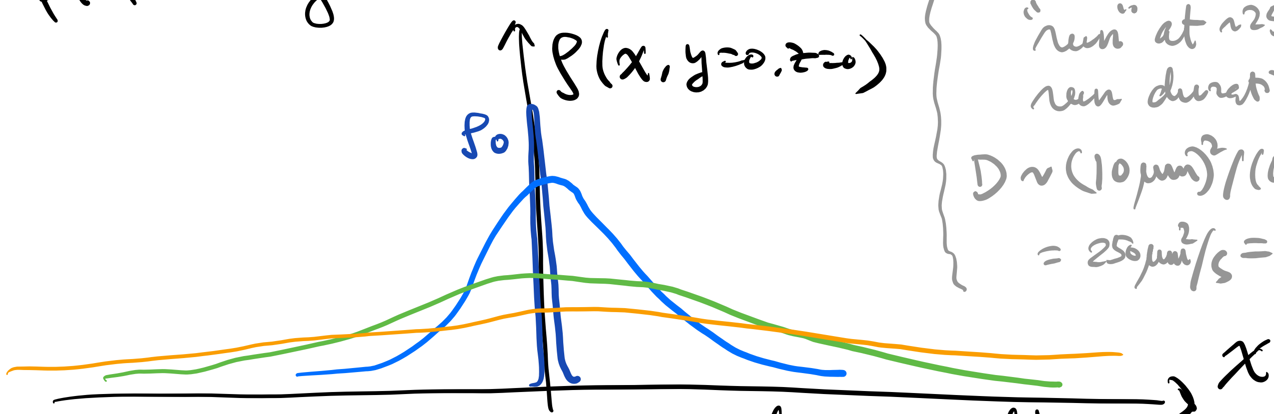
$$\frac{\partial \rho}{\partial t} = D\nabla^2\rho(\vec{r},t);$$ boundary condition: $\rho(\vec{r}\to\infty,t)=0$

initial condition: $\rho_0(\vec{r}) = N_0\,\delta^3(\vec{r})$

(i.e. N_0 individuals placed in a small volume at $\vec{r}=0$)

$$\rho(\vec{r},t) = \frac{N_0}{(4\pi Dt)^{3/2}}\, e^{-\frac{r^2}{4Dt}}$$ – spreading Gaussian

plot along x-axis



E. coli in liquid
"run" at ~25 μm/s
run duration ~ 0.4 s
$D \sim (10\,\mu m)^2/(0.4\text{ sec})$
$= 250\,\mu m^2/s = 0.9\,mm^2/hr$

⇒ the width of the density distribution expands

$$\langle x^2\rangle = \int d^3r\, x^2 \rho(\vec{r},t) = 2Dt; \quad \boxed{W \sim \sqrt{Dt}}$$

⇒ $\int d^3r\,\rho(\vec{r},t) = N_0$ <u>unchanged</u>

2. Range expansion for growing population

- logistic growth of well-mixed population

$$\frac{d\rho}{dt} = r\rho\cdot(1-\rho/\tilde{\rho})$$

- allow random spatial movement

Starting from localized initial spatial dist $\rho_0(\vec{r})$

- Study in 1d for illustration

$$\boxed{\frac{\partial\rho(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\rho + r\rho\cdot(1-\rho/\tilde{\rho})}$$

Fisher-Kolmogorov Equation (1937)

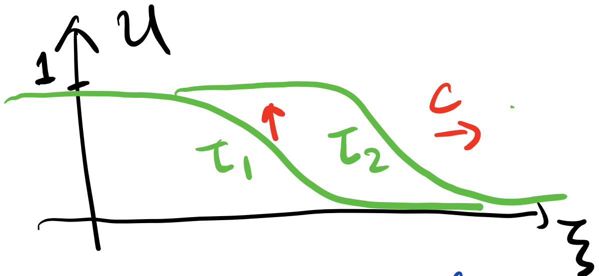
dimensionless form: $u = \rho/\tilde{\rho}$, $\tau = rt$, $\xi = \frac{x}{\sqrt{D/r}}$

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2}{\partial \xi^2}u + u(1-u)$$

