Rigorous derivation of kinetic equations from particle systems

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Outline

Introduction

Derivation of kinetic equations from a reduced Hamiltonian particle system

Derivation of kinetic equations from mechanical models with particle aggregation

Motivation

- Many interesting systems in physics can be described by models with a large number of identical components whose microscopic behavior is based on the fundamental laws of mechanics (Newton equations)
- Huge number of particles $\Rightarrow$ behavior of the particles is too complicated at the microscopic level and impossible to analyze
- Instead: Look at the collective behavior of the system on scales much larger than the ones characterizing the micro dynamics
- On such macro scales the system is much simpler and is described by integro-differential equations for which the analysis is more feasible
- The problem of deriving these equations from the microscopic dynamics through suitable scaling limits is one of the central problems of non-equilibrium statistical mechanics.

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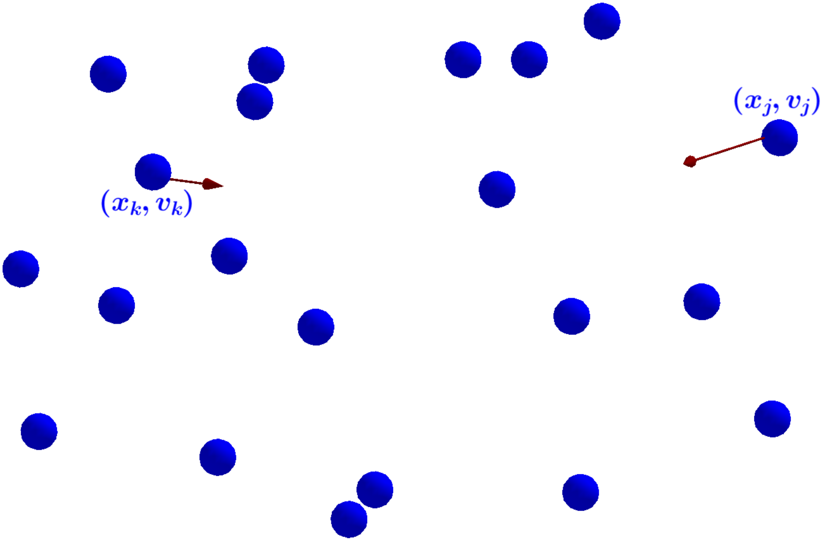

N identical particles in the space $\mathbb{R}^3$ whose physical state is given by their positions $x_1, \ldots, x_N$ and velocities $v_1, \ldots, v_N$. N very large ($N \sim 10^{20}$)

Microscopic description

Mesoscopic description

$$\begin{cases} \dot{x}_j = v_j \\ \dot{v}_j = \sum_{\substack{k=1 \\ j \neq k}}^{N} \mathsf{F}_{jk} \end{cases} \quad \xrightarrow[\text{(Markovian approximation)}]{\text{kinetic limit}} \quad \underbrace{(\partial_t + v \cdot \nabla_x) f}_{transport} = \underbrace{Q(f, f)}_{collisions}$$

Newtonian dynamics

Kinetic equations (Boltzmann/Landau eq.)

- particles interact via a two-body interaction $\phi : \mathbb{R}^3 \to \mathbb{R}^+$
- ϕ spherically symmetric $\Rightarrow$ the force $F_{jk} = -\nabla \phi(x_j - x_k)$ of particle j acting on particle k is directed along $x_j - x_k$
- $f : \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}_+$ probability density in the phase space
- Kinetic limit: suitable rescaling for the number of particles ($N \to \infty$)
  and range/intensity of the potential
  $\rightsquigarrow$ finite/infinite no. of collisions for unit time

Microscopic description

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Newtonian dynamics

kinetic limit $\longrightarrow$ (Markovian approximation)

Mesoscopic description

$$\underbrace{(\partial_t + v \cdot \nabla_x) f}_{\textit{transport}} = \underbrace{Q(f,f)}_{\textit{collisions}}$$

Kinetic equations (Boltzmann/Landau eq.)

