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Travelling Waves for Fully Discretized Bistable Reaction-Diffusion Problems

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Reaction-Diffusion System

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

Rate of change

Diffusion

Mixes points

Reaction

Single point

- **Continuous** spatial variable: $x \in \mathbb{R}$.
- **Continuous** temporal variable: $t \in \mathbb{R}$.
- $0 \le u(x,t) \le 1$
- Prototype for **Pattern formation**.

Reaction Term

$$\partial_t u = \cancel{\Delta u} - G'(u)$$

Rate of change

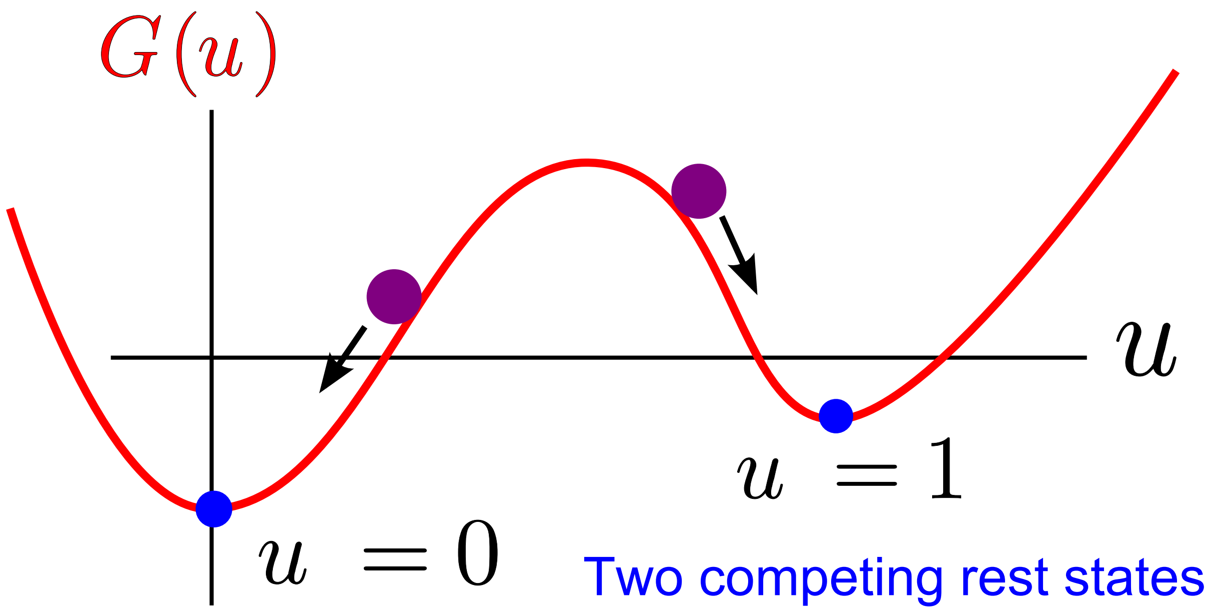
Diffusion

Mixes points

Reaction

Single point

- Think of $G(u)$ as a potential.
- Ignoring spatial variations, u moves through potential landscape.



