Rate-Independent Dynamics and Kramers-Type Phase Transitions in Nonlocal Fokker–Planck Equations with Dynamical Control

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Abstract

The hysteretic behavior of many-particle systems with non-convex free energy can be modeled by nonlocal Fokker–Planck equations that involve two small parameters and are driven by a time-dependent constraint. In this paper we consider the fast reaction regime related to Kramers-type phase transitions and show that the dynamics in the small-parameter limit can be described by a rate-independent evolution equation with hysteresis. For the proof we first derive mass-dissipation estimates by means of Muckenhoupt constants, formulate conditional stability estimates, and characterize the mass flux between the different phases in terms of moment estimates that encode large deviation results. Afterwards we combine all these partial results and establish the dynamical stability of localized peaks as well as sufficiently strong compactness results for the basic macroscopic quantities.

1. Introduction

An ubiquitous and intriguing question in mathematical analysis concerns the conditions under which the dynamics of a given high-dimensional system with small parameters can be described by low-dimensional, reduced evolution equations. In this paper we answer this question, at least partially, for a particular example, namely the Fokker–Planck equation

\[
\tau \partial_t \varrho(t, x) = \partial_x \left( \nu^2 \partial_x \varrho(t, x) + \left( H'(x) - \sigma(t) \right) \varrho(t, x) \right), \quad \text{(FP1)}
\]

where \( \tau \) and \( \nu \) are the small parameters and \( x \in \mathbb{R} \) is a one-dimensional state variable. Moreover, \( H \) is supposed to be a double-well potential and \( \sigma \) is a dynamical multiplier chosen such that the solution complies with

\[
\int_{\mathbb{R}} x \varrho(t, x) \, dx = \ell(t), \quad \text{(FP2)}
\]
where \( \ell \) is a prescribed control function. This dynamical constraint is, for admissible initial data, equivalent to the mean-field formula

\[
\sigma(t) = \int \mathbb{R} H'(x) \varrho(t, x) \, dx + \tau \dot{\ell}(t),
\]

which turns (FP\(_1\)) into a nonlocal, nonlinear, and non-autonomous PDE.

Nonlocal Fokker–Planck equations like (FP\(_1\)) + (FP\(_2\)) have been introduced in [6] in order to model the hysteretic behavior of many-particle storage systems such as modern Lithium-ion batteries (for the physical background, we also refer to [8]). In this context, \( x \in \mathbb{R} \) describes the thermodynamic state of a single particle (nano-particle made of iron-phosphate in the battery case), \( H \) is the free energy of each particle, and \( \nu \) accounts for entropic effects. Moreover, \( \varrho \) is the probability density of a many-particle ensemble and the dynamical control \( \ell \) reflects that the whole system is driven by some external process (charging or discharging of the battery).

Since \( H \) is non-convex, the dynamics of (FP\(_1\)) + (FP\(_2\)) can be rather involved as they are related to three different time scales, namely the small relaxation time \( \tau \), the time scale of the control \( \ell \) (which is supposed to be of order 1), and the Kramers time scale. The latter is given by

\[
\tau \exp \left( \frac{\min\{h_-(\sigma), h_+(\sigma)\}}{\nu^2} \right)
\]

and corresponds, as discussed below, to probabilistic transitions between the different wells of the time-dependent effective potential with energy barriers \( h_-(\sigma), h_+(\sigma) \).

In this paper we restrict our considerations to the fast reaction regime, in which the particular scaling relation between \( \tau \) and \( \nu \) guarantees that the time scale (1) is of order 1 for certain values of \( \sigma \), and study the small-parameter limit \( \tau, \nu \to 0 \). Our main result is that the microscopic PDE (FP\(_1\)) + (FP\(_2\)) can be replaced by a low-dimensional dynamical system which governs the evolution of the dynamical multiplier \( \sigma \) and the phase fraction

\[
\mu(t) := \int_{\text{right stable region}} \varrho(t, x) \, dx - \int_{\text{left stable region}} \varrho(t, x) \, dx,
\]

where the stable regions (or ‘phases’) are the connected components of \( \{ x \in \mathbb{R} : H''(x) > 0 \} \). The micro-to-macro transition studied here has much in common with those in [20, 21, 23], which likewise derive macroscopic models for the dynamics of phase transitions from microscopic gradient flows with non-convex energy and external driving. Our microscopic system, however, is different as it involves the diffusive term \( \nu^2 \partial_x^2 \varrho \), which causes specific effects and necessitates the use of different methods.

**Many-particle interpretation** It is well-known, see for instance [24], that the linear Fokker–Planck equation (FP\(_1\)) with \( \sigma \equiv 0 \) is equivalent to the Langevin equation

\[
\tau \frac{d}{dt} x = -H'(x) \, dt + \sqrt{2} \nu \, dW,
\]

where \( W \) denotes a standard Brownian motion in \( \mathbb{R} \). In other words, \( \varrho \) describes for \( \sigma \equiv 0 \) the statistics of a large ensemble of identical