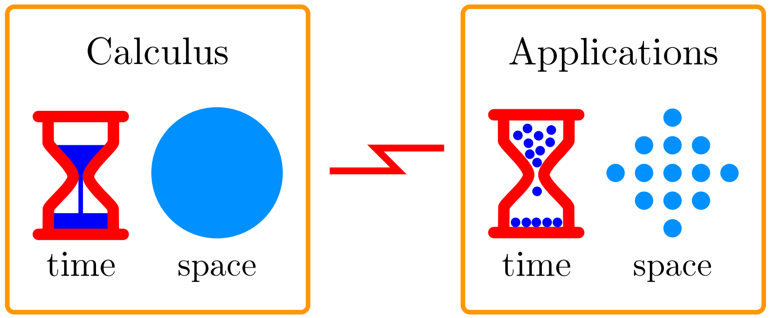
Discretization Schemes vs Travelling Waves for Reaction-Diffusion Systems



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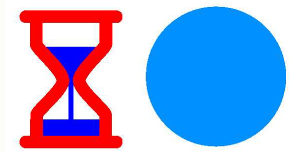
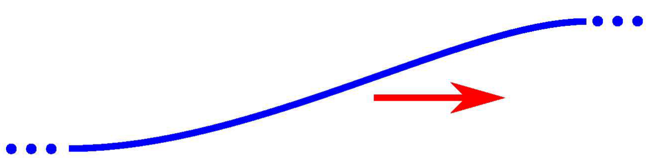
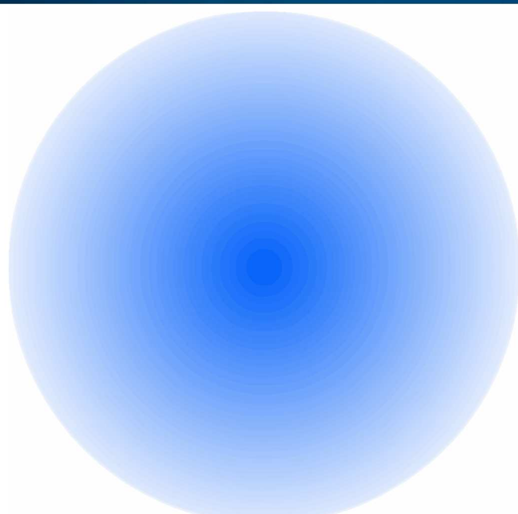
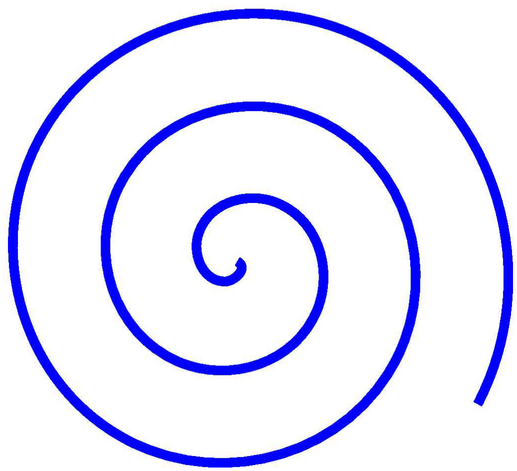
Patterns

PDE $\quad u_t = F(u, \nabla u, \Delta u)$



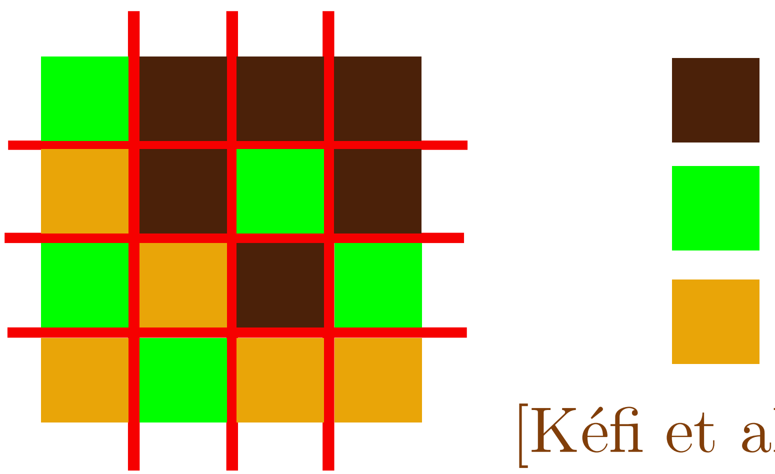






Desertification

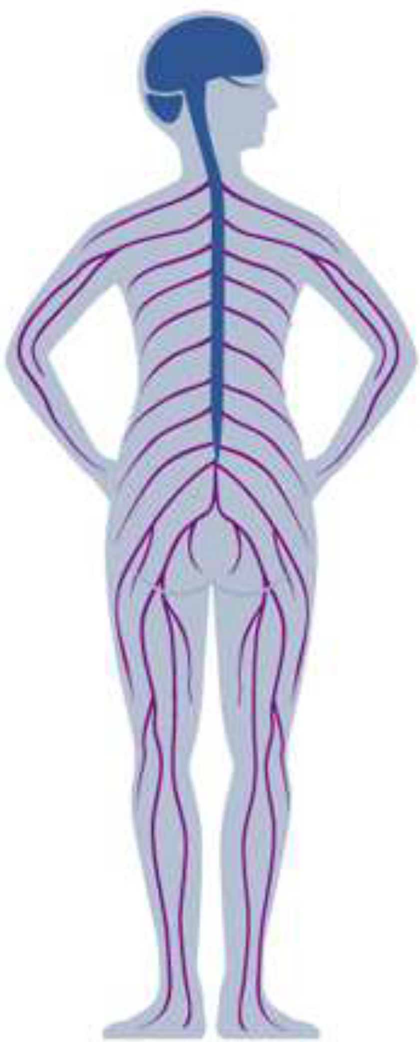
vegetation patch size
$\sim$
power law

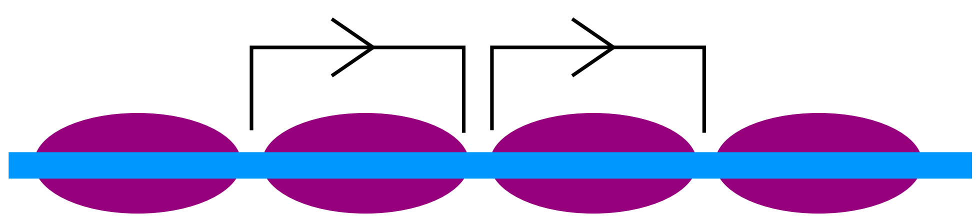


Fertile
Vegetation
Desert

[Kéfi et al; Nature (2007)]

