The Enskog process:

Particle approximation for hard and soft potentials

Martin Friesen

joint work with:
Barbara Rüdiger
Padmanabhan Sundar

October 27, 2017
International Conference on Stochastic Analysis, Stochastic Control and Applications
Hammamet, Tunisia

General setting

- We study a gas in the vacuum in dimension $d \geq 3$.
- Each particle is completely described by position r and velocity v.
- Particles move according to straight lines in the direction of their velocities.
- Particles perform binary, elastic collisions.
  Velocities may be parametarized by $n \in S^{d-1}$ via

$$v^\star = v + (u - v, n)n$$
$$u^\star = u - (u - v, n)n$$

  where u, v incomming velocities and $u^\star, v^\star$ outgoing velocities.
- Conservation of momentum

$$v + u = v^\star + u^\star$$

  Conservation of kinetic energy

$$|v|^2 + |u|^2 = |v^\star|^2 + |u^\star|^2.$$

The space-homogeneous case

Space-homogeneous case corresponds to particles uniformly distributed in $\mathbb{R}^d$.

Sochastic methods

- Tanaka '79, '87
- Horowitz, Karandikar '90
- Fournier, Mouhot '06
- Fournier '15
- Fournier, Mischler '16
- Xu '16

Analytic methods

- Desvillettes, Mouhot '06
- Lu, Mouhot '12
- Morimoto, Wang, Yang '16

What is studied?

- Existence and uniqueness to space-homogeneous Boltzmann equation
- Existence of a density, finiteness of entropy
- Particle approximation, propagation of chaos
- Speed of convergence to equilibrium

But what happens if the particles are not distributed uniformly in space?

The Enskog equation

The time evolution is described by a particle density function $f_t(r,v) \geq 0$ subject to the Enskog equation

$$\frac{\partial f_t(r,v)}{\partial t} + v \cdot (\nabla_r f_t)(r,v) = \mathcal{Q}(f_t, f_t)(r,v), \quad t > 0,\ r, v \in \mathbb{R}^d$$

with non-local and non-linear collision integral

$$\mathcal{Q}(f_t, f_t) = \int_E \left(f_t(r, v^\star) f_t(q, u^\star) - f_t(r,v) f_t(q,u)\right) \beta(r-q) \sigma(|v-u|) du dq Q(d\theta) d\xi$$

where $E = \mathbb{R}^{2d} \times (0, \pi] \times S^{d-2}$, $|(u-v, n)| = \sin(\frac{\theta}{2})|u-v|$.

- If $\beta = \delta_0$, then we get the classical Boltzmann equation.
- If $\beta = 1$, then space-homogeneous Boltzmann equation.
- If $0 < a \leq \beta \in L^\infty$, then similar to space-homogeneous Boltzmann equation.

In this work we consider $\beta \geq 0$ symmetric and **compactly supported around zero**

The physical collision kernel

In the physical dimension $d = 3$ have
Boltzmanns original model

$$\sigma(|z|) = |z| \quad \text{and} \quad Q(d\theta) = \sin(\frac{\theta}{2})\cos(\frac{\theta}{2})d\theta.$$

Most common class of models: $s > 2$

$$\sigma(|z|) = |z|^{\gamma} \quad \text{and} \quad Q(d\theta) = b(\theta)d\theta$$

with

$$\gamma = \frac{s-5}{s-1} \in (-3, 1) \quad \text{and } b(\theta) \sim \theta^{-1-\nu} \quad \text{and} \quad \nu = \frac{2}{s-1} \in (0, 2).$$

One distinguishes between the following:

Table:

Hard potentials	$0 < \gamma < 1$	$0 < \nu < \frac{1}{2}$	$5 < s$
Maxwellian molecules	$\gamma = 0$	$\nu = \frac{1}{2}$	$5 = s$
Soft potentials	$-1 < \gamma < 0$	$\frac{1}{2} < \nu < 1$	$3 < s < 5$
Very soft potentials	$-3 < \gamma < -1$	$1 < \nu < 2$	$2 < s < 3$

Role of angular singularity

- Typically $\int_0^{\pi} Q(d\theta) = \infty$.
- But $\int_0^{\pi} \theta^a Q(d\theta) < \infty$ for all $a > \nu$.