[Boltzmann 1872]

$$\partial_t f + v \cdot \nabla_x f = Q(f,f) \qquad \text{on} \quad f(t,x,v) \geq 0$$

$$Q(f,f)(v) = \int_{S^2} \int_{\mathbb{R}^3} \underbrace{B(v - v_*, \omega)}_{\text{collision kernel } (\geq 0)} \{\underbrace{f(v')f(v'_*)}_{\text{appearing}} - \underbrace{f(v)f(v_*)}_{\text{disappearing}}\} d\omega \, dv_*$$

[Lanford '75 (hard-spheres); Pulvirenti, Saffirio, Simonella (smooth short-range potentials); Pulvirenti, Simonella (hard-spheres); Gallagher, Saint-Raymond, Texier (smooth short-range potentials) . . . **only for short times !!**]

Microscopic description

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$\xrightarrow{\text{kinetic limit}}$

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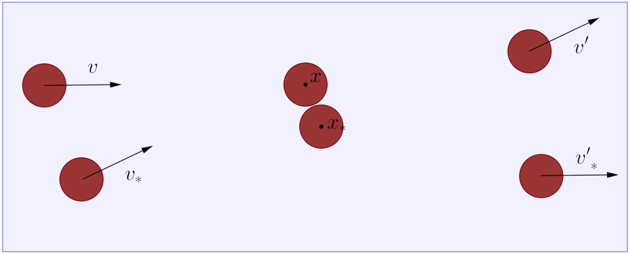

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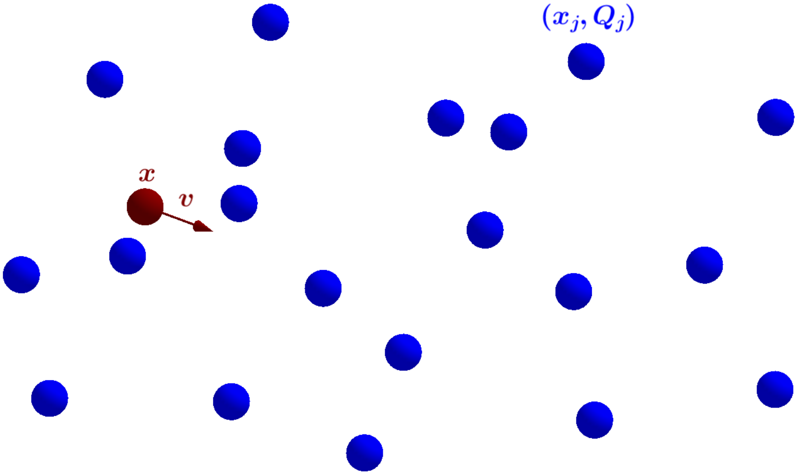
Postulates:

- particles interact via binary collisions (dilute regime)
- collisions are localized in space & time (the duration of a collision is very small)
- collisions are elastic (momentum and kinetic energy are preserved)
- collisions are microreversible (reversibility at microscopic level)
- Boltzmann chaos (velocities of two particles about to collide are uncorrelated)

From a many-body problem into an effective single-particle system



Test particle in a random configuration of obstacles $c_1, \ldots, c_N$ [Lorentz 1905]

Microscopic description

$$\begin{cases} \dot{x} = v \\ \dot{v} = -\sum_i \nabla\Phi(x - x_i) \end{cases}$$

Newtonian dynamics (Lorentz gas)

$\xrightarrow{\text{kinetic limit}}$ (Markovian approximation)

Mesoscopic description

$$\underbrace{(\partial_t + v \cdot \nabla_x) f}_{\textit{transport}} = \underbrace{\mathcal{L}(f)}_{\textit{collisions}}$$

Linear kinetic equations

Linear Boltzmann equation

$$(\partial_t + v \cdot \nabla_x) f(t, x, v) = \int_{\mathbb{S}^2} d\omega\, B(\omega, v)\,[f(t, x, v'(\omega)) - f(t, x, v)]$$

$$v' = v - 2(\omega \cdot v)\omega \quad (\text{collision rule})$$

Lorentz Gas: Poisson distribution of obstacles in $\mathbb{R}^d$ of intensity μ.
ϕ: short-range potential. $\varepsilon > 0$ micro-macro ratio.

