UNIVERSITÄT
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Effective dynamics of many-particle systems with dynamical constraint

joint work with Barbara Niethammer *and* Juan J.L. Velázquez

Workshop *From particle systems to differential equations*

WIAS Berlin, 21 February 2012

Contents

Many-particle storage systems

↓ *Modelling (thermodynamics group at WIAS)*

Nonlocal Fokker-Planck equations with two small parameters

↓ *Asymptotic Analysis (this talk)*

Effective ODEs for small parameter limits

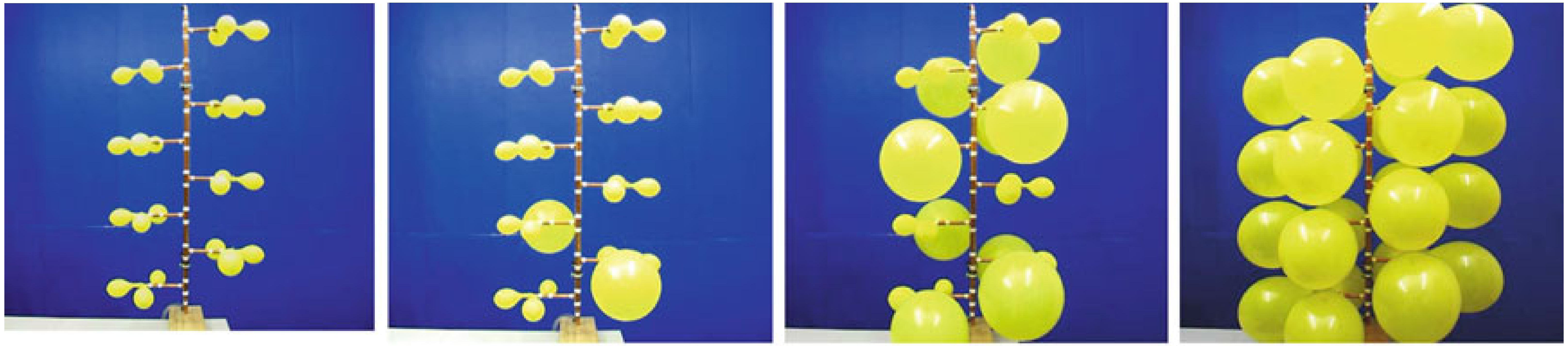
Fast reaction regime via Kramers' formula for large deviations

Slow reaction regime via regular transport and singular events

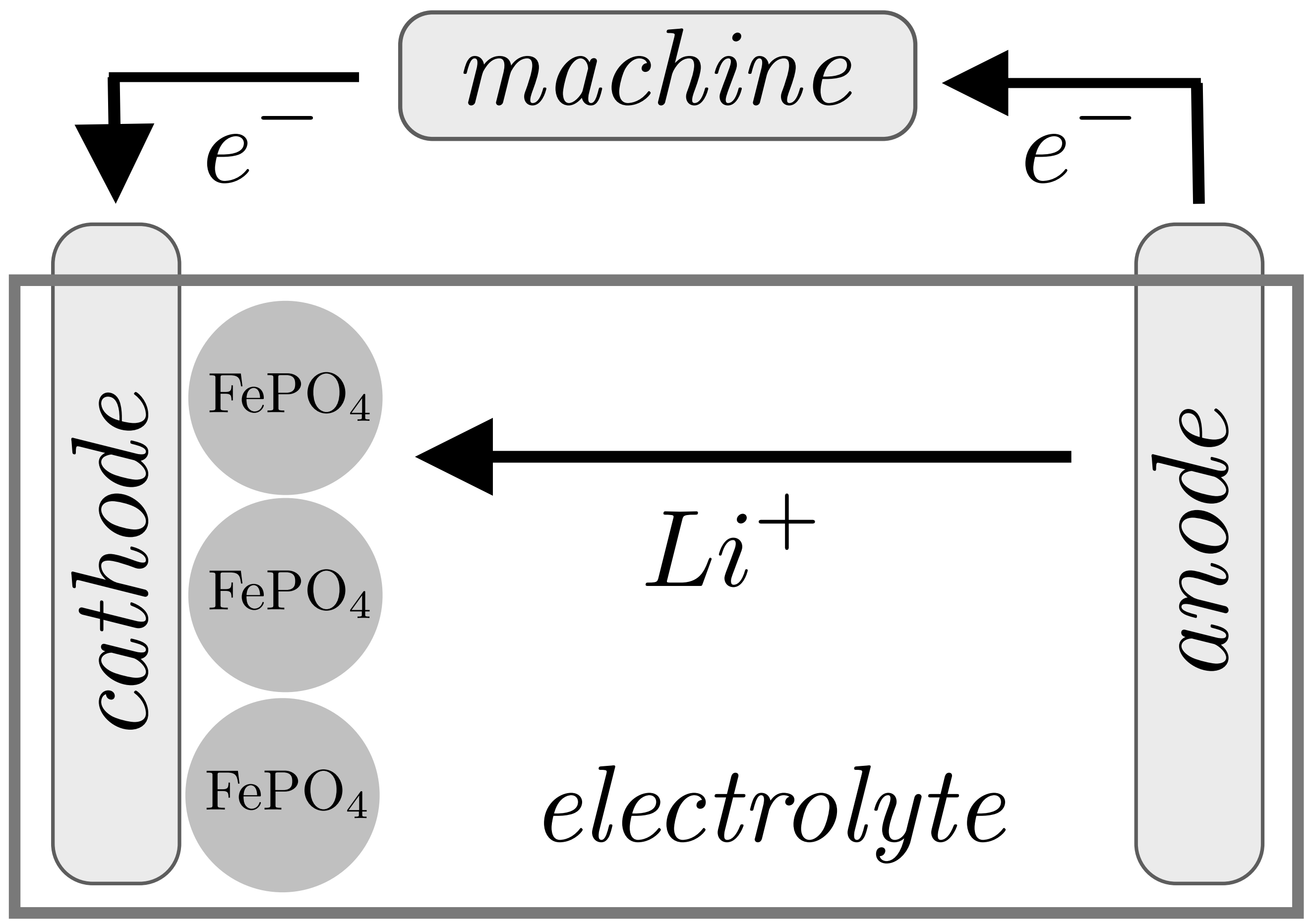
Many-particle storage systems

1. Interconnected rubber balloons

pictures taken by Clemens Guhlke (WIAS)



2. Lithium-ion batteries



Key features

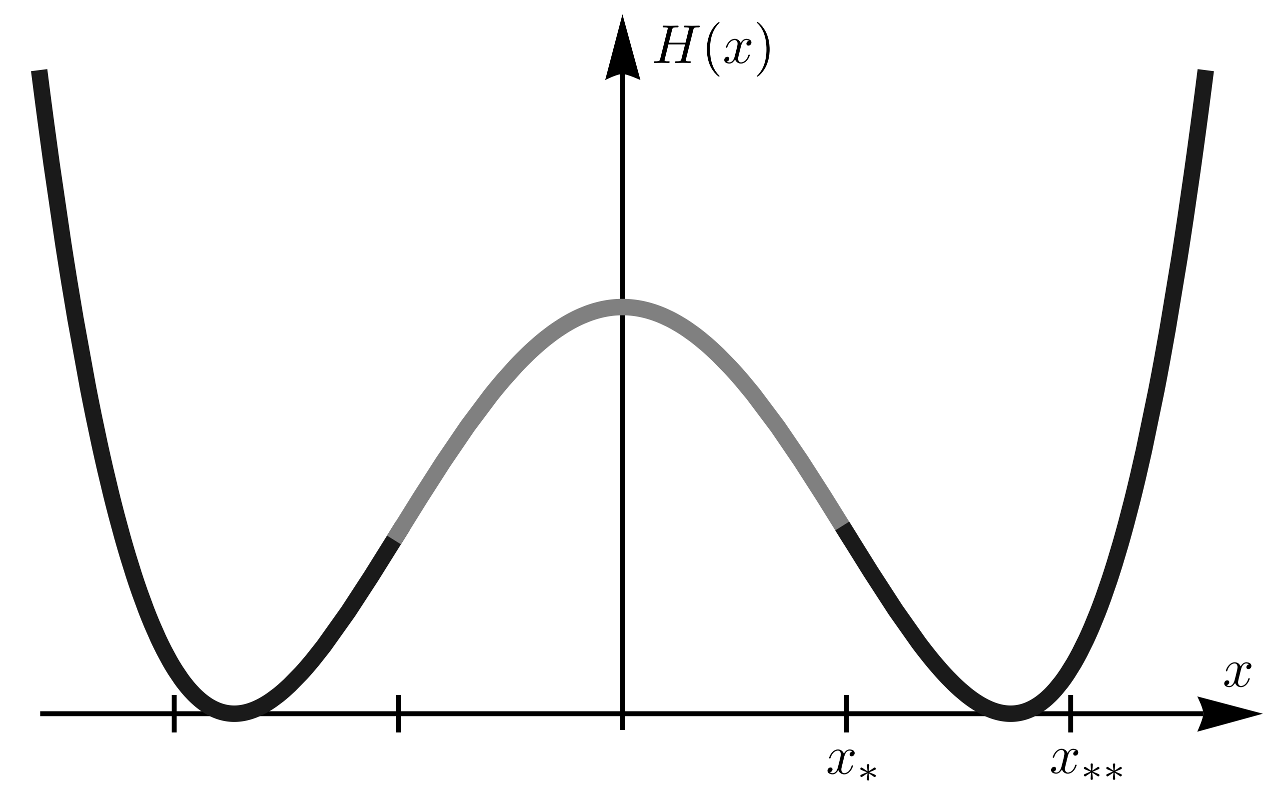
- *fast relaxation* to local equilibrium
- free energy of single-particle system is *double-well potential*
- moment of the many-particle system is controlled (*dynamical constraint*)

First guess for model

simple gradient flow $\tau \dot{x}_i(t) = \sigma(t) - H'\big(x_i(t)\big)$

dynamical constraint $N^{-1} \sum_{i=1}^{N} x_i(t) = \ell(t)$

nonlocal multiplier $\sigma(t) = N^{-1} \sum_{i=1}^{N} H'\big(x_i(t)\big) + \tau \dot{\ell}(t)$



Problem Macroscopic evolution is ill-posed !

Remedy Take into account entropic effects !