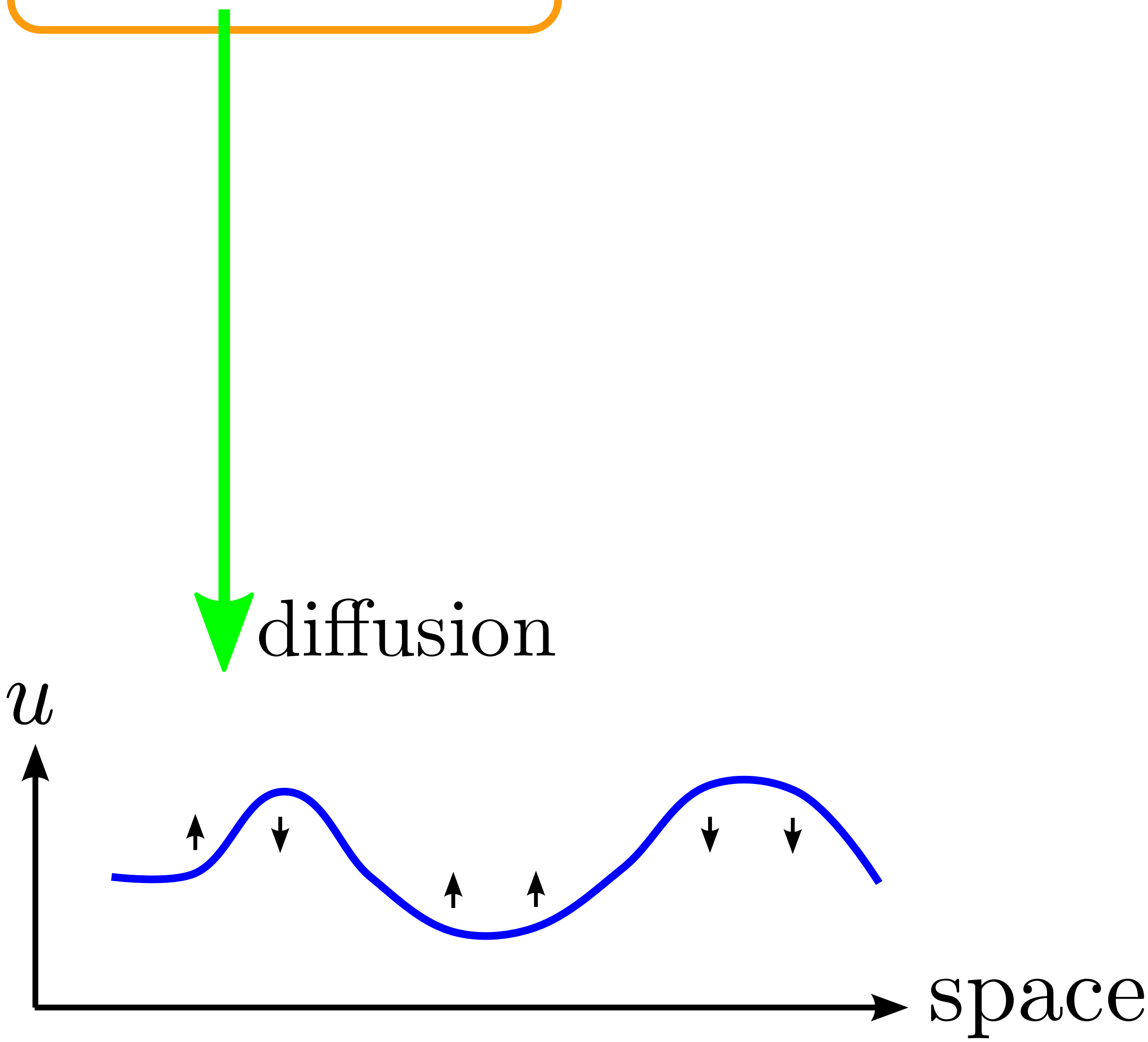
Nerve Conduction





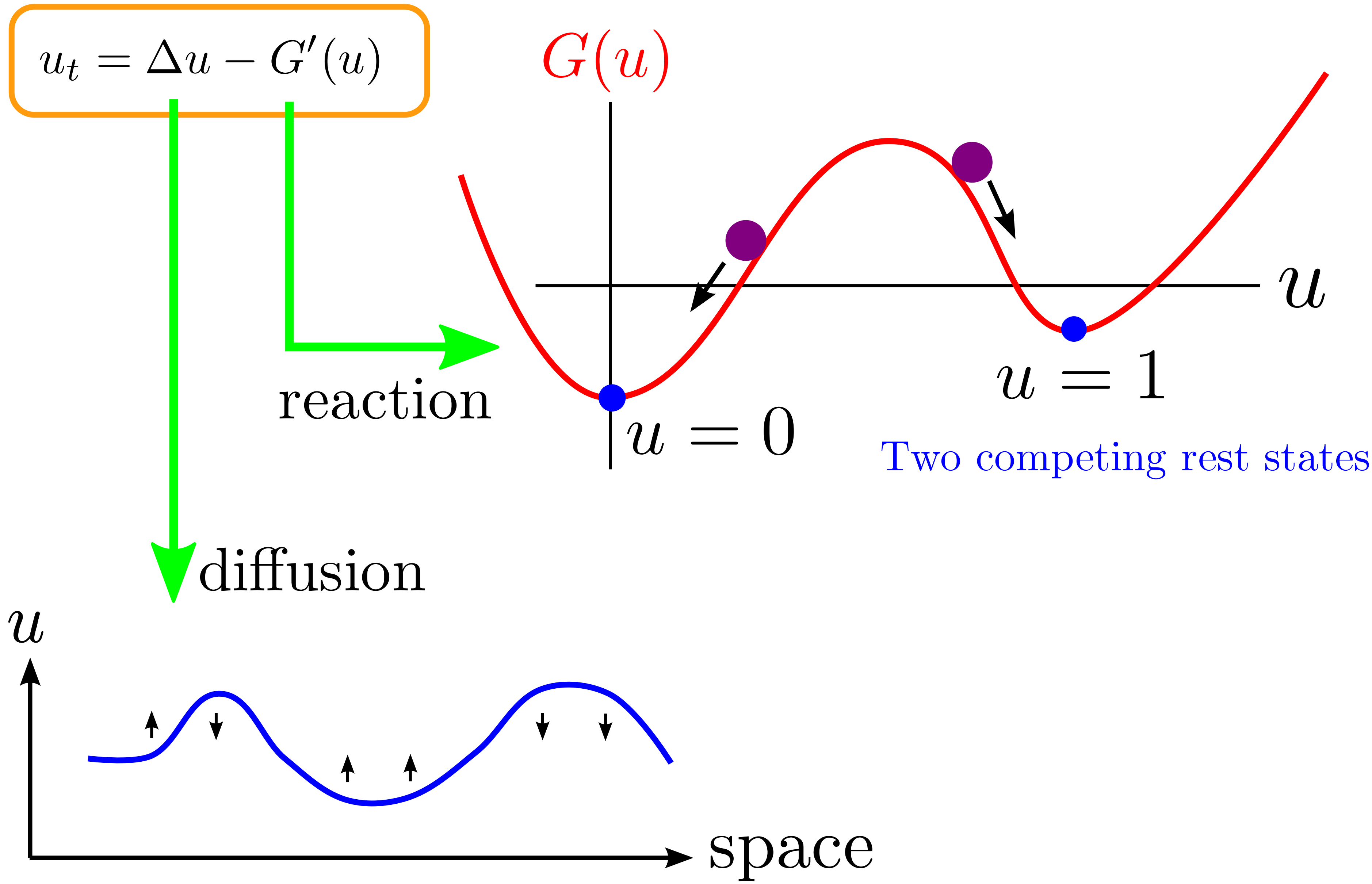
Reaction-diffusion PDE

$$u_t = \Delta u - G'(u)$$



Reaction-diffusion PDE

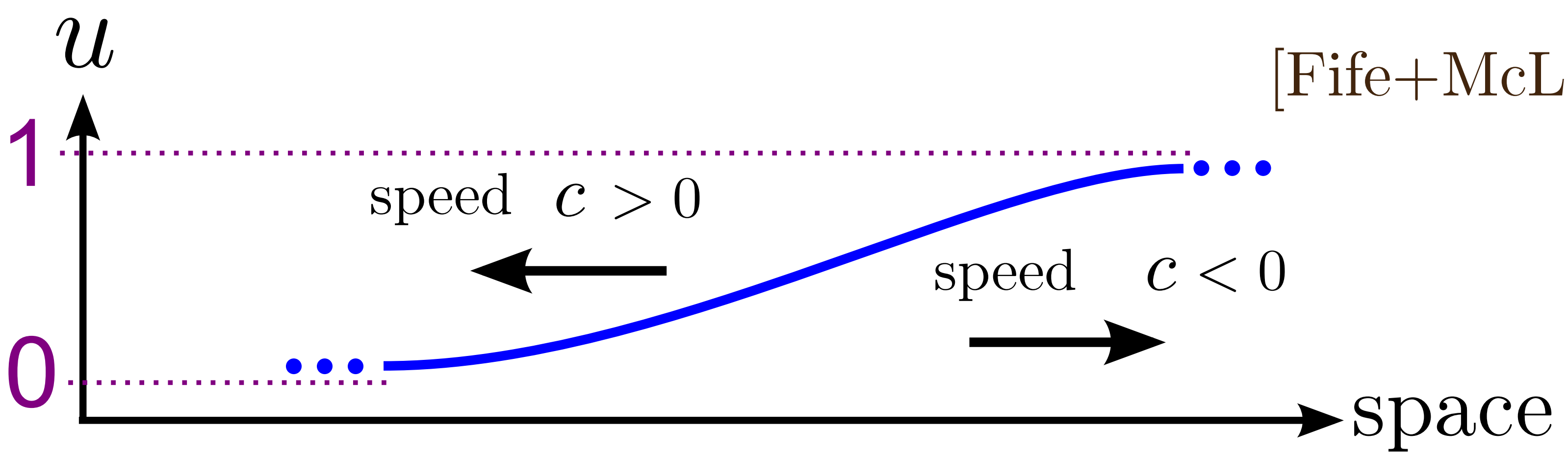
$$u_t = \Delta u - G'(u)$$



Reaction-diffusion PDE

$$u_t = \Delta u - G'(u)$$ PDE

Structure: Invasion wave $u(t,x) = \Phi(x+ct)$

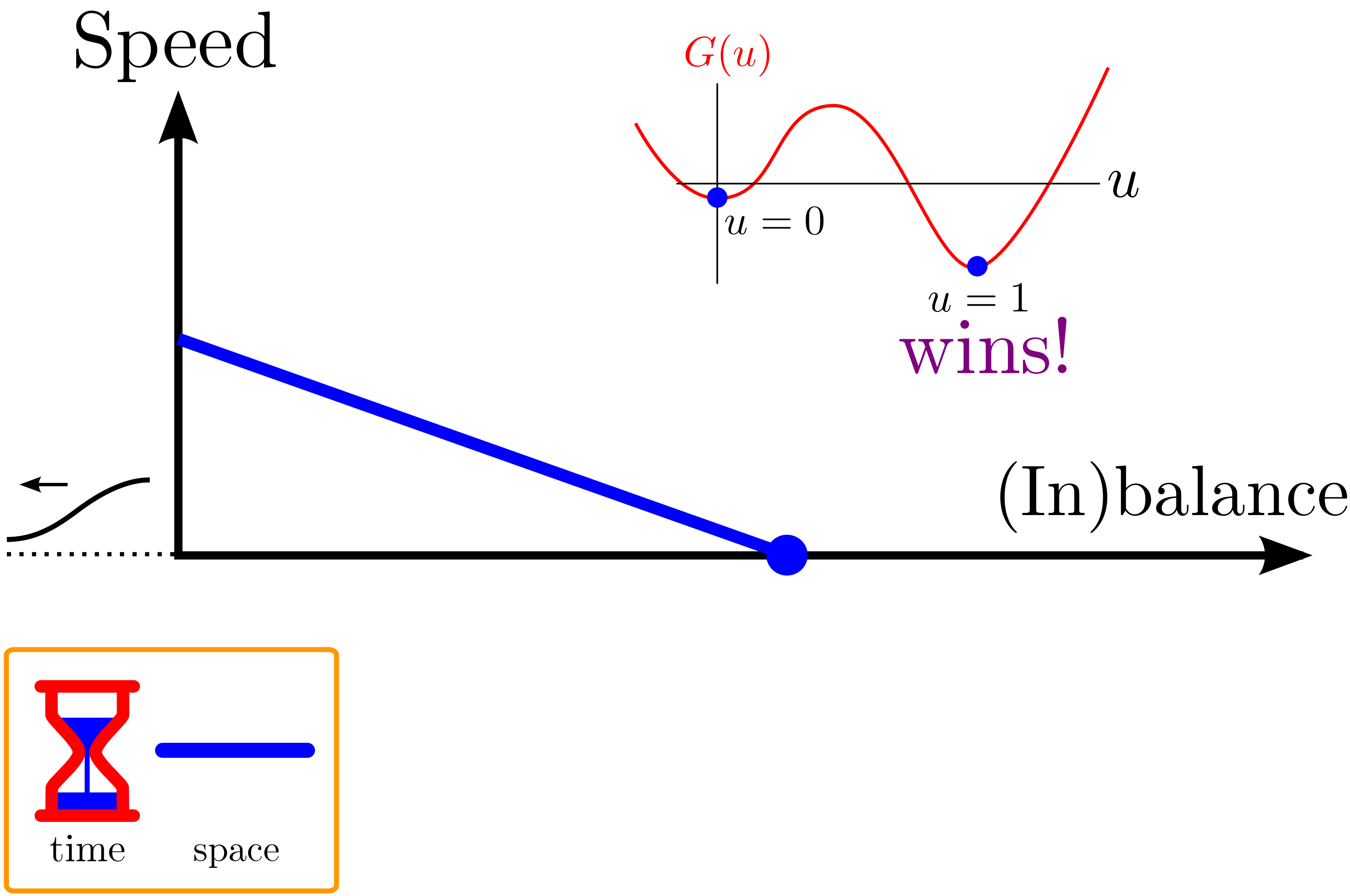


[Fife+McLeod; 1970s]

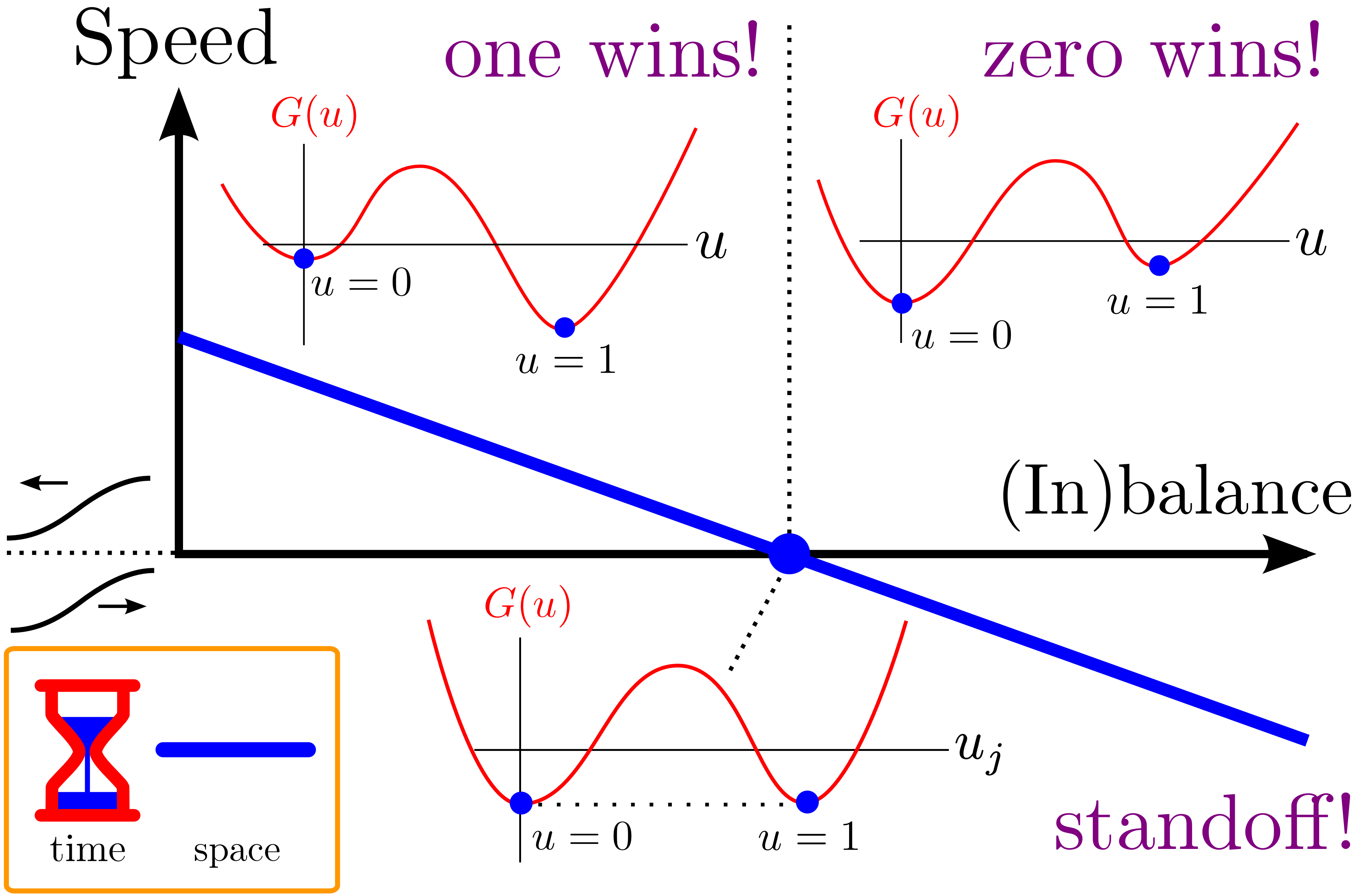
Fixed spatial profile Φ

$$c\Phi'(\xi) = \Phi''(\xi) - G'\big(\Phi(\xi)\big)$$ ODE

Reaction-diffusion - continuous space

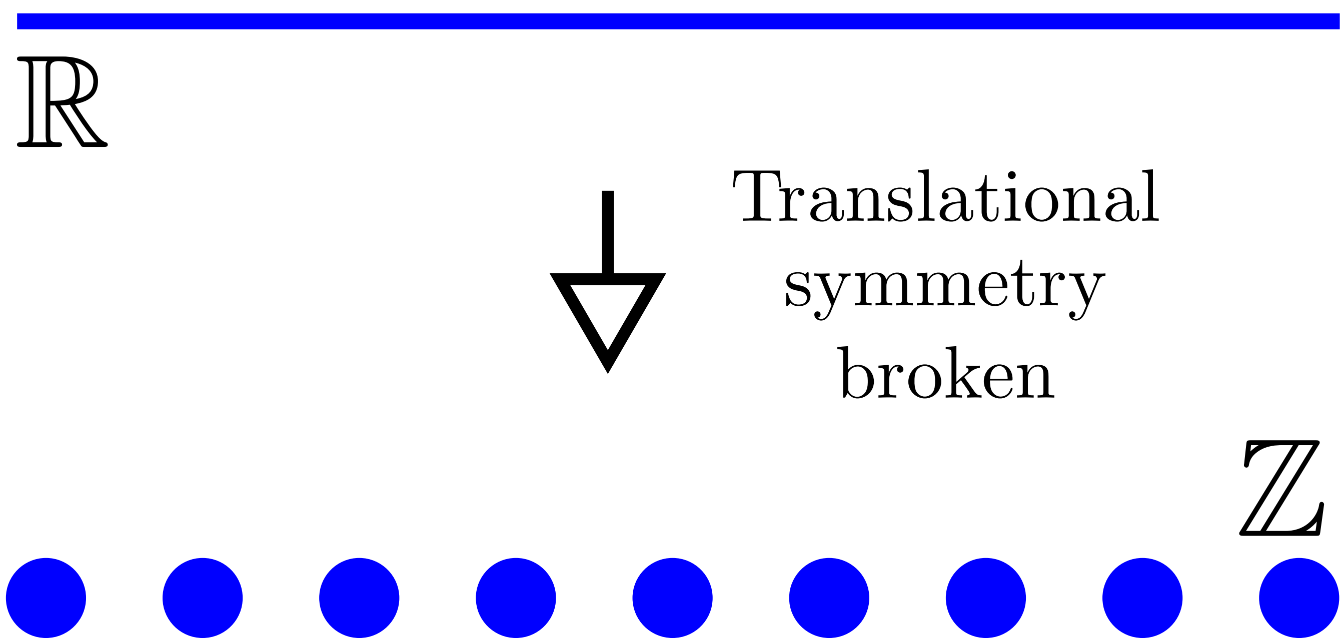


Reaction-diffusion - continuous space



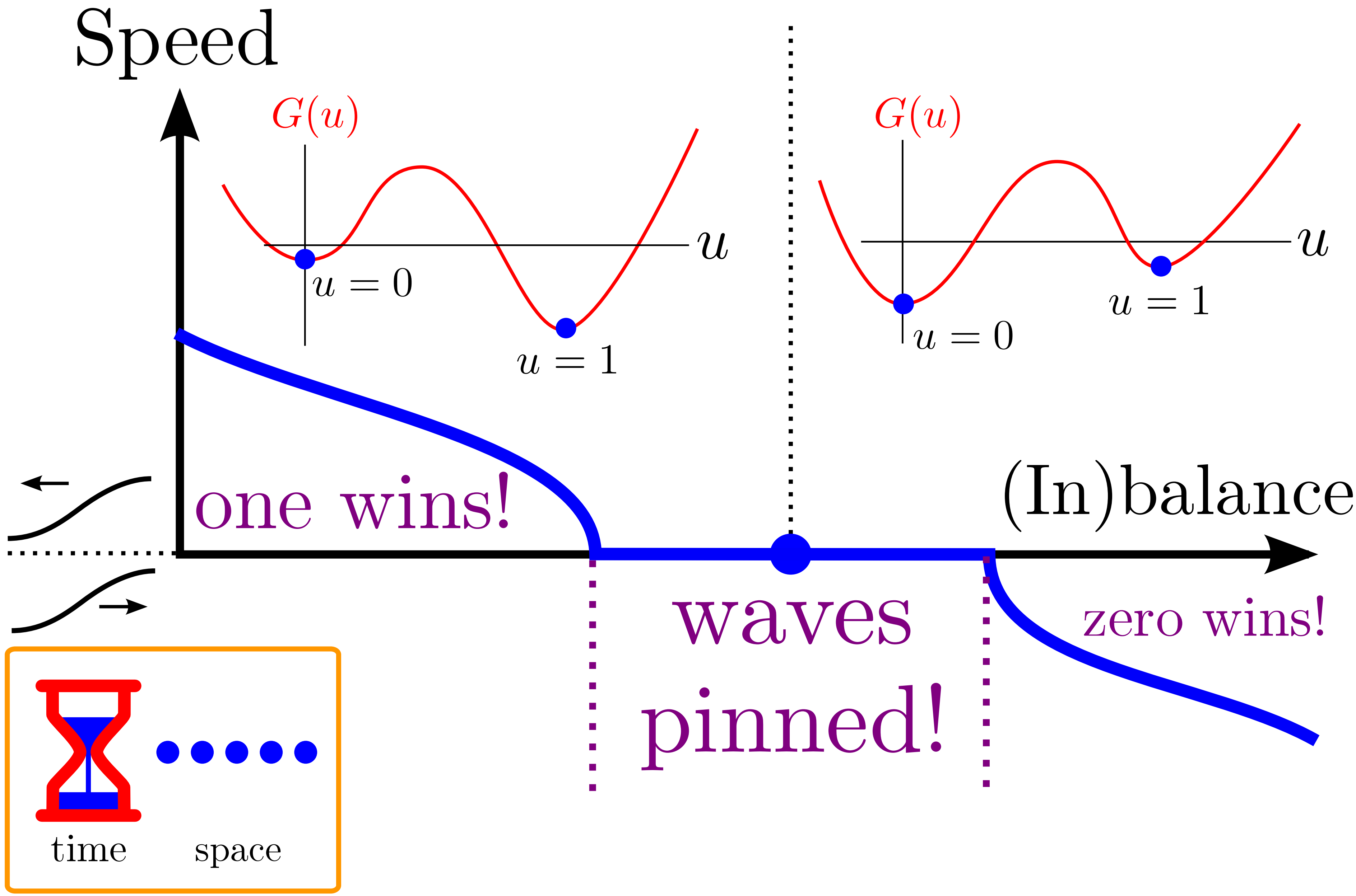
Continuous vs Discrete Space

$$c\Phi'(\xi) = \Phi''(\xi) - G'\big(\Phi(\xi)\big)$$ ODE



$$c\Phi'(\xi) = \Phi(\xi+1) + \Phi(\xi-1) - 2\Phi(\xi) - G'\big(\Phi(\xi)\big)$$ MFDE

