Homogeneous polyatomic Boltzmann flow: wellposedness and integrability

Milana Čolić

Department of Mathematics and Informatics, Faculty of Sciences, University of Novi Sad

in collaboration with R. Alonso & I. M. Gamba

Mathematical models for interacting dynamics on networks

Alexander von Humboldt Stiftung/Foundation

Science Fund of the Republic of Serbia

PROMIS, MaKiPol #6066089

Outline of the talk

- Kinetic model (Boltzmann equation based on the continuous internal energy)
- Space homogeneous problem:
  - Existence and Uniqueness theory

Irene M. Gamba and Milana Pavić-Čolić.
On the Cauchy problem for Boltzmann equation modelling a polyatomic gas,
Journal of Mathematical Physics, 64: 013303, 2023.

Ricardo Alonso, Irene M. Gamba and Milana Pavić-Čolić.
The Cauchy Problem for Boltzmann Bi-linear Systems: The Mixing of Monatomic and Polyatomic Gases, Journal of Statistical Physics, 191:9, 2024.

  - Intregrability propagation

Ricardo Alonso and Milana Pavić-Čolić.
Integrability propagation for a Boltzmann system describing polyatomic gas mixtures,
SIAM Journal on Mathematical Analysis, 56:1, 2024.

Boltzmann equation for a polyatomic gas in the continuous setting

- distribution function $f(t, x, \xi)$ describes the state of a gas
- t time, x space, ξ microscopic (kinetic) variable

  monatomic gas – particle velocity v

  polyatomic gas $\xi = (v, I)$

The Boltzmann equation

$$\partial_t f(t,x,\xi) + v \cdot \nabla_x f(t,x,\xi) = Q(f,f)(\xi)$$
$$= Q^+(f,f)(\xi) - Q^-(f,f)(\xi) = Q^+(f,f)(\xi) - \nu[f](\xi) f(\xi)$$

- two elements: transport operator $v \cdot \nabla_x$ and collision operator $Q(f,f)(\xi)$
- to describe collision operator $Q(f,f)(\xi)$ we need to study collisions (microscopic aspect)
  - even for elastic collisions, kinetic energy is not preserved

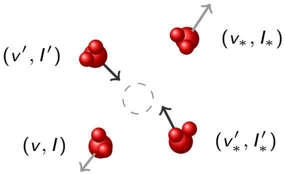
Bridge between molecular dynamics and fluid dynamics (observables=microscopic averages)

mass density $\rho(t,x) = \int_\xi m \, f$ or momentum density $\rho u(t,x) = \int_\xi mv \, f$

- specific internal energy $e(T)$ of a thermally perfect/nonpolytropic gas is related to temperature depended specific heats (macroscopic aspect)

$$\frac{\mathrm{d}\hat{e}(T)}{\mathrm{d}T} = \hat{c}_v(T) \neq \frac{3}{2}$$

Microscopic dynamics - binary collision of polyatomic molecules



$$\xi = (v, I) \in \mathbb{R}^3 \times [0, \infty)$$

$$V = \frac{v + v_*}{2}, \quad \text{center of mass velocity}$$

$$u = v - v_*, \quad \text{relative velocity}$$

$$\text{CL momentum} \quad mv' + mv'_* = mv + mv_*$$

$$\text{CL energy} \quad \frac{m}{2} v'^2 + I' + \frac{m}{2} v'^2_* + I'_* = \frac{m}{2} v^2 + I + \frac{m}{2} v^2_* + I_*$$

$\Leftrightarrow$

$$V' = V$$

$$\frac{m}{4} \left| u' \right|^2 + I' + I'_* = \frac{m}{4} \left| u \right|^2 + I + I_*$$

Borgnakke–Larsen procedure

$$V' = V$$

$$\underbrace{\frac{m}{4}\left|u'\right|^2}_{RE} + \underbrace{I' + I'_*}_{(1-R)E} = \frac{m}{4}\left|u\right|^2 + I + I_* =: E$$