Quenched Disorder

Boltzmann Entropy

Mielke & Truskinovsky (ARMA 2012)

non-local Fokker-Planck eqautions

Nonlocal Fokker-Planck equations

more details in Dreyer, Guhlke, Herrmann (CMAT 2011)

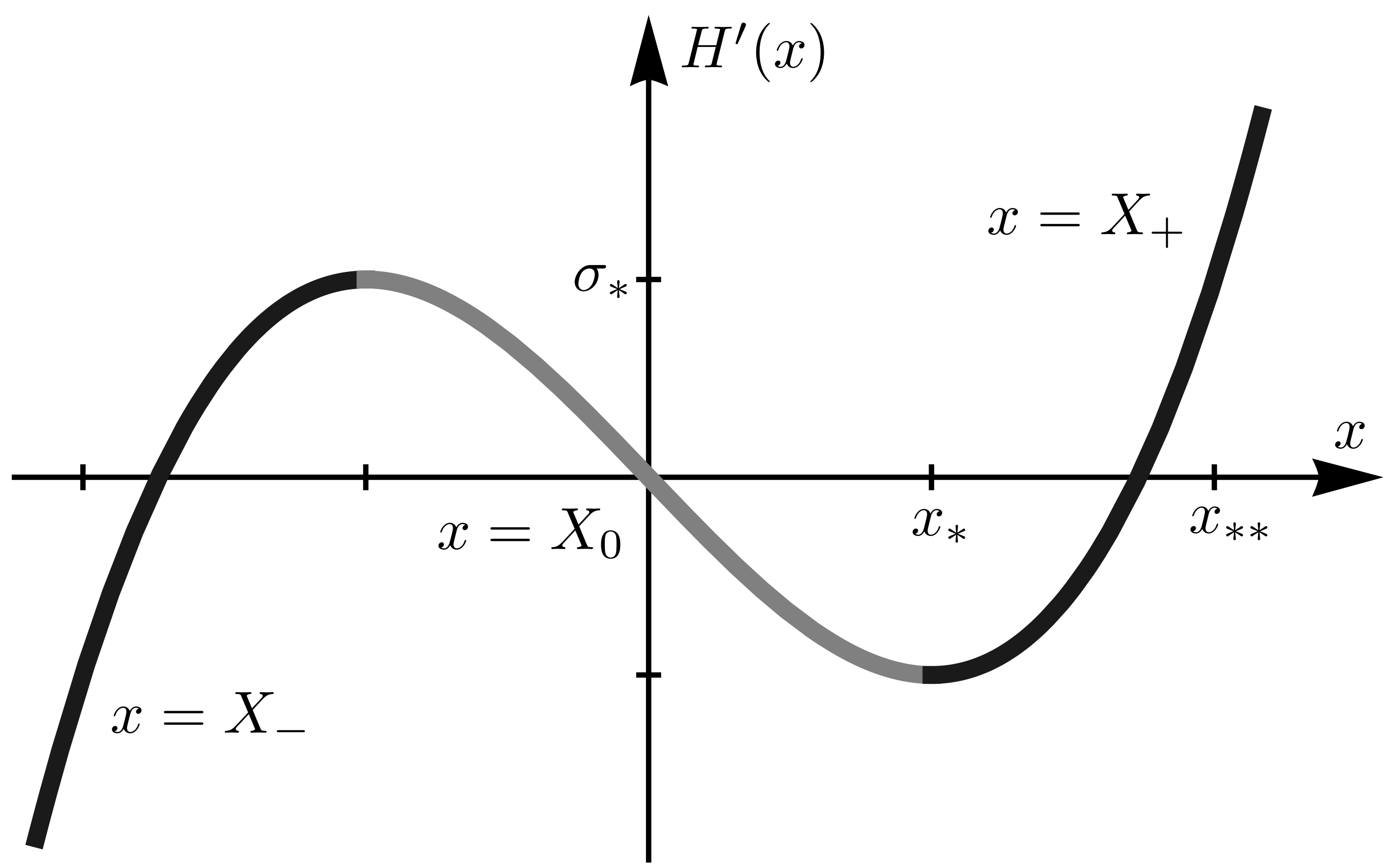
relaxation time *entropy* *dynamical multiplier*

$$\tau \partial_t \varrho = \partial_x \left(\nu^2 \partial_x \varrho + \big(H'(x) - \sigma(t) \big) \varrho \right)$$

$$\int_{\mathbb{R}} x \varrho(x,t) \mathrm{d}x = \ell(t)$$

dynamical constraint

$$\sigma(t) = \int_{\mathbb{R}} H'(x) \varrho(x,t) \mathrm{d}x + \tau \dot{\ell}(t)$$



stable interval *unstable interval* *stable interval*

3 Time scales

$$\tau \partial_t \varrho = \partial_x \left(\nu^2 \partial_x \varrho + \big(H'(x) - \sigma(t) \big) \varrho \right)$$

Goal Understand small parameter dynamics !

$$\tau, \nu \to 0$$

Different times scales:

- relaxation time of single particle system
  (relaxation to metastable state)

  $$\tau$$

- 'chemical reactions' (Kramers' formula)
  (relaxation to equilibrium)

  $$\tau \exp\left(\frac{\triangle H}{\nu^2}\right)$$

- dynamical constraint

  $$\dot{\ell} = O(1)$$

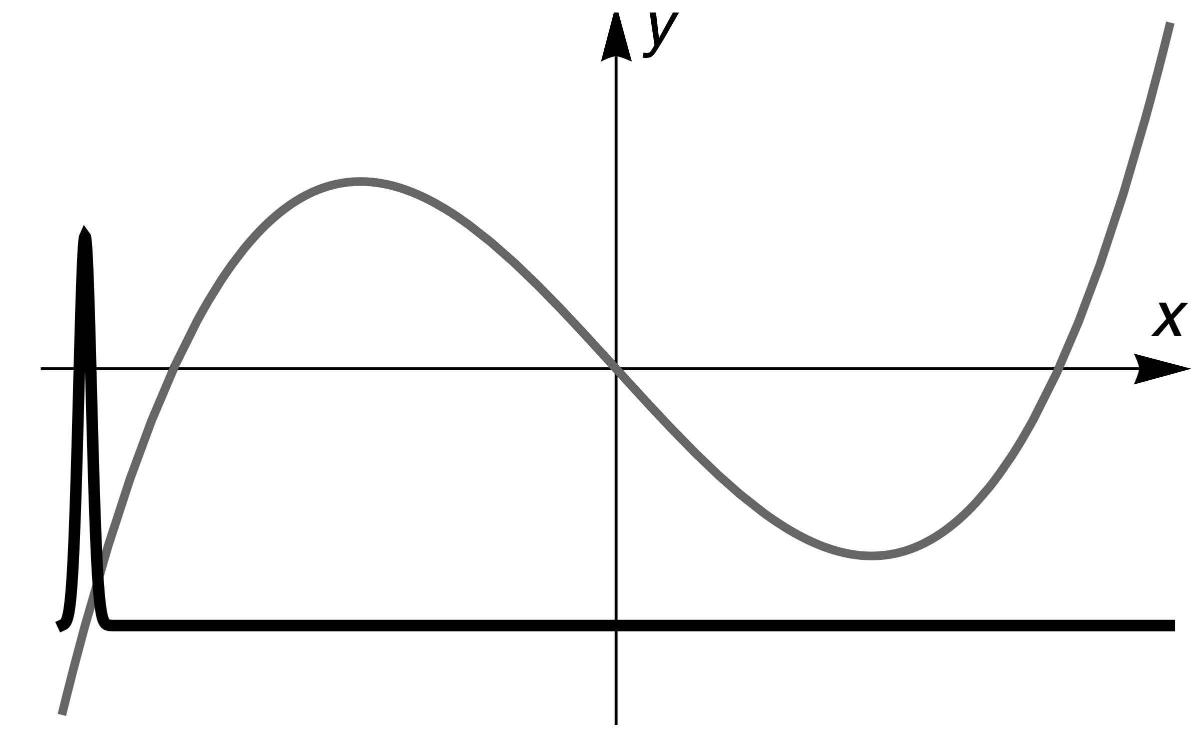
Overview on different scaling regimes

Simple initial value problems

simplifying assumptions

$$\boxed{\dot{\ell} > 0}$$

$$\boxed{\ell(0) < -x_{**},} \qquad \varrho(x,0) \approx \delta_{\ell(0)}(x)$$



macroscopic output

$$t \mapsto \big(\ell(t), \eta(t)\big), \qquad t \mapsto \big(\ell(t), \mu(t)\big)$$

stress-strain relation — *phase-fraction - strain relation*

mean force $$\eta(t) = \int_{\mathbb{R}} H'(x)\varrho(x,t)\mathrm{d}x \;= \sigma(t) - \tau\dot{\ell}$$

phase fraction $$\mu(t) = -\int_{-\infty}^{0} \varrho(x,t)\mathrm{d}x + \int_{0}^{+\infty} \varrho(x,t)\mathrm{d}x$$

