Kramers and non-Kramers Phase Transitions in Many-Particle Systems with Dynamical Constraint

Michael Herrmann

(joint work with Barbara Niethammer and Juan J.L. Velázquez)

We study the different dynamical regimes in a nonlocal Fokker-Planck equation and use formal asymptotics to derive reduced evolutionary models for different small-parameter limits.

Nonlocal Fokker-Planck equations were introduced in [2] to model many-particle storage systems such as lithium-ion batteries or interconnected rubber balloons. In the simplest case, see also [3], the equations read

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

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

Here, ϱ is a time-dependent probability measure, $x \in \mathbb{R}$ denotes the state of a single particle, H is a generic double-well potential, and τ, ν are two parameters. Moreover, ℓ is a prescribed function of time that controls the first moment, that means we have

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

for any solution, provided that the initial data are admissible.

Numerical simulations as displayed in Figure 1, as well as heuristic arguments indicate that for $0 < \tau, \nu \ll 1$ there exists mainly two dynamical regimes.

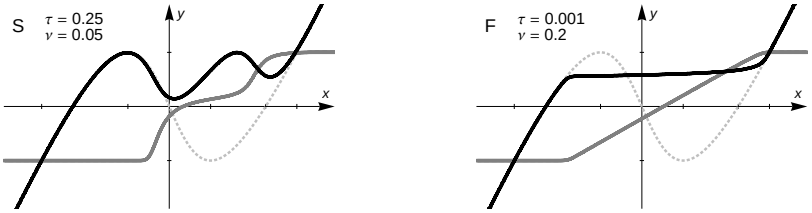

Figure 1. Typical solutions with $\dot{\ell} > 0$ for slow (left) and fast reactions (right). The solid curves in Black and Gray represent the evolution of σ and the phase fraction $\mu = \int_{\mathbb{R}} \mathrm{sgn}(x) \varrho \,\mathrm{d}x$, respectively.

The **fast reaction regime** corresponds to

$$\tau = \exp\left(-\frac{b}{\nu^2} \right), \qquad 0 < b < b_{\mathrm{crit}}, \qquad 0 < \nu \ll 1,$$

so phase transitions due to large deviations are possible. The main difficulty, however, is to understand how Kramers' formula [4] can be applied to an effective potential $H_\sigma(x) = H(x) - \sigma$ that depends implicitly on time t via the dynamical constraint ℓ.

As main result on fast reactions, we show the existence of two constants σ_b and d_b such that the limit dynamics for $\nu \to 0$ and $\dot{\ell} > 0$ is governed by

$$\sigma(t) = \begin{cases} \sigma_b & \text{for } t_1 < t < t_2, \\ H'\big(\ell(t)\big) & \text{else,} \end{cases} \qquad \dot{\mu}(t) = \begin{cases} d_b\, \dot{\ell}(t) & \text{for } t_1 < t < t_2, \\ 0 & \text{else.} \end{cases}$$

Here, the times $t_1 < t_2$ are uniquely defined by $H'\big(\ell(t_i)\big) = \sigma_b$ and $H''\big(\ell(t_i)\big) > 0$.

In the **slow reaction regime** we have

$$\nu = \exp\left(-\frac{a}{\tau}\right), \qquad 0 < a < a_{\mathrm{crit}}, \qquad 0 < \tau \ll 1,$$

and mass exchange according to Kramers' formula is not relevant anymore. Instead, the limit dynamics is governed by (i) quasi-stationary transport of either single-peak or two-peaks configurations, and (ii) a sequence of singular times corresponding to *switching*, *merging*, and *splitting* of peaks. We refer to Figure 2 for an illustration, and to [1] for more details.

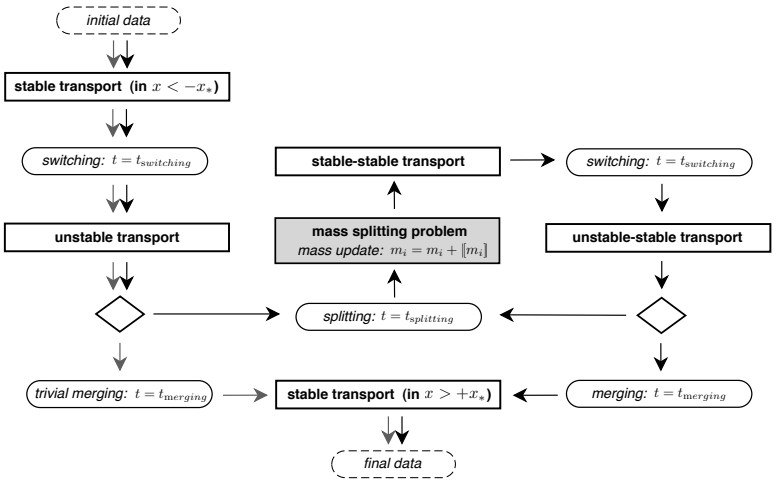

FIGURE 2. Flowchart of the limit dynamics with slow reactions, $\dot{\ell} > 0$, and $\ell(0) \ll 0$. Intervals of quasi-stationary transport are interrupted by several types of singular events.

REFERENCES

[1] M. Herrmann, B. Niethammer, J.J.L Velázquez, *Kramers and non-Kramers phase transitions in many-particle systems with dynamical constraint*, preprint arXiv:1110.3518 (2011).

[2] W. Dreyer, Cl. Guhlke, M. Herrmann, *Hysteresis and phase transition in many-particle storage systems*, Contin. Mech. Thermodyn. **23-3** (2011), 211–231.

[3] W. Dreyer, R. Huth, A. Mielke, J. Rehberg, M. Winkler, *Blow-up versus boundedness in a nonlocal and nonlinear Fokker-Planck equation*, WIAS-Preprint no. 1604 (2011).

[4] H.A. Kramers, *Brownian motion in a field of force and the diffusion model of chemical reactions*, Physica **7** (1940), 284–304.