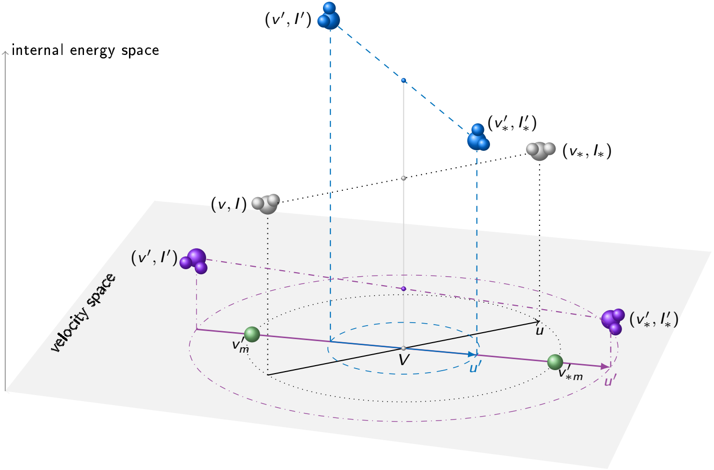
$$\frac{m}{4}\left|u'\right|^2 = RE$$

$$u' = \left|u'\right|\sigma = 2\sqrt{\frac{RE}{m}}\,\sigma$$

$$\iff \begin{cases} v' = V + \sqrt{\frac{RE}{m}}\,\sigma \\ v'_* = V - \sqrt{\frac{RE}{m}}\,\sigma \end{cases}$$

$$I' + I'_* = (1-R)E$$

$$\begin{cases} I' = r(1-R)E \\ I'_* = (1-r)(1-R)E \end{cases}$$



(v, I) and (v_*, I_*) given
prescribe a scattering direction σ and partition functions r and R
calculate the states (v', I') and (v'_*, I'_*) using the collision transformation

$R = 0.1 \Rightarrow$ E weights a bigger proportion to the internal energy for smaller values of R
(limit $R = 0$ renders the total energy E as the pure internal energy)

$R = 0.8 \Rightarrow$ larger values of R give a bigger proportion to the molecular kinetic energy
(limit $R = 1$ shrinks the total energy E to be just the kinetic energy)

v'_m and v'_{*m} - collisions without internal energy, or classical monatomic elastic collision

Boltzmann equation for a polyatomic gas - the continuous approach

- additional argument of the distribution function

$$f := f(t, x, v, I)$$

- the Boltzmann equation

$$\partial_t f + v \cdot \nabla_x f = Q(f,f)(v,I)$$

- collision operator (non-weighted setting)

$$Q(f,g)(v,I) = \int_{(v_*,I_*)} \int_{(\sigma,r,R)} \Bigg(\underbrace{f(v',I')\,g(v'_*,I'_*)}_{Q^+,\ \text{positive=gain}} \left(\frac{I\,I_*}{I'\,I'_*}\right)^{\alpha} - \underbrace{f(v,I)g(v_*,I_*)}_{Q^-,\ \text{negative=loss}} \Bigg) \underbrace{\mathcal{B}}_{\text{collision kernel}} \underbrace{d_\alpha(r,R)}_{\text{micro-reversibility}}$$

$\alpha > -1$ related to the specific heat c_v, $\quad \alpha = \hat{c}_v - \frac{5}{2}$,

$\alpha = \frac{\delta}{2} - 1$, with $\delta > 0$ related to the specific heat c_v, $\quad \delta = 2\hat{c}_v - 3$,

$d_\alpha(r,R) := (r(1-r))^{\alpha}(1-R)^{2\alpha+1}\sqrt{R}$ or $d_\delta(r,R) := (r(1-r))^{\frac{\delta}{2}-1}(1-R)^{\delta-1}\sqrt{R}$

$\mathcal{B} := \mathcal{B}(v, v_*, I, I_*, R, r, \sigma) = \mathcal{B}(v', v'_*, I', I'_*, R', r', \sigma') = \mathcal{B}(v_*, v, I_*, I, R, 1-r, -\sigma) \geq 0$

subject to modelling

- non-weighted setting (internal energy) $\|f\|_{L^1} = \int_{\mathbb{R}^3 \times [0,\infty)} |f(v,I)| \, \mathrm{d}I \mathrm{d}v$

cf. Bourgat&Desvillettes&Le Tallec&Perthame'94

$$Q^{nw}(f,f)(v,I) = \int_{(v_*,I_*)} \int_{(r,R,\sigma)} \left(f' f'_* \left(\frac{I \, I_*}{I' \, I'_*} \right)^{\alpha} - f \, f_* \right) \times \mathcal{B}^{nw} \tilde{d}_{\alpha}(r,R) \, (1-R) \, R^{1/2} \, \mathrm{d}R \, \mathrm{d}r \, \mathrm{d}\sigma \mathrm{d}I_* \, \mathrm{d}v_*,$$