Low density limit: $\mu_\varepsilon = \varepsilon^{-(d-1)}\mu, \quad \phi(x) \to \phi\left(\frac{x}{\varepsilon}\right)$ (rarefied gas)

[Gallavotti '69; Spohn '78; Desvillettes, Pulvirenti '99; Basile, N.,Pezzotti, Pulvirenti CMP'15; Marcozzi, N. JSP '16]

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Newtonian dynamics
(Lorentz gas)

kinetic limit $\longrightarrow$ (Markovian approximation)

Mesoscopic description

$$\underbrace{(\partial_t + v \cdot \nabla_x) f}_{transport} = \underbrace{\mathcal{L}(f)}_{collisions}$$

Linear kinetic equations

Linear Landau equation

$$(\partial_t + v \cdot \nabla_x) f(t,x,v) = k\, \Delta_{v_\perp} f(t,x,v)$$

$\Delta_{v_\perp}$: Laplace Beltrami op. on $\mathbb{S}^2$; $k > 0$: diffusion coefficient

Weak-coupling limit: $\mu_\varepsilon = \varepsilon^{-d}\mu$, $\phi(x) \to \sqrt{\varepsilon}\phi\left(\frac{x}{\varepsilon}\right)$ (high density, weak inter.)

[Kesten, Papanicolau '78, Dürr, Goldstein, Lebowitz '87, Desvillettes, Ricci '01; Komorowski, Ryzhik '06; Basile, N., Pulvirenti JSP'14; Marcozzi, N. JSP '16]

The Markovian approximation

- Linear Boltzmann equation

$$\{v(t)\}_{t\geq 0} \text{ Markov jump process,} \quad x(t) = \int_0^t v(s)ds$$

- Linear Landau equation

$$\{v(t)\}_{t\geq 0} \text{ Brownian motion on } S^d_{|v|}, \quad x(t) = \int_0^t v(s)ds$$

(Diffusion on the energy sphere)

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Why a diffusion?

- Momentum transferred in a single scattering: $O(\sqrt{\varepsilon})$
- Number of obstacles met by a test particle in the unit time: $O(\frac{1}{\varepsilon})$
- Total momentum variation in unit time: zero in the average,

  variance $\frac{1}{\varepsilon} O(\sqrt{\varepsilon})^2 = O(1)$

$$|v| \text{ preserved (elastic collisions)} \Rightarrow \text{diffusion on } S^d_{|v|}$$

Diffusion coefficient? Variance of the transferred momentum in each collision.

The Markovian approximation

Initial probability distribution $f_0 = f_0(x, v)$.

$$f_\varepsilon(x, v, t) = \mathbb{E}_\varepsilon[f_0(T_{\mathbf{c}_N}^{-t}(x, v))], \quad T_{\mathbf{c}_N}^{t}(x, v) \text{ Hamiltonian flow}$$

Goal: $f_\varepsilon(x, v, t) \to f(x, v, t)$ as $\varepsilon \to 0$?

Strategy: constructive approach [Gallavotti '79]

Technical difficulty: some random configurations

$\rightsquigarrow$ trajectories that "remember" too much (*unphysical trajectories*)

Key tools:

- suitable **change of variables**
  $\rightsquigarrow$ Markovian approximation (given by the Boltzmann eq.)
- control of **memory effects:**
  the set of bad configurations (**recollisions**, **interferences**) is negligible as $\varepsilon \to 0$ (*quantitative estimates*!)