E. coli: $D \simeq 1\,\mathrm{mm^2/h}$; $r \simeq 1/\mathrm{hr}$.
$\sqrt{D\cdot r} = 1\,\mathrm{mm/hr}$.

$$\frac{x}{\sqrt{D/r}} - crt = \frac{x - \overbrace{c\sqrt{D\cdot r}}^{v}\,t}{\sqrt{D/r}}$$

a) look for propagating sol'n:



$$u(\xi,\tau) = y(\underbrace{\xi - c\tau}_{z}); \quad v = c\sqrt{D\cdot r}$$

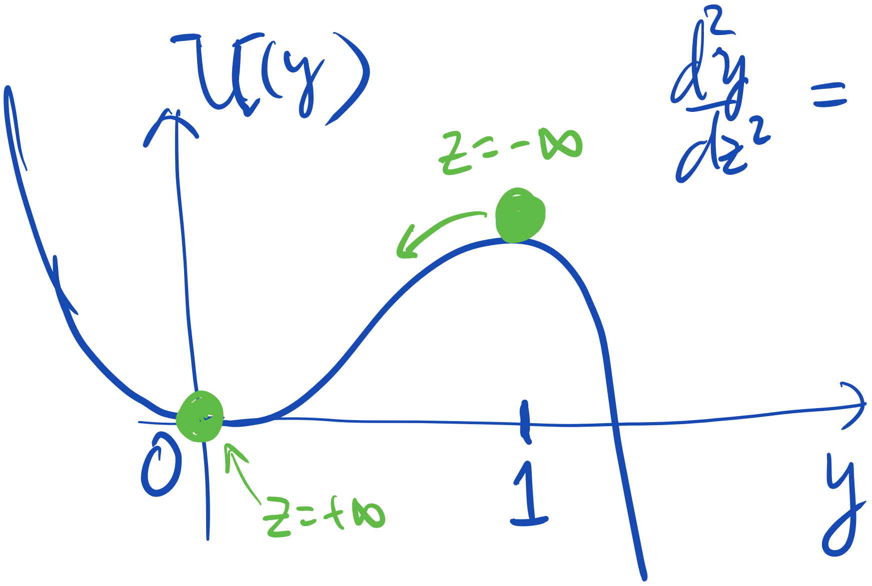
$$\frac{\partial u}{\partial \xi} = \frac{dy}{dz} \qquad \frac{\partial u}{\partial \tau} = -c\frac{dy}{dz}$$

$$\frac{d^2y}{dz^2} + c\frac{dy}{dz} + y\cdot(1-y) = 0 \qquad (3)$$

$\Rightarrow$ What is the propagating speed c or $v = c\cdot\sqrt{D\cdot r}$?

→ find c such that $y(z) > 0$ exist with $y(z \to -\infty) = 1$, $y(z \to \infty) = 0$.

- Can visualize ③ as Newton's eqn of motion for a "particle" at "position" y at "time" z



friction coeff

"velocity"

$$\frac{d^2y}{dz^2} = \underbrace{-c\frac{dy}{dz}}_{\text{friction}} \underbrace{- y(1-y)}_{F(y) = -\frac{dU}{dy}}$$

$$U(y) = \frac{y^2}{2} - \frac{y^3}{3}$$

- expect two types of motion:
  - if "friction" (c) is small, get "damped oscillation" around $y=0$ (unphysical since y cannot be -ve)
  - if friction (c) suff large (over damped) then expect $y(z) > 0$

⇒ a range of allowed c?

• quantify the above conditions by doing linear stability analysis around $y=0$ (front)

for $y \ll 1$. $\dfrac{d^2y}{dz^2} = -c\dfrac{dy}{dz} - y$.

let $y = y_0 e^{-\lambda z}$, $\lambda^2 - c\lambda + 1 = 0$

$$\lambda_\pm = \frac{c \pm \sqrt{c^2-4}}{2} \rightarrow \begin{cases} \frac{c}{2} \pm i\sqrt{1-\left(\frac{c}{2}\right)^2} & c<2 \\ >0 & c \geq 2 \end{cases}$$

→ damped osc if $c<2$; Stable if $c \geq 2$

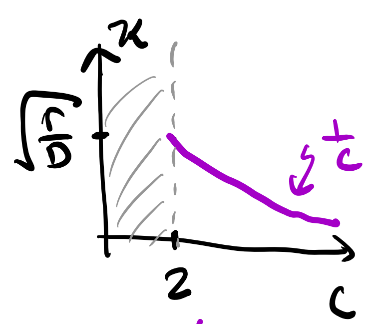
⇒ propagating sol'n exist for $c \geq 2$