Numerical simulations - macroscopic view

slow reactions

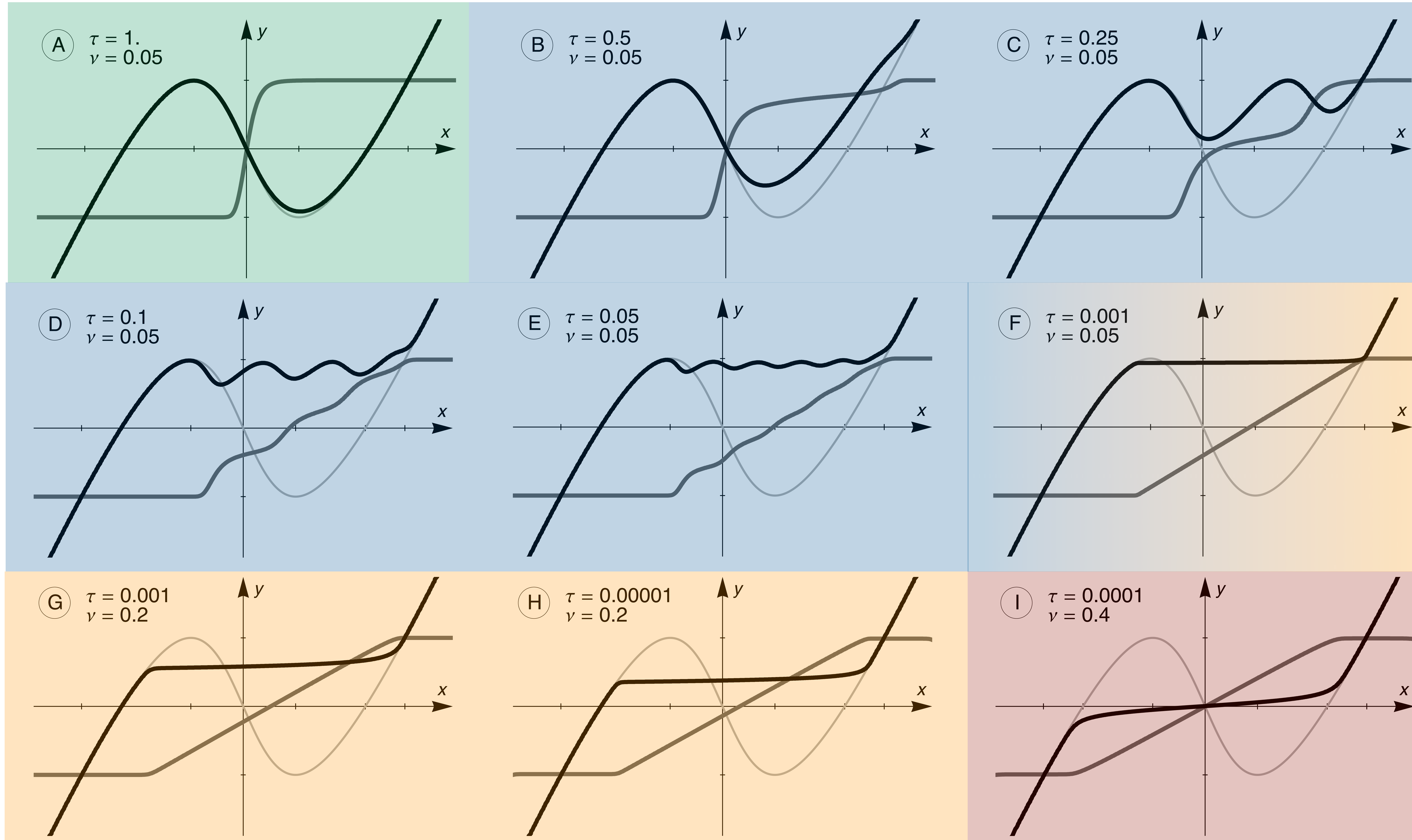
Type I

Type II

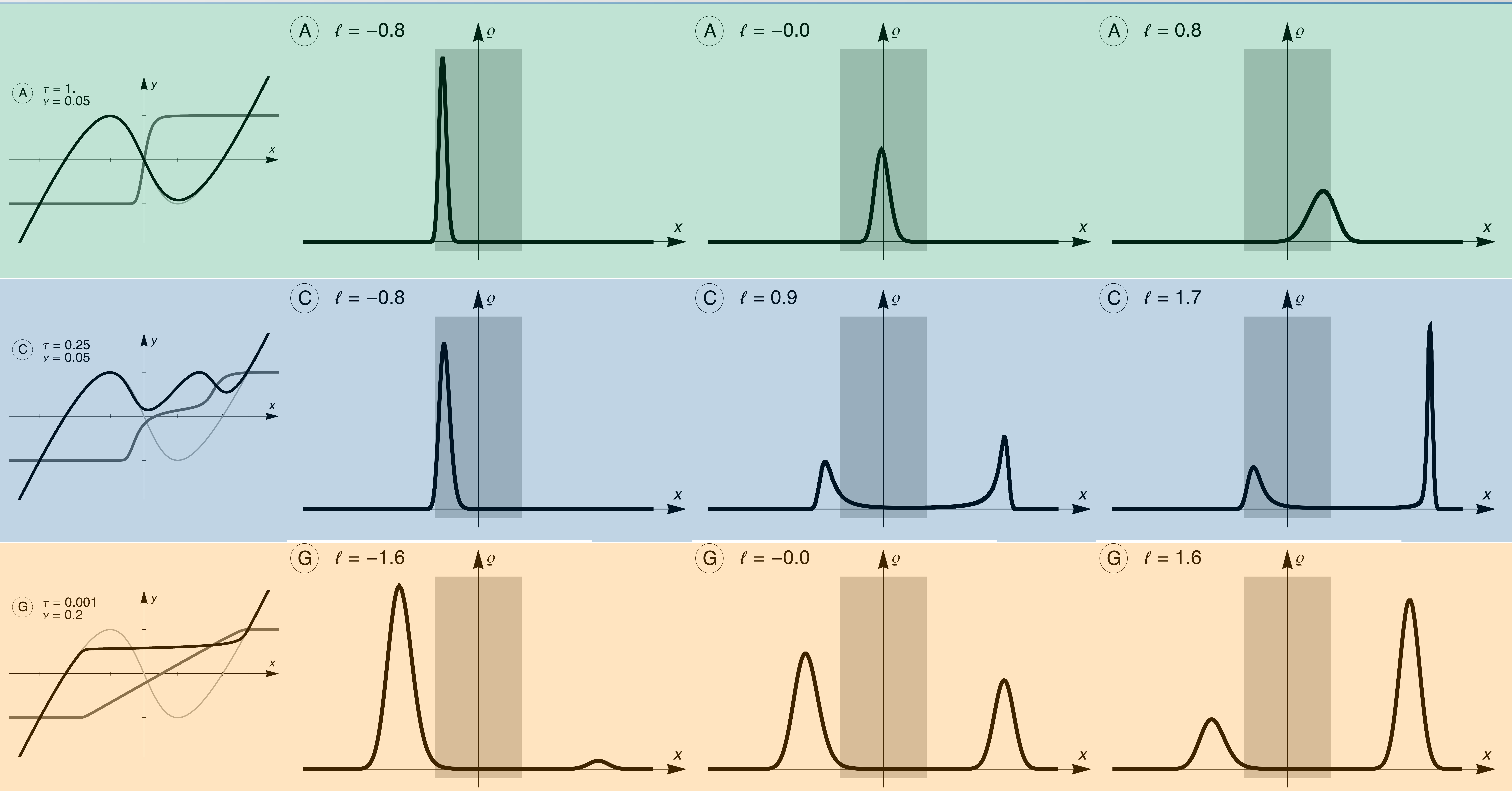
fast reactions

Type III

Type IV



Numerical simulations - microscopic view

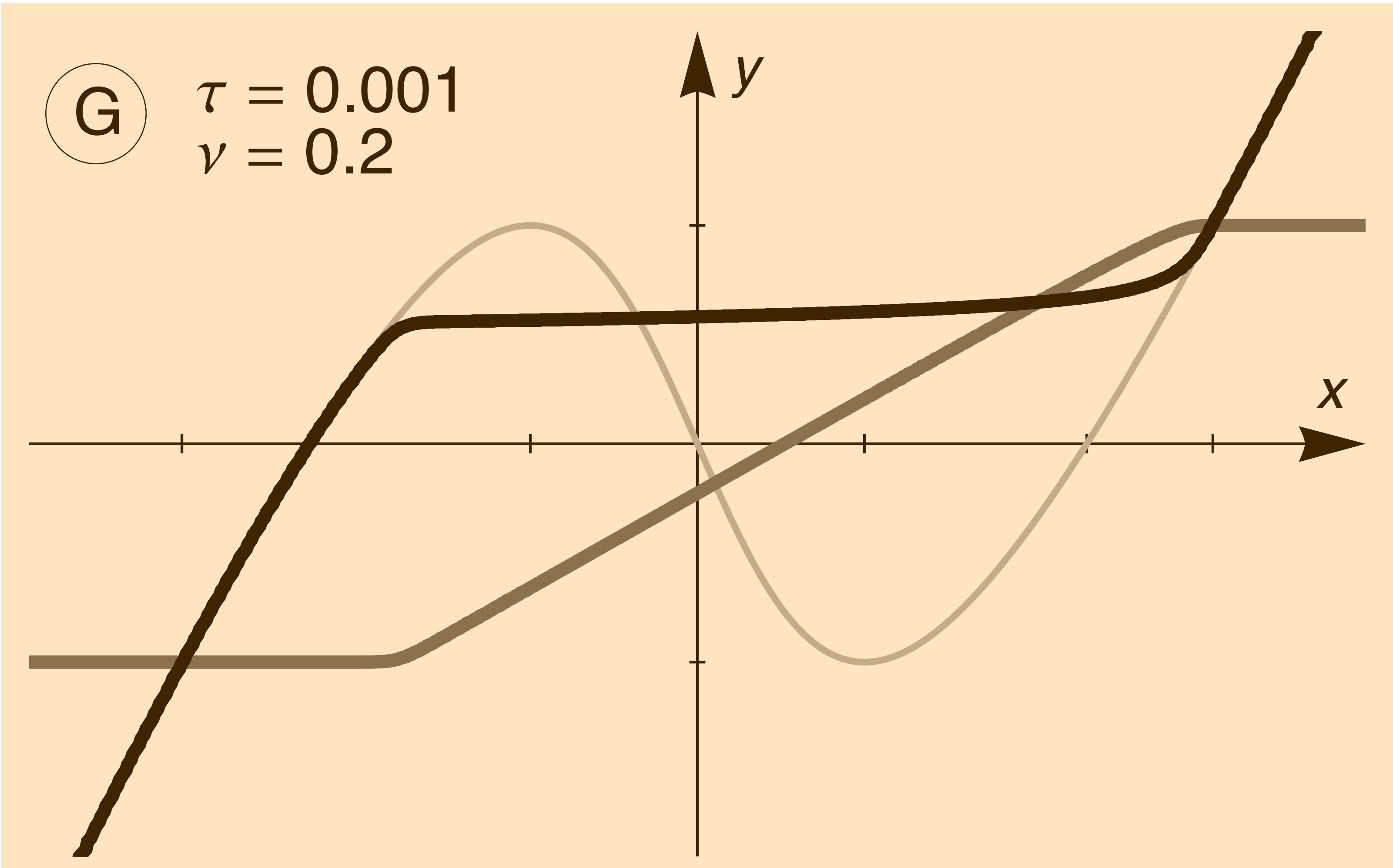


Scaling regimes for parameters

$\tau, \nu \to 0$

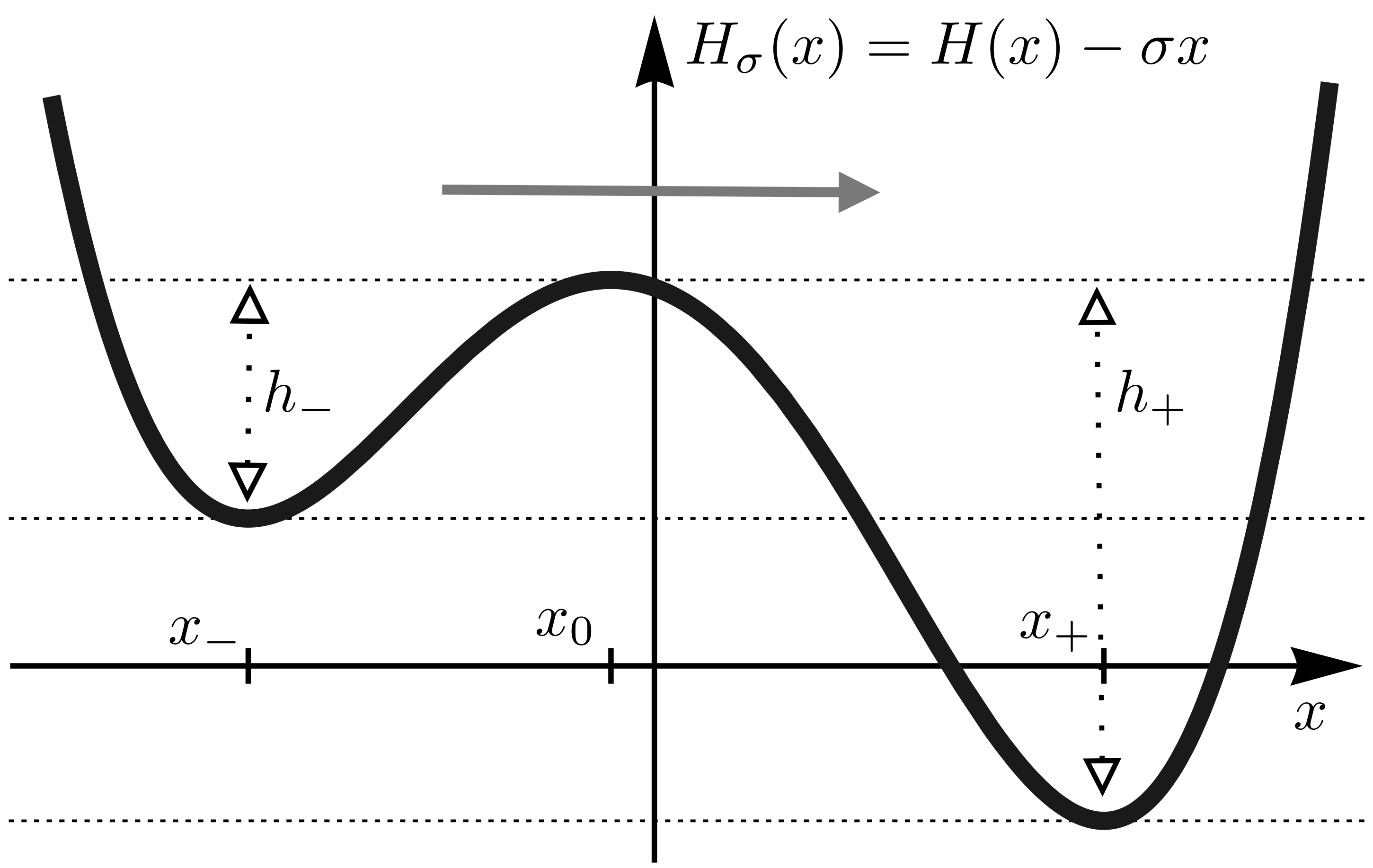
$\tau \log 1/\nu \to \infty$		single-peak evolution
$\tau = \dfrac{a}{\log 1/\nu}$	$0 < a < a_{\mathrm{crit}}$	piecewise continuous two-peaks evolution
$\tau = \nu^p$	$0 < p < 2/3$	open problem
$\tau = \nu^p$	$2/3 < p < \infty$	limit of Kramers' formula
$\tau = \exp\left(-\dfrac{b}{\nu^2}\right),$	$0 < b < b_{crit}$	Kramers' formula
$\nu^2 \log 1/\tau \to \infty$		quasi-stationary limit

