Effective Dynamics of Nonlocal Many-Particle Systems with Dynamical Constraint

Joint work with Barbara Niethammer and Juan J.L. Velázquez

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Lattice and Nonlocal Dynamical Systems and Applications

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Lattice and Nonlocal Dynamical Systems and Applications

Contents

- Nonlocal Fokker-Planck equations driven by a dynamical constraint
  - Arise in modelling of Lithium-ion batteries
  - Complicate dynamics due to 3 different time scales
  - Involve two small parameters
- Reduced models for small parameter limits
  - Form rigorous proofs for fast and slow reactions driven and to be found, resp.
    - Formal and heuristic arguments only
  - Slow reaction regime with splitting of unstable peaks
  - Fast reaction regime driven by Kramers formula for time-dependent potentials
- This talk
  - Formal and heuristic arguments only
Model and Motivation

Nonlocal Fokker-Planck equation with dynamical constraint
Lithium-ion batteries

How to derive the hysteresis from the properties of nano-particles? (made of iron phosphate) powder of nano-particles

.. image:: lithium-ion.png
   :width: 100%

charging
discharging

capacity of powder

electrolyte

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powder of nano-particles (made of iron phosphate)
Assumptions on dynamics

Dreyer, Gührike, Herrmann: Continuum Mechanics and Thermodynamics (2011)

1. Energy per particle has two local minima
2. Each particle minimizes its energy quickly
3. Mean position is prescribed by $\langle x \rangle (t)$
4. Evolution of ensemble
5. Stochastic fluctuations

Forces = chemical potential
"Position" = Li-concentration
"Position" = Li-concentration

Microscopic quantities

Modeling assumptions

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Evolution equation

\[
\frac{\partial}{\partial t} \rho(x,t) + \nabla \cdot \left( \nabla \rho(x,t) \rho_0(x) \right) = \int H(x) \rho(x,t) dx = \rho(t) \phi
\]

Equivalent mean-field formula

\[
\rho(t) = \rho_0(x) \int H(x) \rho(x,t) dx
\]

Dynamical constraint

Energy per particle \((x) H\)

Dynamical multiplier \((t) \phi\)

Probability density of powder \((x,t) \rho\)

Nonlocal Fokker-Planck equation

\[
\left( \frac{\partial}{\partial t} \rho(t) - (x,H) \right) + \nabla \cdot \left( \nabla \phi \right) = \nabla \cdot \left( \rho(t) \right)
\]
Three time scales

- Relaxation to meta-stable state
- Convergence to equilibrium
- Dynamics constraint

Reduced models for small parameter limit

Goal

Which times scales are relevant?

\[ \frac{1}{\tau} \left( \frac{\tau^2}{\beta H \nabla} \right) \exp \left( \frac{\tau}{\beta H \nabla} \right) \]

side comment: what about lattices?


similar equations

chain of bistable units + hard-loading device + overdamped limit + thermal fluctuations

bi-stable spring

dashpot

bi-stable spring

dashpot
Heuristics and Simulations
How is the mass transferred between the stable intervals?

\[ \dot{\rho}(t) = 1, \quad \rho(0) = \rho_f, \quad (t_\rho) = \rho(\rho_f) \]

Phase fraction

\[ \dot{u}(t) = (t)u, \quad u_0 = (t)u_f \]

Negative voltage

\[ \dot{\varphi}(t) = (t)\varphi, \quad \varphi_0 = (t)\varphi_f \]

Capacity of powder

Macroscopic quantities

Simplifying assumptions

Final dynamics

Initial and final dynamics

Overview
Type II Lattice and Nonlocal Dynamical Systems and Applications

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Simulations - macroscopic view

A: \( t = 1 \), \( n = 0.05 \), \( x, y \)

B: \( t = 0.5 \), \( n = 0.05 \), \( x, y \)

C: \( t = 0.25 \), \( n = 0.05 \), \( x, y \)

D: \( t = 0.1 \), \( n = 0.05 \), \( x, y \)

E: \( t = 0.05 \), \( n = 0.05 \), \( x, y \)

F: \( t = 0.001 \), \( n = 0.05 \), \( x, y \)

G: \( t = 0.001 \), \( n = 0.2 \), \( x, y \)

H: \( t = 0.00001 \), \( n = 0.2 \), \( x, y \)

I: \( t = 0.0001 \), \( n = 0.4 \), \( x, y \)