Diffusion Term

$$\partial_t u = \Delta u - \xcancel{G'(u)}$$

Rate of change

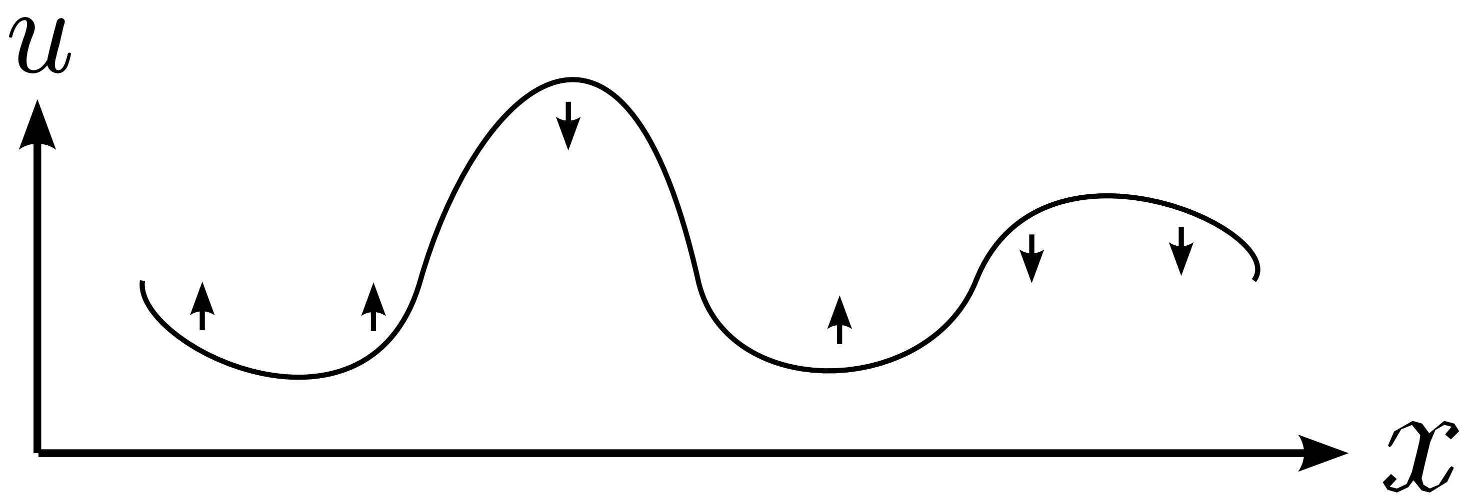
Diffusion

Mixes points

Reaction

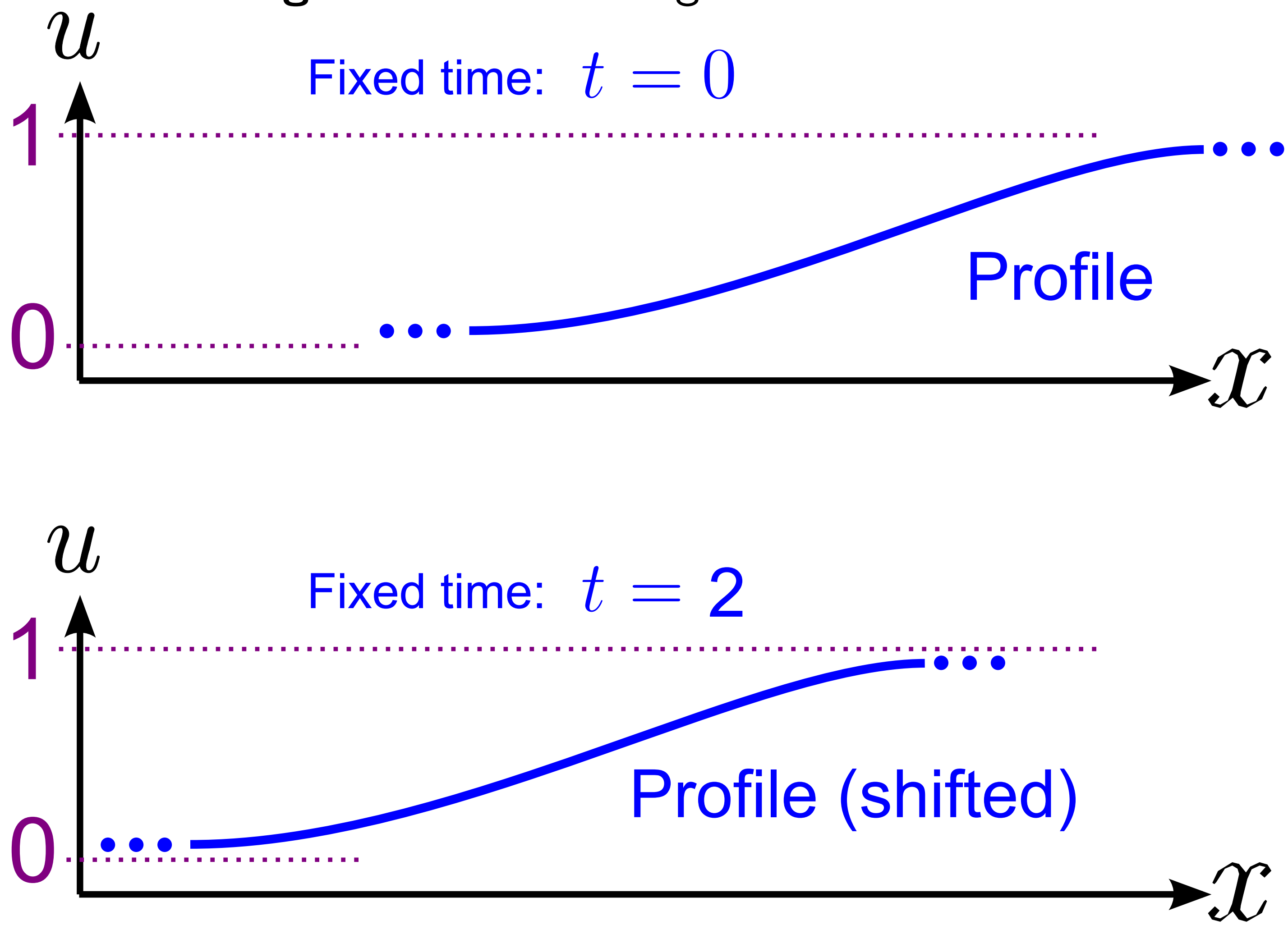
Single point

- Diffusion: flattens wrinkles.



Travelling Waves

Basic pattern: **travelling waves** connecting $u = 0$ to $u = 1$.

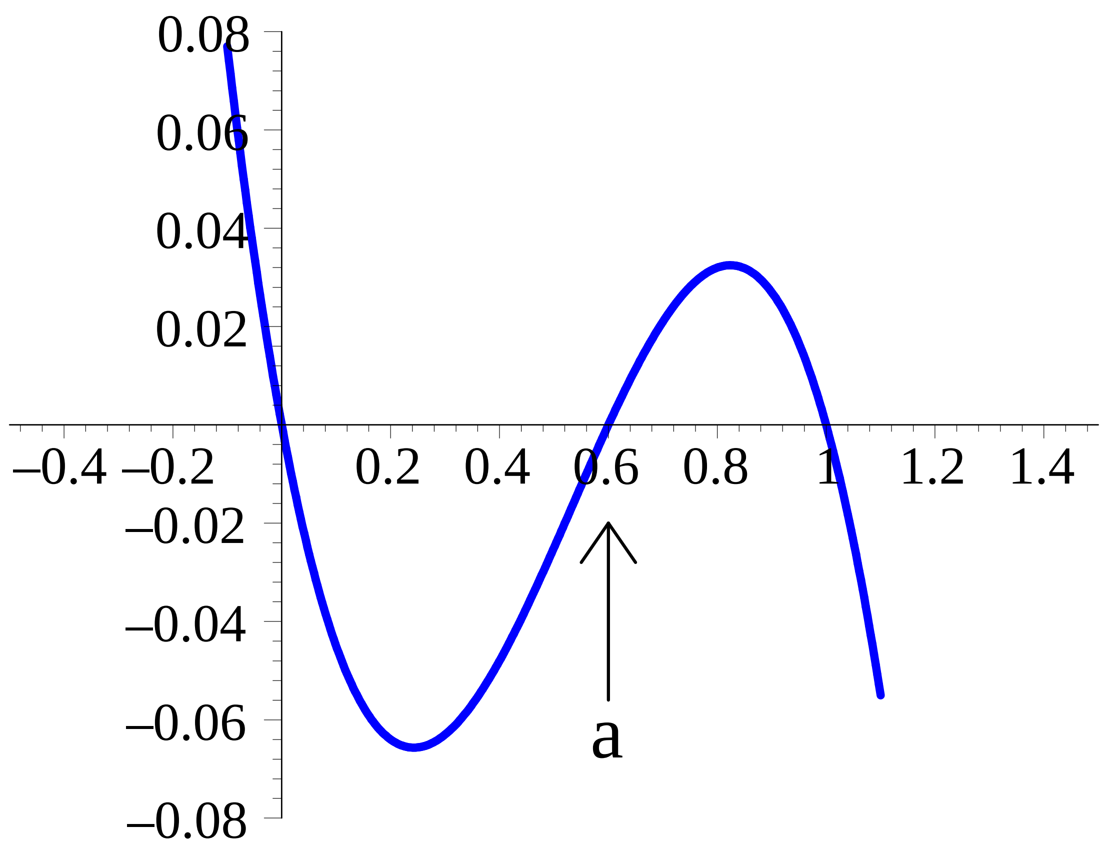


- Building blocks for more complex patterns.

Nonlinearity

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

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



Travelling wave: PDE

Nagumo PDE with $g_{\mathrm{cub}}(\cdot; a)$:

$$\partial_t u = \partial_{xx} u + u(1-u)(u-a).$$

Starting step [Fife, McLeod]: travelling waves.

Travelling wave $u(x,t) = \Phi(x+ct)$ satisfies:

$$c\Phi'(\xi) \quad = \quad \Phi''(\xi) + \Phi(\xi)\big(1-\Phi(\xi)\big)\big(\Phi(\xi)-a\big).$$

Interested in pulse solutions connecting 0 to 1, i.e.

$$\lim_{\xi\to-\infty} \Phi(\xi) = 0, \qquad \lim_{\xi\to+\infty} \Phi(\xi) = 1.$$