Kramers' formula and Type-II transitions



$$\tau = \exp\left(-\frac{b}{\nu^2}\right)$$

Kramers formula



particles can cross the energy barrier due to stochastic fluctuations (*large deviations*, *tunneling*)

Kramers' formula provides mass flux between wells

$$\boxed{\text{time scale} = \tau \exp\left(\frac{+\triangle H_\sigma}{\nu^2}\right) = \tau \exp\left(\frac{\min\{h_-, h_+\}}{\nu^2}\right)}$$

Observation For $\tau = \exp(-b/\nu^2)$ there exists σ_b, such that

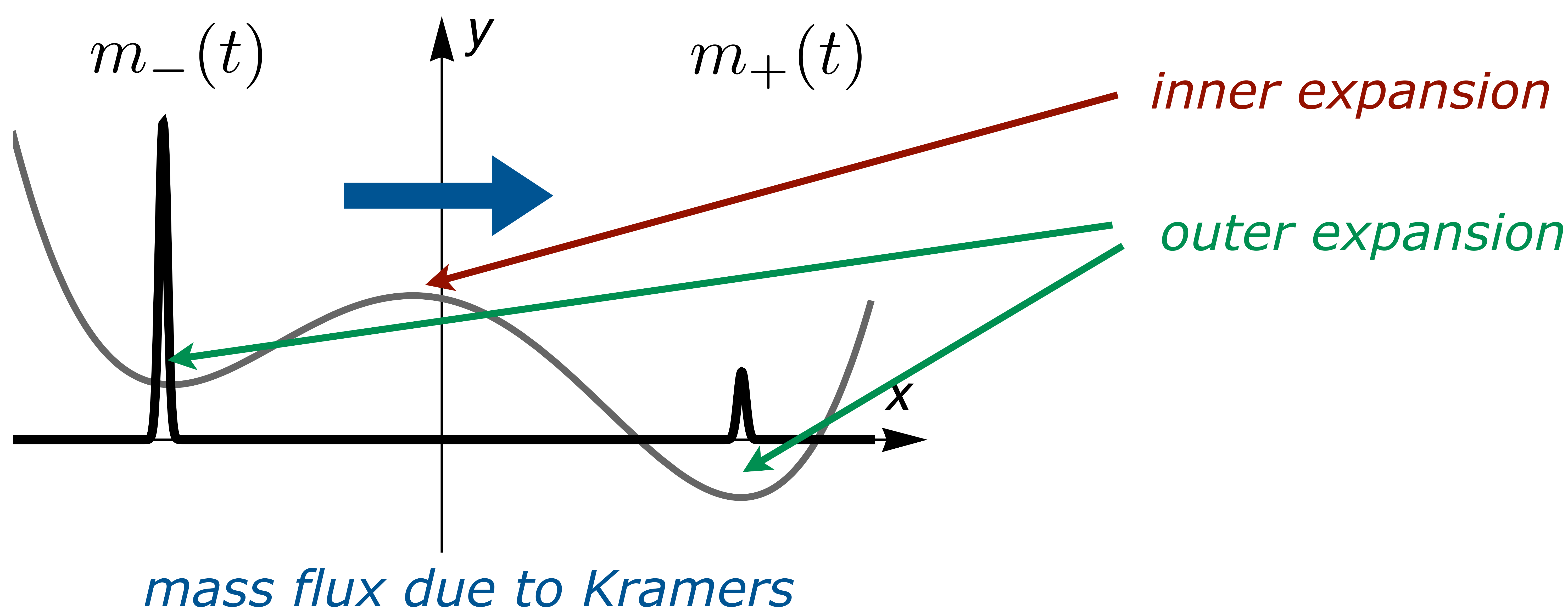
(1) mass flux is of order 1 provided that $\sigma(t) = \sigma_b + \nu^2 \psi(t)$

(2) small fluctuations of σ are sufficient to satisfy the constraint

Inner and outer expansions

Idea (1) for each σ we have three positions x_-, x_0, x_+ with $H'(x_{-/0/+}) = \sigma$

(2) two narrow peaks with masses $m_\pm(t)$ at $x_\pm(t)$



$$\nu^2 \partial_x \varrho + H'_{\sigma(t)}(x)\varrho = \begin{cases} 0 & \text{for} \quad x \approx x_\pm(t)\,, \\ R(t) & \text{for} \quad x \approx x_0(t)\,. \end{cases}$$

outer expansion
inner expansion

Matching of inner and outer expansions

Outer expansion

$$\varrho(x,t) \approx \begin{cases} \mu_-(t)\exp\left(\dfrac{-H_{\sigma(t)}(x)}{\nu^2}\right) & \text{for} \quad x < x_0(t)\,, \\ \mu_+(t)\exp\left(\dfrac{-H_{\sigma(t)}(x)}{\nu^2}\right) & \text{for} \quad x > x_0(t)\,. \end{cases}$$

$$m_\pm(t) = \pm\int_{x_0(t)}^{\pm\infty} \varrho(x,t)\mathrm{d}x \approx c_\pm(t)\mu_\pm(t)\nu\exp\left(-\frac{H_{\sigma(t)}(x_\pm(t))}{\nu^2}\right)$$

Inner expansion

$$\varrho\big(x_0(t)\pm\delta,t\big) \approx \exp\left(-\frac{H_{\sigma(t)}\big(x_0(t)\pm\delta\big)}{\nu^2}\right)\left(C(t) \mp \frac{R(t)}{\nu^2}\exp\left(\frac{H_{\sigma(t)}\big(x_0(t)\big)}{\nu_2}\right)\right)$$

Matching conditions result from equating the time-dependent pre-factors !

Kramers formula for mass flux

$$\boxed{\frac{R(t)}{\tau} = m_-(t) r_-(t) - m_+(t) r_+(t)}$$

$$r_\pm(t) = c_\pm(t) \exp\left(\frac{b - h_\pm(t)}{\nu^2}\right)$$

$$h_\pm(t) = H_{\sigma(t)}(x_0(t)) - H_{\sigma(t)}(x_\pm(t))$$

$$x_i(t) = X_i(\sigma(t))$$

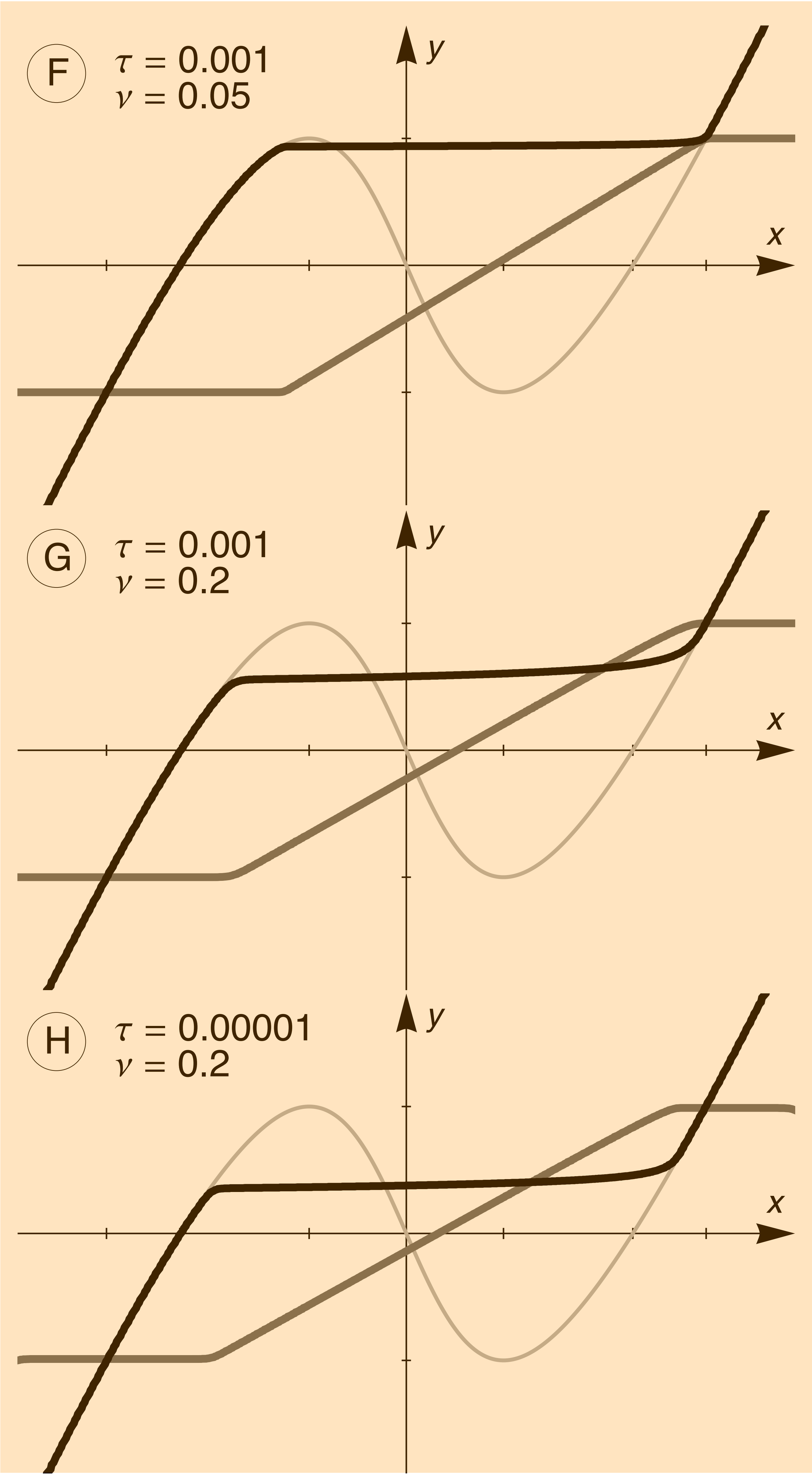
Observation For each $0 < b < b_{crit}$ there exists $0 < \sigma < \sigma_*$ such that

$$\boxed{\begin{array}{lcl} \sigma(t) < \sigma_b & \Longrightarrow & r_-(t) \ll 1 \\ \sigma(t) = \sigma_b + \nu^2 \psi(t) & \Longrightarrow & r_-(t) \sim \exp(\psi(t)) \\ \sigma(t) > \sigma_b & \Longrightarrow & r_-(t) \gg 1 \end{array}}$$

$$|r_+(t)| \ll 1 \quad \text{if} \quad \sigma > 0$$

Strategy Adjust ψ according to dynamical constraint

Main result for fast reactions



Main result. *Suppose that the dynamical constraint and the initial data satisfies* (4) *and* (5), *and that* τ *and* ν *are coupled by*

$$\tau = \exp\left(-\frac{b}{\nu^2}\right)$$

for some constant $b \in (0,\, h_{\mathrm{crit}})$. *Then there exists a constant* $\sigma_b \in (0,\, \sigma_*)$ *such that*

1. *the dynamical multiplier satisfies*

$$\sigma(t) \quad \xrightarrow{\nu \to 0} \quad \begin{cases} H'\big(\ell(t)\big) & \text{for} \quad t < t_1\,, \\ \sigma_b & \text{for} \quad t_2 < t < t_2\,, \\ H'\big(\ell(t)\big) & \text{for} \quad t > t_2 \end{cases}$$

where t_1 *and* t_2 *are uniquely determined by* $\ell(t_1) = X_-(\sigma_b)$ *and* $\ell(t_2) = X_+(\sigma_b)$,

