KRAMERS AND NON-KRAMERS PHASE TRANSITIONS IN MANY-PARTICLE SYSTEMS WITH DYNAMICAL CONSTRAINT

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In [2] we study the different dynamical regimes in a nonlocal Fokker-Planck equation with two parameters and use formal asymptotics to derive reduced evolutionary models for different small-parameter limits.

1. Fokker-Planck equation with dynamical constraint

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

$$\text{(FP)} \qquad \begin{aligned} \tau\partial_t\varrho(t,\,x) &= \partial_x\Big(\nu^2\partial_x\varrho(t,\,x) + \big(H'(x)-\sigma(t)\big)\varrho(t,\,x)\Big),\\ \sigma(t) &= \int_{\mathbb{R}} H'(x)\varrho(t,\,x)\,\mathrm{d}x + \tau\dot\ell(t), \end{aligned}$$

where 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 the small parameters. Moreover, ℓ is a prescribed function of time that controls the first moment, that means we have

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

for any solution to (FP), provided that the initial data are admissible.

From a mathematical point of view, (FP) can be regarded as a Wasserstein gradient flow that is driven by the dynamical constraint (C), and we readily verify the energy law $\tau\dot{\mathcal{E}} = -\mathcal{D}+\tau\dot\ell$. Here, $\mathcal{D}$ is the Wasserstein dissipation and $\mathcal{E}$ denotes the usual energy of the unconstrained Fokker-Planck equation with potential H, see [5, 1] for details. We also refer to [4] for existence and uniqueness results on bounded domains.

2. Different dynamical regimes

The PDE (FP) exhibits rather complicated dynamics as it involves three different time scales: (*i*) the scale of the dynamical constraint, which is supposed to be of order 1, (*ii*) the small relaxation time $\tau \ll 1$, and (*iii*) Kramers' time scale $\tau\exp\big(\triangle H_\sigma/\nu^2\big)$, on which particles can move between the different wells of H_σ due to stochastic fluctuations. Here, H_σ defined by $H_\sigma(x) = H(x) - \sigma x$ is the time-dependent effective potential and $\triangle H_\sigma$ denotes the energy barrier.

In order to identify relevant scaling regimes and to derive reduced limit models we specialize to strictly increasing constraints and always suppose that initial data

Date: December 10, 2011.

are well prepared in the sense that $\varrho(0, x)$ can be approximated by a narrow peak located at $\ell(0) \ll 0$ with $H''\big(\ell(0)\big) > 0$.

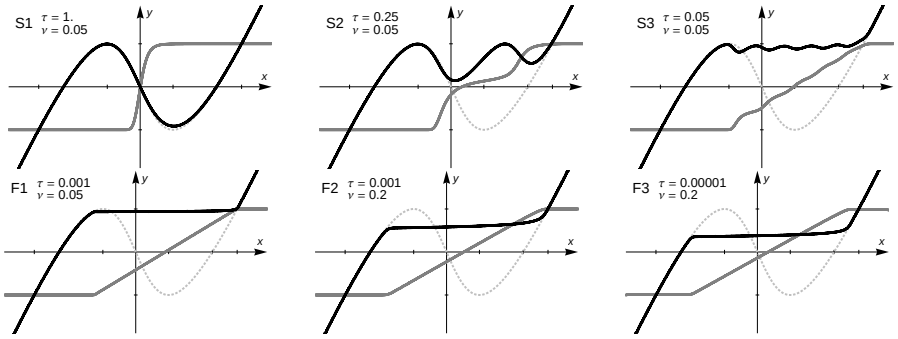

FIGURE 1. Numerical solutions with $\dot\ell > 0$ in the slow reaction regime (top row) and the fast reaction regime (bottom row). The solid curves in Black and Gray represent $t \mapsto \big(\ell(t),\, \eta(t)\big)$ and $t \mapsto \big(\ell(t),\, \mu(t)\big)$, respectively, where $\eta = \int_{\mathbb{R}} H'(x)\varrho(t,\, x)\,\mathrm{d}x$ and $\mu = \int_{\mathbb{R}} \mathrm{sgn}(x)\varrho(t,\, x)\,\mathrm{d}x$ are the *macroscopic force* and the *phase fraction*, respectively.

Numerical simulations as displayed in Figure 1, as well as heuristic arguments combined with formal expansions, indicate that there exist mainly two dynamical regimes, which we refer to as *fast reactions* and *slow reactions*, depending on whether mass exchange according to Kramers' formula is relevant or not; the motivation for these nomenclatures is that Kramers derived his large deviations formula in the context of chemical reactions [6].

condition	*parameter*	*reactions*	
$\tau = a/\log(1/\nu)$	$0 < a < \infty$	slow	*limit dynamics as in Figure 2*
$\tau = \nu^p$	$0 < p < \frac{2}{3}$	slow	open problem
$\tau = \nu^p$	$\frac{2}{3} < p < \infty$	fast	*limit in Kramers' formula*
$\tau = \exp(-b/\nu^2)$	$0 < b < b_{\mathrm{crit}}$	fast	*Kramers' formula*
$\tau < \exp(-b_{\mathrm{crit}}/\nu^2)$		fast	*quasi-stationary limit*

TABLE 1. The different scaling regimes for $0 < \tau, \nu \ll 1$.