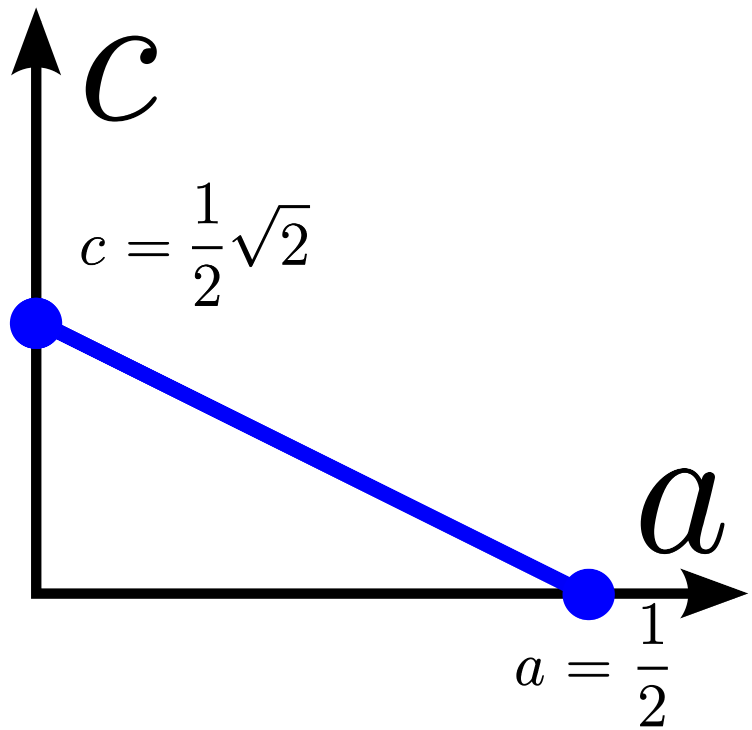
Signal Propagation: PDE

Recall travelling wave ODE

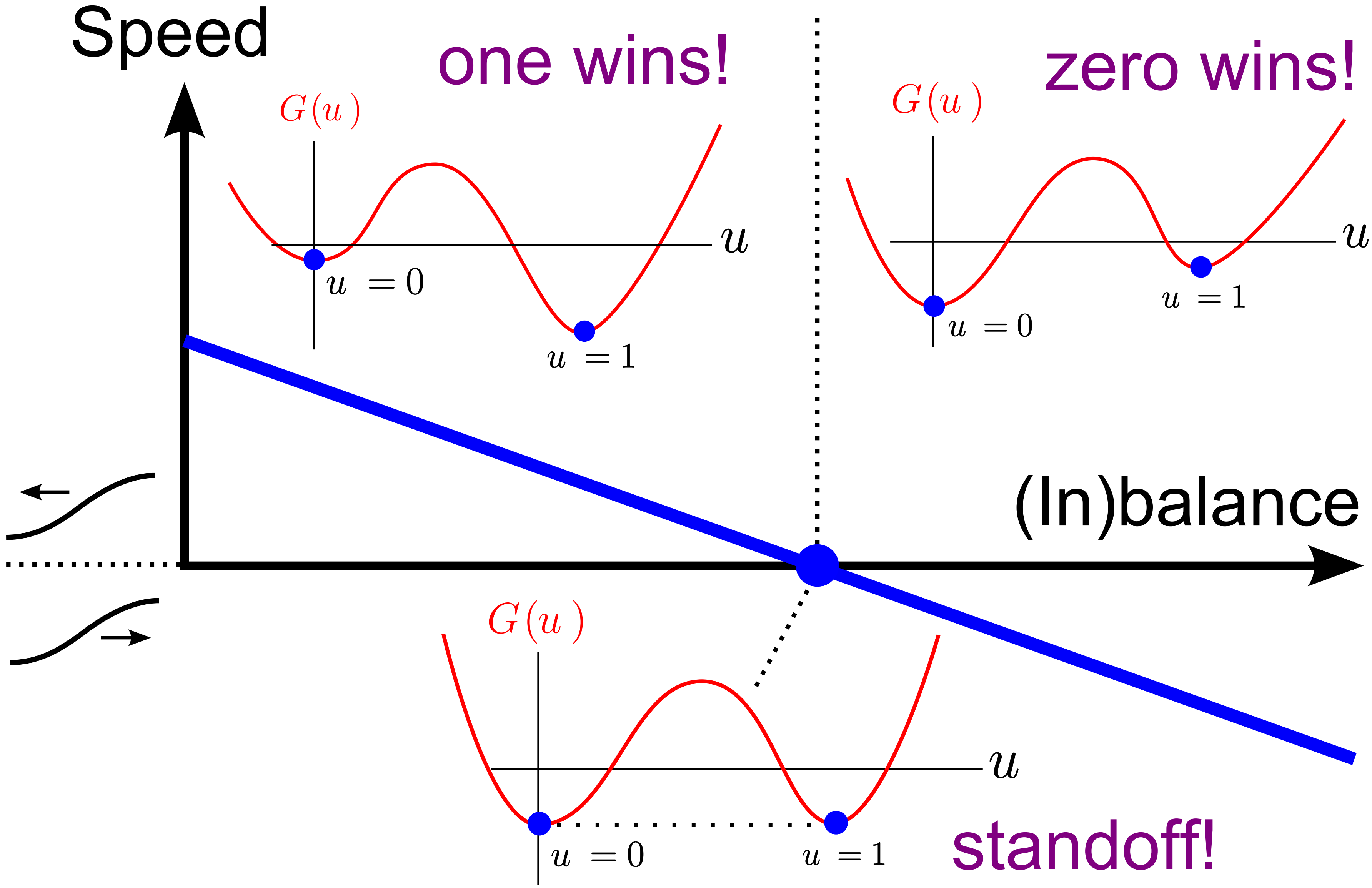
$$
\begin{aligned}
c\Phi'(\xi) &= \Phi''(\xi) + \Phi(\xi)\big(a - \Phi(\xi)\big)\big(\Phi(\xi) - 1\big). \\
\lim_{\xi \to -\infty} \phi(\xi) &= 0, \\
\lim_{\xi \to +\infty} \phi(\xi) &= 1.
\end{aligned}
$$

Explicit solutions available:

$$
\begin{aligned}
\Phi(\xi) &= \tfrac{1}{2} + \tfrac{1}{2}\tanh\left(\tfrac{1}{4}\sqrt{2}\,\xi\right), \\
c(a) &= \tfrac{1}{\sqrt{2}}(1 - 2a).
\end{aligned}
$$

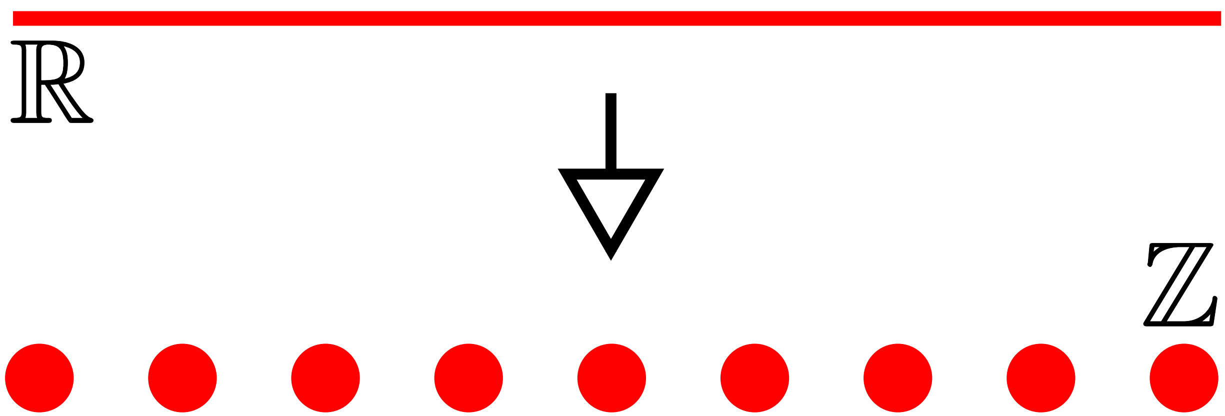


Continuous space



Step 1 - Spatial Discretization

- Translational symmetry broken



- Gaps in discrete space: barriers

- Fundamental difference between Moving Waves and Standing Waves

Reaction-Diffusion System

$$\dot{u}_j(t) = [\Delta_{\mathbb{Z}}\, u(t)]_j - G'\big(u_j(t)\big).$$

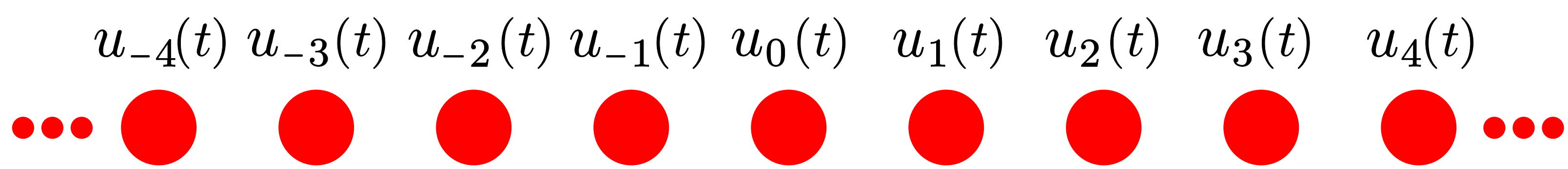
Rate of change

Diffusion

Mixes neighbours

Reaction

Single grid site



- **Discrete** spatial variable: $j \in \mathbb{Z}$.
- **Continuous** temporal variable: $t \in \mathbb{R}$.
- $0 \leq u_j(t) \leq 1$