2. *the state of the system satisfies*

$$\varrho(x,\, t) \quad \xrightarrow{\nu \to 0} \quad m_-(t)\delta_{X_-(\sigma(t))}(x) + m_+(t)\delta_{X_+(\sigma(t))}(x)\,.$$

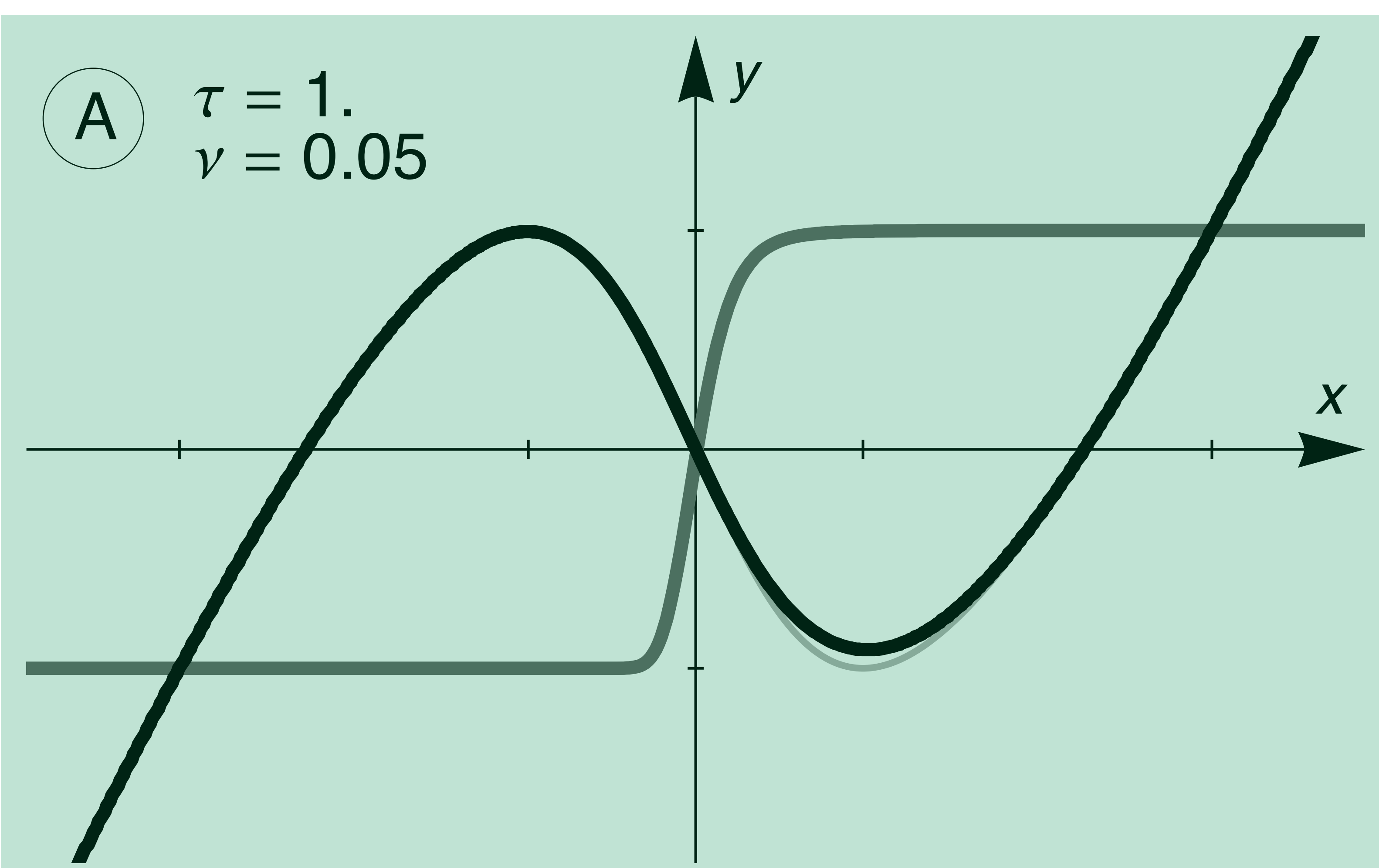
where $m_+(t) = 1 - m_-(t)$ *and*

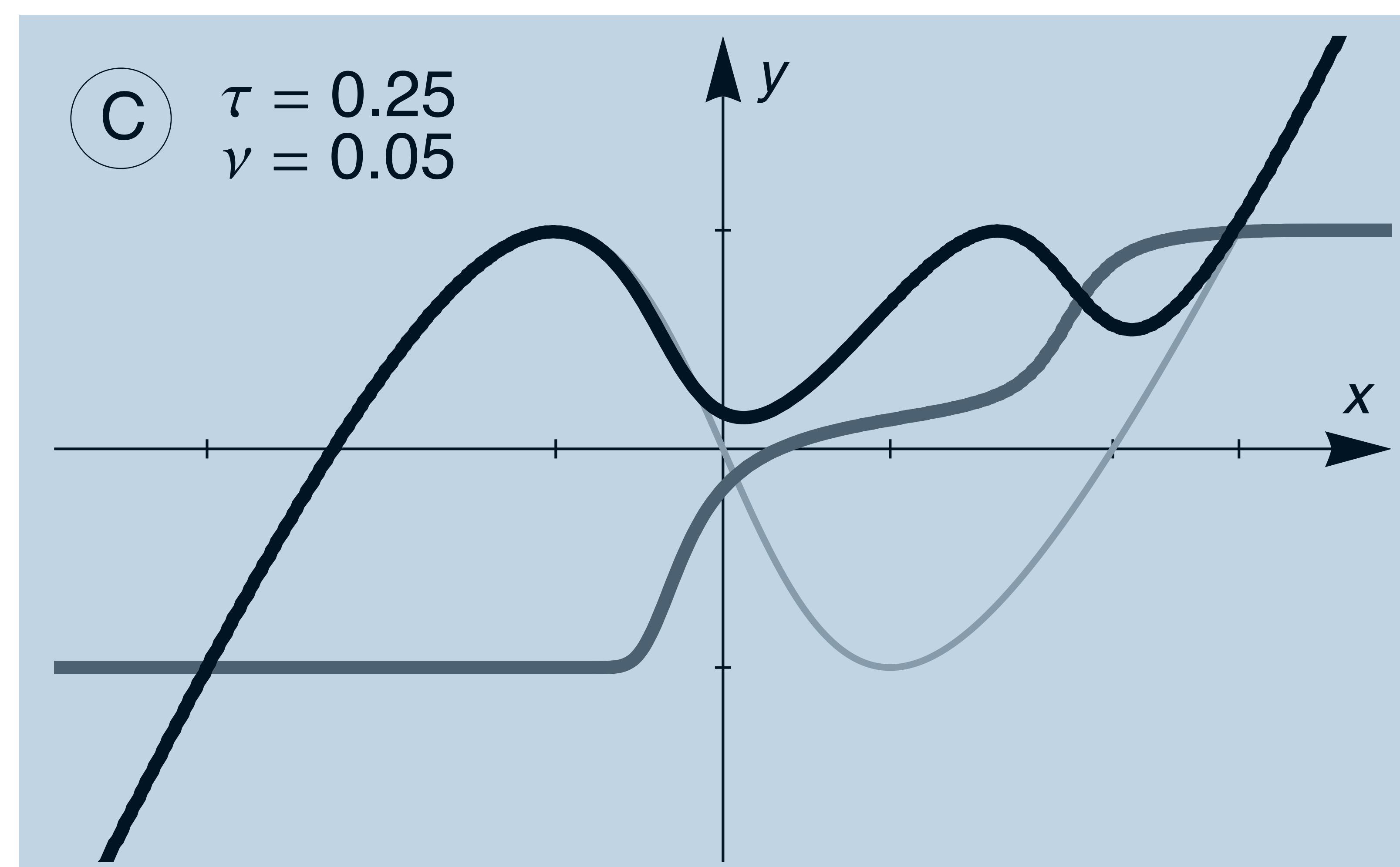
$$m_-(t) = \begin{cases} 1 & \text{for} \quad t < t_1\,, \\ \dfrac{X_+(\sigma_b) - \ell(t)}{X_+(\sigma_b) - X_-(\sigma_b)} & \text{for} \quad t_1 < t < t_2\,, \\ 0 & \text{for} \quad t > t_2\,. \end{cases}$$

Moreover, the assertions remain true

1. *with* $\sigma_b = 0$ *if* $\tau \leq \exp\left(-\frac{h_{\mathrm{crit}}}{\nu^2}\right)$,
2. *with* $\sigma_b = \sigma_*$ *if* $\tau \ll \nu^{\frac{2}{3}}$ *but* $\tau > \exp\left(-\frac{b}{\nu^2}\right)$ *for all* $b > 0$.

Slow reaction limit: Type-I/II transitions

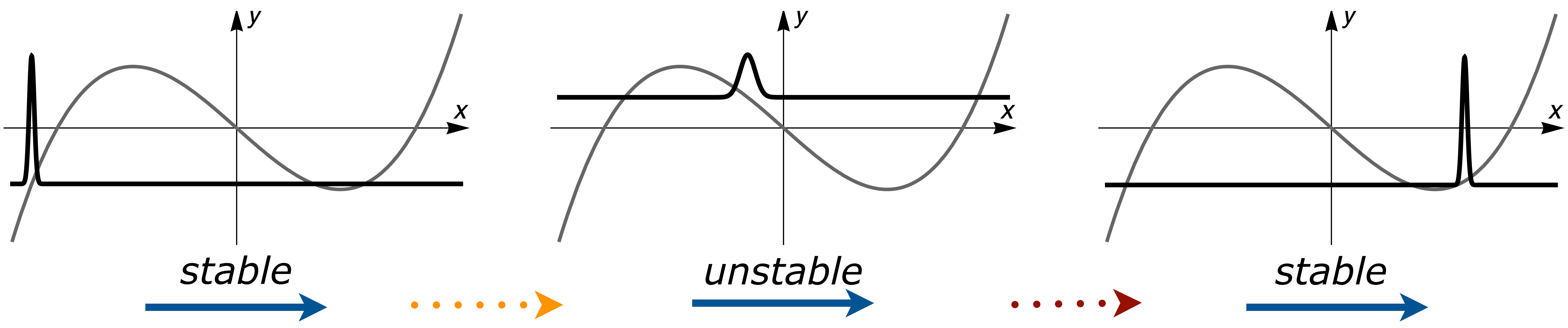




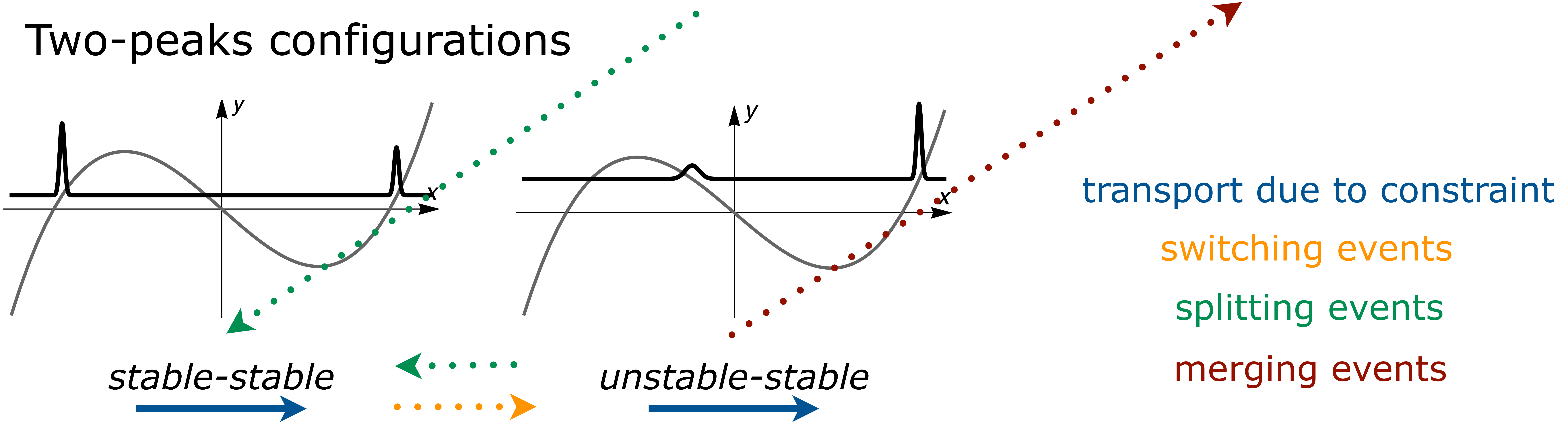
$$\nu = \exp\left(-\frac{a}{\tau}\right)$$