$c \geq 2$, $y \sim A e^{-\lambda_+ z} + B e^{-\lambda_- z} \overset{\text{large } z}{\simeq} B e^{-\lambda_- z}$ (since $\lambda_- < \lambda_+$)

$$u(\xi, \tau) = y(\xi - c\tau) \propto e^{-\lambda_-(\xi - c\tau)}$$

$$= e^{-\lambda_- \frac{x - c\sqrt{D\cdot r}\,t}{\sqrt{D/r}}} = e^{-\kappa(x - vt)}$$

allowed speed: $\boxed{v = c\sqrt{Dr} \geq 2\sqrt{D\cdot r}}$



Steepness of front:

$$\boxed{\kappa = \frac{\lambda_-}{\sqrt{D/r}} = \sqrt{\frac{r}{D}}\cdot\left(\frac{c}{2} - \sqrt{\left(\frac{c}{2}\right)^2 - 1}\right) \leq \sqrt{\frac{r}{D}}}$$

⇒ broader front for faster prop.

for $c \gg 2$, $\frac{c}{2} - \sqrt{\left(\frac{c}{2}\right)^2 - 1} = \frac{c}{2}\left(1 - \sqrt{1 - \left(\frac{2}{c}\right)^2}\right) \simeq \frac{1}{c}$ ⇒ $\kappa \propto \frac{1}{c}$.

b) selection of propagating speed

in general, propagating speed c can depend on the initial profile $u(\xi, \tau=0)$

- examine the sol'n at the front
  (u^2 term can be neglected at front)

$$\frac{\partial u}{\partial \tau} = u + \frac{\partial^2}{\partial \xi^2} u$$

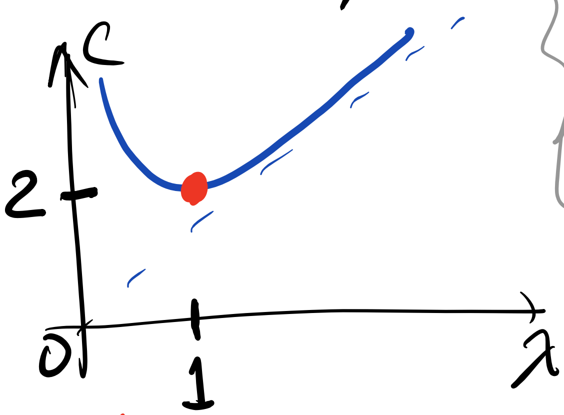
suppose init cond is $u(\xi, 0) \overset{\xi \to \infty}{\sim} u_0 e^{-\lambda \xi}$

for $\tau > 0$, look for traveling sol'n

$$u(\xi, \tau) = u_0 e^{-\lambda(\xi - c\tau)}$$

then $\lambda c = 1 + \lambda^2$

$$\Rightarrow \quad c = \lambda + \frac{1}{\lambda}$$

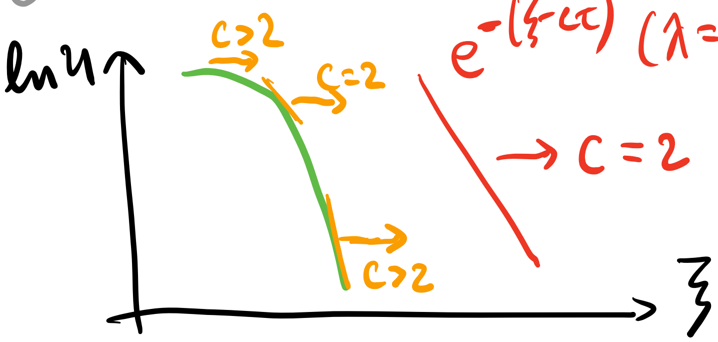


- $\frac{dc}{d\lambda} = 1 - \frac{1}{\lambda^2}$
- $\frac{d^2c}{d\lambda^2} = \frac{2}{\lambda^3} > 0$
  $\to$ at most one min
- $\frac{dc}{d\lambda} = 0 \to \lambda^* = 1$.
  $\to c(\lambda^*) = 2$

$\to$ speed depends on steepness of init profile (λ)

• Stability of propagating front w/ different slope λ

[heuristics given below; formal sol'n via stability analysis]