Diffusion Term

$$\dot{u}_j(t) = [\Delta_{\mathbb{Z}}\, u(t)]_j - \cancel{G'\big(u_j(t)\big)}.$$

Rate of change

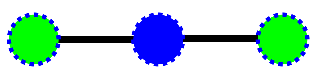
Diffusion

Mixes neighbours

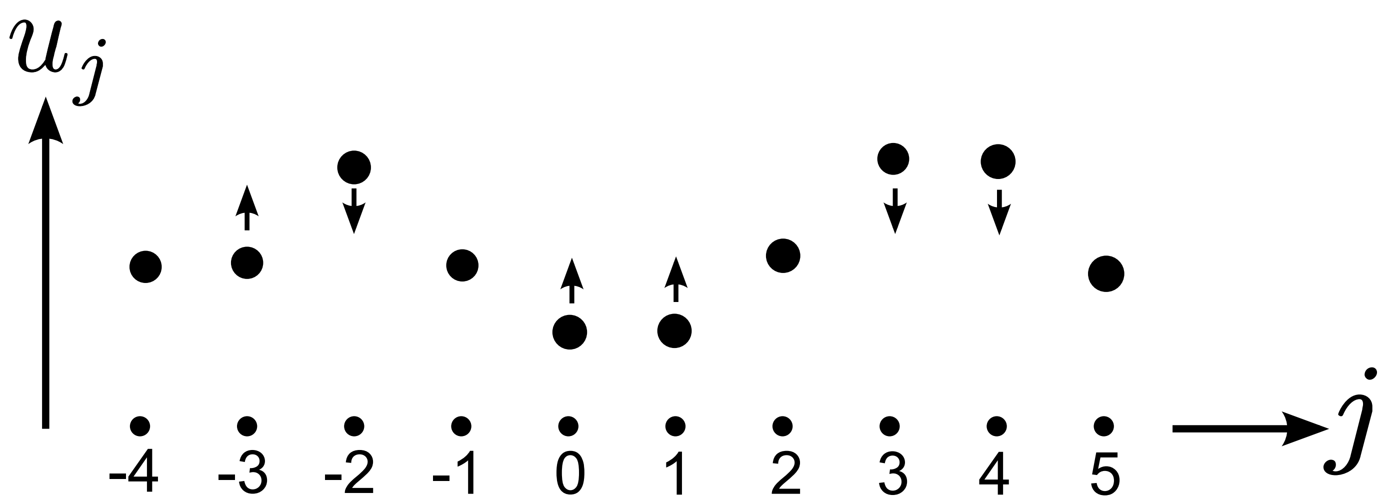
Reaction

Single grid site

- Diffusion: flattens variations between neighbours.

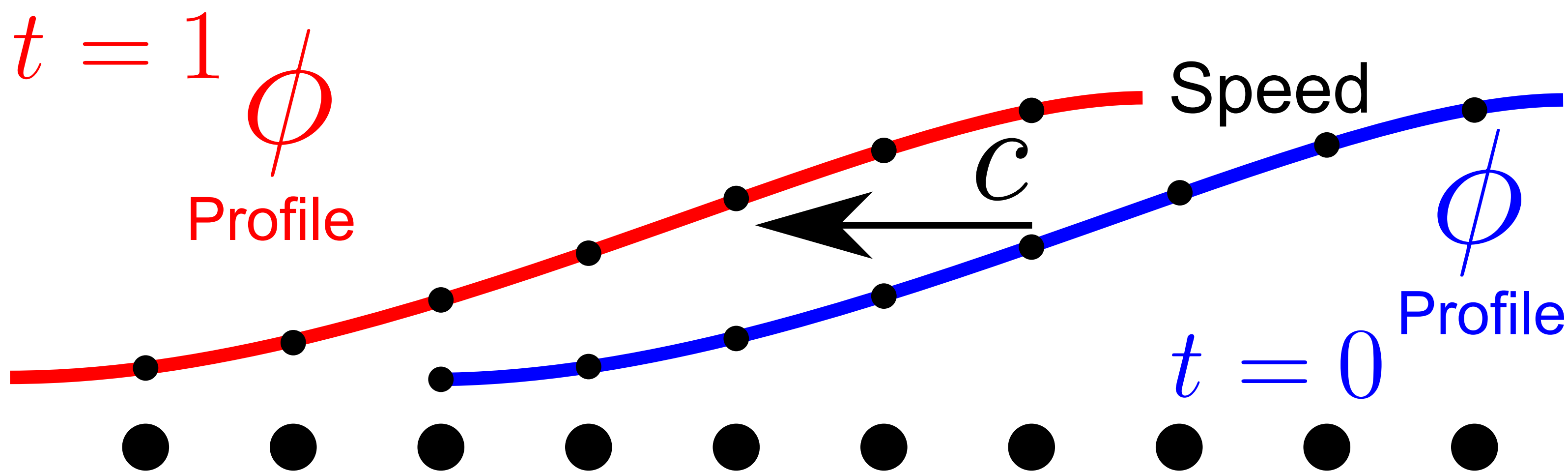


$$[\Delta_{\mathbb{Z}} u(t)]_j = u_{j+1}(t) + u_{j-1}(t) - 2u_j(t)$$



Travelling Waves

Again: Basic pattern: **travelling waves** connecting $u = 0$ to $u = 1$.



Different times see different **discrete samples** of **smooth** underlying profile.

Signal Propagation: LDE

Consider the Nagumo LDE

$$\frac{d}{dt}u_j(t) = [u_{j+1}(t) + u_{j-1}(t) - 2u_j(t)] + g_{\mathrm{cub}}(u_j(t);a), \qquad j \in \mathbb{Z}.$$

Travelling wave profile $u_j(t) = \Phi(j + ct)$ must satisfy:

$$\begin{aligned} c\Phi'(\xi) &= \Phi(\xi+1) + \Phi(\xi-1) - 2\Phi(\xi) + g_{\mathrm{cub}}\big(\Phi(\xi);a\big) \\ \lim_{\xi\to-\infty}\Phi(\xi) &= 0, \\ \lim_{\xi\to+\infty}\Phi(\xi) &= 1. \end{aligned}$$

- Notice that wave speed c enters in singular fashion.
- When $c \neq 0$, this is a functional differential equation of mixed type (MFDE).
- When $c = 0$, this is a difference equation.

Propagation Failure

Recall travelling wave MFDE:

$$
\begin{array}{rcl}
c\Phi'(\xi) & = & [\Phi(\xi+1) + \Phi(\xi-1) - 2\Phi(\xi)] + g_{\mathrm{cub}}\big(\Phi(\xi); a\big) \\
\lim_{\xi \to -\infty} \phi(\xi) & = & 0, \\
\lim_{\xi \to +\infty} \phi(\xi) & = & 1.
\end{array}
$$

When $c = 0$, can restrict to $\xi \in \mathbb{Z}$: recurrence relation!

With $p_j = \Phi(j)$ and $r_j = \Phi(j+1)$, we find

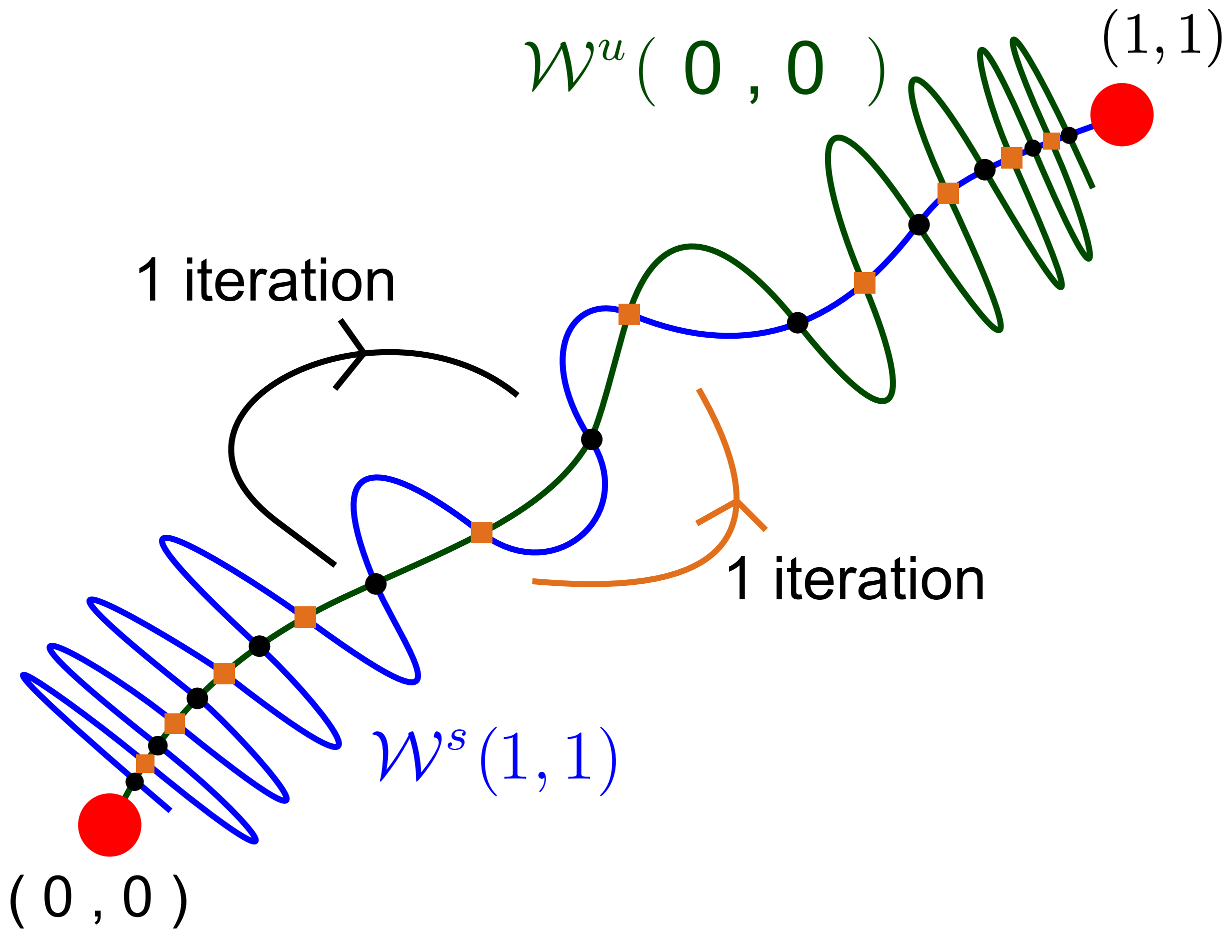
$$
\begin{array}{rcl}
p_{j+1} & = & r_j \\
r_{j+1} & = & -p_j + 2r_j - r_j(r_j - a)(1 - r_j).
\end{array}
$$