- weighted setting (internal state) $\|f\|_{L^1_\varphi} = \int_{\mathbb{R}^3 \times [0,\infty)} |f(v,I)| \, \varphi(I) \mathrm{d}I \mathrm{d}v$

cf. Desvillettes'97, Desvillettes&Monaco&Salvarani'05

$$Q^{w}(g,g)(v,I) = \int_{(v_*,I_*)} \int_{(r,R,\sigma)} \left(g' g'_* - g g_* \right) \, \mathcal{B}^{w} (1-R) R^{1/2} \frac{1}{\varphi(I)} \, \mathrm{d}R \, \mathrm{d}r \, \mathrm{d}\sigma \mathrm{d}I_* \, \mathrm{d}v_*$$

- equivalence for $\varphi(I) = I^{\alpha}$ provided that
  - $f = g \, I^{\alpha}$
  - $\mathcal{B}^{nw} = \dfrac{\mathcal{B}^{w}}{I^{\alpha} I_*^{\alpha} \, \tilde{d}_{\alpha}(r,R)}$

  cf. Djordjić, MČ, Spasojević, KRM, 2021

Comment. $\varphi(I) = I^{\alpha}$ good choice for the polytropic case.
To find another $\varphi(I)$ that reproduces correct experimental data and provides accessible computation —> challenging !

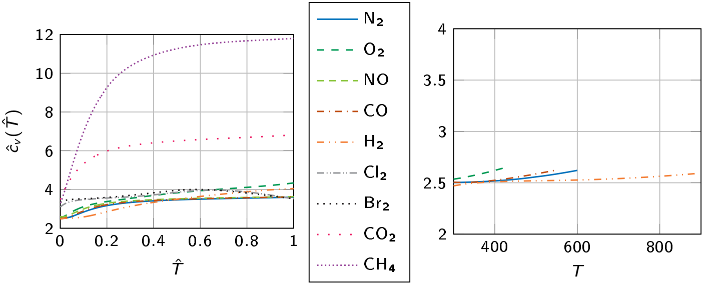
Polyatomic gases and parameter α – macroscopic picture

Thermally perfect gases (non-polytropic)

- thermal equation of state $p = (\rho/m)\, k\, T$ (thermally perfect/nonpolytropic gases)
- temperature depended specific heats connected with the specific internal energy $\hat{e}(T)$,

$$\frac{\mathrm{d}\hat{e}(T)}{\mathrm{d}T} = \hat{c}_v(T)$$

- Polytropic assumption $\hat{c}_v(T)$ =const $\Rightarrow \hat{e}(T) = \hat{c}_v T \Rightarrow \alpha = \hat{c}_v - \frac{5}{2}$



cf. Djordjić, MPČ, Torrilhon, PRE, 2021; MPČ, Simić PRF, 2022;
Djordjić, Oblapenko, MPČ, Torrilhon, CMT, 2023

Polyatomic gases and measure $d_\alpha(r,R)\,\mathrm{d}r\,\mathrm{d}R$

$\xi_{\mathbf{tr}} \geq 3$ number of effective translational degrees of freedom

dependent on the collision kernel, for us $\xi_{\mathbf{tr}} = 3+\zeta$

$\delta > 0$ number of internal degrees of freedom

- algorithm for sampling post-collisional energies of particles within DSMC
  - first sample $\frac{I'}{E} \sim \text{Beta}[\frac{\delta}{2}, \frac{\delta+\xi_{\mathbf{tr}}}{2}]$
  - sample $\phi \sim \text{Beta}[\frac{\delta}{2}, \frac{\xi_{\mathbf{tr}}}{2}]$ and set $\frac{I'_*}{E} = (1-\frac{I'}{E})\phi$
  - the remaining energy is $\frac{\frac{m}{4}|u'|^2}{E} = 1 - \frac{I'}{E} - \frac{I'_*}{E}$
- the scaled energies $(\frac{I'}{E}, \frac{I'_*}{E}, \frac{\frac{m}{4}|u'|^2}{E} = \frac{E'_{\mathbf{tr}}}{E} = 1-\frac{I'}{E}-\frac{I'_*}{E})$ understood as random variables follow Dirichlet/multi-variable Beta distribution with pdf