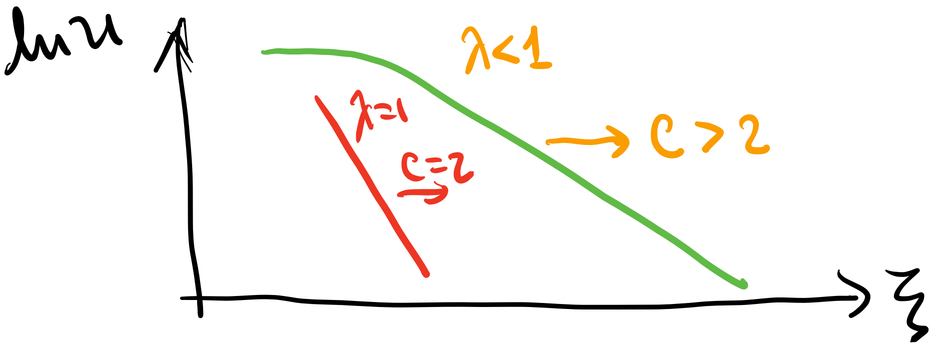


Sharply declining init cond

$\to$ $c = c_{min} = 2$

"marginal stability"

the above does not apply to broader init cond.



Thus for any init cond $u(\xi,0)$

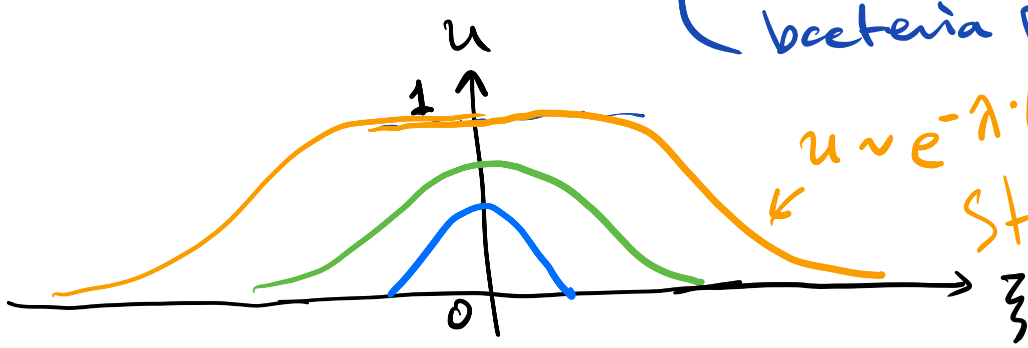
such that $u(\xi,0)=0$ for $\xi>\xi_0$

(i.e. init pop confined to a certain region $\xi<\xi_0$)

then eventually the speed of the front

approaches $c = c_{min} = 2$ or $v^* = 2\sqrt{D\cdot r}$.

(validation for motile bacteria population, Cremer 2019)



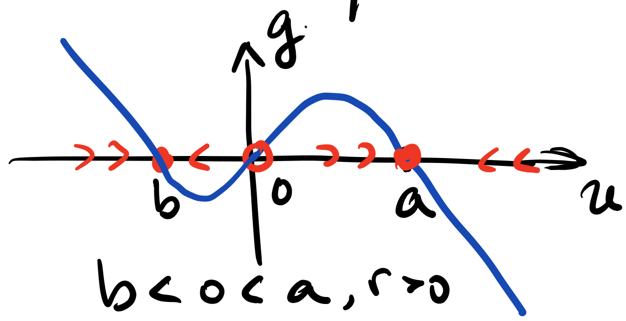
$u \sim e^{-\lambda\cdot(\xi-2\tau)}$; $\lambda(c=2)=1$

Steepness $\kappa = \lambda\sqrt{\frac{r}{D}} = \sqrt{\frac{r}{D}}$

3. Trigger wave:

u = "order parameter" of a "bistable system"

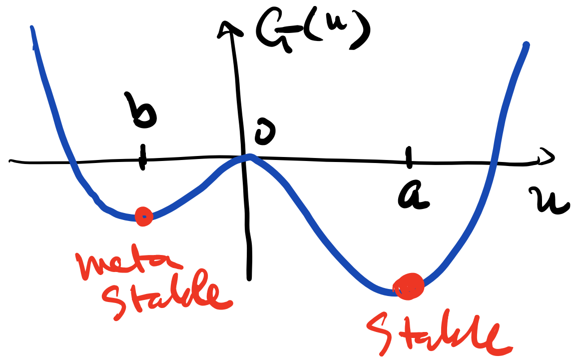
$$\frac{du}{dt} = \underbrace{r\,u\,(a-u)\cdot(u-b)}_{g(u) = -\frac{\partial G}{\partial u}}$$



$b < 0 < a,\ r > 0$

e.g. magnetization (ferromagnet)

mitotic wave, chromosome mod, ...