Overview - states for increasing constraints

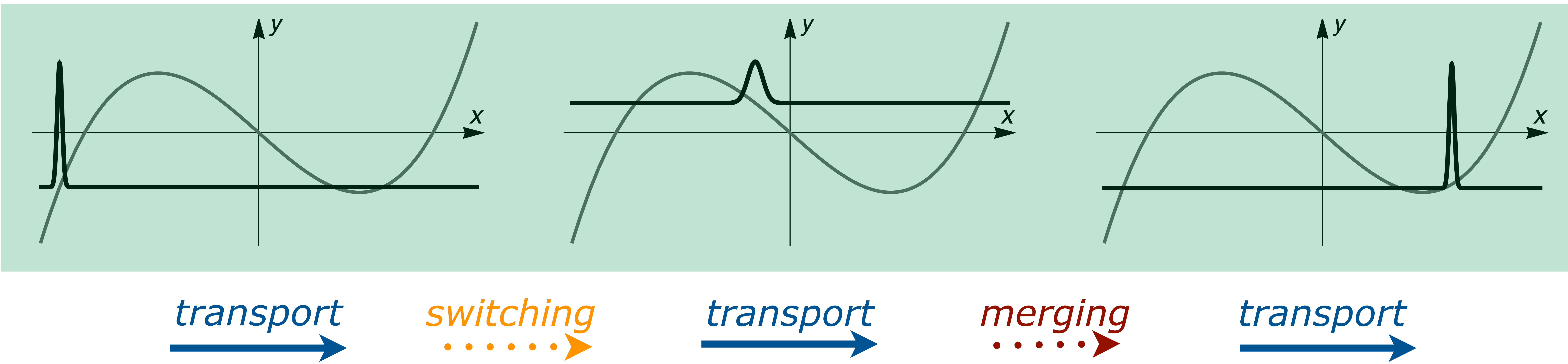
Single-peak configurations



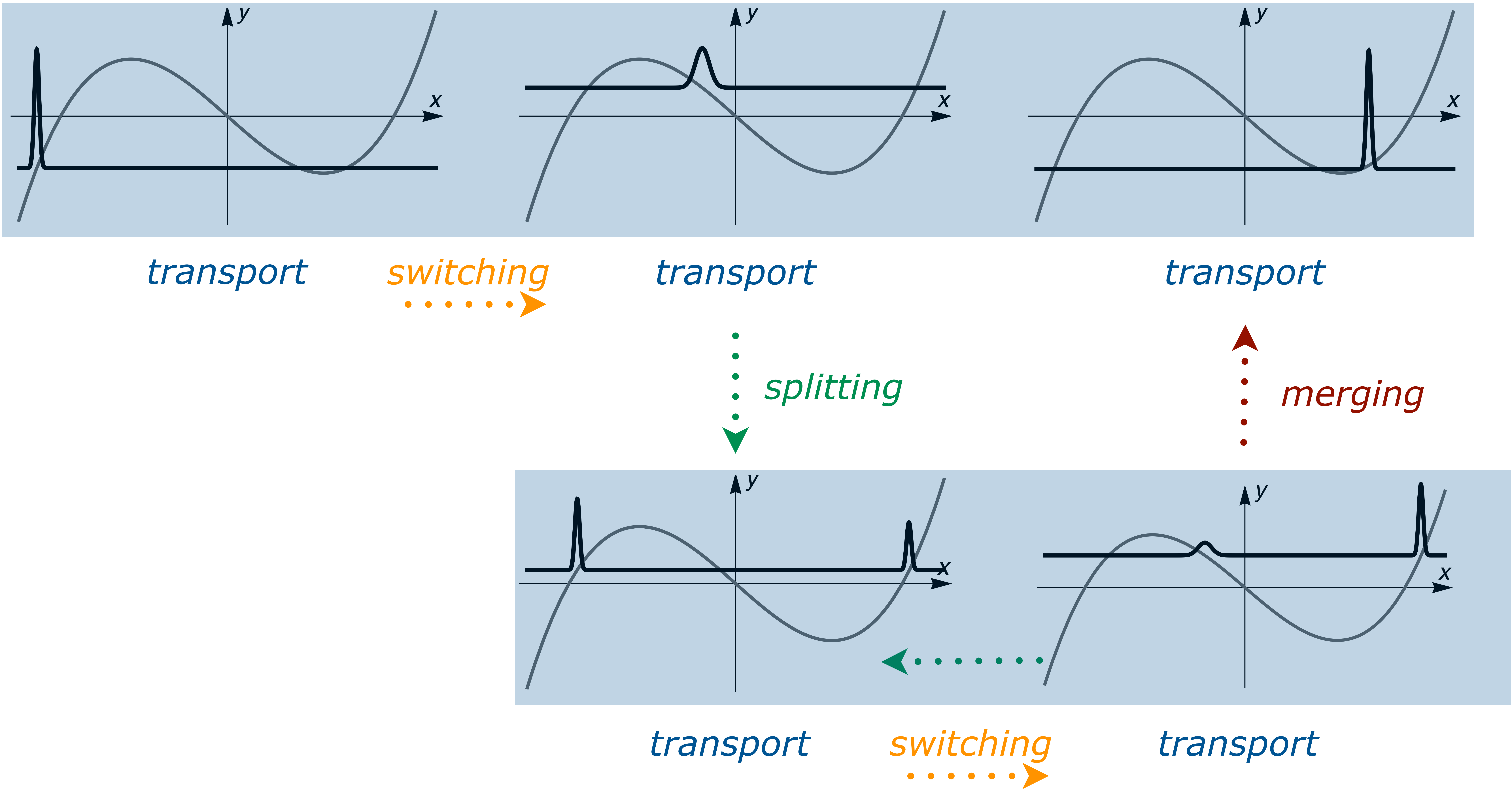
Two-peaks configurations



Overview - Type-I phase transitions



Overview - Type-II phase transitions



Overview - Simplified models

transport

localised peaks move due to the constraint

switching

stable peaks enter unstable interval

merging

unstable peaks merge rapidly with stables ones

splitting

unstable peaks split rapidly into two stables ones

two-peaks ODE

peak-widening model

mass-splitting problem

two-peaks approximation

transport, switching, and merging of peaks

Two-peaks approximation to FP

Dynamical model

$$\boxed{\begin{aligned} \tau \dot{x}_1 &= \sigma - H'(x_1) \\ \tau \dot{x}_2 &= \sigma - H'(x_2) \\ \sigma &= m_1 H'(x_1) + m_2 H'(x_2) + \tau \dot{\ell} \end{aligned}}$$