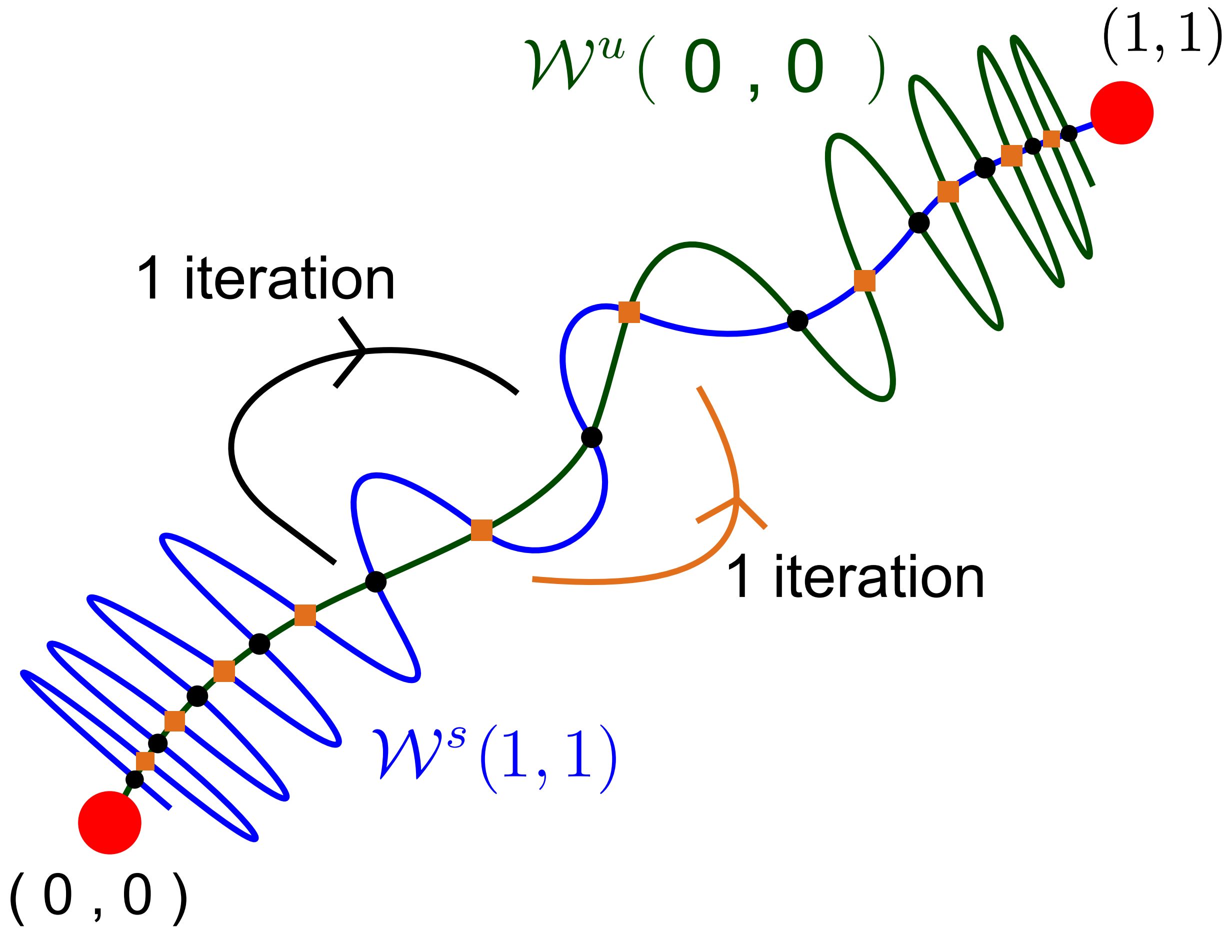
Reaction-diffusion - discrete space



Propagation Failure

At $c = 0$, planar recurrence relation for pair $\Big(\Phi(j), \Phi(j+1)\Big)$.

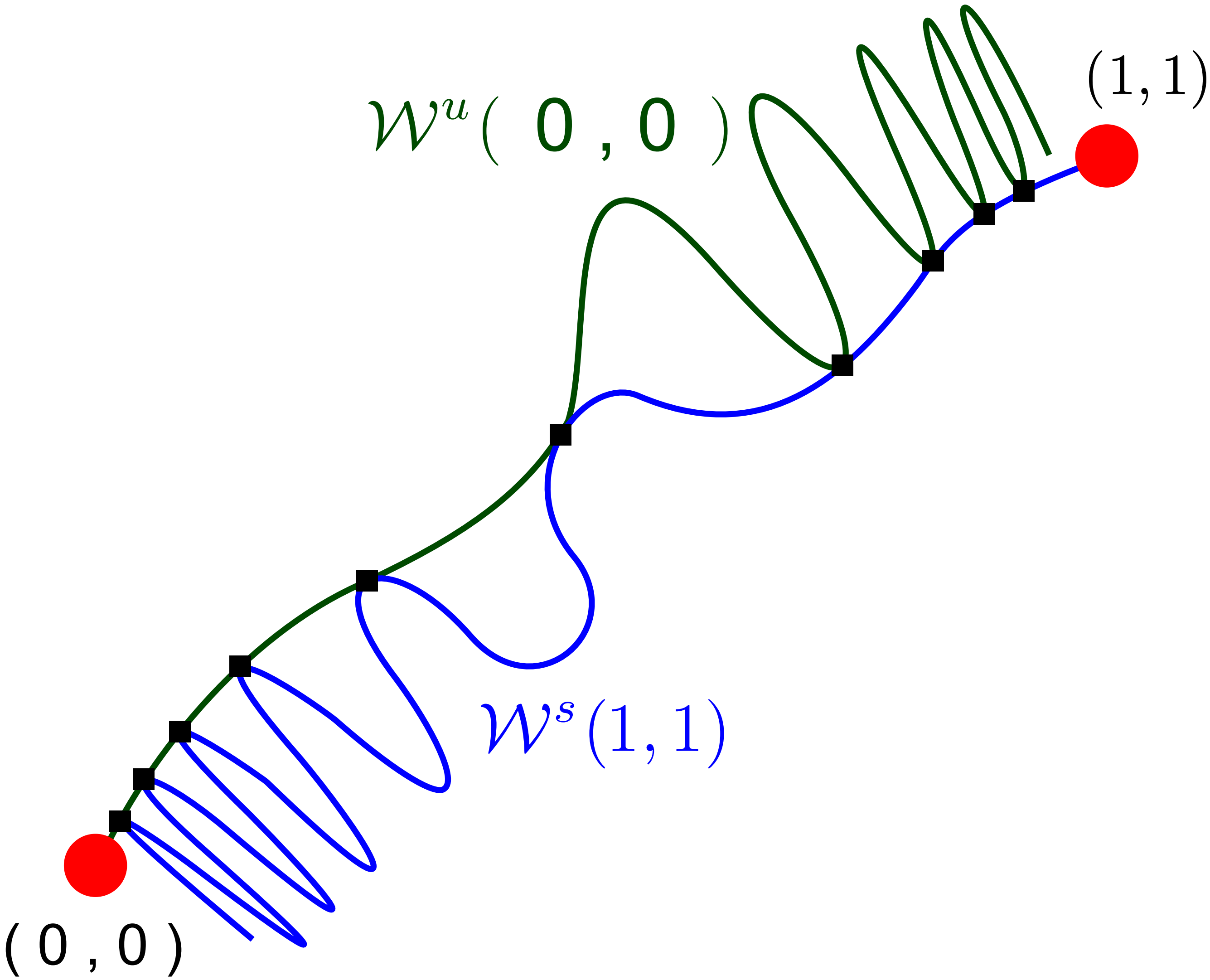
Typical at balance:



Heteroclinic for recursion relation ↔ standing wave for LDE.

Propagation Failure

Edge of pinning region:

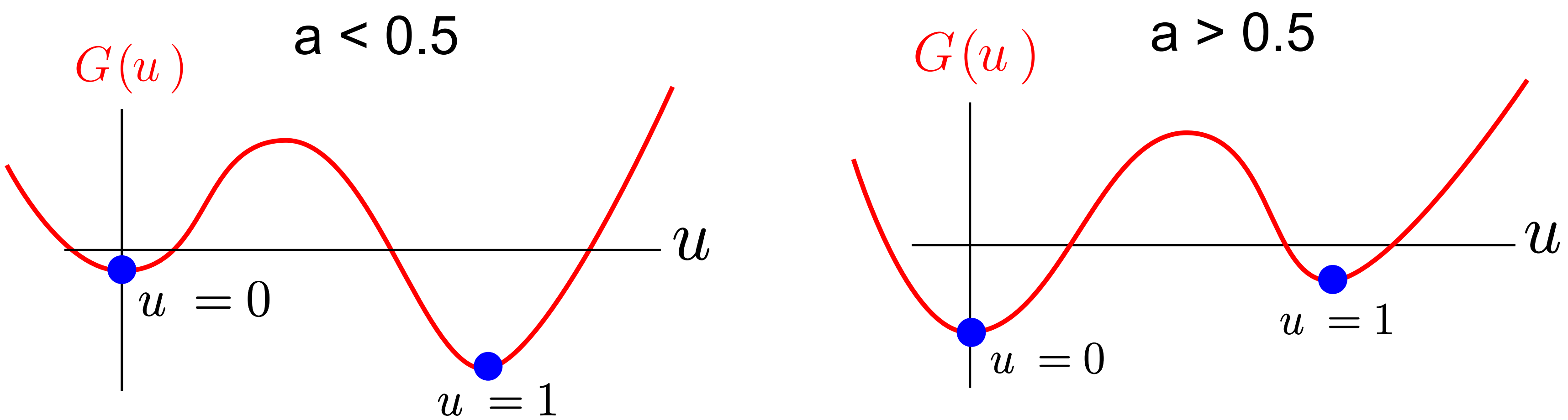


[Keener, Hoffman, Mallet-Paret, Van Vleck, Elmer, Scheel, ...]

Nonlinearity

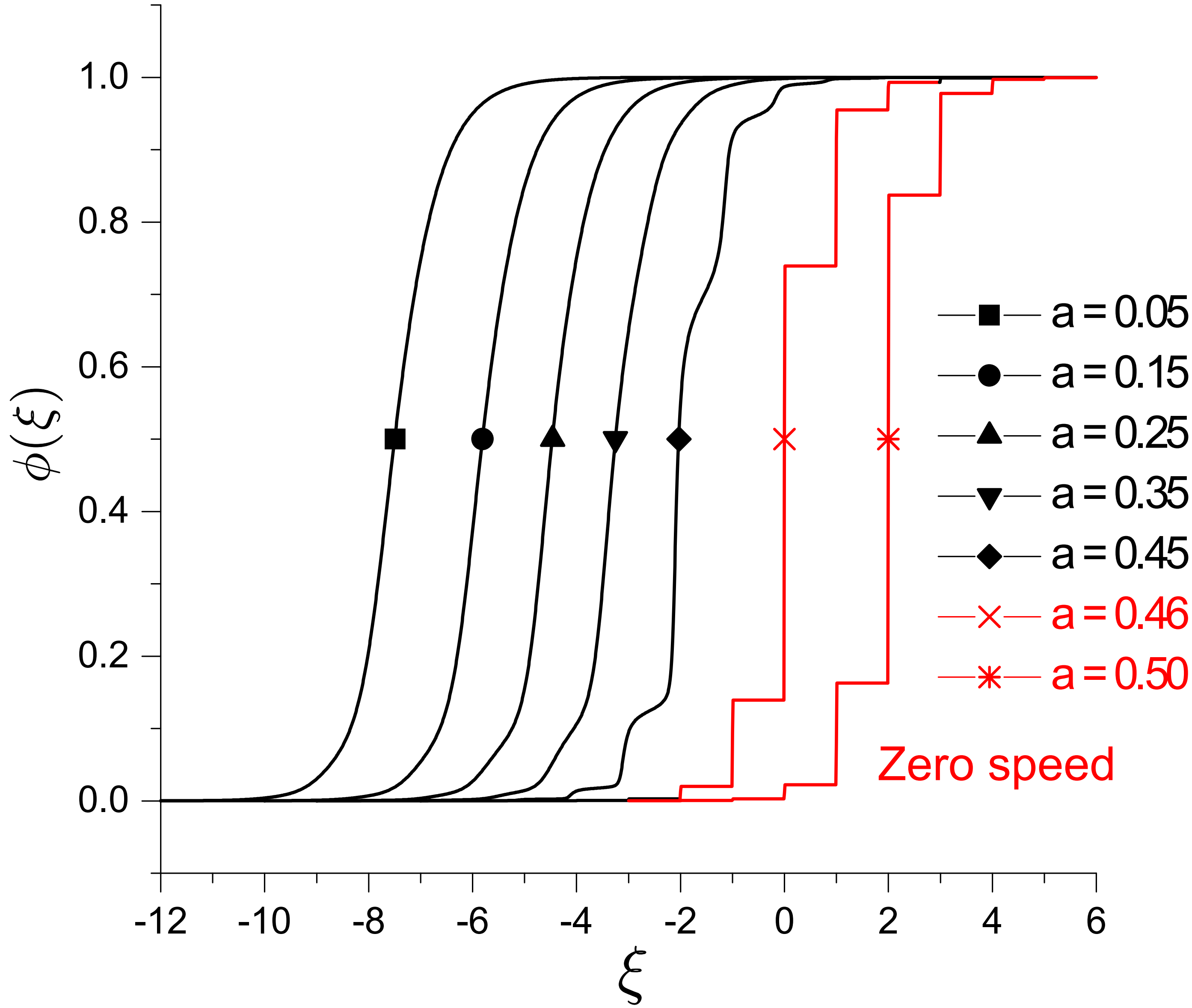
For concreteness, will use quartic potential; i.e.

$$-G'(u) = -G'(u; a) = g_{\mathrm{cub}}(u; a) = u(1-u)(u-a)$$



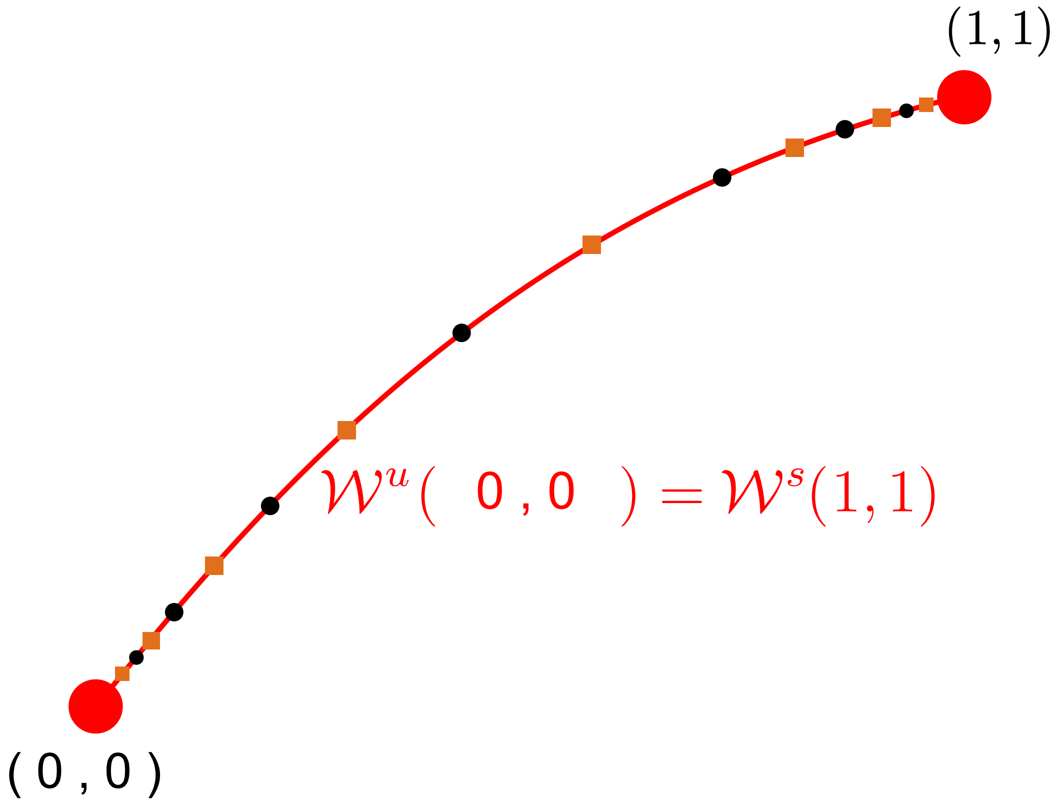
Discrete Nagumo LDE - Propagation failure

Wave profiles:



Propagation Failure - Discrete map

Special multi-site discretizations:

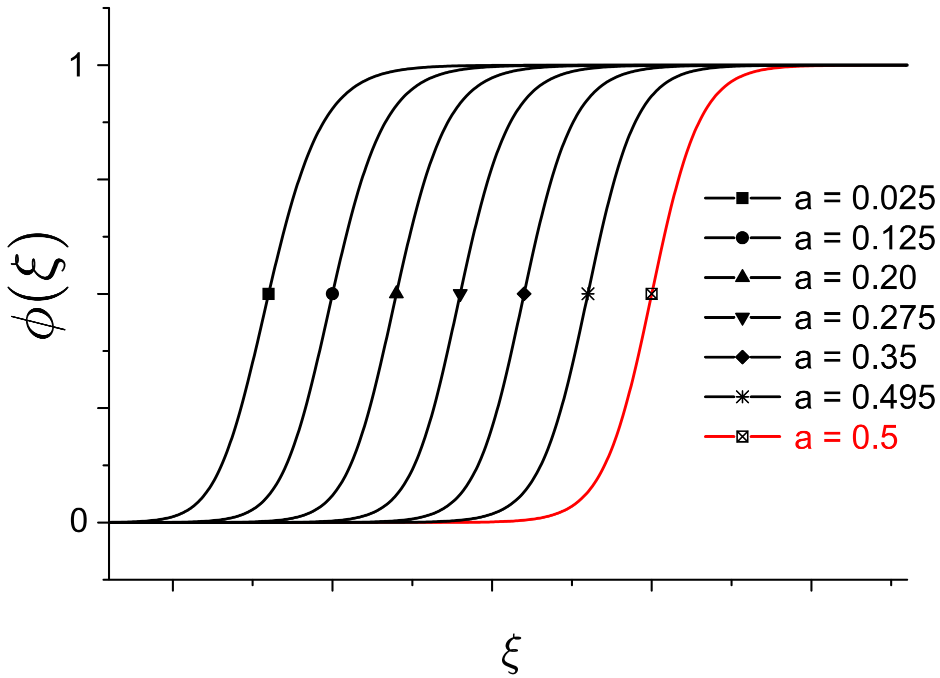


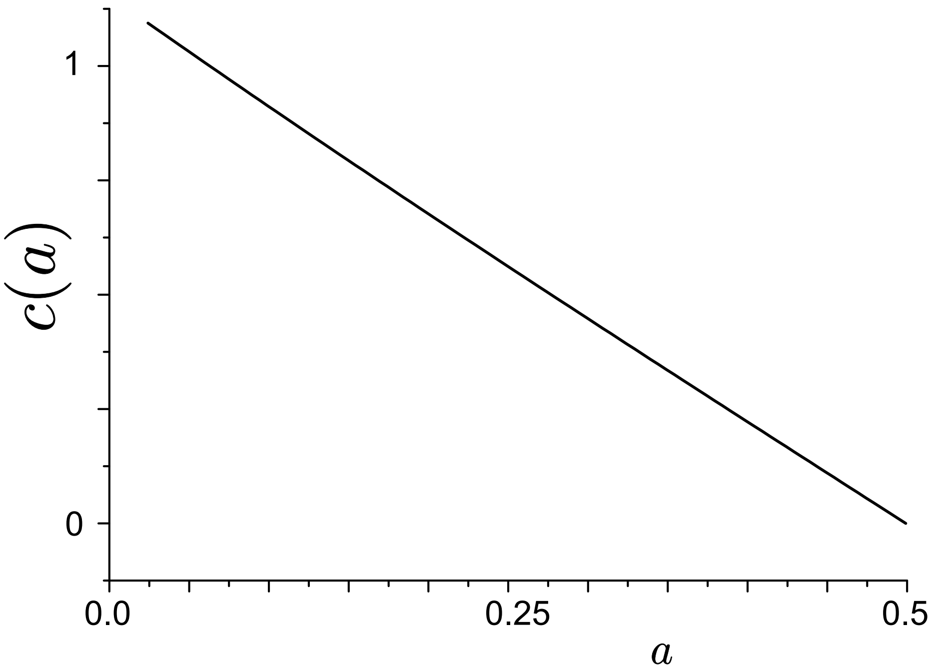
Continuous family of standing waves instead of just two flavours.

Propagation Failure

Thm. [H., Sandstede, Pelinovsky] No pinning for LDE

$$\frac{d}{dt}u_j = u_{j-1} + u_{j+1} - 2u_j + (u_j - a)\Big(u_{j-1}(1 - u_{j+1}) + u_{j+1}(1 - u_{j-1})\Big)$$

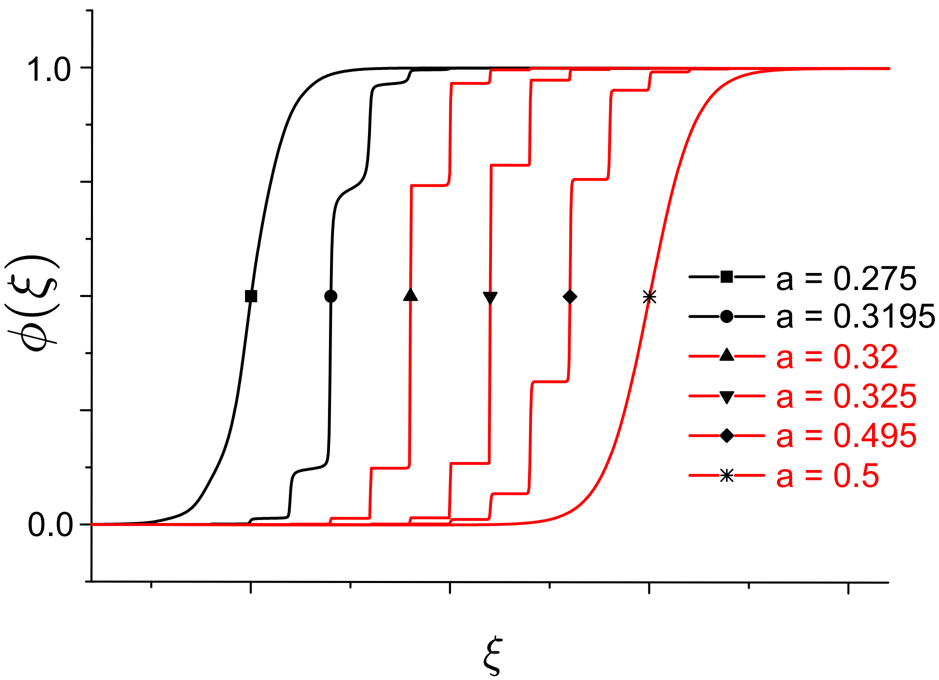


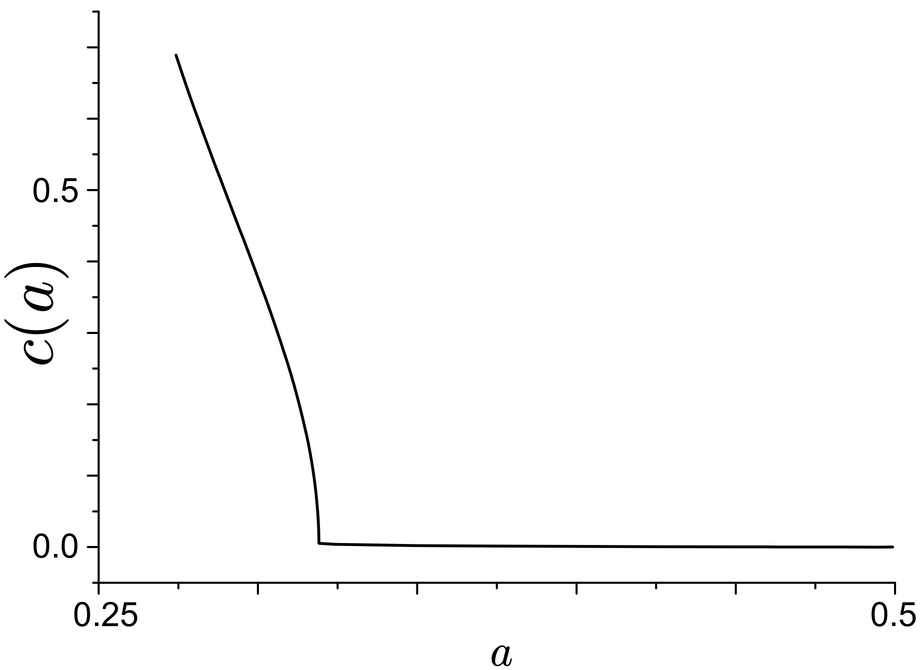


Propagation Failure

Thm. [H., Sandstede, Pelinovsky] Do have pinning for LDE

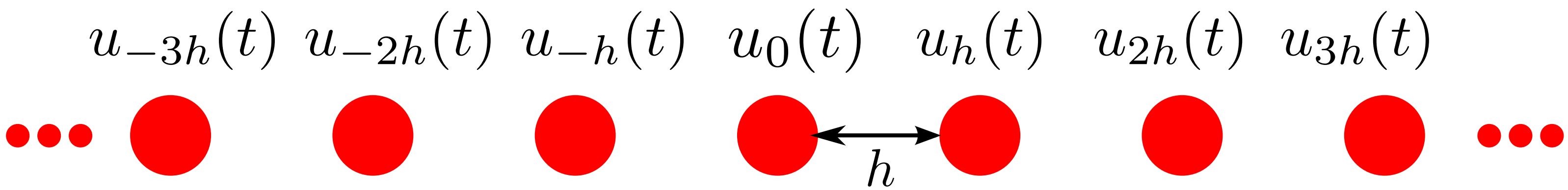
$$\frac{d}{dt}u_j = u_{j-1} + u_{j+1} - 2u_j + 4u_j(1-u_j)(u_{j-1} + u_{j+1} - 2a) \\ -5(a - \tfrac{1}{2})\sin(2\pi u_j)(\tfrac{6}{5} + \tfrac{8}{5}u).$$





Continuum regime

Rescale grid: $\mathbb{Z} \mapsto h\mathbb{Z}$.



Rescale LDE:

$$\frac{d}{dt}u_{jh}(t) = \frac{1}{h^2}\big[u_{(j+1)h}(t) + u_{(j-1)h}(t) - 2u_{jh}(t)\big] - G'\big(u_{jh}(t)\big)$$

Travelling wave $u_{jh}(t) = \Phi(jh + ct)$ must satisfy

$$c\Phi'(\xi) = [\Delta_h \Phi](\xi) - G'\big(\Phi(\xi)\big)$$

with

$$[\Delta_h \Phi](\xi) = \frac{1}{h^2}\Big[\Phi(\xi + h) + \Phi(\xi - h) - 2\Phi(\xi)\Big]$$

Lifting waves

Recall

$$[\Delta_h \Phi] = \frac{1}{h^2}\big[\Phi(\xi + h) + \Phi(\xi - h) - 2\Phi(\xi)\big]$$

Goal: bifurcate off PDE waves

$$c_0 \phi_0'(\xi) = \phi_0''(\xi) - G'(\phi(\xi))$$

to get LDE waves

$$c\Phi'(\xi) = [\Delta_h \Phi](\xi) - G'\big(\Phi(\xi)\big)$$

for $0 < h \ll 1$.

[Bates, Chen, Chmaj (2003)]: 'spectral convergence'.

The perturbation

Bifurcation problem

$$\Phi(\xi) = \phi_0(\xi) + v(\xi), \qquad c = c_0 + \widetilde{c}$$

where (c_0, ϕ_0) is PDE wave.

The perturbation is **singular**, in the sense that one must solve

$$\mathcal{L}_h v = O(v^2 + h + \widetilde{c}),$$

with $\mathcal{L}_h : H^1 \to L^2$ given by

$$[\mathcal{L}_h v](\xi) = -c_0 v'(\xi) + [\Delta_h v](\xi) - G''(\phi_0(\xi))v(\xi).$$

Compare with PDE operator $\mathcal{L}_0 : H^2 \to L^2$

$$[\mathcal{L}_0 v](\xi) = -c_0 v'(\xi) + v''(\xi) - G''(\phi_0(\xi))v(\xi).$$

Note: operators act on different spaces.

Spectral Convergence

Recall

$$[\mathcal{L}_h v](\xi) = -c_0 v'(\xi) + [\Delta_h v](\xi) - G''(\phi_0(\xi))v(\xi).$$

Want to show: $\mathcal{L}_h - 1$ invertible for $0 < h \ll 1$.

- Assume $(\mathcal{L}_h - 1)v_h = w_h$ with $\|v_h\|_{H^1} = 1$.
- Goal: show $\|w_h\|_{L^2} \gtrsim 0$ as $h \downarrow 0$.
- Take **weak** limits:

$$v_h \rightharpoonup v_0 \in H^1, \qquad w_h \rightharpoonup w_0 \in L^2$$

- Observe: $[\mathcal{L}_0 - 1]v_0 = w_0$ so

$$v_0 = [\mathcal{L}_0 - 1]^{-1} w_0$$

- Danger: v_0 and w_0 could be zero.

Continued

- For compact $K \subset \mathbb{R}$, we have (after subsq) strong convergence

$$v_h \rightarrow v_0 \in L^2(K)$$

Can we exclude $v_0 = 0$? **Danger:**

$$v_h = h \sin(\xi/h), \qquad v_h' = \cos(\xi/h)$$

Notice:

$$\|v_h\|_{L^2([-\pi;\pi])} = h\sqrt{\pi}$$

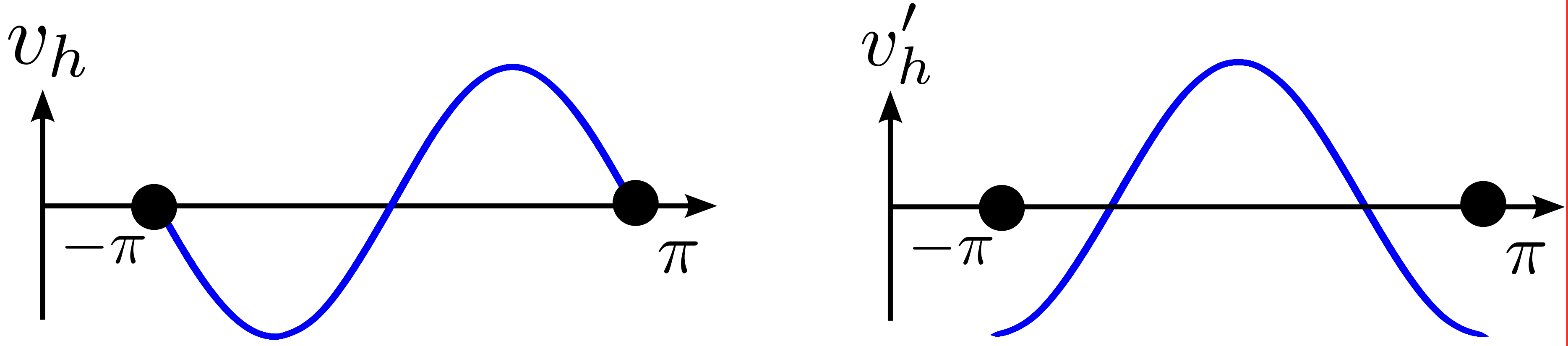
while

$$\|v_h'\|_{L^2([-\pi;\pi])} = \sqrt{\pi}$$

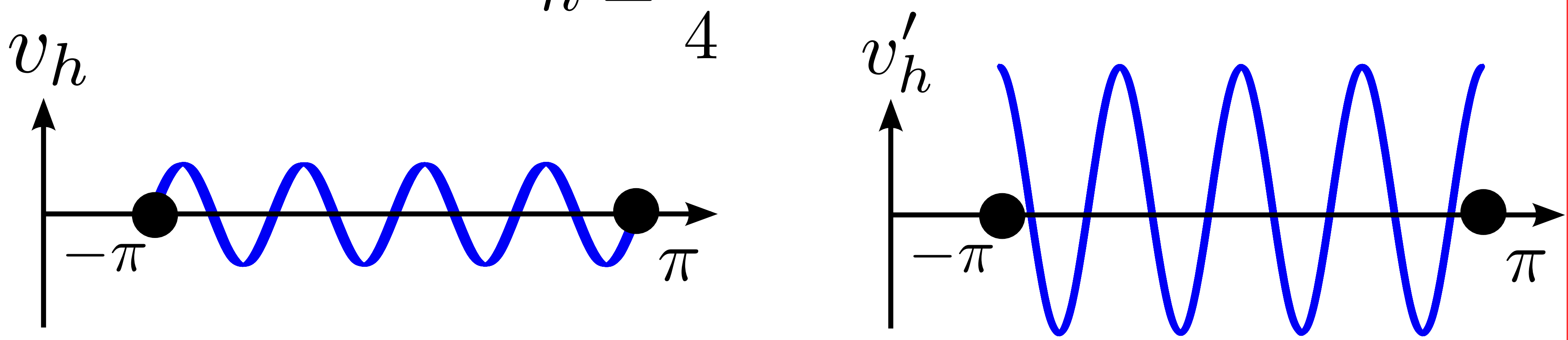
So: $\|v_h\|_{L^2(K)} \sim O(h)$ while $\|v_h\|_{H^1(K)} \sim O(1)$