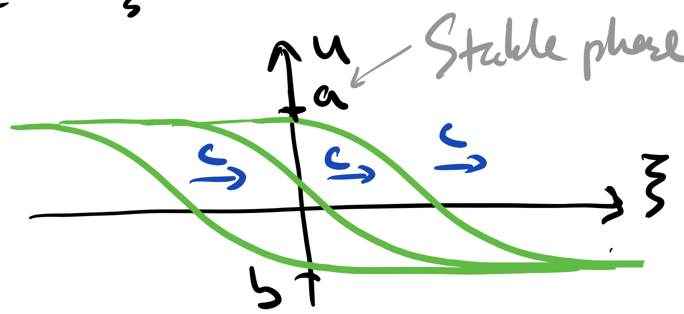


Spatially coupled dynamics:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + r\,u\,(a-u)(u-b)$$

$$\tau = rt;\ \xi = \sqrt{\frac{r}{D}}\,x \rightarrow \frac{\partial u}{\partial \tau} = \frac{\partial^2}{\partial \xi^2}u + u(a-u)(u-b)$$

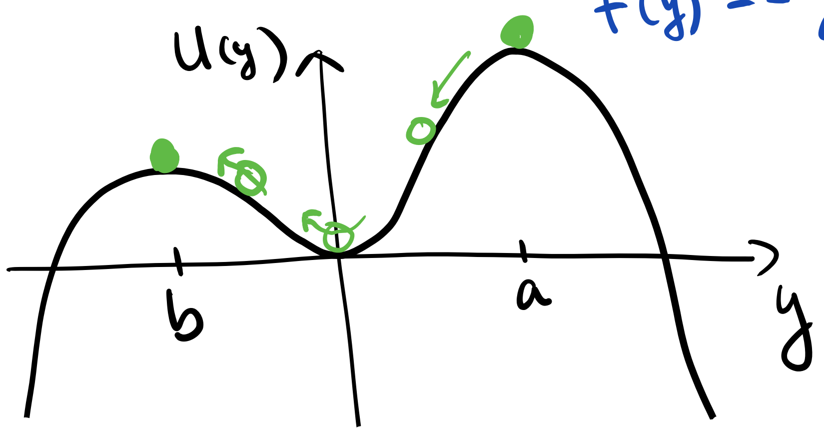
Propagation from stable to metastable phase ("trigger wave")



$$u(\xi,\tau) = y(\underbrace{\xi - c\tau}_{z})$$

$$\Rightarrow \frac{d^2y}{dz^2} = -c\frac{dy}{dz}\ \underbrace{-\,y(a-y)(y-b)}_{f(y) = -\frac{dU}{dy}} \quad (4)$$

Note: $f = -g$. fictitious dynamics always from stable to metastable phase



Mechanical analogy: a ball rolling down from a, move pass origin, and stop exactly at b.

$\Rightarrow$ "dissipation energy", proportional to c,
must be exactly equal to $\Delta U \equiv U(a) - U(b)$
(unique criterion for prop. speed c)

$\rightarrow$ multiply Eq ④ by $\frac{dy}{dz}$ and integrate over z:

$$\frac{d^2y}{dz^2}\frac{dy}{dz} = -c\left(\frac{dy}{dz}\right)^2 - \frac{dU}{dy}\cdot\frac{dy}{dz}$$

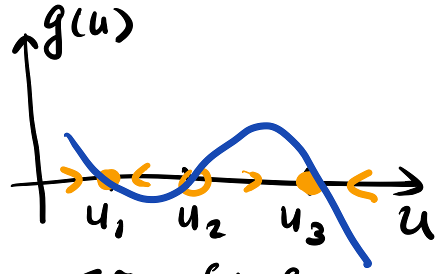
$$\underbrace{\int_{-\infty}^{\infty} dz \frac{d}{dz}\left(\frac{dy}{dz}\right)^2}_{=(y')^2\big|_{-\infty}^{\infty} = 0} = -c\int_{-\infty}^{\infty} dz \left(\frac{dy}{dz}\right)^2 - \int_{-\infty}^{\infty} dz \frac{dU}{dz}$$

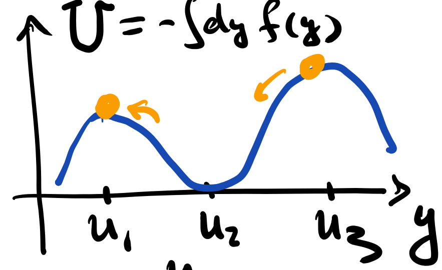
$$c\cdot\int_{-\infty}^{\infty} dz\left(\frac{dy}{dz}\right)^2 = U(-\infty) - U(\infty) = U(a) - U(b).$$

