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**

\[ \tau \dot{x}_i(t) = \sigma(t) - H'(x_i(t)) \]

**dynamical constraint**

\[ N^{-1} \sum_{i=1}^{N} x_i(t) = \ell(t) \]

**nonlocal multiplier**

\[ \sigma(t) = N^{-1} \sum_{i=1}^{N} H'(x_i(t)) + \tau \dot{\ell}(t) \]

**Problem**

Macroscopic evolution is ill-posed !

**Remedy**

Take into account entropic effects !

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Quenched Disorder
Boltzmann Entropy

Mielke & Truskinovsky (ARMA 2012)

*non-local Fokker-Planck equations*
Nonlocal Fokker-Planck equations

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

\[ \tau \partial_t \varrho = \partial_x (\nu^2 \partial_x \varrho + (H'(x) - \sigma(t)) \varrho) \]
\[ \int_{\mathbb{R}} x \varrho(x, t) \, dx = \ell(t) \]

relaxation time \hspace{1cm} entropy \hspace{1cm} dynamical multiplier

dynamical constraint

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

stable interval \hspace{1cm} unstable interval \hspace{1cm} stable interval
3 Time scales

Goal: Understand small parameter dynamics!

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

Different times scales:

- relaxation time of single particle system
  (relaxation to metastable state)
  \[ \tau \]

- 'chemical reactions' (Kramers’ formula)
  (relaxation to equilibrium)
  \[ \tau \exp \left( \frac{\Delta H}{\nu^2} \right) \]

- dynamical constraint
  \[ \dot{\ell} = O(1) \]
Overview on different scaling regimes
Simple initial value problems

simplifying assumptions

\[ \ell(0) < -x_{**}, \quad \varrho(x, 0) \approx \delta_{\ell(0)}(x) \]

\[ \dot{\ell} > 0 \]

macroscopic output

\[ t \mapsto (\ell(t), \eta(t)), \quad t \mapsto (\ell(t), \mu(t)) \]

stress-strain relation

phase-fraction - strain relation

mean force

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

phase fraction

\[ \mu(t) = -\int_{-\infty}^{0} \varrho(x, t) dx + \int_{0}^{+\infty} \varrho(x, t) dx \]
Type II

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Numerical simulations - macroscopic view

slow reactions

Type I

Type II

fast reactions

Type III

Type IV

A \( \tau = 1 \)
\( \nu = 0.05 \)

B \( \tau = 0.5 \)
\( \nu = 0.05 \)

C \( \tau = 0.25 \)
\( \nu = 0.05 \)

D \( \tau = 0.1 \)
\( \nu = 0.05 \)

E \( \tau = 0.05 \)
\( \nu = 0.05 \)

F \( \tau = 0.001 \)
\( \nu = 0.05 \)

G \( \tau = 0.001 \)
\( \nu = 0.2 \)

H \( \tau = 0.00001 \)
\( \nu = 0.2 \)

I \( \tau = 0.0001 \)
\( \nu = 0.4 \)
Numerical simulations - microscopic view

\[ \begin{align*}
C(t) &= -0.8 \sum_i C_i \\
G(t) &= 0.9 \sum_i G_i \\
A(t) &= 1.7 \sum_i A_i \\
\end{align*} \]

\[ \begin{align*}
t &= 0.25 \\
n &= 0.05 \\
\end{align*} \]

\[ \begin{align*}
\tau &= 1.0, y = 0.05 \\
\tau &= 0.25, y = 0.05 \\
\tau &= 0.001, y = 0.2 \\
\end{align*} \]
### Scaling regimes for parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\tau \log 1/\nu \to \infty$</td>
<td>single-peak evolution</td>
</tr>
<tr>
<td>$\tau = \frac{a}{\log 1/\nu}$</td>
<td>$0 &lt; a &lt; a_{\text{crit}}$</td>
</tr>
<tr>
<td>$\tau = \nu^p$</td>
<td>$0 &lt; p &lt; 2/3$</td>
</tr>
<tr>
<td>$\tau = \nu^p$</td>
<td>$2/3 &lt; p &lt; \infty$</td>
</tr>
<tr>
<td>$\tau = \exp\left(-\frac{b}{\nu^2}\right)$,</td>
<td>$0 &lt; b &lt; b_{\text{crit}}$</td>
</tr>
<tr>
<td>$\nu^2 \log 1/\tau \to \infty$</td>
<td>quasi-stationary limit</td>
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</tbody>
</table>
Kramers’ formula and Type-II transitions