Weak Limits

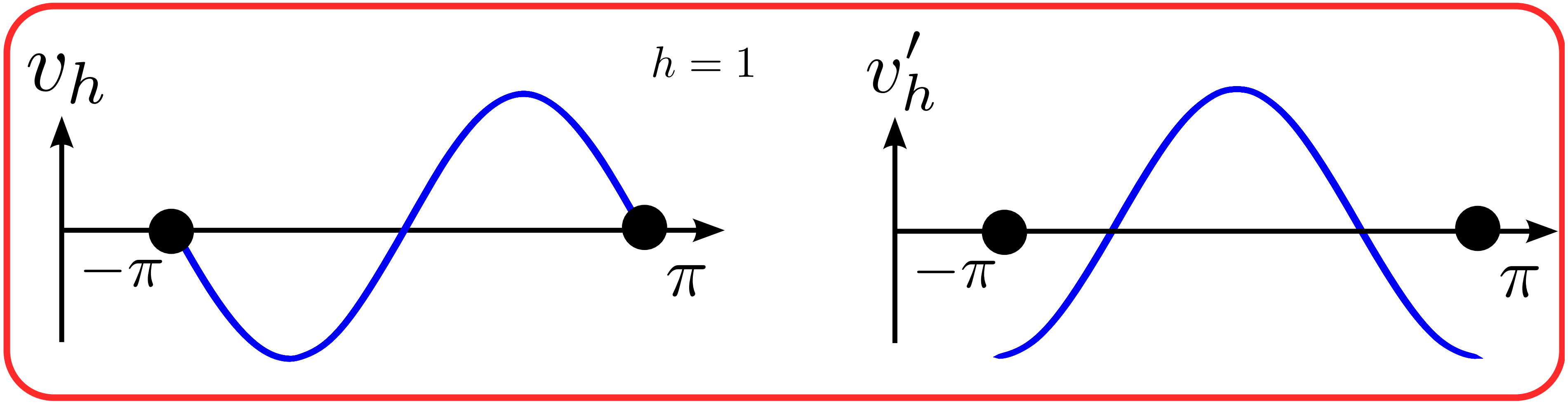
$$h = 1$$



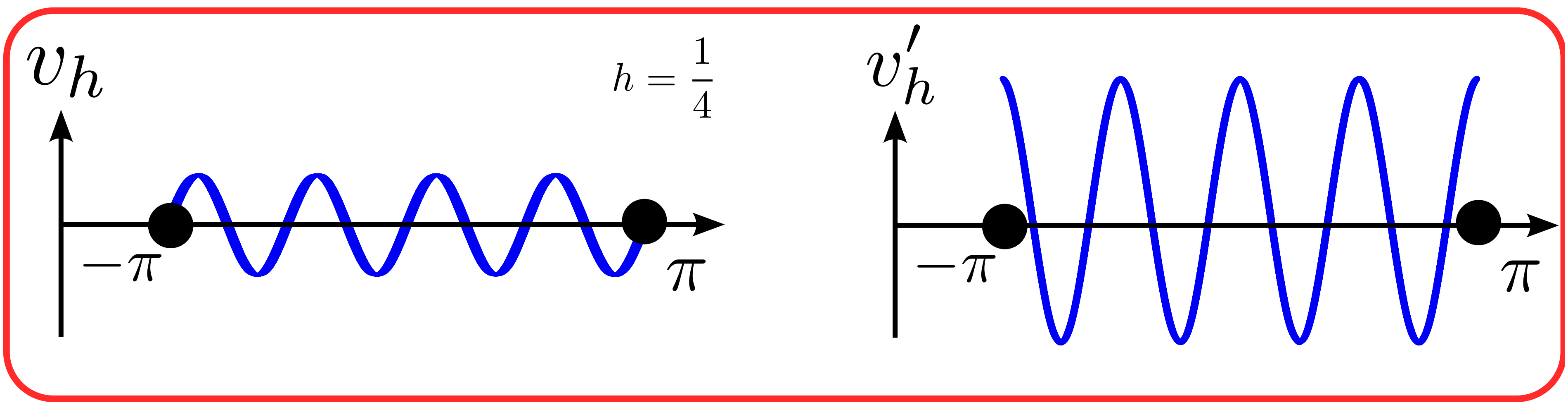
$$h = \frac{1}{4}$$



Weak Limits

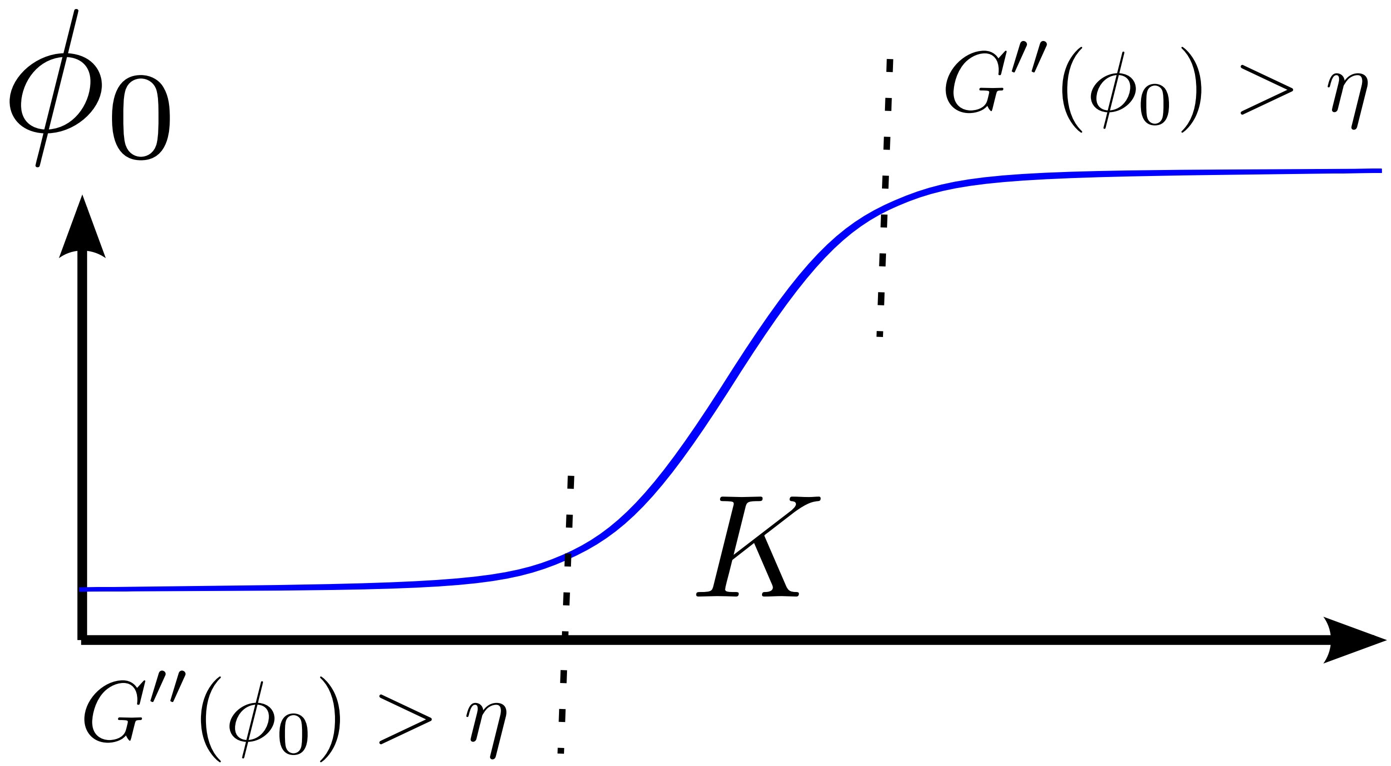


$$\|v_h\|_2 = O(h) \qquad\qquad \|v_h'\|_2 = O(1)$$

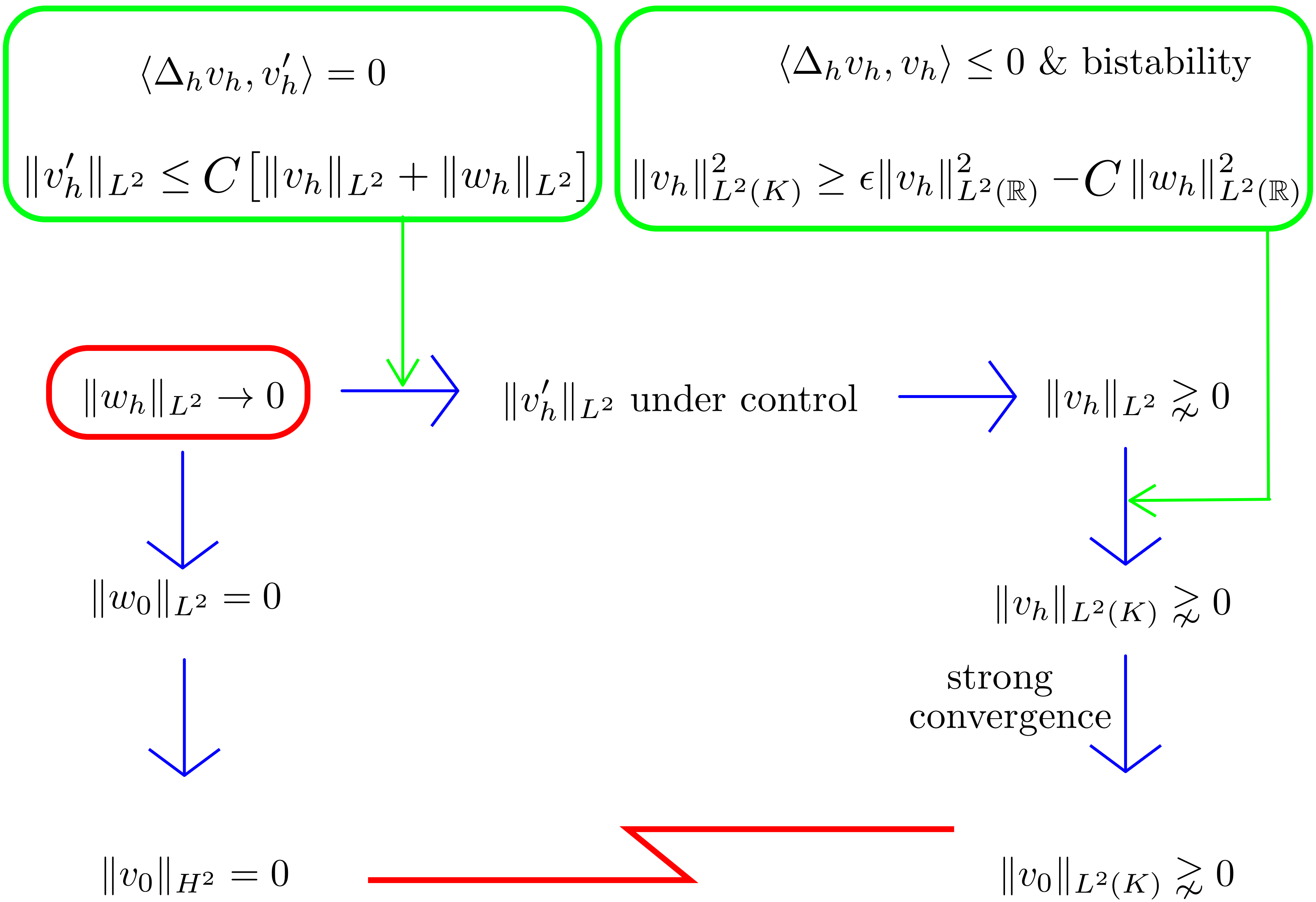


Compact Interval

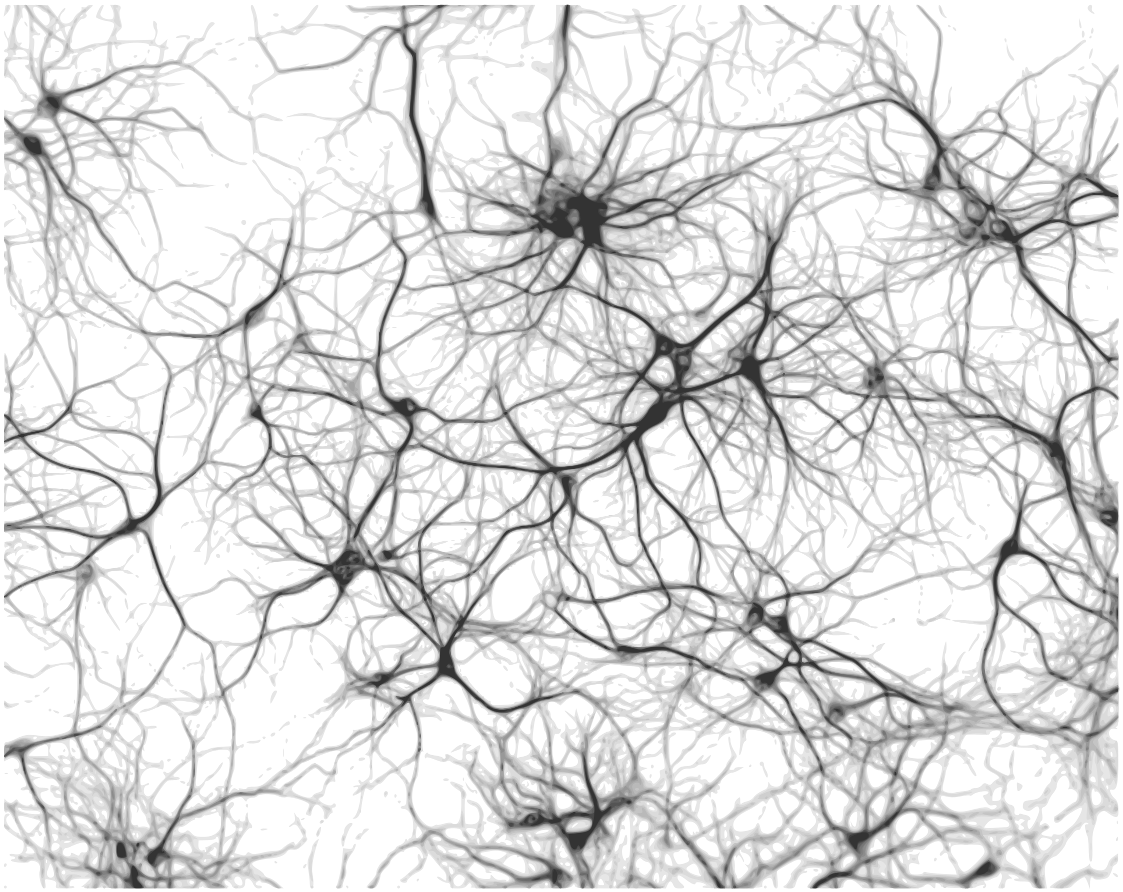
Pick K large so that $G'' > \eta$ outside K:



Spectral convergence [Bates, Chen, Chmaj (2003)]



Neural Fields



Complex (discrete) topology

Longe range interactions

[Bressloff (2012)]

Search for effective eqns

Infinite-Range FitzHugh-Nagumo LDE

Discrete FitzHugh-Nagumo

$$\begin{aligned} \dot{u}_{jh} &= \tfrac{1}{h^2} \sum_{k>0} \alpha_k \big[u_{(j+k)h} + u_{(j-k)h} - 2u_{jh} \big] - G'\big(u_{jh}\big) - w_{jh} \\ \dot{w}_{jh} &= \rho \big[u_{jh} - \gamma w_{jh} \big] \end{aligned}$$

- Coefficients α_k decay sufficiently fast
- Not necessarily positive
- Spectral conditions ensure Laplace-like properties

Infinite-range discretization of FHN PDE

$$\begin{aligned} u_t &= u_{xx} - G'\big(u\big) - w \\ w_t &= \rho \big[u - \gamma w \big] \end{aligned}$$