$\Rightarrow$ $c \propto U(a) - U(b)$,
Thermodynamic potential $(U(a) - U(b) = -\Delta G)$
is the driving force for propagation

Analysis of trigger wave dynamics:

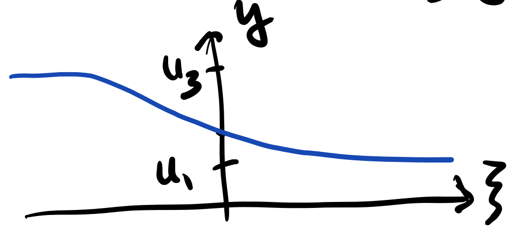
$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial \xi^2} u + \underbrace{(u-u_1)\cdot(u_2-u)(u-u_3)}_{g(u):\ u_1 < u_2 < u_3}$$





let $u(\xi,\tau) = y(\xi - c\tau)$

$$L[u] = \frac{d^2y}{dz^2} + c\frac{dy}{dz} + \underbrace{(y-u_1)\cdot(u_2-y)(y-u_3)}_{g(y) = -f(y) = \frac{dU}{dy}} = 0$$



Soln: try $\frac{dy}{dz} = \underbrace{\alpha(y-u_1)\cdot(y-u_3)}_{h(y)}$.

$$\frac{d^2y}{dz^2} = \frac{d}{dz}h(y(z)) = \frac{dy}{dz}\cdot\frac{dh}{dy}$$

$$= \frac{dy}{dz}\cdot\alpha\cdot(y-u_1+y-u_3)$$

$$= \alpha^2(y-u_1)(y-u_3)\cdot(2y-u_1-u_3)$$

$$\rightarrow L(u) = (y-u_1)\cdot(y-u_3)\cdot\left[\alpha^2(2y-u_1-u_3) + c\alpha + (u_2-y)\right]$$

$$\rightarrow [\ \ ] = 0 \rightarrow 2\alpha^2 = 1; \quad \alpha = \pm\frac{1}{\sqrt{2}}$$

$$\alpha^2(u_1+u_3) = c\alpha + u_2$$

$$\rightarrow c = \frac{1}{2\alpha}(u_1+u_3-2u_2)$$

y(z) from direct integration: $\frac{dy}{dz} = \alpha(y-u_1)(y-u_3)$.

$$\rightarrow y(z) = \frac{u_3 + u_1 e^{\alpha(u_3-u_1)(z-z_0)}}{1+e^{\alpha(u_3-u_1)(z-z_0)}}$$

z_0 is arbitrary shift of z-axis

$$= \frac{u_1+u_3}{2} + \frac{u_1-u_3}{2}\tanh\left[\frac{\alpha}{2}(u_3-u_1)(z-z_0)\right]$$

boundary condition: $y(z \to -\infty) = u_3$, $y(z \to +\infty) = u_1$ $\Big\}$ $\alpha > 0$.

$$\rightarrow \quad \boxed{c = \frac{1}{\sqrt{2}}(u_1 + u_3 - 2u_2)}$$

$\Rightarrow$ propagation to the right if $\frac{u_1 + u_3}{2} > u_2$

left if $< u_2$

direction of propagation:

$$U(u_3) - U(u_1) = -\int_{u_1}^{u_3} dy\, f(y) = \int_{u_1}^{u_3} dy\, (y-u_1)(u_2-y)(y-u_3)$$

$$= -\frac{1}{12}(u_3-u_1)^2 \left[(u_2-u_1)^2 - (u_3-u_2)^2\right]$$

$$= \frac{1}{12}\underbrace{(u_3-u_1)^3}_{>0 \text{ for } u_3 > u_1}(u_1 + u_3 - 2u_2)$$

$$c = \frac{6\sqrt{2}}{(u_3-u_1)^3}\left[U(u_3) - U(u_1)\right]$$

propagation from stable to metastable state

$\Rightarrow$ Why does the system know about metastability even though the dynamics is deterministic?

existence of Lyapunov function

$$\mathcal{L}[u] = \int dx \left[\frac{1}{2} D \left(\frac{\partial u}{\partial x}\right)^2 - U(u)\right]$$

$$\frac{\partial u}{\partial t} = -\frac{\delta}{\delta u(x,t)}\mathcal{L}[u]$$

can show $\frac{d}{dt}\mathcal{L} < 0$ except when u solves PDE.