\[ \tau = \exp\left(-\frac{b}{v^2}\right) \]
Kramers formula

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

Kramers’ formula provides mass flux between wells

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

Observation

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

1. mass flux is of order 1 provided that \( \sigma(t) = \sigma_b + \nu^2 \psi(t) \)
2. small fluctuations of \( \sigma \) are sufficient to satisfy the constraint
Inner and outer expansions

Idea
1. For each $\sigma$ we have three positions $x_-, x_0, x_+$ with $H'(x_-/0/+ x_0) = \sigma$
2. Two narrow peaks with masses $m_\pm(t)$ at $x_\pm(t)$

\[ \nu^2 \partial_x \varrho + H'_{\sigma(t)}(x) \varrho = \begin{cases} 
0 & \text{for } x \approx x_\pm(t), \\
R(t) & \text{for } x \approx x_0(t).
\end{cases} \]
Matching of inner and outer expansions

**Outer expansion**

\[ \rho(x, t) \approx \begin{cases} 
\mu_-(t) \exp \left( \frac{-H_\sigma(t)(x)}{\nu^2} \right) & \text{for } x < x_0(t), \\
\mu_+(t) \exp \left( \frac{-H_\sigma(t)(x)}{\nu^2} \right) & \text{for } x > x_0(t). 
\end{cases} \]

\[ m_\pm(t) = \pm \int_{x_0(t)}^{\pm \infty} \rho(x, t) \, dx \approx c_\pm(t) \mu_\pm(t) \nu \exp \left( - \frac{H_\sigma(t)(x_\pm(t))}{\nu^2} \right) \]

**Inner expansion**

\[ \rho(x_0(t) \pm \delta, t) \approx \exp \left( - \frac{H_\sigma(t)(x_0(t) \pm \delta)}{\nu^2} \right) \left( C(t) \mp \frac{R(t)}{\nu^2} \exp \left( \frac{H_\sigma(t)(x_0(t))}{\nu^2} \right) \right) \]

**Matching conditions** result from equating the time-dependent pre-factors!
Kramers formula for mass flux

\[ \frac{R(t)}{\tau} = m_-(t)r_-(t) - m_+(t)r_+(t) \]

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

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

\[ x_i(t) = X_i(\sigma(t)) \]

Observation

For each \( 0 < b < b_{\text{crit}} \) there exists \( 0 < \sigma < \sigma_* \) such that

\[ \sigma(t) < \sigma_b \quad \implies \quad r_-(t) \ll 1 \]

\[ \sigma(t) = \sigma_b + \nu^2 \psi(t) \quad \implies \quad r_-(t) \sim \exp(\psi(t)) \]

\[ \sigma(t) > \sigma_b \quad \implies \quad r_-(t) \gg 1 \]

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

Strategy

Adjust \( \psi \) according to dynamical constraint
Main result. Suppose that the dynamical constraint and the initial data satisfies (4) and (5), and that $\tau$ and $\nu$ are coupled by

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

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

1. the dynamical multiplier satisfies

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

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

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

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

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

Moreover, the assertions remain true

1. with $\sigma_b = 0$ if $\tau \leq \exp \left( - \frac{h_{\text{crit}}}{\nu^2} \right)$,

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

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Slow reaction limit: Type-I/II transitions

\[ \tau = 1, \quad \nu = 0.05 \]

\[ \tau = 0.25, \quad \nu = 0.05 \]

\[ \nu = \exp \left( -\frac{a}{\tau} \right) \]
Overview - states for increasing constraints