Saddles $(0, 0)$ and $(1, 1)$.

Propagation Failure

$$\begin{aligned} p_{j+1} &= r_j \\ r_{j+1} &= -p_j + 2r_j - r_j(r_j - a)(1 - r_j). \end{aligned}$$

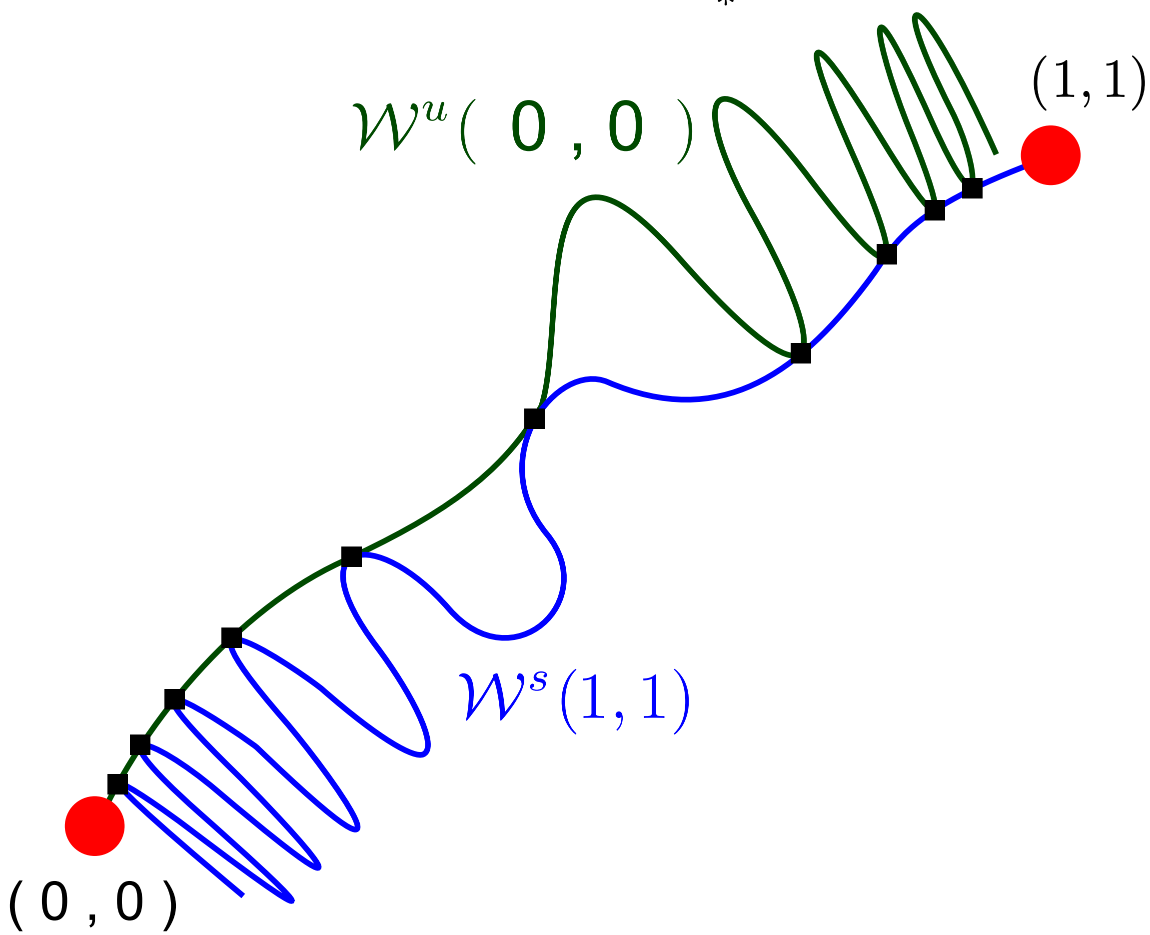
For $a = \frac{1}{2}$, site-centered (orange) and bond-centered (black) solutions. Generically:



Propagation Failure

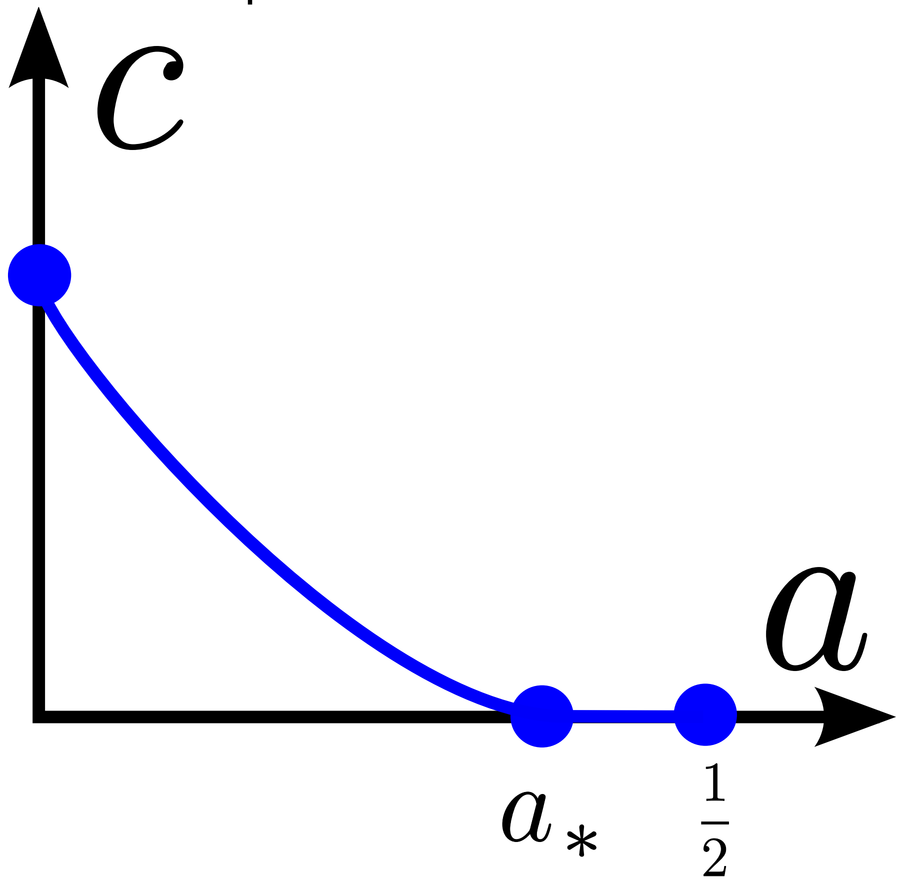
$$
\begin{aligned}
p_{j+1} &= r_j \\
r_{j+1} &= -p_j + 2r_j - r_j(r_j - a)(1 - r_j).
\end{aligned}
$$

Two branches coincide and annihilate at $a = a_*$.