$$\begin{aligned} m_1 + m_2 &= 1 \\ \dot{m}_i &= 0 \end{aligned}$$

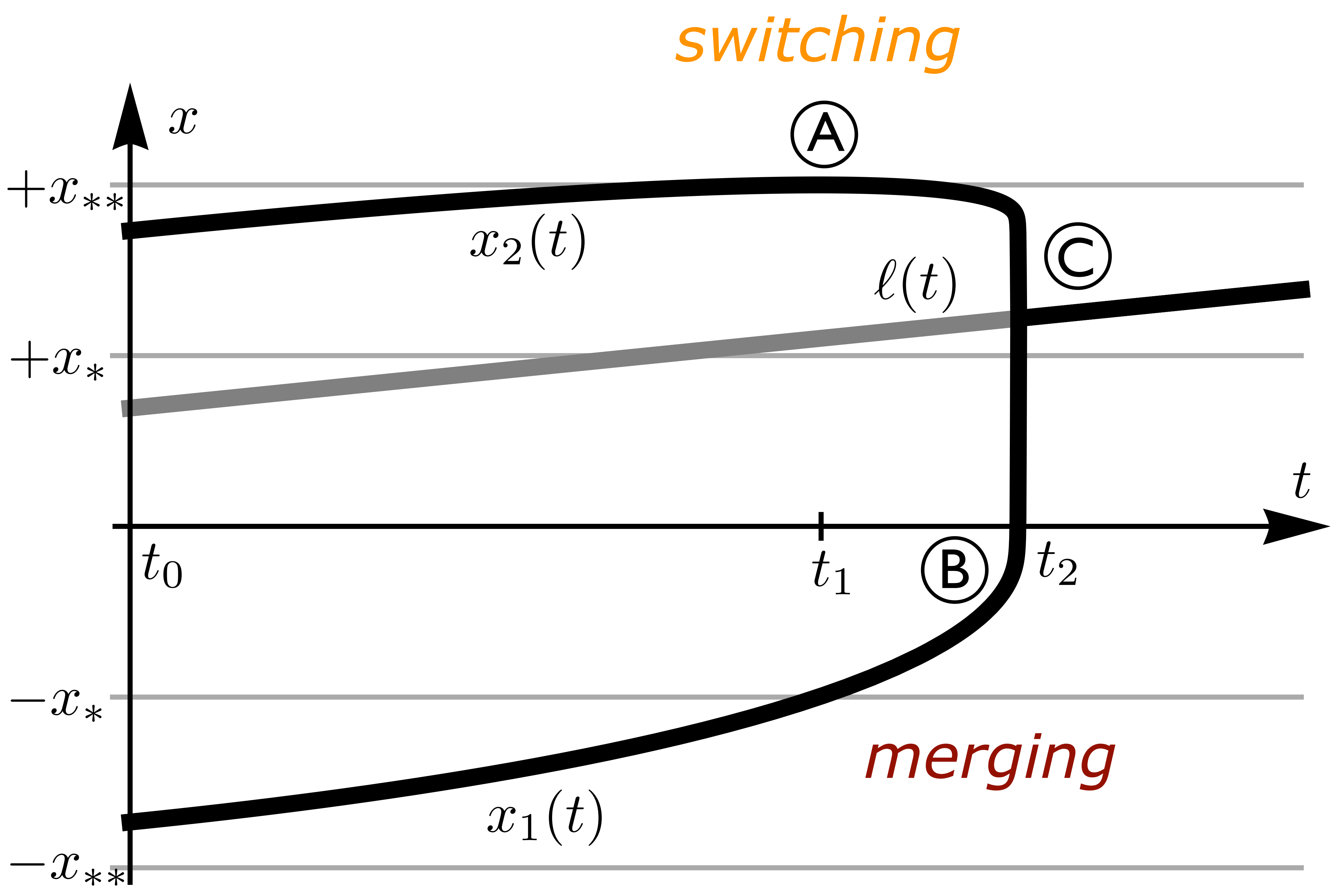
Quasi-stationary limit

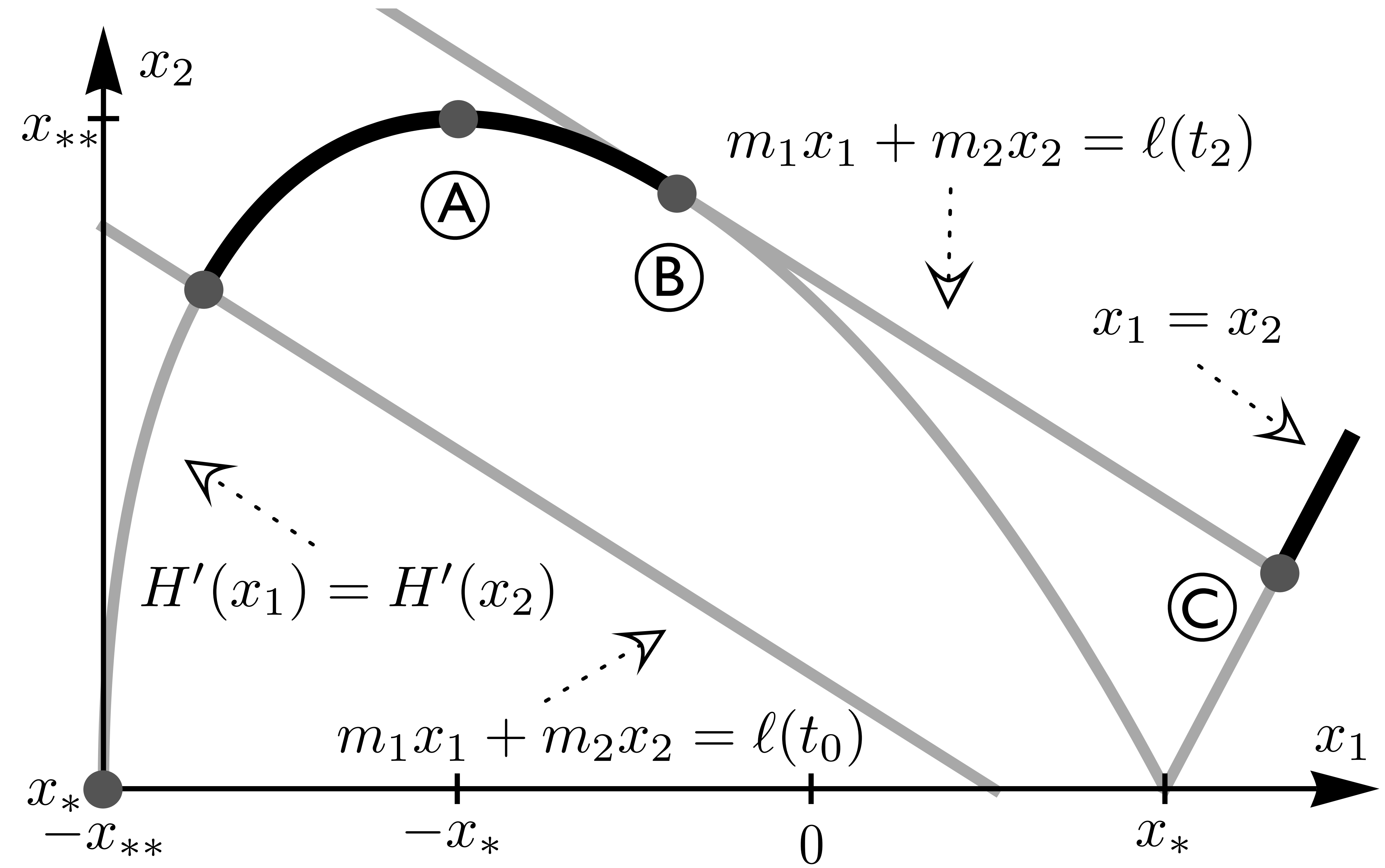
$$\tau \to 0$$

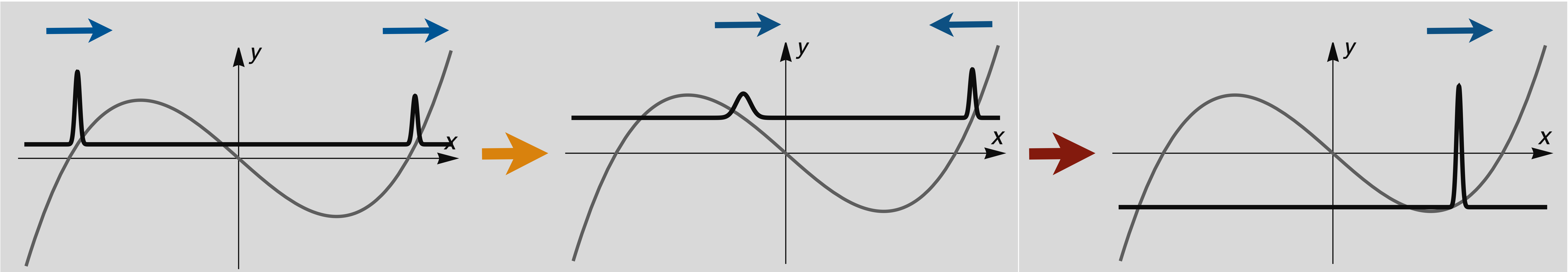
$$\boxed{\begin{aligned} H'(x_1) &= H'(x_2) \\ m_1 x_1 + m_2 x_2 &= \ell \end{aligned}}$$

Multiple solution branches ! Which ones are selected by dynamics ?

Two-peaks approximation to FP





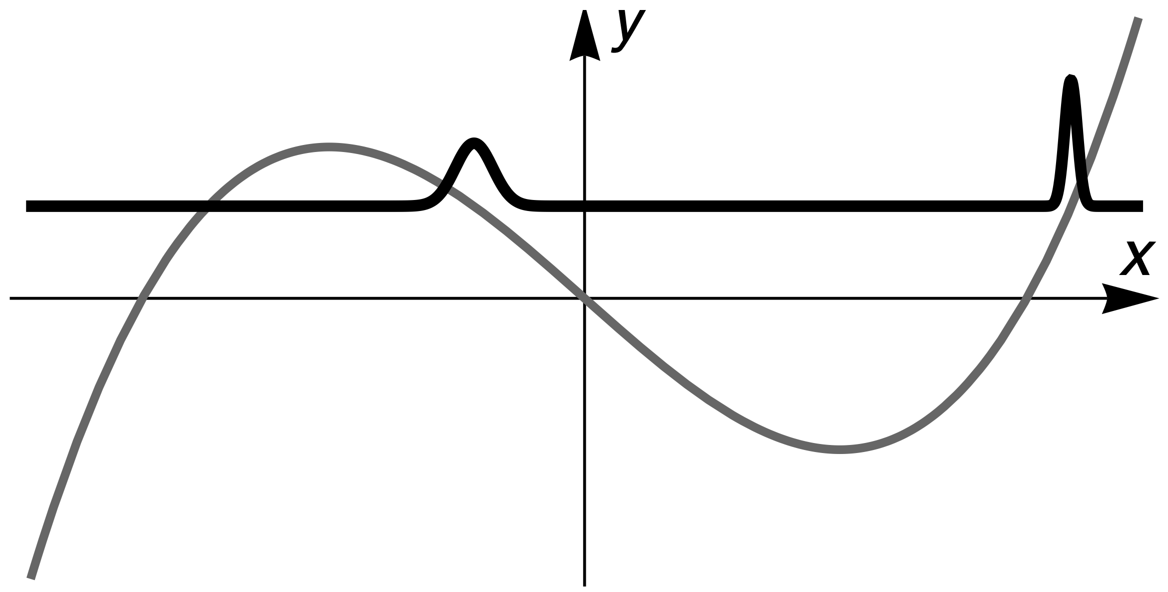


entropic effects

widening and splitting of unstable peaks

- peak-widening model: width of unstable peaks blows up (almost) instantaneously, determines splitting time
- mass splitting problem: system forms (almost) instantaneously two stable peaks determines jump of the system

Peak-widening model



$$\varrho = m_1 \hat\varrho + m_2 \delta_{x_2}$$
$$\ell = m_1 \int_{\mathbb{R}} x \hat\varrho \, \mathrm{d}x + m_2 x_2$$

$$\boxed{\begin{aligned} \tau \partial_t \hat\varrho &= \partial_x \left(\nu^2 \partial_x \hat\varrho + \big(H'(x) - \sigma \big) \hat\varrho \right) \\ \tau \dot x_2 &= \sigma - H'(x_2) \\ \sigma &= m_1 \int_{\mathbb{R}} H'(x) \hat\varrho \mathrm{d}x + m_1 H'(x_2) + \tau \dot\ell \end{aligned}}$$

position of peak

$$\boxed{\tau \dot x_1 = \sigma - H'(x_1)}$$

width of peak

$$\boxed{w(t) = \nu \lambda(t) W\big(\theta(t)\big)}$$

$$\hat\varrho(x,t) =: \frac{1}{\nu\lambda(t)} R\left(-\frac{\big(x - x_1(t)\big)^2}{\nu\lambda(t)}, \theta(t) \right)$$

Formula for width of unstable peaks

- define scaling factors
- expand nonlinearity (fine if width is small)

as long as width is small

$$\partial_\theta R = \partial_y^2 R$$

$$R(y,\theta) \approx \frac{1}{\sqrt{4\pi\zeta}} \exp\left(-\frac{y^2}{4\theta}\right), \; W(\theta) \sim \sqrt{\theta}$$

evolution of width

$$\begin{array}{rcl} 0 < t < t_{\mathrm{sw}} & : & w(t) = \mathcal{O}(\nu) \\ t_{\mathrm{sw}} < t < t_{\mathrm{sp}} & : & \nu \ll w(t) \ll 1 \\ t_{\mathrm{sp}} < t & : & w(t) \gg 1 \end{array}$$

$$\int_{t_{sw}}^{t_{sp}} H''\big(x_1(t)\big)\mathrm{d}t + a = 0$$

can be computed by quasi-stationary two-peaks approximation

Mass splitting problem

ansatz

$$\nu = 0, \qquad t = t_{sp} + \tau s$$

$$l(s) = \text{const} = l(t_{sp})$$

$$\boxed{\begin{aligned} \partial_s \hat{\varrho} &= \partial_x \Big(\big(H'(x) - \sigma(s)\big) \hat{\varrho} \Big) \\ \dot{x}_2 &= \sigma(s) - H'(x_2) \\ \sigma(s) &= m_1 \int_{\mathbb{R}} H'(x) \hat{\varrho} \,\mathrm{d}x + m_2 H'(x_2) \end{aligned}}$$

asymptotic initial data

$$\boxed{\hat{\varrho}(x,s) \xrightarrow{s \to -\infty} \frac{1}{2\beta\sqrt{\pi}} \exp\left(- \frac{x - x_1(t_{sw})}{4\exp(2\beta s)} \right),} \qquad \beta = -H''\big(x_1(t_{sw})\big) > 0$$

Mass splitting problem

Conjecture

Data at $s = +\infty$ depend continuously on data at $s = -\infty$.