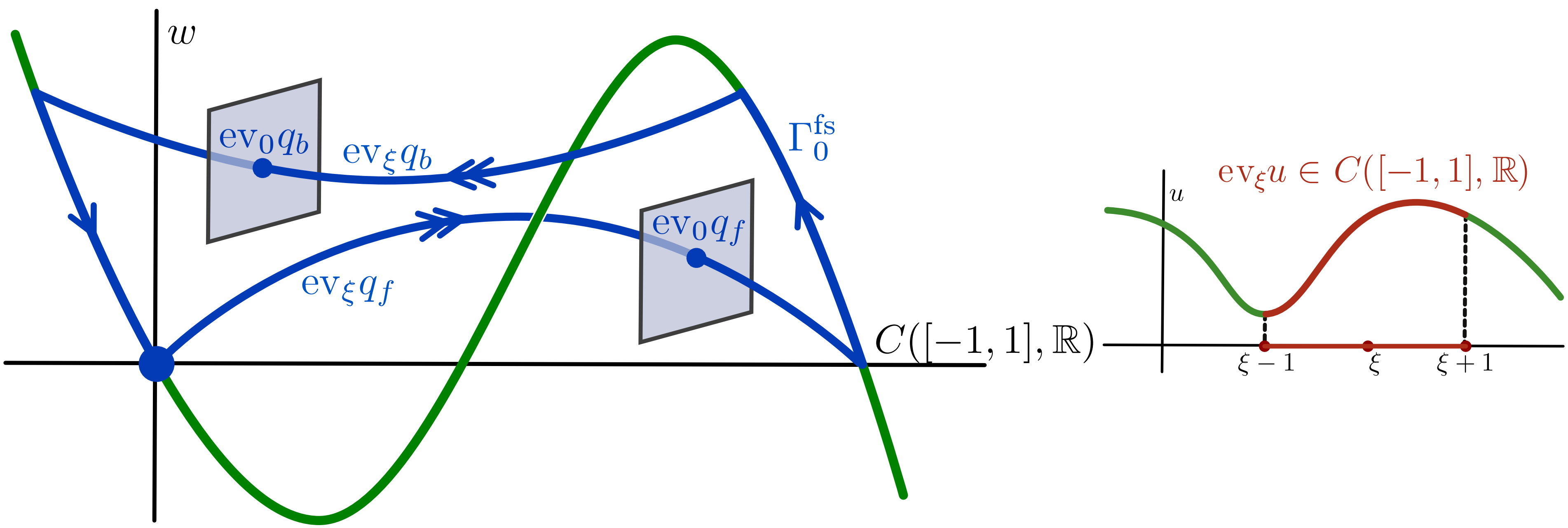
Goal: transfer existence and stability of PDE waves to LDE (for $0 < h \ll 1$)

Infinite-Range FitzHugh-Nagumo LDE

Discrete FitzHugh-Nagumo

$$\begin{aligned} \dot{u}_{jh} &= \frac{1}{h^2}\sum_{k>0}\alpha_k\big[u_{(j+k)h} + u_{(j-k)h} - 2u_{jh}\big] - G'\big(u_{jh}\big) - w_{jh} \\ \dot{w}_{jh} &= \rho\big[u_{jh} - \gamma w_{jh}\big] \end{aligned}$$

When $\alpha_k = 0$ for $k > 1$: Lin's method [Sandstede + H.].



Wave Equation

LDE travelling wave equation:

$$\begin{aligned} c\overline{u}'(\xi) &= [\Delta_{h;inf}\overline{u}](\xi) - G'\big(\overline{u}(\xi)\big) - \overline{w}(\xi) \\ c\overline{w}'(\xi) &= \rho\big[\overline{u}(\xi) - \gamma\overline{w}(\xi)\big] \end{aligned}$$

with

$$[\Delta_{h;inf}\Phi](\xi) = \frac{1}{h^2}\sum_{k>0}\big[\Phi(\xi + kh) + \Phi(\xi - kh) - 2\Phi(\xi)\big]$$

PDE waves:

$$\begin{aligned} c_0\overline{u}_0' &= u_0'' - G'\big(\overline{u}_0\big) - \overline{w}_0 \\ c_0\overline{w}_0' &= \rho\big[\overline{u}_0 - \gamma\overline{w}_0\big] \end{aligned}$$

Assumption: PDE waves exist and spectrally stable.

Results

Recall travelling wave MFDE

$$\begin{aligned} c\overline{u}'(\xi) &= [\Delta_{h;inf}\overline{u}](\xi) - G'\big(\overline{u}(\xi)\big) - \overline{w}(\xi) \\ c\overline{w}'(\xi) &= \rho\big[\overline{u}(\xi) - \gamma\overline{w}(\xi)\big] \end{aligned}$$

Thm. [H. and W. Schouten 2017] Suppose $\sum k^2 \alpha_k < \infty$. For every $0 < h \ll 1$ there is a travelling pulse solution which converges to $(c_0, \overline{u}_0, \overline{w}_0)$ as $h \downarrow 0$.

Thm. [H. and W. Schouten 2017] Suppose

$$\sum e^{\nu k} \alpha_k < \infty$$

for some $\nu > 0$. Then the travelling pulses above are **nonlinearly stable**.

Remark: Existence of pulses obtained earlier by [Scheel and Faye] **without** restriction on h, but with exponential decay on α_k.

Linear operators

Proofs hinge on understanding transition from PDE operator $\mathcal{L}_0 : H^2 \times H^1 \to L^2 \times L^2$:

$$\mathcal{L}_0 = \begin{pmatrix} -c_0\frac{d}{d\xi} + \frac{d^2}{d\xi^2} - G''(u_0) & 1 \\ \rho & -c_0\frac{d}{d\xi} - \gamma\rho \end{pmatrix}$$

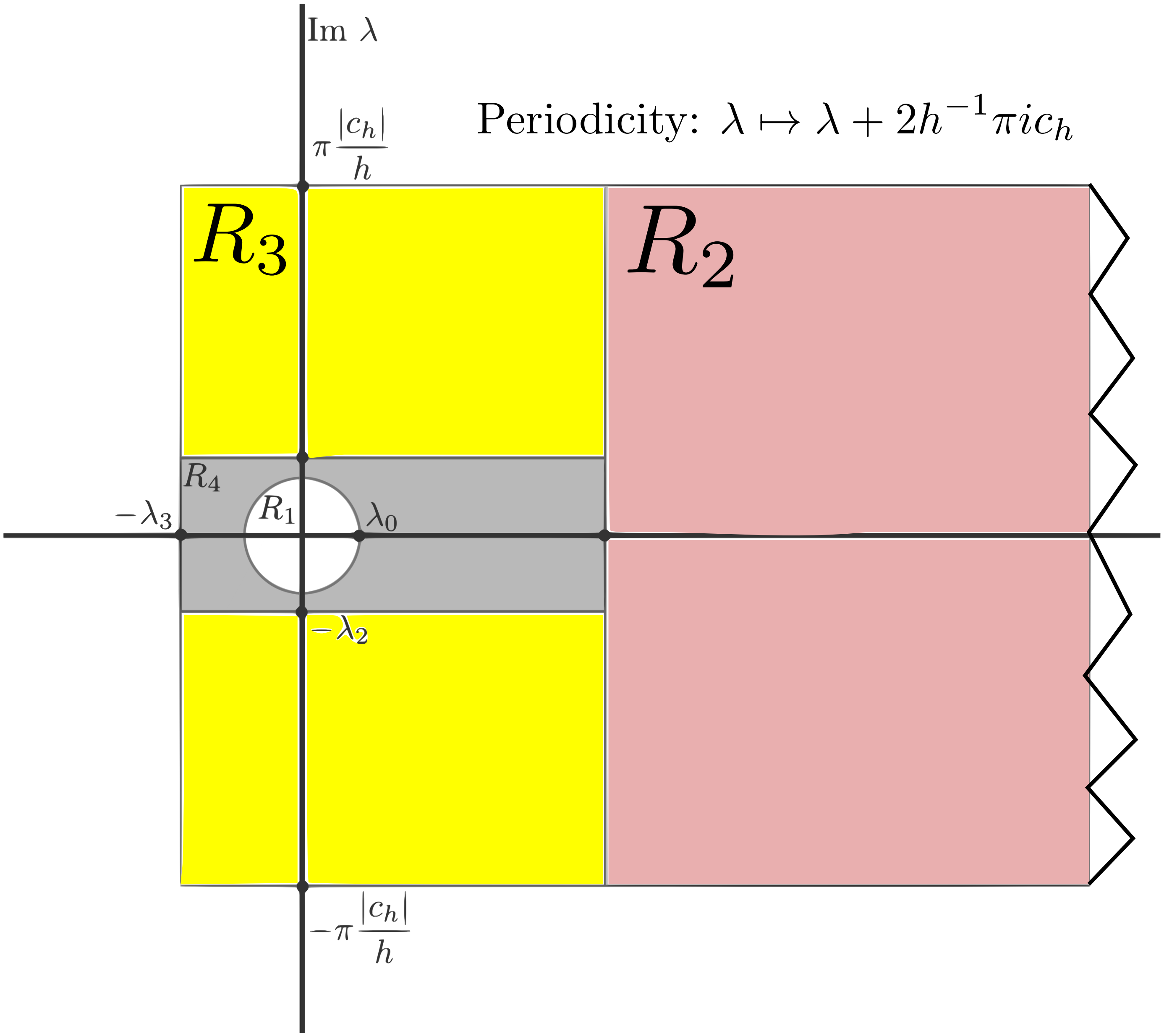
to LDE operator $\mathcal{L}_h : H^1 \times H^1 \to L^2 \times L^2$:

$$\mathcal{L}_h = \begin{pmatrix} -c_0\frac{d}{d\xi} + \Delta_h - G''(u_0) & 1 \\ \rho & -c_0\frac{d}{d\xi} - \gamma\rho \end{pmatrix}.$$

As before: operators act on different spaces

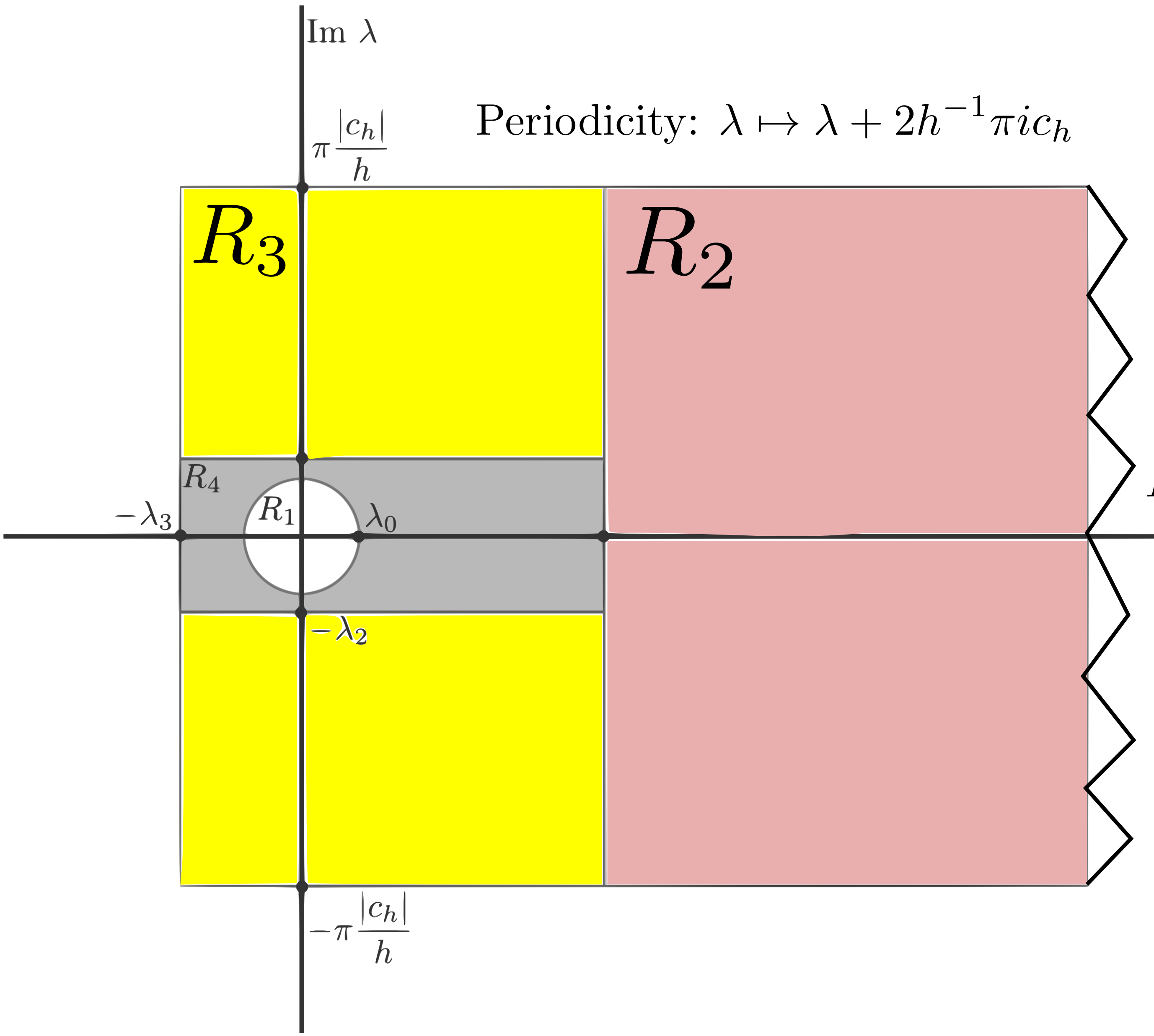
- 'Spectral convergence' can be extended
- Cross-terms needs to be kept under control
- Very useful: slow system is **linear**

Spectral Stability



Need to understand $\mathcal{L}_h - \lambda$ uniformly in λ as $h \downarrow 0$

Spectral Stability



R_1 : delicate

R_2 : standard

R_3 : Fourier transform

R_4 : Modified 'Bates'

Near $\lambda = 0$ - Beyond 'Bates'

PDE: $\mathcal{L}_0$ is Fredholm with index zero; simple eigenvalue $\lambda = 0$.

In particular, given $\mathbf{f} = (f_1, f_2) \in L^2 \times L^2$, there exist $(v, w) \in H^2 \times H^1$ and $\gamma \in \mathbb{R}$ for which

$$\mathcal{L}_0(v, w) = \mathbf{f} + \gamma(\overline{u}_0', \overline{w}_0')$$

with orthogonality condition

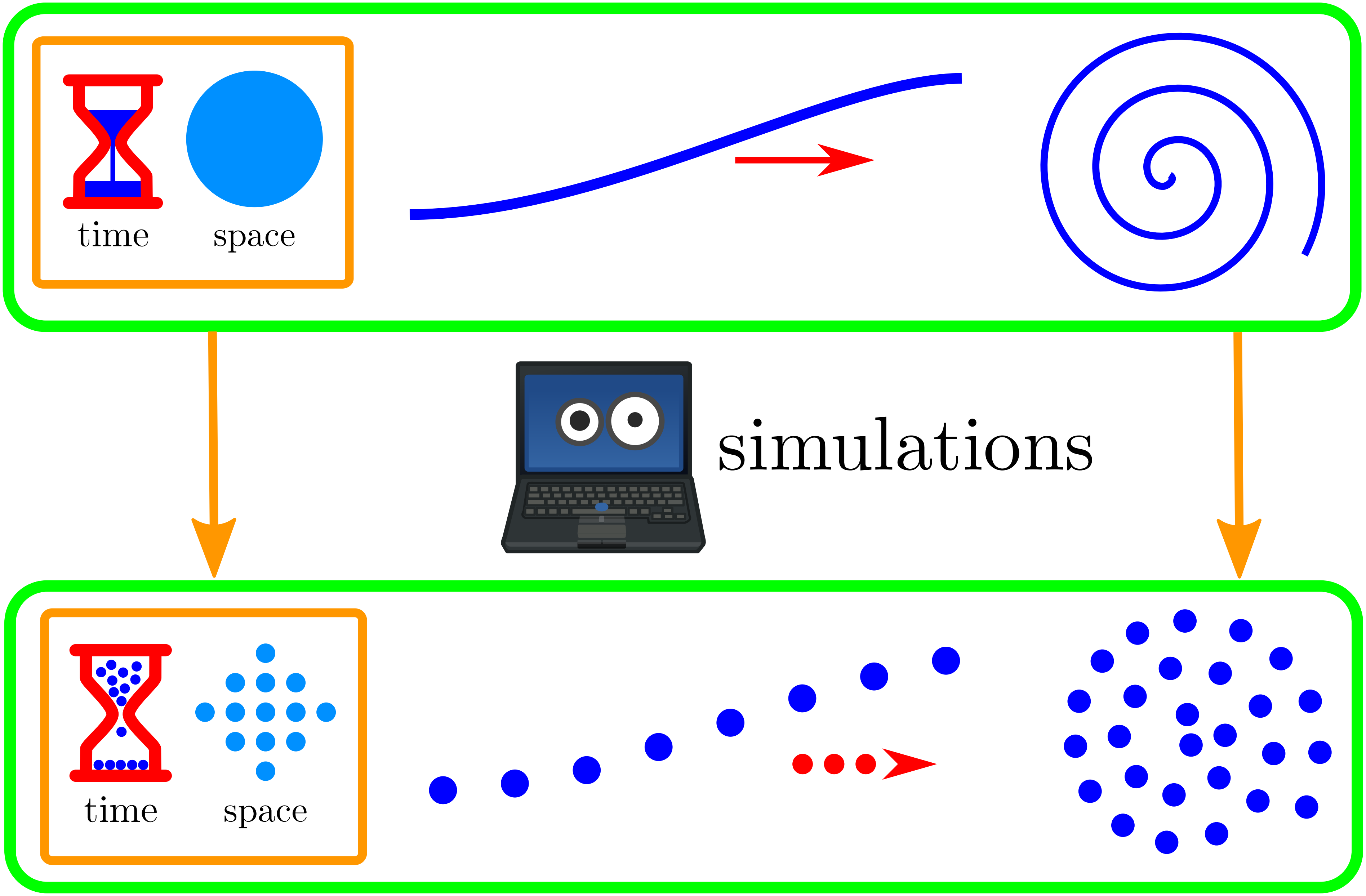
$$\Big\langle (\overline{u}_0', \overline{w}_0'), (v, w) \Big\rangle_{L^2 \times L^2} = 0.$$

Thm. [H., Schouten] For all $0 < h \ll 1$ and all $\mathbf{f} = (f_1, f_2) \in L^2 \times L^2$ there are $(v, w) = (v_h, w_h)(\mathbf{f}) \in H^1 \times H^1$ and $\gamma = \gamma_h(\mathbf{f}) \in \mathbb{R}$ so that

$$\mathcal{L}_h(v, w) = \mathbf{f} + \gamma(\overline{u}_0', \overline{w}_0')$$

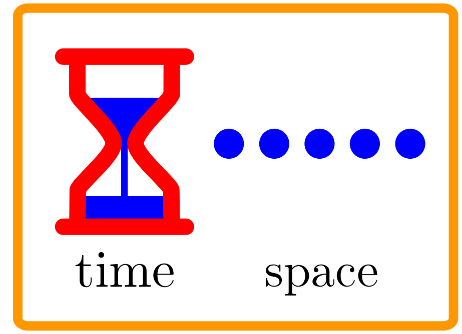
with same orthogonality condition as above.