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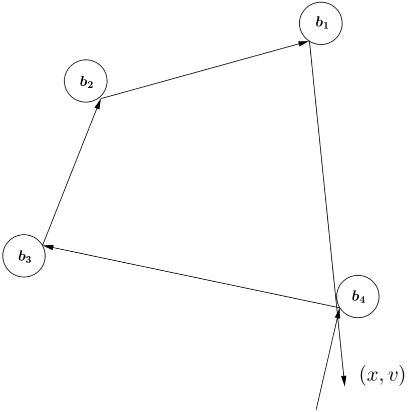
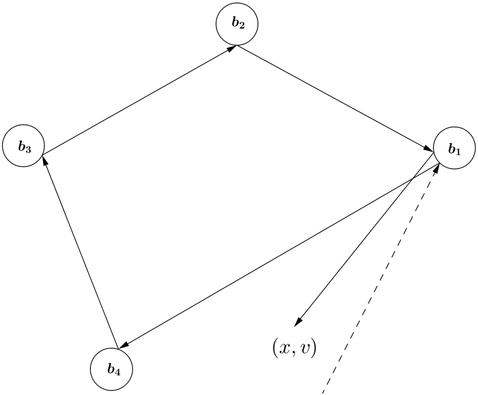
Pathological configurations in the Markovian approximation



Backward Interference

$\exists b_j$ s.t. $\xi_\varepsilon(-s) \in B(b_j, \varepsilon)$
for $s \in (t_{i+1}, t_i)$, $j > i$



Backward Recollision

$\exists b_i$ s.t. for $s \in (t_{j+1}, t_j)$, $j > i$,
$\xi_\varepsilon(-s) \in \partial B(b_i, \varepsilon)$

Microscopic description **Macroscopic description**

$$\begin{cases} \dot{x} = v \\ \dot{v} = -\sum_i \nabla\Phi(x - x_i) \end{cases} \quad \Longrightarrow \quad \partial_t \varrho = D\Delta\varrho, \quad \varrho = \int f\, dv$$

[Bunimovich and Sinai '81]

Newtonian dynamics (Lorentz gas)

Hydrodynamic equation (diffusion equation)

$\searrow$ $\nearrow$

Mesoscopic description

kinetic limit $\nearrow$ $\nwarrow$ fast relaxation limit

$$(\partial_t + v \cdot \nabla_x) f(x, v, t) \sim \mu_\varepsilon \varepsilon\, \mathcal{L} f(x, v, t)$$

Scaling limit: $\phi(x) \to \phi\left(\frac{x}{\varepsilon}\right)$, $\mu_\varepsilon \to \infty$ s.t. $\mu_\varepsilon \varepsilon \to \infty$ & $\mu_\varepsilon \varepsilon^2 \to 0$ ("Low density")

Look at a longer time scale in which the equilibrium starts to evolve
$\Longrightarrow$ diffusion for the position variable

[Erdos, Salmhofer, Yau, '08 (Quantum Boltzmann); [Bodineau, Gallagher, Saint-Raymond '13 (Boltzmann); Basile, N., Pulvirenti JSP'13 (Landau); Basile, N.,Pezzotti, Pulvirenti CMP'15 (Boltzmann; **nonequilibrium**; **Fick Law**)]

Short-range vs. long-range interactions.
The role of correlations

Test particle in random force fields with long range interactions

$$\frac{dx}{dt} = v, \quad \frac{dv}{dt} = F_\varepsilon(x;\omega); \quad x(0) = x_0,\ v(0) = v_0$$

Kinetic limit?