Assumptions

Our assumptions

1. $\beta \in C_c^1(\mathbb{R}^d)$ and moderate angular singularity

$$\int_0^\pi \theta Q(d\theta) < \infty.$$

2. $\sigma(|z|) = |z|^\gamma$ or $\sigma(|z|) = (1 + |z|^2)^{\frac{\gamma}{2}}$ with $\gamma \in (-1, 2]$

Some remarks:

- Only an upper bound and some Lipschitz-type estimate is imposed on σ.
- In the physical dimension $d = 3$ we cover all cases where $s > 3$ (Hard potentials, Maxwell molecules and Soft potentials).
- For Very soft potentials several technical difficulties have to be overcome.

Posing the problem

Main question:
Find the stochastic process **(Enskog process)** behind the Enskog equation.

Use such a representation to study:

- Existence and uniqueness theory.
- Particle approximation scheme / propagation of chaos.

This is an extension / continuation of

(Albeverio, Rüdiger, Sundar, '17, *The Enskog process*, J. Stat. Phys.)

Our methods are mainly stochastic, but different to the previous work.

Weak formulation of the Enskog equation

Do not know that every solution has a density $\Rightarrow$ study weak formulation.

Definition

$(\mu_t)_{t\geq 0}$ (weak) solution to Enskog equation, if

- Has enough moments, i.e.

$$\sup_{t\in[0,T]} \int_{\mathbb{R}^{2d}} \left(|v| + |v|^{1+\gamma}\right) d\mu_t(r,v) < \infty, \quad \forall T > 0.$$

- Satisfies the equation, i.e. for all $\psi \in C_b^1(\mathbb{R}^{2d})$

$$\langle \psi, \mu_t \rangle = \langle \psi, \mu_0 \rangle + \int_0^t \langle A(\mu_s)\psi, \mu_s \rangle ds.$$

with $\langle \psi, \mu \rangle = \int_{\mathbb{R}^{2d}} \psi(r,v) d\mu(r,v)$ and

$$(A(\mu_s)\psi)(r,v) = v \cdot (\nabla_r \psi)(r,v)$$
$$+ \int_{\mathbb{R}^{2d}} \int_{S^{d-1}} \left(\psi(r,v^\star) - \psi(r,v)\right) \beta(r-q)\sigma(|v-u|)Q(d\theta)d\xi d\mu_s(q,u)$$

Stochastic representation Theorem

Let $(\mu_t)_{t\geq 0}$ solution to Enskog equation such that

$$t \longmapsto \int_{\mathbb{R}^{2d}} |v|^{1+\gamma} d\mu_t(r,v)$$

is continuous. Then:

- There exists a stochastic process (R_t, V_t) such that

$$\psi(R_t, V_t) - \psi(R_0, V_0) - \int_0^t (A(\mu_s)\psi)(R_s, V_s) ds$$

  is a martingale for all $\psi \in C_b^1(\mathbb{R}^{2d})$ and $(R_t, V_t) \sim \mu_t$.
- Moment estimates for $p \geq 1$ (where $\gamma^+ = \max\{\gamma, 0\}$)

$$\mathbb{E}(\sup_{s\in[0,t]} |V_s|^p) \leq \left(\mathbb{E}(|V_0|^p) + C \sup_{s\in[0,T]} \mathbb{E}(|V_s|^{p+\gamma^+}) \right) e^{Ct}, \quad t \in [0,T], \ T > 0.$$

- If V_t has $3+\gamma$ moments, then conservation of momentum and energy holds.

Above condition is satisfied if μ_t has $2+2\gamma$ finite moments in v.