Numerical Analysis



Full discretization

$$\dot{u}_j = u_{j+1} + u_{j-1} - 2u_j - G'(u_j)$$



$$\frac{1}{\Delta t}[u_j(t) - u_j(t-\Delta t)] = u_{j+1}(t) + u_{j-1}(t) - 2u_j(t) - G'(u_j(t))$$

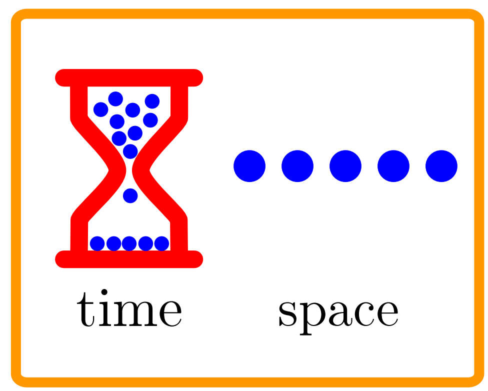
BDF-1 (Backward-Euler)

$$\frac{3}{2\Delta t}[u_j(t) - \frac{4}{3}u_j(t-\Delta t) + \frac{1}{3}u_j(t-2\Delta t)] = u_{j+1}(t) + u_{j-1}(t) - 2u_j(t) - G'(u_j(t))$$

BDF-2

$\vdots$

BDF-6



Full discretization

Travelling waves under BDF-k must solve:

$$c[\mathcal{D}_{k,c,\Delta t}\Phi](\zeta) = \Phi(\zeta+1) + \Phi(\zeta-1) - 2\Phi(\zeta) - G'\big(\Phi(\zeta)\big)$$

BDF-1:

$$[\mathcal{D}_{1,c,\Delta t}\Phi](\zeta) = \frac{1}{c\Delta t}\Big[\Phi(\zeta) - \Phi(\zeta - c\Delta t)\Big]$$

BDF-2:

$$[\mathcal{D}_{2,c,\Delta t}\Phi](\zeta) = \frac{3}{2c\Delta t}\Big[\Phi(\zeta) - \frac{4}{3}\Phi(\zeta - c\Delta t) + \frac{1}{3}\Phi(\zeta - 2c\Delta t)\Big]$$

For smooth functions Φ:

$$[\mathcal{D}_{k,c,\Delta t}\Phi](\zeta) - \Phi'(\zeta) \sim (\Delta t)^k \left\|\Phi^{(k+1)}\right\|_\infty .$$

Full discretization

Travelling waves under BDF-k must solve:

$$c[\mathcal{D}_{k,c,\Delta t}\Phi](\zeta) = \Phi(\zeta+1) + \Phi(\zeta-1) - 2\Phi(\zeta) - G'\big(\Phi(\zeta)\big)$$

Write (Φ_*, c_*) for spatially discrete wave (assume $c_* > 0$).

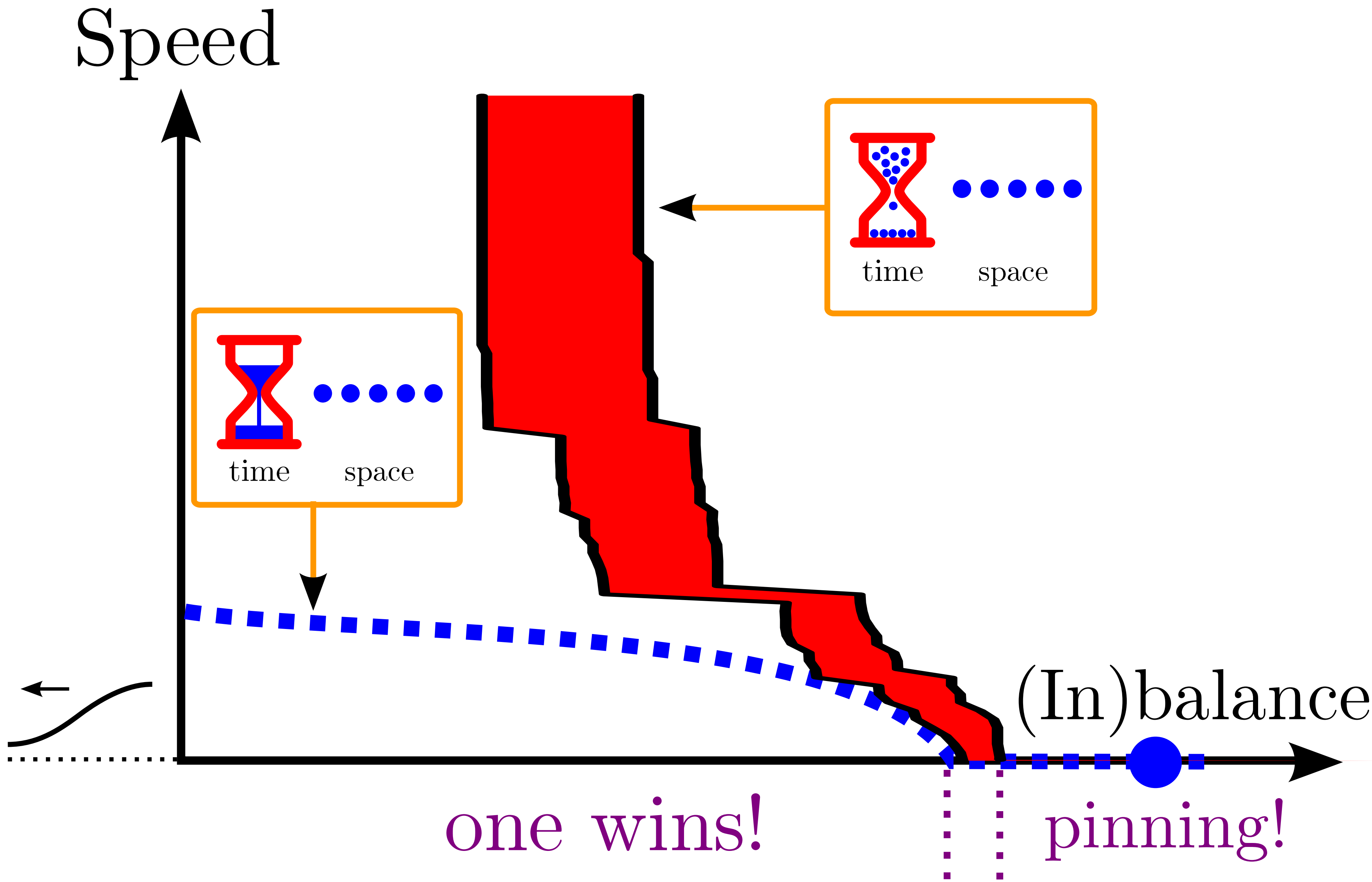
Thm. [H. and Van Vleck 2015] Fix integer $P \geq 1$. For all small

$$\epsilon \in \frac{P}{\mathbb{N}_{>0}}$$

there exists a **family** of travelling waves (Φ, c) near (Φ_*, c_*) for BDF-k with timestep $\Delta t = \frac{\epsilon}{c}$.

Observation The wavespeed loses its uniqueness. (We have a proof for BDF-1 in anti-continuum regime).

Reaction-diffusion - discrete time+space



Bifurcation

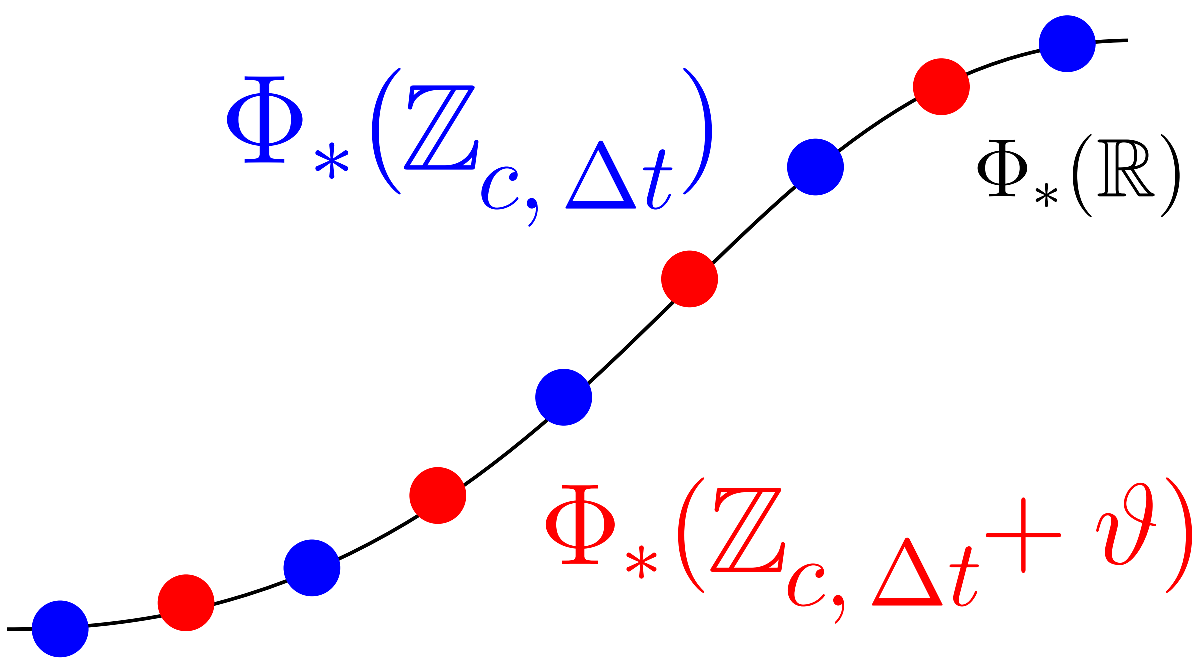
Bifurcate from spatially discrete wave Φ_* by writing

$$\Phi(\zeta) = \Phi_*(\vartheta + \zeta) + v(\zeta).$$

Pair (c, Φ) must solve fully discrete travelling wave system

$$c[\mathcal{D}_{k,c,\Delta t}\Phi](\zeta) = \Phi(\zeta+1) + \Phi(\zeta-1) - 2\Phi(\zeta) - G'\big(\Phi(\zeta); a\big).$$

Write $\mathbb{Z}_{c,\Delta t}$ for domain of ζ. For $c\Delta t = \frac{p}{q}$ we have $\mathbb{Z}_{c,\Delta t} = q^{-1}\mathbb{Z}$. Otherwise dense.



Singular perturbation

Fix $\vartheta = 0$ and concentrate on bifurcation problem

$$\Phi(\zeta) = \Phi_*(\zeta) + v(\zeta), \qquad c = c_* + \widetilde{c}$$

where (c_*, Φ_*) is **spatially discrete** wave.

The perturbation is **singular**, in the sense that one must solve

$$\mathcal{L}_{k,c,\Delta t} v = O(v^2 + c\Delta t + \widetilde{c}),$$

with $\mathcal{L}_{k,c,\Delta t} : \ell^2(\mathbb{Z}_M; \mathbb{R}) \to \ell^2(\mathbb{Z}_M; \mathbb{R})$ given by

$$[\mathcal{L}_{k,c,\Delta t} v](\zeta) = -c_* \mathcal{D}_{k,c,\Delta t} v + v(\zeta + 1) + v(\zeta - 1) - 2v(\zeta) + g'(\Phi_*(\zeta))v(\zeta).$$

Want to exploit spatially-discrete linearization $\mathcal{L}_* : H^1(\mathbb{R}; \mathbb{R}) \to L^2(\mathbb{R}; \mathbb{R})$

$$[\mathcal{L}_* v](\xi) = -c_* v'(\xi) + v(\xi + 1) + v(\xi - 1) - 2v(\xi) + g'(\Phi_*(\xi))v(\xi).$$

Note: operators act on different spaces.

Spectral convergence

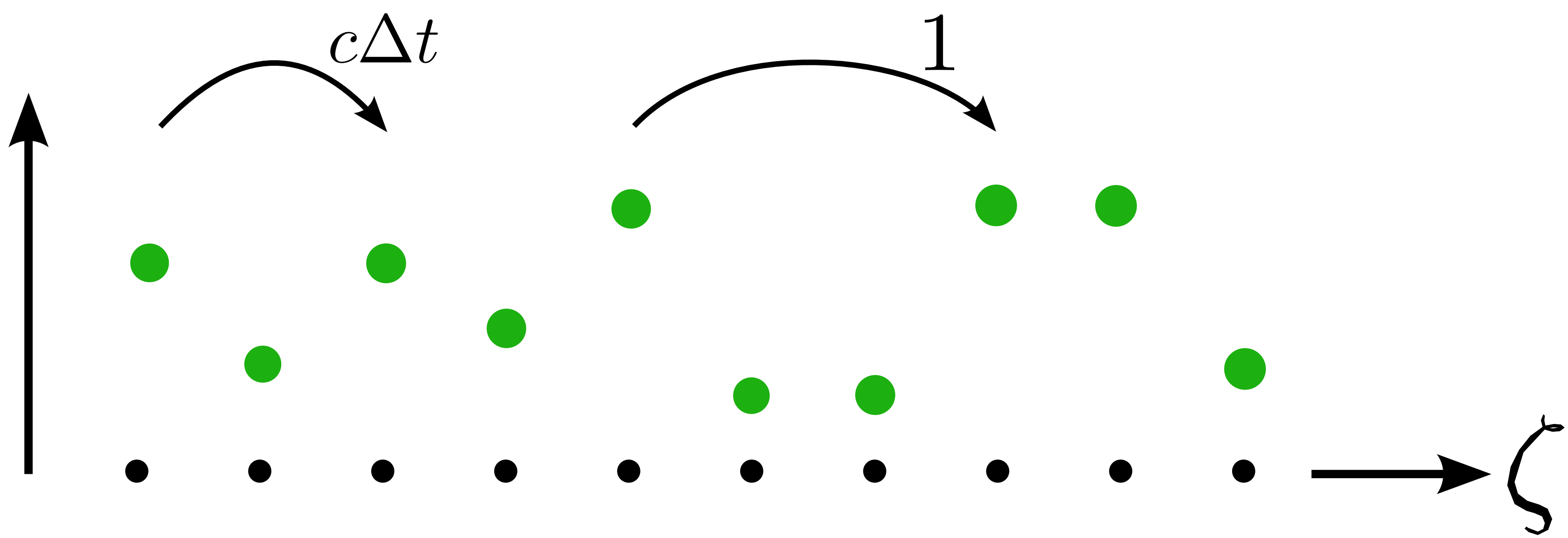
- Proof based on adaptation of 'spectral convergence' technique [Bates, Chen, Chmaj].