Single-peak configurations

- Stable configurations
- Unstable configurations

Two-peaks configurations

- Stable-stable configurations
- Unstable-stable configurations

Transport due to constraint
Switching events
Splitting events
Merging events
Overview - Type-I phase transitions

- transport
- switching
- transport
- merging
- transport
Overview - Type-II phase transitions

Transport

Switching

Transport

Transport

Splitting

Merging

Transport

Switching

Transport
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

\[ \begin{align*}
\tau \dot{x}_1 &= \sigma - H'(x_1) \\
\tau \dot{x}_2 &= \sigma - H'(x_2) \\
\sigma &= m_1 H'(x_1) + m_2 H'(x_2) + \tau \ell
\end{align*} \]

\[ m_1 + m_2 = 1 \]
\[ \dot{m}_i = 0 \]

Quasi-stationary limit

\[ \tau \to 0 \]

\[ \begin{align*}
H'(x_1) &= H'(x_2) \\
m_1 x_1 + m_2 x_2 &= \ell
\end{align*} \]

Multiple solution branches! Which ones are selected by dynamics?
Two-peaks approximation to FP

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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

\[ \tau \partial_t \hat{\rho} = \partial_x \left( \nu^2 \partial_x \hat{\rho} + (H'(x) - \sigma) \hat{\rho} \right) \]
\[ \tau \dot{x}_2 = \sigma - H'(x_2) \]
\[ \sigma = m_1 \int_{\mathbb{R}} H'(x) \hat{\rho} \, dx + m_1 H'(x_2) + \tau \ell \]

\( \rho = m_1 \hat{\rho} + m_2 \delta_{x_2} \)
\( \ell = m_1 \int_{\mathbb{R}} x \hat{\rho} \, dx + m_2 x_2 \)

position of peak

\[ \tau \dot{x}_1 = \sigma - H'(x_1) \]

width of peak

\[ w(t) = \nu \lambda(t) W(\theta(t)) \]

\[ \hat{\rho}(x, t) =: \frac{1}{\nu \lambda(t)} R \left( -\frac{(x - x_1(t))^2}{\nu \lambda(t)}, \theta(t) \right) \]
Formula for width of unstable peaks

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

\[
\partial_\theta R = \partial_y^2 R \\
R(y, \theta) \approx \frac{1}{\sqrt{4\pi \zeta}} \exp \left(-\frac{y^2}{4\theta}\right), \ W(\theta) \sim \sqrt{\theta}
\]

as long as width is small

evolution of width

\[
0 < t < t_{sw} : \quad w(t) = \mathcal{O}(\nu) \\
t_{sw} < t < t_{sp} : \quad \nu \ll w(t) \ll 1 \\
t_{sp} < t : \quad w(t) \gg 1
\]

\[
\int_{t_{sw}}^{t_{sp}} H''(x_1(t)) \, dt + a = 0
\]

can be computed by quasi-stationary two-peaks approximation
Mass splitting problem

ansatz

\[ \nu = 0, \quad t = t_{sp} + \tau s \]

\[ \hat{\rho} = \partial_x \left( (H'(x) - \sigma(s)) \hat{\rho} \right) \]

\[ \dot{x}_2 = \sigma(s) - H'(x_2) \]

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

\[ \sigma(s) = m_1 \int_{\mathbb{R}} H'(x) \hat{\rho} \, dx + m_2 H'(x_2) \]

asymptotic initial data

\[ \hat{\rho}(x, s) \xrightarrow{s \to -\infty} \frac{1}{2\beta \sqrt{\pi}} \exp \left( -\frac{x - x_1(t_{sw})}{4 \exp(2\beta s)} \right), \quad \beta = -H''(x_1(t_{sw})) > 0 \]
Mass splitting problem

Conjecture

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

Mass Splitting Function

\[
(m_1, m_2) \mapsto (\mu m_1, m_2 + (1 - \mu)m_1)
\]

\[\mu = M(\ell, m_1)\]

data just before splitting \hspace{1cm} data just after splitting
Main result for slow reactions

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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!