Propagation

Typical wave speed c versus a plot for discrete reaction-diffusion systems:

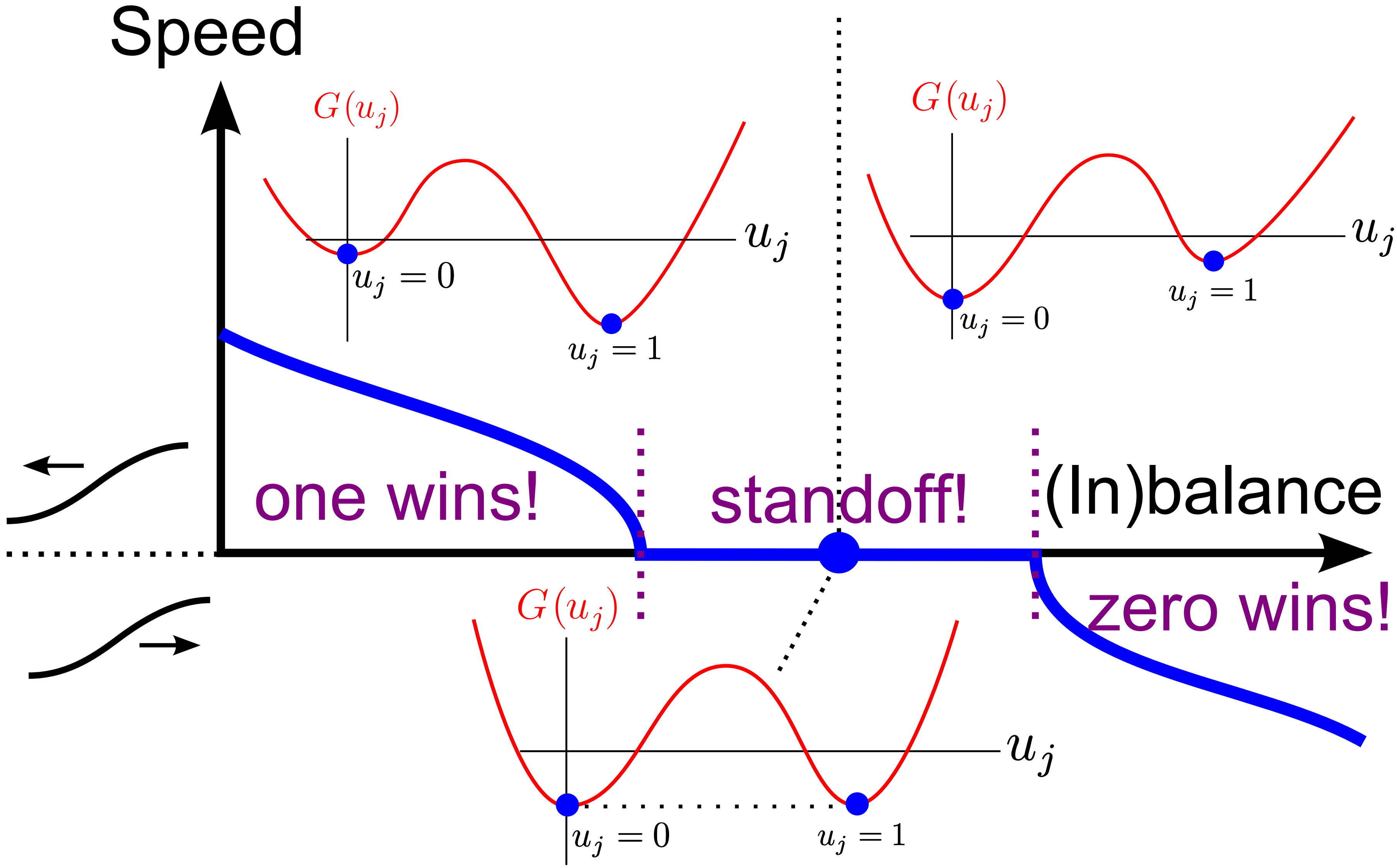


Wave speed c depends **uniquely** on a.

In case $a_* < \frac{1}{2}$, then we say that LDE suffers from propagation failure.

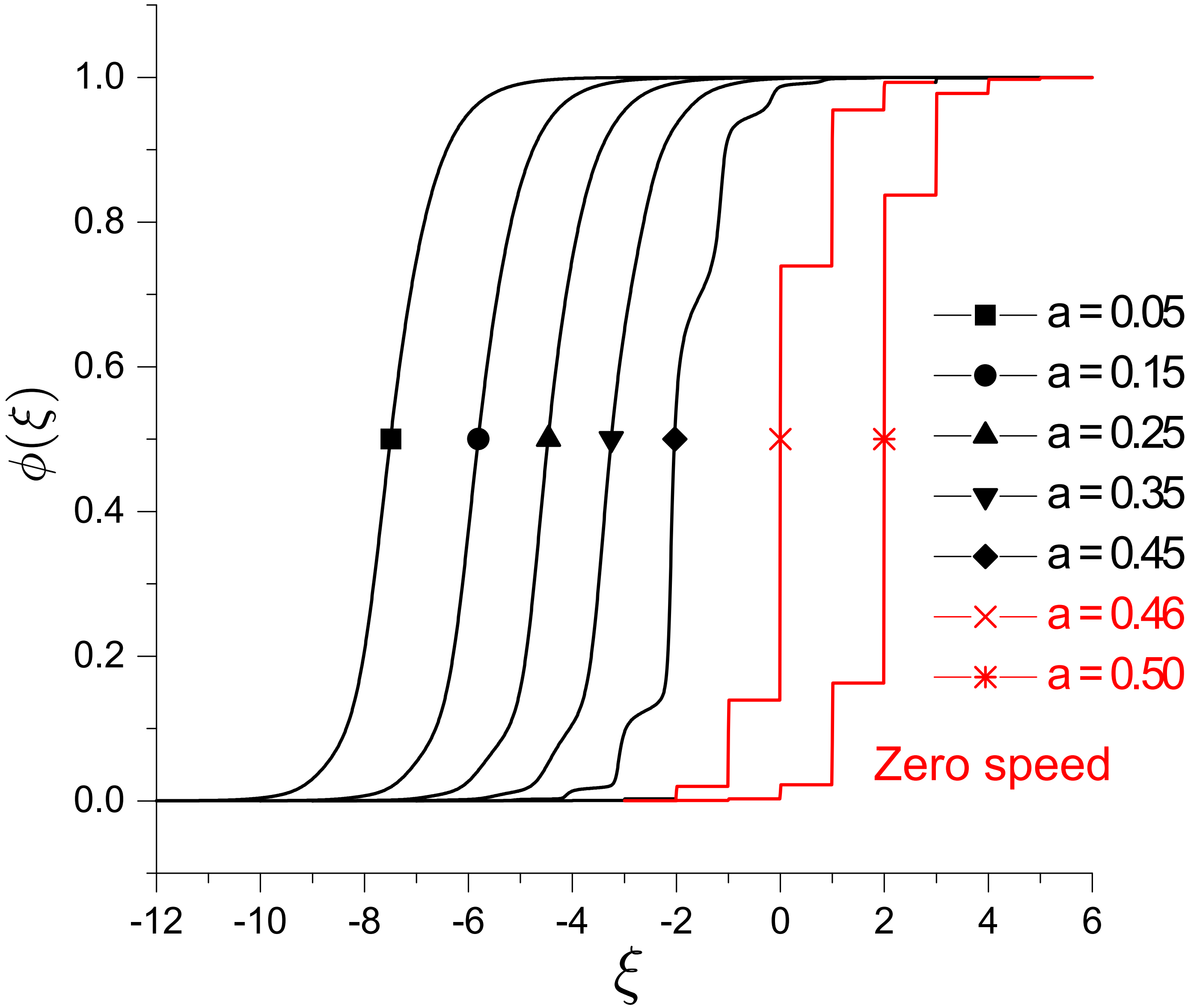
Propagation failure common for LDEs [Keener, Mallet-Paret, Hoffman, ...].

Discrete space



Discrete Nagumo LDE - Propagation failure

Travelling waves for the discrete Nagumo LDE connecting $0 \to 1$.