- Step A: Assuming $(\mathcal{L}_{k,c_j,(\Delta t)_j} - \delta)v_j \to 0$, use interpolation to pass to a weak limit $V \in H^1$.

- Step B: recover 'missing' information on V by exploiting bistable structure.

Step A: Weak Convergence

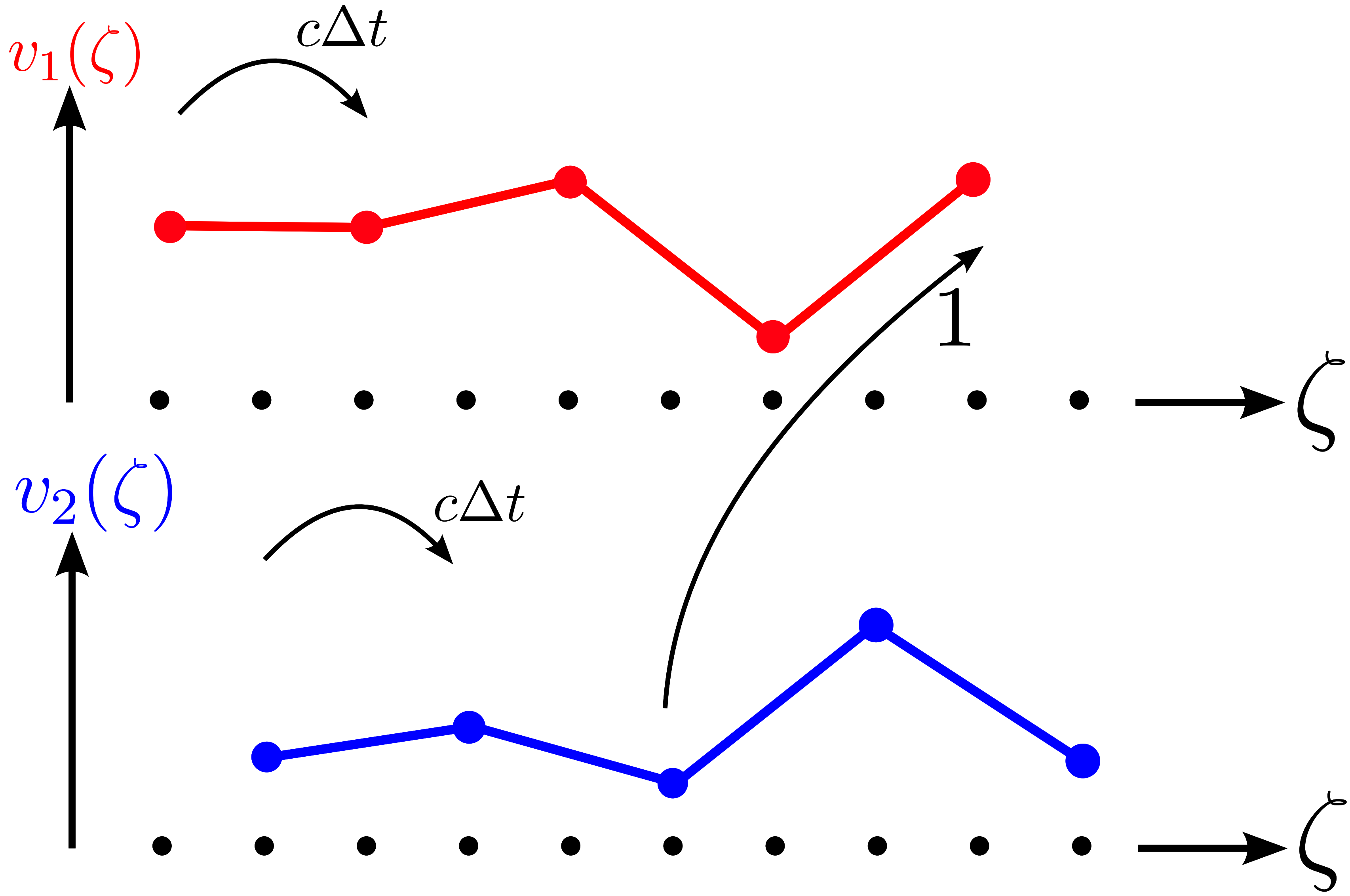
Need to build an H^1-function from sequence



Here $c\Delta t = \frac{2}{3}$ so $\zeta \in \mathbb{Z}_{c,\Delta t} = \frac{1}{3}\mathbb{Z}$.

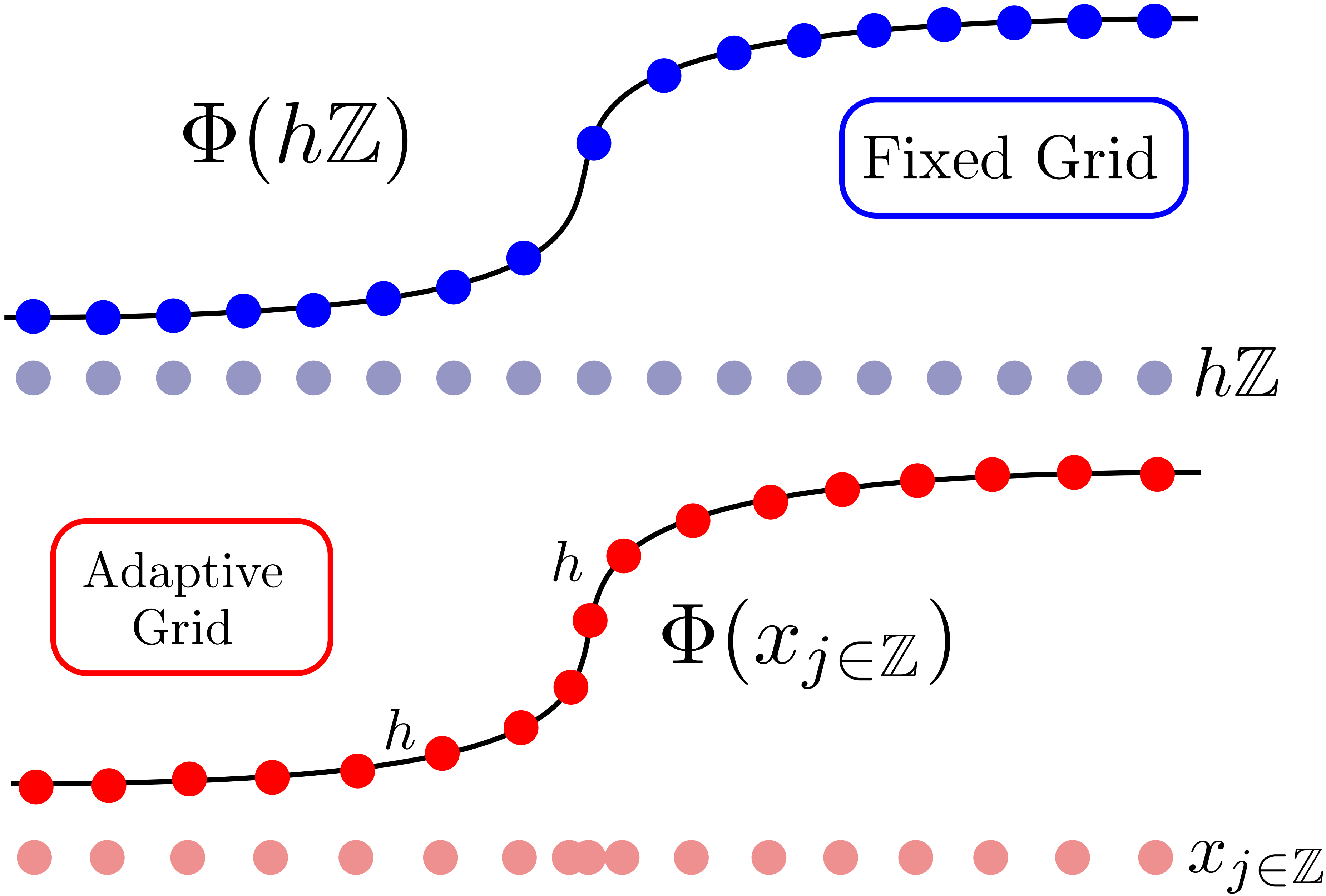
Cannot directly do interpolation in a **controlled** fashion.

Step A: Weak Convergence



After splitting; can interpolate. Size of derivative controlled by $\mathcal{D}_{k,c,\Delta t} v$.

Adaptive Grid



Adaptive Grid

Lattice system:

$$\begin{aligned}\dot{u}_j &= \left(\frac{u_{j+1}-u_{j-1}}{x_{j+1}-x_{j-1}}\right)\dot{x}_j \\ &\qquad + \frac{2}{x_{j+1}-x_{j-1}}\left[\frac{u_{j-1}-u_j}{x_j-x_{j-1}} + \frac{u_{j+1}-u_j}{x_{j+1}-x_j}\right] - G'(u_j;a).\end{aligned}$$

Starting point: instant equidistribution of arclength:

$$h^2 = (x_{j+1}-x_j)^2 + (u_{j+1}-u_j)^2 \qquad \text{for all } j \in \mathbb{Z}$$

Boundary condition:

$$x_j \to jh \qquad \text{as } j \to -\infty$$

(only local movement of grid-points)

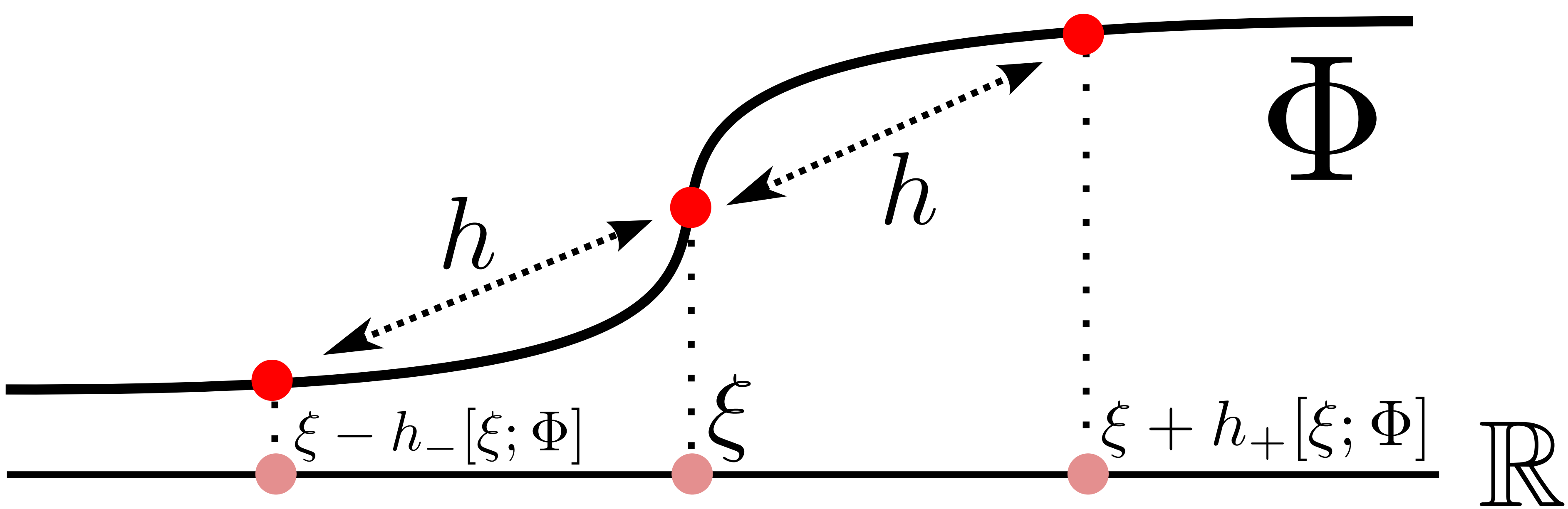
Adaptive Grid

$$\dot{u}_j \quad = \quad \left(\frac{u_{j+1}-u_{j-1}}{x_{j+1}-x_{j-1}}\right)\dot{x}_j + \frac{2}{x_{j+1}-x_{j-1}}\left[\frac{u_{j-1}-u_j}{x_j-x_{j-1}} + \frac{u_{j+1}-u_j}{x_{j+1}-x_j}\right] - G'(u_j;a).$$

Ansatz: $u_j(t) = \Phi(x_j(t) + ct) = \Phi(\xi)$.

Implicitly define grid distance in terms of wave-coordinate ξ:

$$x_{j+1}(t) - x_j(t) = h_+[\xi;\Phi], \qquad x_j(t) - x_{j-1}(t) = h_-[\xi;\Phi]$$

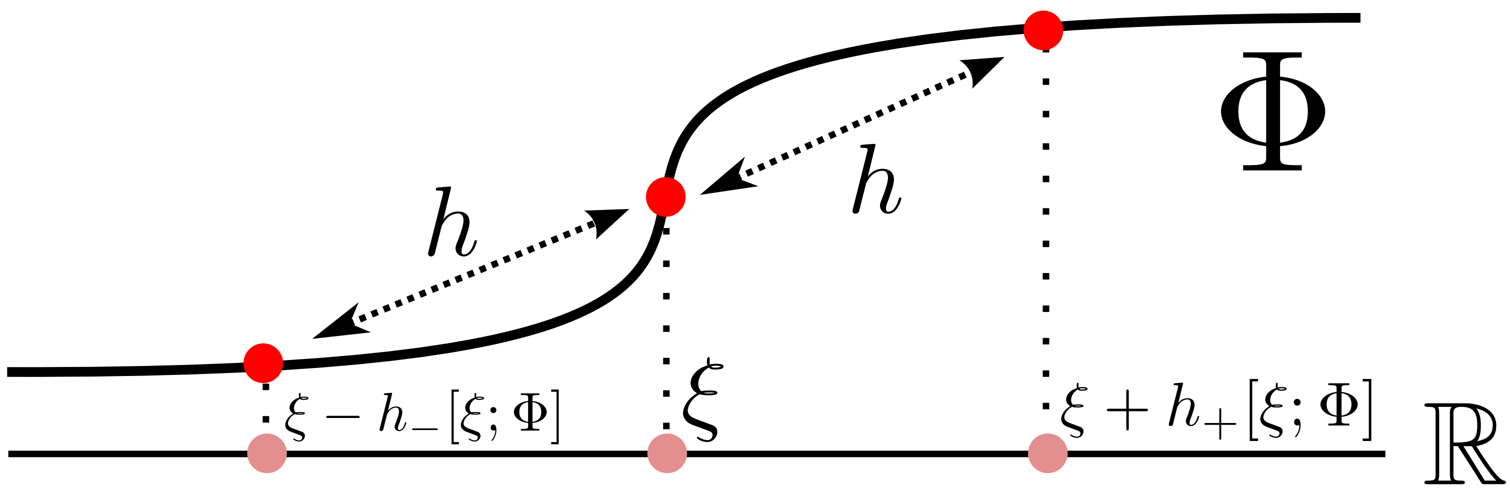


Adaptive Grid

Travelling wave equation is state-dependent MFDE with infinite shifts.

Example: diffusive term Φ'' becomes:

$$\frac{2}{h_+[\xi;\Phi] + h_-[\xi;\Phi]}\Big[\frac{\Phi(\xi + h_+[\xi;\Phi]) - \Phi(\xi)}{h_+[\xi;\Phi]} - \frac{\Phi(\xi - h_-[\xi;\Phi]) - \Phi(\xi)}{h_-[\xi;\Phi]}\Big]$$



Thm. [H., Van Vleck and Huang, 2017]: For $0 < h \ll 1$ the adaptive scheme has travelling waves.

Observation: Pinning region is significantly smaller with adaptive grids.

Outlook

- Transfer of stability properties?
- Wavespeed (non)-uniqueness hidden in exponentially small terms
- Can we handle fast (but non-instantaneous) grid movement:

$$\tau \dot{x}_j \quad = \quad \sqrt{(x_{j+1} - x_j)^2 + (u_{j+1} - u_j)^2} - \sqrt{(x_{j-1} - x_j)^2 + (u_{j-1} - u_j)^2},$$

- Other structural perturbations: di-atomic lattices