Main feature: Mixing properties of the random field (short-range potentials)
$\Rightarrow$ statistical independence of trajectories in the limit

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Main difficulty: Slow decay of the correlations of the random field

- Construct the random field determined by a Poisson distr. of sources generating potentials $\Phi(x) \sim |x|^{-s}$, $s > 1/2$ (with different charges)

[Chandrasekhar '43, Holtsmark '19]

$$F(x;\omega) = \lim_{R\to\infty} F_U^{(R)}(x;\omega) = \lim_{R\to\infty}\left[-\sum_{x_n\in RU} Q_{j_n}\nabla\Phi(x-x_n)\right]$$

- Estimate the diffusive timescale and identify conditions for the vanishing of correlations to obtain the correct Markovian approximation.

[N., Simonella, Velázquez RMP '18]

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Kinetic description: $\phi(x) \sim |x|^{-s}$ for $|x|$ large

Which is the fastest process determining particle deflections?

$s > 1$	$s = 1$	$1/2 < s < 1$
Boltzmann eq. $(T_{BG} \ll T_L)$	Landau eq. $(T_L \ll T_{BG})$	Stochastic diff. eq. with correlations $x(\tau + d\tau) - x(\tau) = v(\tau)d\tau$ $v(\tau + d\tau) - v(\tau) = D(x(\tau), v(\tau); d\tau)$ $D = O(d\tau^{\beta}) \;\; \beta \in (0, 1)$

- binary collisions with single scatterers $\Rightarrow$ linear Boltzmann eq.
- many small interactions before a binary collision $\Rightarrow$ linear Landau eq. (the deflections over times of order T_L should be uncorrelated!!)
- if the lack of correlations does not take place $\Rightarrow$ stochastic diff. eq. (macroscopic deflections must be taken into account !)

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Key tool: analysis of the **correlations** for the deflections

$$D(x_0, v; \tilde{T}_L) = \int_0^{\tilde{T}_L} \nabla_x \Phi_L\left(x_0 + vt, \varepsilon\right) \omega\, dt \qquad (\tilde{T}_L = hT_L)$$

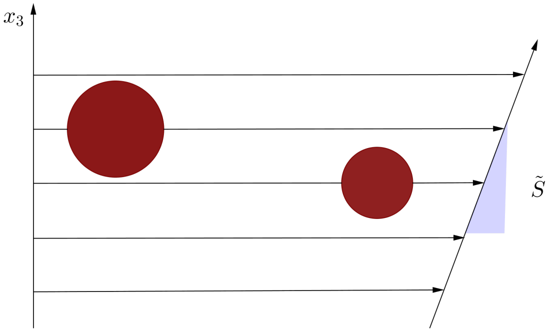
Perspectives . . . . . .

- Rigorous derivation of the linear Landau eq. for Coulombian interactions
- Rigorous derivation of the linear Boltzmann eq. for $\phi(|x|) \sim |x|^{-s}$, $s > 1$
- Extension to the analysis of long-range potentials in the nonlinear case.
- Analysis of the stochastic differential eq. with correlated noise $\quad (s \leq \frac{1}{2})$

Coagulation vs. collision dynamics

Microscopic irreversibility No Detailed Balance	vs.	Microscopic reversibility Detailed Balance

Coagulation processes in shear flows



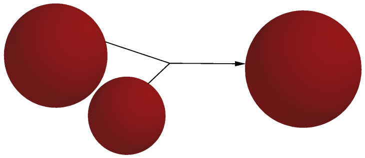
- spherical particles in $\mathbb{R}^3$
- $u(x) = \left(\tilde{S}x_3, 0, 0\right)$ speed

  $\tilde{S} = \frac{\partial u_1}{\partial x_3}$ shear coeff.
- position of particle center

  $x_1 = x_{1,0} + Ux_3 t$

- Collisions between pairs of particles with different values of x_3

  $\Rightarrow$ instantaneous coalescence



Smoluchowski Equation in a shear flow (1916)