Type IV

Type III

Type II

Type I

Fast reactions

Slow reactions
Simulations - microscopic view
<table>
<thead>
<tr>
<th>Scaling Regimes</th>
<th>$\infty \leftarrow 1/\log 1+a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Quasi-stationary Limit</td>
<td>$q &gt; q &gt; 0$</td>
</tr>
<tr>
<td>Kramers Formula</td>
<td>$\left(1-\frac{q}{a}\right) \exp = \frac{1}{x}$</td>
</tr>
<tr>
<td>Limit of Kramers Formula</td>
<td>$\infty &gt; d &gt; 3/2$, $\frac{d}{\sqrt{a}} = 1$</td>
</tr>
<tr>
<td>Open Problem</td>
<td>$3/2 &gt; d &gt; 0$, $d/\sqrt{a} = 1$</td>
</tr>
<tr>
<td>Two-peak Evolution</td>
<td>$q &gt; q &gt; 0$, $\frac{q}{\log 1+a} = 1$</td>
</tr>
<tr>
<td>Piecewise Continuous</td>
<td>$b &gt; b &gt; 0$, $b/\log 1 = 1$</td>
</tr>
<tr>
<td>Single-peak Evolution</td>
<td>$\infty \leftarrow a/\log 1+a$</td>
</tr>
<tr>
<td>$0 \leftarrow a/\log 1+a$</td>
<td></td>
</tr>
</tbody>
</table>
Fast reactions regime: Type-III Transitions

\[ \frac{\epsilon}{q} \int \exp \left( -\frac{\epsilon}{q} \right) dx \equiv \mathcal{T} \]
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Kramers formula

\[
\begin{align*}
(p)_t &= H = x^n_x - x^n
\\
0 &= H = x^n_x
\end{align*}
\]

Key Observation

Particles diffuse in a time-dependent effective potential

\[
\varphi - (x)H = (x)^\varphi H
\]

Asymptotics

- singe-well for \( \varphi < |(x)\varphi| \)
- double-well for \( \varphi > |(x)\varphi| \)

Effective potential

Particles diffuse in a time-dependent effective potential

FP-flux = 0

inner expansion

outer expansion

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Singular ODE for the masses and the constraint:

\[ (\varphi, -m) \frac{d}{dt} I = \gamma, \quad (\varphi, -m) = \frac{1}{(t) \mathcal{R}}, \quad I = \mp m + w \]

Further observations:

\[ \left( \frac{q}{(\varphi)^q - q} \right) \exp (\varphi)^ \pm c = (\varphi)^ \pm \lambda \]

Effective mass flux (via asymptotic analysis):

\[ \left( \frac{q}{q} \right) \exp = \lambda \]

Kramers formula

Small deviations from critical values determined by constraint.

Critical values (corresponding to increasing or decreasing constraint, resp.)

Mass flux is of order 1 if and only if multiplier is close to one of two
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**Limit model for type-I/II transitions**

- • describes numerical observations very well
- • is rate-independent
- predicts the plateau height

\[
0 = \left( \left( t \right) \eta^l, \left( t \right) \gamma, \left( t \right) \phi \right) \in \mathcal{C} \\
\left( \left( t \right) \eta^l \right) \mathcal{I}^\eta \psi + \left( \left( t \right) \eta^l \right) \mathcal{R} \phi \subseteq \left( t \right) \phi
\]

\[
\left( t \right) \gamma \phi = \left( t \right) \eta^l, \quad \gamma \phi = \left( t \right) \eta^l = \left( t \right) \phi
\]

Intermediate (plateau) dynamics

\[
0 = \left( t \right) \eta^l, \quad \left( \left( t \right) \gamma \right), \mathcal{H} = \left( t \right) \eta^l = \left( t \right) \phi
\]

Initial and final dynamics
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PDE techniques for fast reactions

• gradient flow structure, energy-dissipation estimates
• mass-dissipation estimates via Muckenhoupt functionals
• large deviations results
• dynamical peak stability estimates
• a priori and moment estimates

Herrmann, Niethammer, Velázquez: in preparation
Slow Reactions Regime: Type-I/II Transitions

\[
\left( \int_0^\infty \frac{t}{v} \exp{\xi} \, d\xi \right) = \alpha
\]
Type-II transitions
Simplified models