Step Two - Temporal Discretization

Apply Backward-Euler time discretization with time-step Δt:

$$\frac{1}{\Delta t}\big[u_j(t) - u_j(t-\Delta t)\big] = [\Delta_{\mathbb{Z}} u(t)]_j - G'(u_j(t)).$$

- Temporal variable t now in $(\Delta t)\mathbb{Z}$ (discrete).
- Spatial variable $j \in \mathbb{Z}$ still discrete.

Travelling wave Ansatz $u_j(t) = \Phi(j + ct)$ now yields

$$c[\mathcal{D}_{1,M}\Phi](\zeta) = \Phi(\zeta+1) + \Phi(\zeta-1) - 2\Phi(\zeta) - G'\big(\Phi(\zeta)\big)$$

in which $M = (c\Delta t)^{-1}$ and

$$[\mathcal{D}_{1,M}\Phi](\zeta) = M[\Phi(\zeta) - \Phi(\zeta - M^{-1})]$$

Domain of ζ depends on M. Dense in $\mathbb{R}$ if M irrational; otherwise periodic.

BDF Methods

- Backward-Euler discretization is the order $k = 1$ BDF (Backward Differentiation Formula) method.
- These methods are L-stable (slightly worse than A-stable); much better than forward Euler.
- Methods available up to order $k = 6$.

With BDF order k discretization, wave must solve:

$$c[\mathcal{D}_{k,M}\Phi](\zeta) = \Phi(\zeta+1) + \Phi(\zeta-1) - 2\Phi(\zeta) - G'\big(\Phi(\zeta)\big).$$

Example for $k = 2$:

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

For smooth functions ϕ:

$$[\mathcal{D}_{k,M}\phi - \phi'](\zeta) = O(M^{-k}\left\|\phi^{(k+1)}\right\|_{\infty}).$$

Backward-Euler: restatement

For backward-Euler one can look for solutions to

$$\widetilde{c}\Phi'(\xi) = \frac{1}{\Delta t}\big[\Phi(\xi - c\Delta t) - \Phi(\xi)\big] + \Phi(\xi+1) + \Phi(\xi-1) - 2\Phi(\xi) - G'\big(\Phi(\xi);a\big)$$

with $\widetilde{c} = 0$.

All shifted terms have **positive** coefficients. Allows framework of Mallet-Paret for **spatial discretization** to be applied for **fixed** c and Δt.

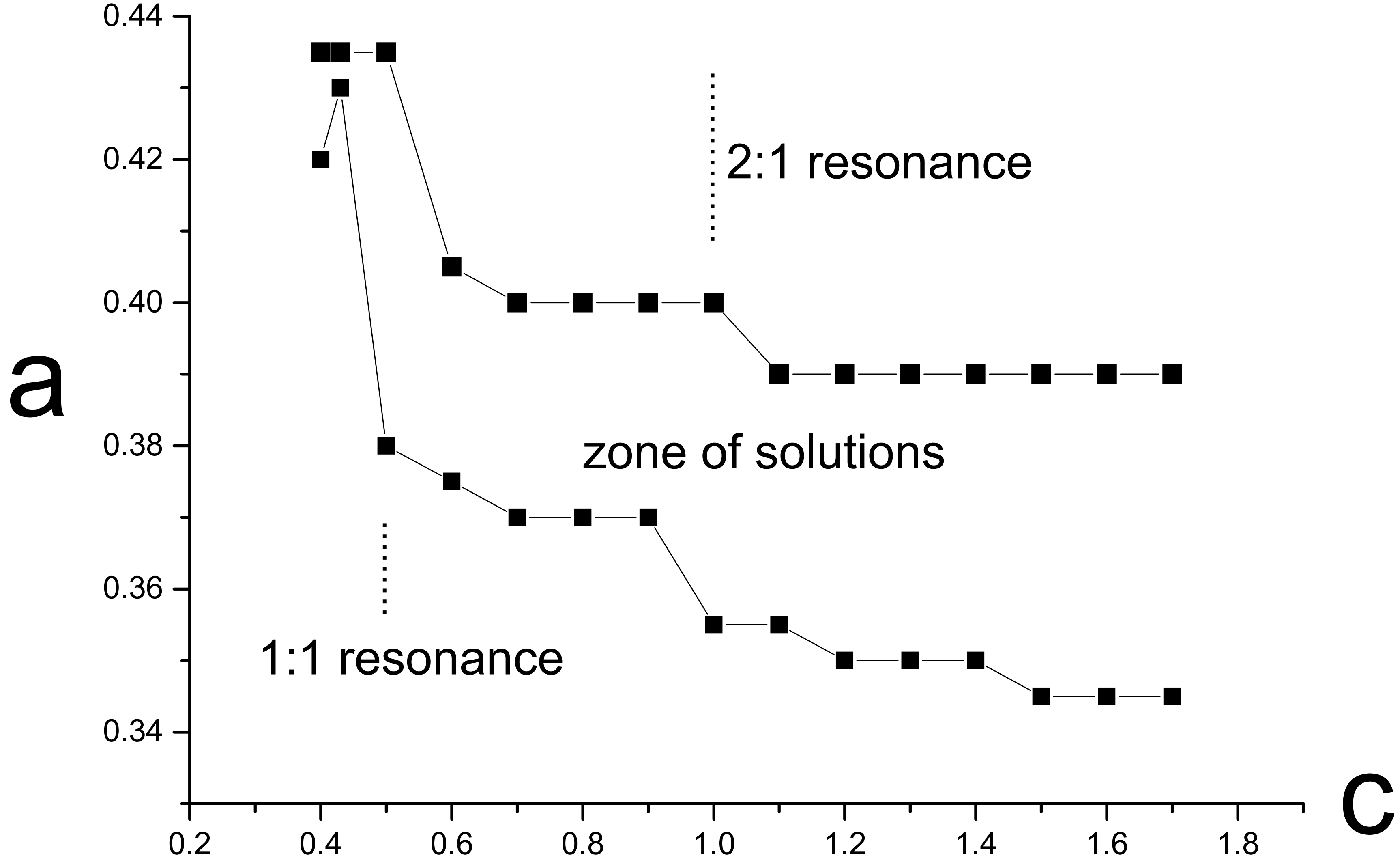
This gives unique $\widetilde{c} = \widetilde{c}(c,a)$.

Thm. [H., Van Vleck based on Mallet-Paret] Fix Δt. For all c sufficiently small, there is at least one a for which $\widetilde{c}(c,a) = 0$.

Numerical insights Generically, $\widetilde{c}(c,a) = 0$ for range of a [propagation failure]. Wave speed c is no longer a unique function of a. [Critical intervals $[a_-(c), a_+(c)]$ overlap for different values of c]

Backward-Euler: non-uniqueness of wave speed

Regions in (c, a) space where solutions exist.



Singular perturbation

For orders $2, 3, \ldots 6$, this monotonic structure is not available.

Goal here is to fix a and look at $cT \to 0$, writing

$$\Phi(\zeta) = \Phi_*(\zeta) + v(\zeta), \qquad c = c_* + c'$$

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

However the bifurcation is **singular**, in the sense that one must solve

$$\mathcal{L}_{k,M} v = O(v^2 + M^{-1} + c'),$$

with

$$[\mathcal{L}_{k,M} v](\zeta) = -c_* \mathcal{D}_{k,M} v + v(\zeta + 1) + v(\zeta - 1) - 2v(\zeta) + g'(\Phi_*(\zeta))v(\zeta).$$

We only know that

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

is Fredholm with index zero as $H^1 \to L^2$ map, with $\mathrm{Ker}\, \mathcal{L}_* = \{\Phi_*\}$. Can we lift?

Spectral convergence

- Comparison between $\mathcal{L}_{k,M}$ and $\mathcal{L}_*$ can be studied based by adapting 'spectral convergence' technique [Bates, Chen, Chmaj].