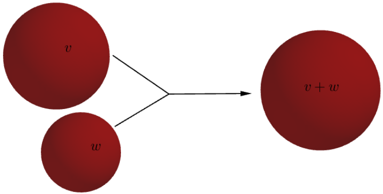
- Suitable rescaling for shear, particle density and volume fraction (one collision for unit of time)
- The particle distribution in the space of positions and volumes f in the scaling limit satisfies

$$\partial_t f(t,x,v) + Ux_3\partial_{x_1} f(t,x,v) = \frac{1}{2}\int_0^v K(v-w,w)f(t,x,v-w)f(t,x,w)dw - \int_0^\infty K(v,w)f(t,x,v)f(t,x,w)dw$$

Coagulation kernel

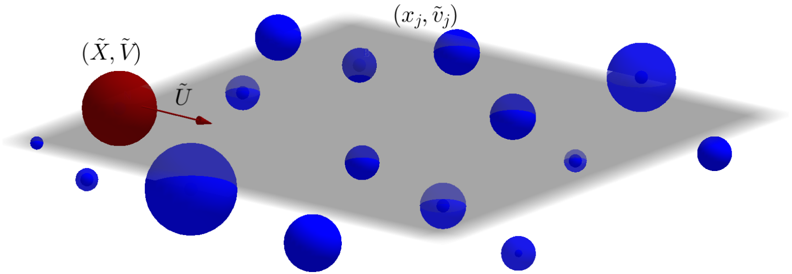
$$K(v,w) = \frac{4}{3}S(v^{\frac{1}{3}} + w^{\frac{1}{3}})^3$$

(collision frequency)



[Smoluchowski 1916]

A coalescing particle in a random background



- Random distribution of obstacles: $\{x_j\}_{j \in N}$ positions, $\{\tilde{v}_j\}_{j \in N}$ volumes
- Average no. of particles for unit of volume is 1. Volume fraction $\phi > 0$
- $\{x_k\} \sim \mathcal{P}_1$ in $\mathbb{R}^3$ and $\{v_k\} \sim G(v)$ prob. distr. in $[0, \infty)$. $G(v) \sim v^{-\sigma}$

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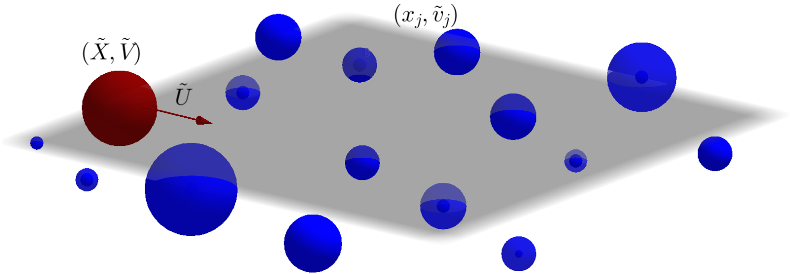
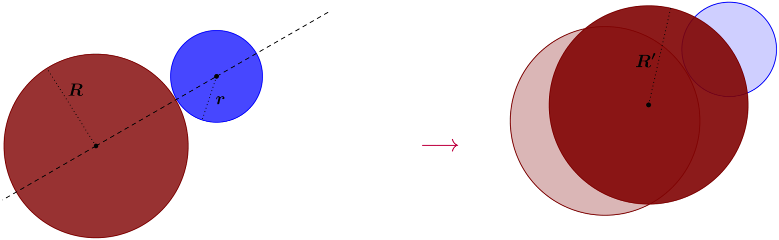


- The tagged particle moves freely with speed $\tilde{U}$ along $e_1 = (1, 0, 0)$
- $(\tilde{Y}_0, \tilde{V}_0)$ initial configuration. $\tilde{Y}(t) = \tilde{X}(t) - \tilde{U}te_1$ (moving background)
- Merging dynamics: new volume $\tilde{V} + \sum_j \tilde{v}_j$; new position in the center of mass.