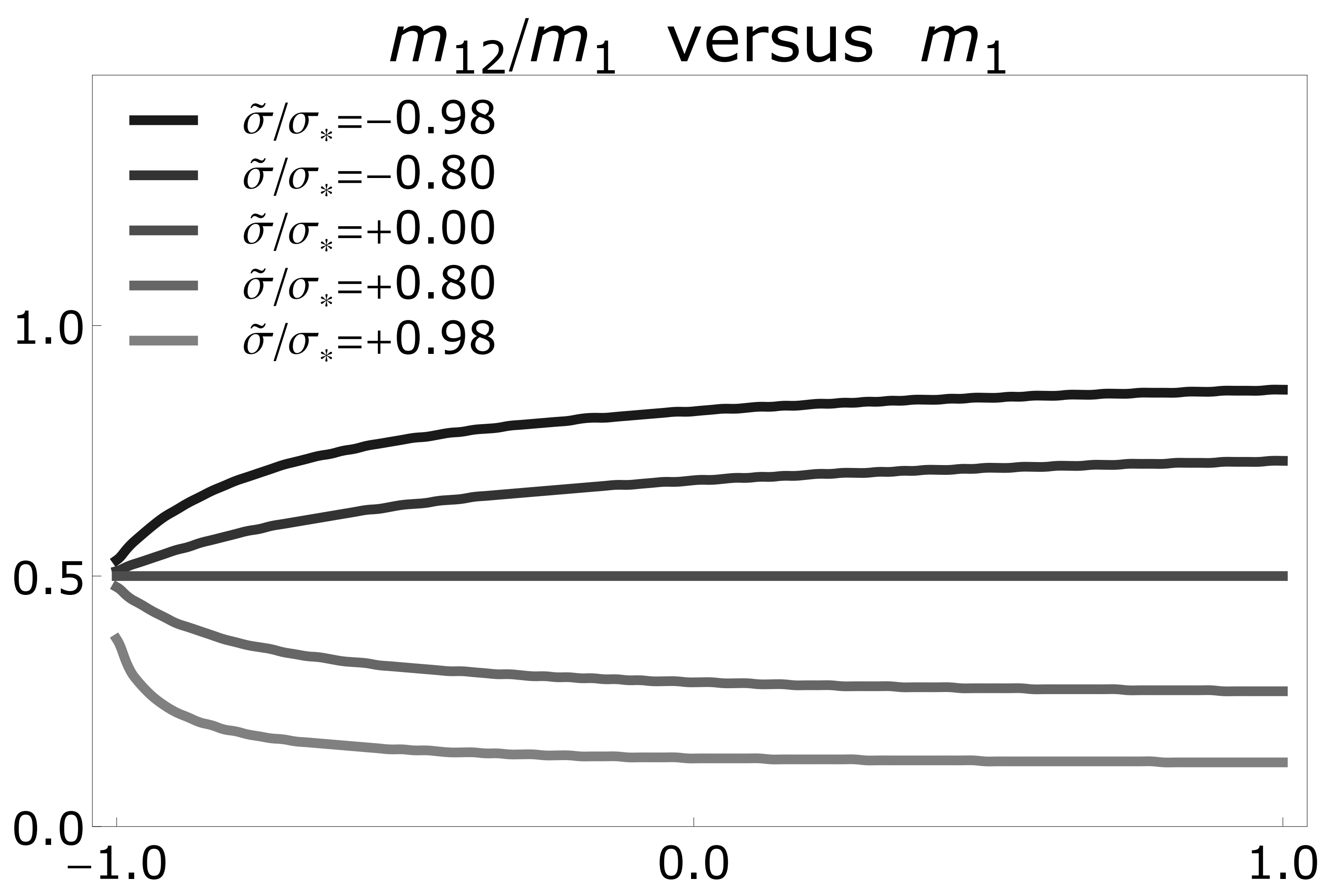
Mass Splitting Function

$$\boxed{(m_1, m_2) \quad \mapsto \quad (\mu m_1, m_2 + (1-\mu) m_1)}$$

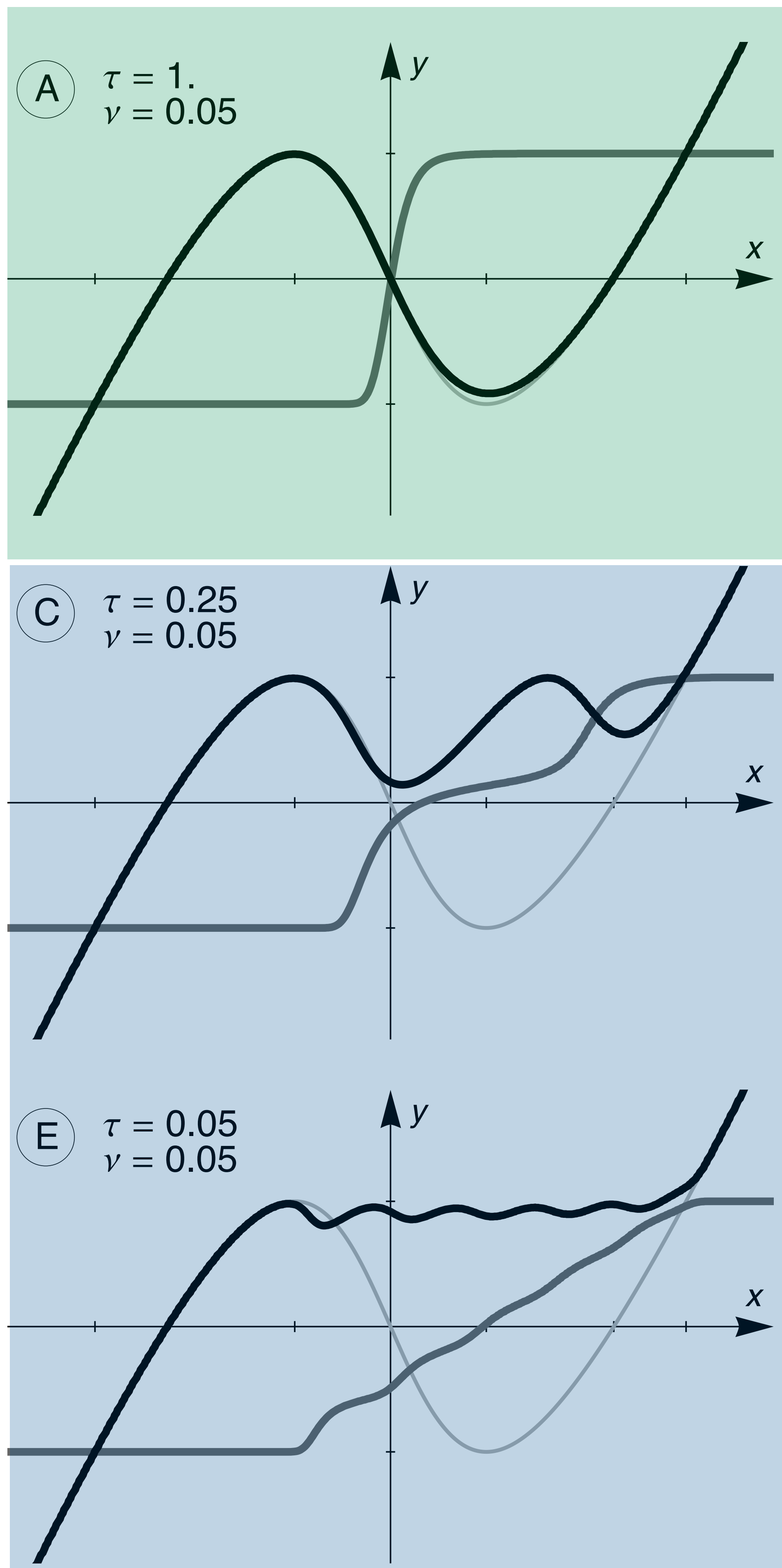
$$\mu = M(\ell, m_1)$$

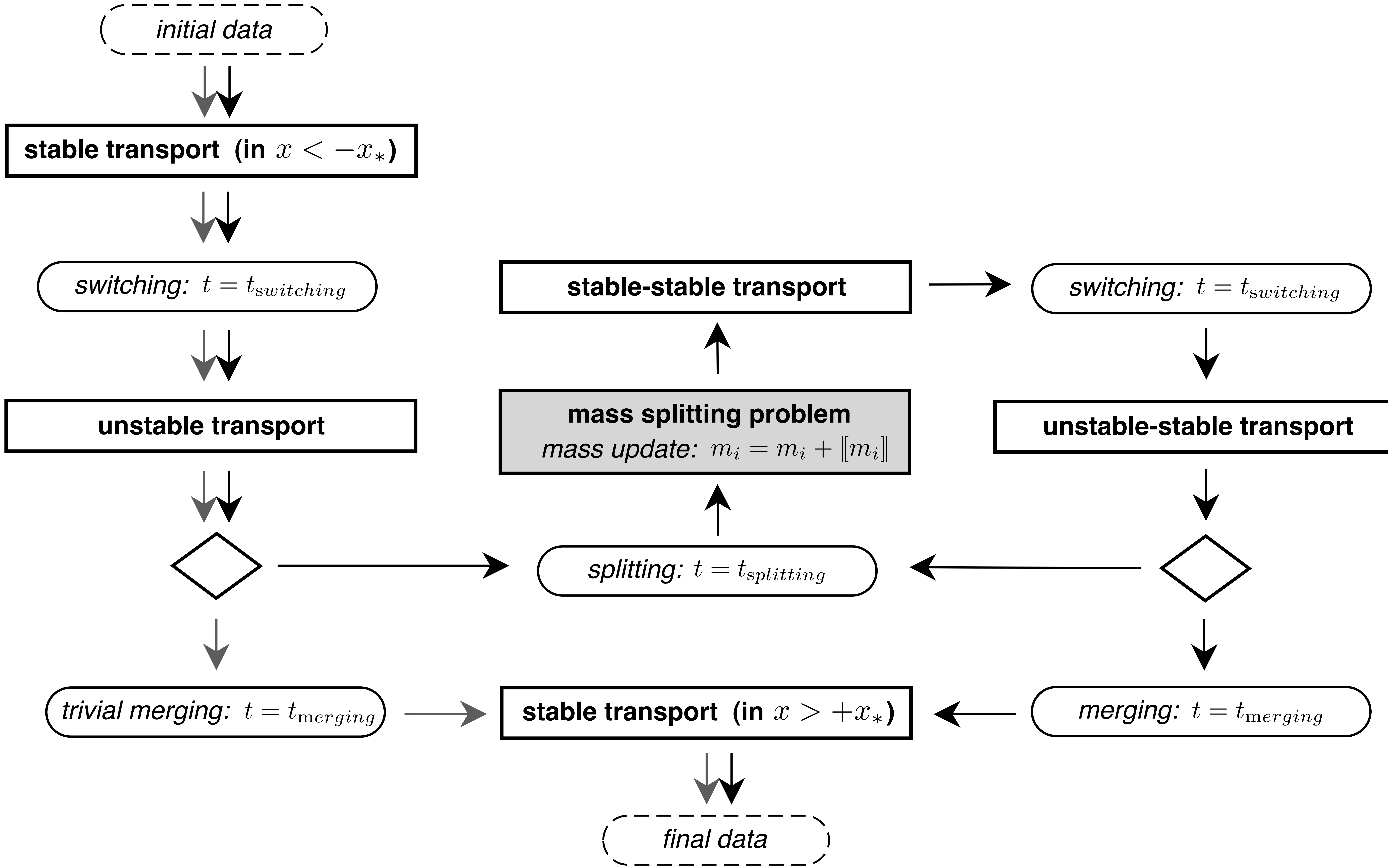
data just before splitting

data just after splitting



Main result for slow reactions





Summary

Fast reaction regime

- Kramers formula describes Type-II transitions
- Type-I transitions as limiting case

Slow reaction regime

- Type-I and Type-II transitions can be described by
  - intervals of quasi-stationary transport
  - singular times corresponding to *switching*, *splitting*, *merging*
- Splitting events require to solve *Mass Splitting Problem*

Open problems

- Find rigorous proofs !
- Fill the gap in the scaling regimes !

Thank you for listening !