On the existence of solutions

Yet do not know whether such a solution to the Enskog equation exists!
Case $Q((0,\pi]) < \infty$ and σ nice

- Illner, Shinbrot '84
- Bellomo, Toscani '87
- Mischer, Perthame '97
- Boudin, Desvillettes '00

Case physical cases: we have some recent progress

- Alexandre, Morimoto, Ukai, Xu , Yang '11, '12 (several works)
- Solution is $f_t = \nu + g_t\sqrt{\nu}$ where $\nu(v) = (2\pi)^{-\frac{3}{2}} e^{-\frac{|v|^2}{2}}$.
- g_t is small in a suitable weighted anisotropic Sobolev norm.
- Alexandre, Morimoto, Ukai, Xu , Yang '13 also solution of the form $f_t = \nu g_t \ldots$

These are **Theories in the small**, i.e. close to Maxwellian.
Why Gaussian ν? Corresponds to equilibrium in the velocity space, i.e.

$$\mathcal{Q}(\nu,\nu) = 0.$$

Existence Enskog process: Soft potentials, Maxwellian molecules

Consider the case $\gamma \in (-1, 0]$, i.e. soft potentials or Maxwellian molecules.
Let μ_0 be such that $\exists p > 2$ and $\exists \varepsilon > 0$ with

$$\int_{\mathbb{R}^{2d}} (|r|^{\varepsilon} + |v|^{p})\, d\mu_0(r, v) < \infty.$$

Then:

- There exists an Enskog process (R_t, V_t) such that

$$\mathbb{E}(\sup_{s \in [0,t]} |V_s|^p) \leq \mathbb{E}(|V_0|^p) e^{Ct}, \quad t \geq 0.$$

- This solution satisfies the conservation laws

$$\mathbb{E}(V_t) = \mathbb{E}(V_0), \quad \mathbb{E}(|V_t|^2) = \mathbb{E}(|V_0|^2).$$

- $\mu_t \sim (R_t, V_t)$ is a solution to the Enskog equation.

Existence Enskog process: Hard potentials

Consider the case $\gamma \in (0, 2]$, i.e. hard potentials.
Let μ_0 be such that $\exists \varepsilon > 0$ and $\exists a > 0$ with

$$C(\mu_0, a) := \int_{\mathbb{R}^{2d}} \left(|r|^{\varepsilon} + e^{a|v|^2} \right) d\mu_0(r, v) < \infty.$$

Then:

- There exists an Enskog process (R_t, V_t) such that for all $p \geq 1$

$$\mathbb{E}(\sup_{s \in [0,t]} |V_s|^p) \leq K_p C(\mu_0, c_p t), \quad t \geq 0.$$

- Solution satisfies the conservation laws.
- $\mu_t \sim (R_t, V_t)$ solves the Enskog equation.

Particle approximation

Let $n \geq 2$ be the number of particles in the gas.
We consider an IPS with Markov generator on $F \in C_c^1(\mathbb{R}^{2dn})$

$$(L_n F)(r,v) = \sum_{k=1}^{n} v_k \cdot (\nabla_{r_k} F)(r,v)$$
$$+ \frac{1}{n} \sum_{k,j=1}^{n} \sigma(|v_k - v_j|)\beta(r_k - r_j) \int_{S^{d-1}} \Big(F(r, v_{kj}) - F(r,v)\Big)\, Q(d\theta)d\xi$$

where $r = (r_1, \ldots, r_n)$, $v = (v_1, \ldots, v_n)$ and $v_{kj} = v + e_k(v_k^\star - v_k) + e_j(v_j^\star - v_j)$.

- The martingale problem $(L, C_c^1(\mathbb{R}^{2dn}), \rho^{(n)})$ is well-posed.
- The transition semigroup leaves C_b invariant and is pointwisely continuous in t.
- The transition semigroup leaves C_0 invariant and is strongly continuous.
- Study moment estimates with constants uniformly in $n \geq 2$.