Kinematic of coalescing processes

Binary coagulation: [tagged particle with a single obstacle]



$V = \frac{4}{3}\pi R^3$, $v = \frac{4}{3}\pi r^3$ $\quad$ $V' = V + v, \;\; R' = (r^3 + R^3)^{\frac{1}{3}}$

Multiple coagulation: merging operator $\mathcal{M}$

$$\mathcal{M}(Y, V; \omega) = \left(\frac{VY + \sum_{k \in J} x_k v_k}{V + \sum_{k \in J} v_k}, V + \sum_{k \in J} v_k ; \omega \setminus J \right)$$

Linear Smoluchowski Equation in a shear flow

- Suitable rescaling for the speed of the tagged particle, position and sizes (one collision for unit of time)
- The distribution function f for the particle position and volume in the scaling limit satisfies

$$\partial_t f(Y,V,t) = U\int_0^{\frac{\pi}{2}} d\theta \int_0^{2\pi} d\varphi \Big[\int_0^V dv\, K(V-v,v,\theta) f(Y - \frac{v}{V-v} R\, n(\theta,\varphi), V-v, t) - \int_0^{\infty} dv\, K(V,v,\theta) f(Y,V,t) \Big] \equiv \mathcal{Q}[f](Y,V,t)$$

$$R = \left(\tfrac{3V}{4\pi}\right)^{\frac{1}{3}}, \qquad n(\theta,\varphi) = (\cos\theta, \sin\theta\cos\varphi, \sin\theta\sin\varphi)$$

$$K(V,v,\theta) = \left(\frac{3}{4\pi}\right)^{\frac{2}{3}} \sin\theta\cos\theta\, G(v)(V^{\frac{1}{3}} + v^{\frac{1}{3}})^2 \qquad \text{(coagulation kernel)}$$

Features of the model

Main source of technical difficulties:

- coalescing particles could trigger sequences of coagulation events
  (formation of an infinite cluster)
- the free flights between coagulation events become shorter
  due to the increasing volume of the tagged particle
  (runaway growth of the tagged particle in finite time)

Main feature of the CTP model:

- The displacement of the center of the tagged particle is not too large
  as the size increases $\rightsquigarrow$ no finite time blow-up with probability one !

Main results

Global well-posedness

- **If** the coalescence events have a finite no. of steps with probability one
- **If** the total length of the free flights of the tagged particle is infinite with probability one ($\sum_j l_j = \infty$)

$\Rightarrow$ the motion of the tagged particle is defined globally in time with probability one.

Rigorous validation of the kinetic equation

$f_0(Y, V)$: initial probability distribution $\quad f_0 \in \mathcal{P}(\mathbb{R}^3 \times \mathbb{R}^+)$

$f_\phi(Y, V, t)$: sol. of the microscopic process $\quad f_\phi \in L^\infty([0, T); \mathcal{M}_+(\mathbb{R}^3 \times \mathbb{R}^+))$

$f(Y, V, t)$: weak sol. of the linear Smoluchowski equation

$$\Rightarrow \quad f_\phi(Y, V, t) \to f(Y, V, t) \quad \text{as} \quad \phi \to 0$$

Main results

Global well-posedness

$\Rightarrow$ the motion of the tagged particle is defined globally in time with probability one.

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Asymptotic behavior of solutions for different values of the power law σ

Self-similarity for $\frac{5}{3} < \sigma < 2$: [Niethammer, N., Throm, Velázquez JDE '18]

- Existence and uniqueness of self-similar profiles
- Stability

Conjectures:

- $\sigma \leq \frac{5}{3}$: instantaneous explosive growth of the volume of the tagged particle
- $\sigma > 2$: the volume of the tagged particle increases like t^3 as $t \to \infty$ (critical exponents for the "fluctuations")

Perspectives . . . . . .

- Characterization of the asymptotic behavior for the solutions (for different σ)
- Rigorous derivation of the nonlinear Smoluchowski eq. in a laminar shear flow
- Rigorous derivation of the Smoluchowski eq. for Brownian particles

  (in the mass-dependent diffusivity and interaction radius case)

Thank you for your attention !!!