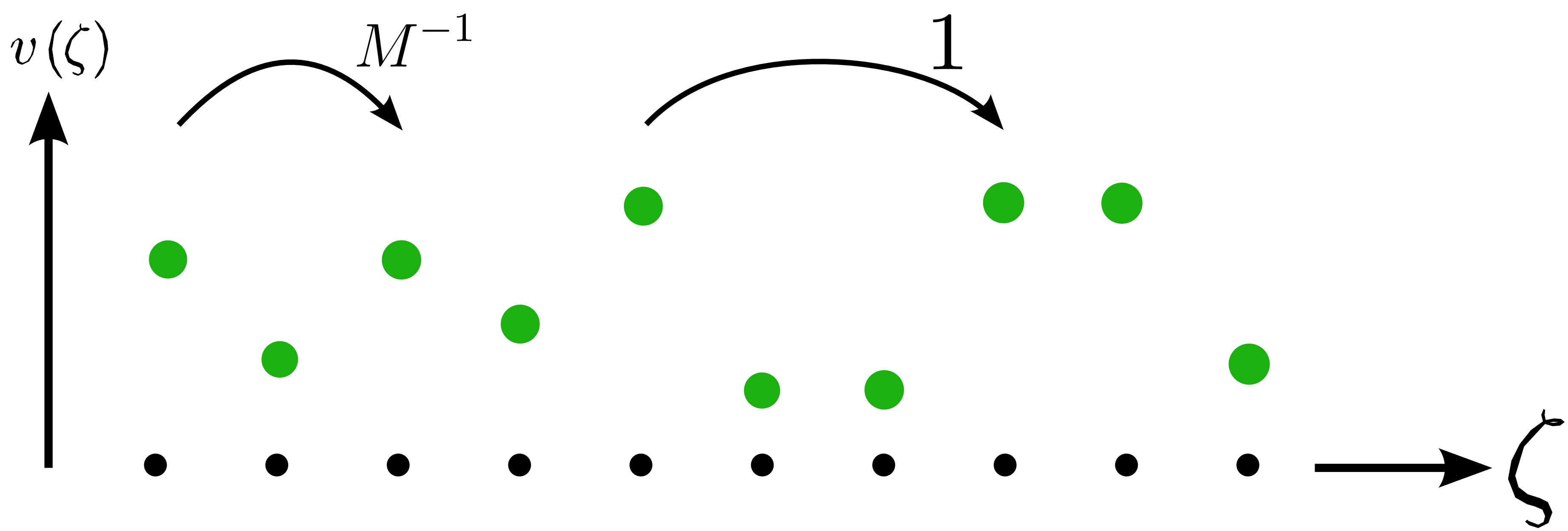
- Compares **resolvents** of linear operators $\mathcal{A}$ and $\mathcal{A}_M$ assuming that $\sigma(\mathcal{A}_M) \to \sigma(\mathcal{A})$ as $M \to \infty$ **on compact subsets** of $\mathbb{C}$.

- Step A: use weak convergence to pass to a weak limit.

- Step B: recover 'missing' information by exploiting equation.

Step A: Weak Convergence

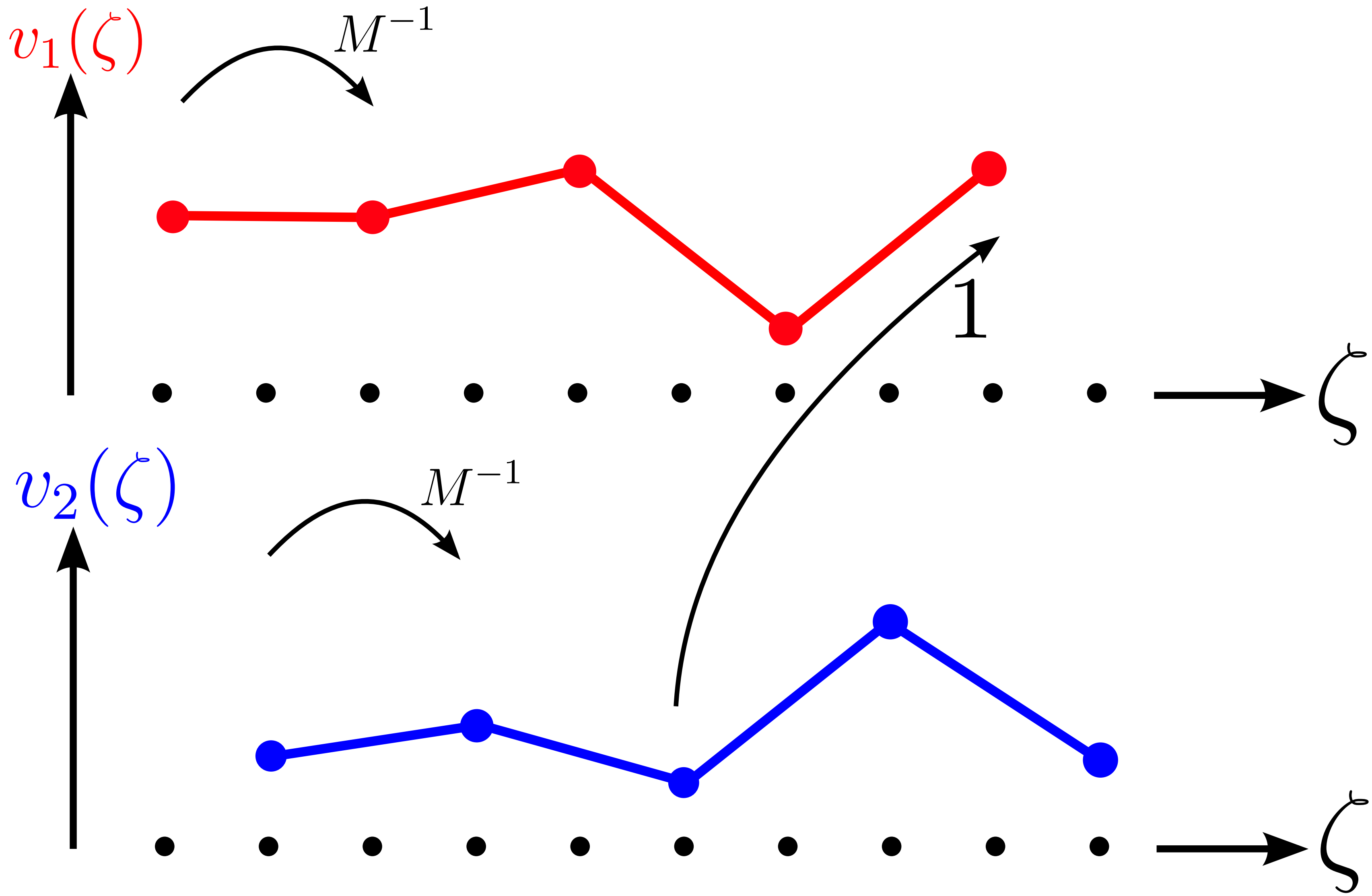
Need to build an H^1-function from sequence



Here $M = \frac{3}{2}$ so $\zeta \in \frac{1}{3}\mathbb{Z}$.

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

Step A: Weak Convergence



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

Step B: Missing information

- Bounded sequence of H^1 functions converge (after subsequence) weakly in H^1 and **strongly** on $L^2([a, b])$.
- Weak limit V satisfies limiting problem $\mathcal{L}_* V = 0$.
- Task: rule out $V = 0$.
- Here exploit **bistable** nature of equation plus monotonic structure of discrete Laplacian
- Can show that $\mathcal{D}_{k,M} v$ can not get too big as $M \to \infty$
- This gives lower bound on $L^2([a, b])$ norm of limit V.

The result

Looking for travelling wave (c, v) of form

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

to system

$$c\mathcal{D}_{k,M}\Phi = \Phi(\zeta+1) + \Phi(\zeta-1) - 2\Phi(\zeta) + g_{\mathrm{cub}}\big(\Phi(\zeta); a\big)$$

Thm. [H., Van Vleck] Fix integer $q_* > 1$. There exists $M_* \gg 1$ so that for all $M \geq M_*$ **and** $M = \frac{p}{q}$ **with** $q \leq q_*$ there are **unique** solutions $c_M(a, \vartheta)$ and $v_M(a, \vartheta)$.

- Δt can be recovered via $M^{-1} = c\Delta t$
- Speed $c_M(a, \vartheta) = c_* + O(M^{-1})$
- Periodicity $c_M(a, \vartheta + M^{-1}) = c_M(a, \vartheta)$.
- Monotonicity $\partial_a c_M(a, \vartheta) < 0$.

We have **non-uniqueness** of wave speed c as a function of a **and** a as a function of c provided we can show that $\partial_\vartheta c_M(a, \vartheta) \neq 0$. But this is $O(e^{M^{-1}})$.