As summarized in Table 1, each regime covers a certain range of possible scaling relations between τ and ν, where the fast reaction regime connects naturally to the quasi-stationary limit given by $\nu > 0$ and $\tau \to 0$. We also emphasize, that the limit model for $\tau, \nu \to 0$ turns out to be rate-independent in the fast reaction regime, whereas it is rate-dependent in the slow reaction regime.

3. Fast reaction regime and Kramers' formula

Since $\tau = \exp(-b/\nu^2)$ is exponentially small in ν^2, large deviations can provide a mass flux of order 1, but the main difficulty is to understand how Kramers' formula can be applied to an effective potential H_σ that depends implicitly on the time via the dynamical constraint.

Our main findings can be described as follows. Relying on suitable inner and outer expansions for ϱ, we compute the mass flux F between the local wells of H_σ

by

$$F(t) \approx m_-(t) r_-\big(\sigma(t)\big) - m_+(t) r_+\big(\sigma(t)\big), \qquad r_\pm(\sigma) = c_\pm(\sigma) \exp\left(\frac{b - h_\pm(\sigma)}{\nu^2}\right).$$

Here $m_\pm$ approximate the masses in the wells, b is the scaling parameter, $c_\pm$ are some constants of order 1, and $h_\pm$ denote the energy barriers between the local maximum and either one of the wells.

Combining the asymptotic formula for the mass flux with the dynamical constraint (C) reveals that there is some σ_b such that $F(t)$ is of order 1 if and only if $\sigma(t) \approx \sigma_b$, and that small perturbation via $\sigma(t) = \sigma_b + \nu^2 \psi(t)$ are sufficient to accommodate the dynamical constraint. In this way we arrive at the following self-consistent limit model that complies very well with the numerical results in the bottom row of Figure 1.

Main result. *For each fast reaction parameter $0 < b < b_{\mathrm{crit}}$ there exist constants σ_b and d_b such that the limit dynamics for $\nu \to 0$ with $\dot{\ell} > 0$ 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 $H''\big(\ell(t_i)\big) > 0$.

4. Limit dynamics in the slow reaction regime

In this regime, $\nu = \exp(-a/\tau)$ is much smaller than τ and mass exchange according to Kramers' formula is not relevant anymore. Instead, the key dynamical effect is that localized peaks can enter the unstable interval, which consists of all x with $H''(x) < 0$. When this happens, the width of the peak starts to widen very rapidly, but since the initial width is of order ν, the peak remains localized for some time of order 1.

Due to the presence of *unstable peaks*, the dynamics of (FP) is rather complicated. However, in the limit $\tau \to 0$ it is possible to derive a reduced dynamical model that characterizes the evolution in terms of single-peak configurations (either *stable* or *unstable*) and two-peaks configurations (either *stable-stable* or *unstable-stable*). We refer to Figure 2 for an illustration, and to [2] for more details.

Main result. *In the slow reaction limit with $\dot{\ell} > 0$, there are time intervals of quasi-stationary* transport*, where either a single or two separated peaks just move according to the dynamical constraint. These intervals are interrupted by singular times corresponding to the following events.*

1. Switching*: A stable peak becomes unstable by entering the unstable interval.*
2. Merging*: The peaks of an unstable-stable configuration merge almost instantaneously to form a single stable peak. A special case of merging is that an unstable peak becomes stable by leaving the unstable interval.*
3. Splitting*: An unstable peak disintegrates very rapidly and the system jumps almost instantaneously to a stable-stable two-peaks configuration.*

Transport, switching, and merging of peaks can all be understood in terms of the *two-peaks approximation*, a rather simple ODE that describes how two particles interact via the dynamical constraint. Splitting events, however, are much more complicated and we have to employ several asymptotic methods to describe them in detail. At first we rely on a simplified *peak-widening model* to derive an effective

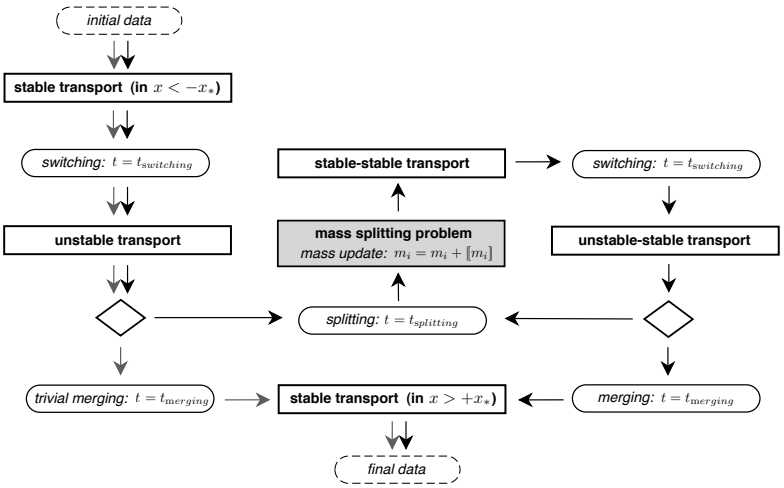

FIGURE 2. Flowchart of the limit dynamics in the slow reaction regime with $\dot{\ell} > 0$. Intervals of quasi-stationary transport are interrupted by singular events corresponding to switching, splitting, and merging of peaks.

formula for the width of an unstable peak, which in turn allows us to compute the (next) splitting time. We then introduce the *mass splitting problem* on a rescaled time scale, which consists of solving a nonlinear and nonlocal transport equation with well-prepared asymptotic initial data. This model serves as a black box to determine the mass distribution between the emerging stable peaks.

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