Particle approximation

Let $(R_1^n, V_1^n), \ldots, (R_n^n, V_n^n)$ be the corresponding Markov process.
The sequence of empirical measures

$$\mu^{(n)} = \frac{1}{n} \sum_{k=1}^{n} \delta_{(R_k^n, V_k^n)}$$

is a random probability measure on $D(\mathbb{R}_+; \mathbb{R}^{2d})$. Denote by $\pi^{(n)}$ the law of $\mu^{(n)}$.
Then:

- $\mu^{(n)}$ is tight, i.e. $\pi^{(n)}$ is relatively compact.
- Let $\pi^{(\infty)}$ be any accumulation point of $\pi^{(\infty)}$. Then for any $P \in \mathrm{supp}(\pi^{(\infty)})$

  $$\psi(r(t), v(t)) - \psi(r(0), v(0)) - \int_0^t (A(\mu_s)\psi)(r(s), v(s))ds, \quad \psi \in C_b^1(\mathbb{R}^{2d})$$

  is a martingale w.r.t. P. Here $(r(t), v(t))$ coordinate process in $D(\mathbb{R}_+; \mathbb{R}^{2d})$.
- Moment estimates for the IPS remain valid for all $P \in \mathrm{supp}(\pi^{(\infty)})$.

Final remarks

- If uniqueness holds for the Enskog equation,
  then typically uniqueness holds for the Enskog process, i.e. $\pi^{(\infty)} = \delta_P$.
  This implies classically *Propagation of chaos*, i.e. $\mu^{(n)} \Longrightarrow P$.
- Some uniqueness is avaliable, but far from satisfactory. Work in progress...

- The moment assumptions for hard potentials are too strong.
- Existence of densities should be different to space-homogeneous case.

Thank You

Thank You!

Stochastic representation Theorem

Such an Enskog process can be obtained as a weak solution to the SDE

$$R_t = R_0 + \int_0^t V_s ds$$

$$V_t = V_0 + \int_0^t \int_E \alpha(V_s, u_s(\eta), \theta, \xi) 1_{[0,\sigma(|V_s - u_s(\eta)|)\beta(R_s - q_s(\eta))]}(z) dN(\eta, z, \theta, \xi, s)$$

where $E = [0,1] \times \mathbb{R}_+ \times (0,\pi] \times S^{d-2}$

- $\alpha(v, u, \theta, \xi) = v^\star - v$ and $-\alpha(v, u, \theta, \xi) = u^\star - u$
- N is a Poisson random measure with compensator on $\mathbb{R}_+ \times E$.

$$d\widehat{N} = d\eta dz Q(d\theta) d\xi$$

- (q_s, u_s) RCLL-process on $([0,1], dz)$ such that $(q_s, u_s) \sim (R_s, V_s) \sim \mu_s$.

Idea of proof: Stochastic representation Theorem

The assertion follows from

Kurtz, Stockbridge '01, Electron. J. Probab.,

Stationary solutions and forward equations for controlled and singular martingale problems

provided we can show

(a) $A(\mu_t)\psi$ is continuous in (t, r, v) for any $\psi \in C_b^1(\mathbb{R}^{2d})$.

(b) There exists a solution to the martingale problem $(A(\delta_{(q,u)}), C_b^1(\mathbb{R}^{2d}), \delta_{(r_0,v_0)})$, for all $(q, u),\ (r_0, v_0) \in \mathbb{R}^{2d}$.

(c) $A(\mu_t)$ satisfies the technical separability condition:
There exists $(\psi_k)_{k\geq 1} \subset C_b^1(\mathbb{R}^{2d})$ such that

$$\left\{ \frac{1}{\zeta} A(\mu_t)\psi \mid \psi \in C_b^1(\mathbb{R}^{2d}) \right\} \subset \overline{\left\{ \frac{1}{\zeta} A(\mu_t)\psi_k \mid k \geq 1 \right\}}$$

with $\zeta(v, u) = (1 + |v|^2)(1 + |u|^2)$.
Closure is taken w.r.t. bounded pointwise convergence.

In contrast to other methods **no uniqueness statement** is needed!

- **But:** Yet do not know whether such a solution to the Enskog equation exists!