1. Mass-splitting problem
2. Peak-widening model
3. Two-peaks ODE

- To mass distribution after splitting
- To compute the next splitting time

- Unstable peaks merge rapidly with stable ones
- Stable peaks enter unstable interval
- Localised peaks move due to constraint
- Switching
- Transport
- Splitting
- Splitting
- Unstable peaks split rapidly

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Two-peaks approximation

\[ \dot{x} = \varepsilon x \varepsilon w + \mathbf{1} x \mathbf{1} w \]

Quasi-stationary limit \( \varepsilon \to 0 \)

Multiple solution branches:

\[ \mathbf{j} = \varepsilon x \varepsilon w + \mathbf{1} x \mathbf{1} w \]

\[ \mathbf{j} = (\varepsilon x, H = (\mathbf{1} x, H) \]

\[ \mathbf{j} \perp + (\varepsilon x, H \varepsilon w + (\mathbf{1} x, H \mathbf{1} w = \mathbf{0} \]

\[ \varepsilon x \mathbf{j} - \mathbf{0} = \varepsilon x \]

\[ \mathbf{1} x \mathbf{j} - \mathbf{0} = \mathbf{1} x \]

\[ \dot{x} = \mathbf{m} \]
\[
\left( (t) \theta, \frac{(t) H}{(t) I} x - x \right) \mathcal{U} \frac{(t) H}{I} := (t, x) \tilde{\varphi}
\]

\[
((t) \theta) \Lambda(t) H = (t) m
\]

Width of peak

\[
(x)_I H - \varrho = x_I \perp
\]

Position of peak

\[
\int x w = y
\]

\[
\int \varphi \cdot x w + \varphi \cdot x \varphi \cdot x w = \varphi
\]

Peak-widening model
can be computed by quasi-stationary two-peaks approximation

\[ 0 = u + \tau p((\frac{\partial}{\partial x})^\perp x) \int_{\Delta t} H \frac{\partial \psi}{\partial \xi} \]

\[ I \ll (\tau) \eta : \tau \gg ds \eta \]
\[ I \gg (\tau) \eta \gg \alpha : ds \eta \gg \tau \gg ms \eta \]
\[ \alpha Q = (\tau) \eta : ms \eta \gg \tau \gg 0 \]

\[ \theta^\wedge \sim (\theta) M \left( \frac{\theta \psi}{\xi \bar{\psi}} - \right) dx \exp \frac{\int \psi \psi^\wedge}{\alpha} \approx (\theta, \tilde{\psi}) H \]
\[ H^{\tilde{\psi} Q} = H^{\theta Q} \]

- only one reasonable choice for time and space scaling
- expand nonlinearity fine as long as width is small
- formula for width of unstable peaks

Formulas for width of unstable peaks
Asymptotic initial data (reminiscent of diffusion) from a curve of possible ones

\[
(t \varepsilon x, s, \hat{z}, \hat{z} x) \text{ for } s \to 1
\]

unstable steady state

unstable steady state

unstable manifold has codim=1

(unstable manifold has codim=1 )

(unstable manifold has codim=1 )

Splitting = heteroclinic connection

\[
(\forall x, H \varepsilon u + x \varepsilon 0(x), H \int \varepsilon u = (s) \varepsilon 0
\]

\[
(s) \varepsilon 0 = \varepsilon x
\]

\[
(\varepsilon (s) \varepsilon 0 - (x) \varepsilon H)^x = \varepsilon s \varepsilon q
\]

(\forall s, \varepsilon 0 = \varepsilon q + \varepsilon s \varepsilon t = t
\]

Simplified

Simplified

Equations

Mass splitting problem
Mass splitting function

\[
(m_1^2/m_1^1)\text{ versus } m_1^1
\]

Heteroclinic connection is well-defined and depends continuously on the parameters. Conjecture (for nonlocal but autonomous transport equation)

\[
(m_{11}, m_2) \leftrightarrow (m_1^1, m_2^1)
\]
Flowchart is numerical integrator!

Main result for slow reactions
Summary

• Kramers formula describes Type-III transitions
• Type-IV transitions as limiting case
• Type-I and Type-II transitions can be described by intervals of quasi-stationary transport
• Fast reaction regime
• Nonlocal Fokker-Planck equations with dynamical constraint involve 3 time scales

and preprint on rigorous PDE analysis (to appear on ArXiv soon).
For more details see paper in SIAM MMS (or arXiv:1110.3518).
Thank you!