$$\varphi(i', i'_*; \delta, \xi_{\mathbf{tr}}) = \frac{\Gamma[\delta + \frac{\xi_{\mathbf{tr}}}{2}]}{\Gamma[\frac{\delta}{2}]^2 \Gamma[\frac{\xi_{\mathbf{tr}}}{2}]} (i')^{\frac{\delta}{2}-1} (i'_*)^{\frac{\delta}{2}-1} (e'_{tr} = 1 - i' - i'_*)^{\frac{\xi_{\mathbf{tr}}}{2}-1}$$

and have marginal distributions $\frac{I'}{E}, \frac{I'_*}{E}$: $\text{Beta}[\frac{\delta}{2}, \frac{\delta+\xi_{\mathbf{tr}}}{2}]$ and $\frac{\frac{m}{4}|u'|^2}{E}$: $\text{Beta}[\frac{\xi_{\mathbf{tr}}}{2}, \frac{\delta}{2}]$

- cross section $\Sigma(E, I, I_* \to I', I'_*)$ is assumed to be related to the probability of obtaining post-collisional energies I', I'_* given the total collision energy E

$$\Sigma(E, I, I_* \to I', I'_*) \approx \varphi(i', i'_*; \delta, \xi_{\mathbf{tr}}) |u|^{\gamma-1}$$

$$\mathcal{B}_{\mathbf{DSMC}} \mathrm{d}i' \mathrm{d}i'_* = \Sigma(E, I, I_* \to I', I'_*) |u| \mathrm{d}i' \mathrm{d}i'_* \approx (R|u|^2)^{\gamma/2} d_\alpha(r,R)\,\mathrm{d}r\,\mathrm{d}R$$

$$Q(f,g)(v,I) = \int_{(v_*,I_*)} \int_{(\sigma,r,R)} \left(\underbrace{f(v',I')\,g(v'_*,I'_*)}_{Q^+,\,\text{positive=gain}} \left(\frac{I\,I_*}{I'\,I'_*}\right)^{\alpha} - \underbrace{f(v,I)g(v_*,I_*)}_{Q^-,\,\text{negative=loss}} \right) \underbrace{\mathcal{B}}_{\text{interaction law}} \; \underbrace{d_\alpha(r,R)}_{\text{micro-reversibility}}$$

- allows for the weak form

Weak form of the collision operator

$$\int_{(v,I)} Q(f,g)(v,I)\,\chi(v,I)$$

$$= \frac{1}{2} \int_{(v,I)} \int_{(v_*,I_*)} \int_{(\sigma,r,R)} f\,g_* \left(\chi(v',I') + \chi(v'_*,I'_*) - \chi(v,I) - \chi(v_*,I_*)\right) \mathcal{B}\, d_\alpha(r,R)$$

Conservation for

$$\chi(v,I) = m, \qquad \chi(v,I) = m\,v, \qquad \chi(v,I) = \frac{m}{2}\,|v|^2 + I.$$

Macroscopic observables defined as moments of the distribution function f

$$\int_{(v,I)} \chi(v,I)\,f\,, \quad \text{in particular} \quad \begin{pmatrix} \rho \\ \rho\,U \\ \frac{\rho}{2}\,|U|^2 + \rho\,e \end{pmatrix} = \int_{(v,I)} \begin{pmatrix} m \\ mv \\ \frac{m}{2}\,|v|^2 + I \end{pmatrix} f$$

The H-theorem

Let the transition function $\mathcal{B}$ be positive function almost everywhere, and let $f \geq 0$ such that the collision operator $Q(f,f)$ and entropy production $\mathcal{D}(f)$ are well defined. Then the following properties hold

i. Entropy production is non-positive, that is

$$\mathcal{D}(f) := \int_{\mathbb{R}^{4+}} Q(f,f)(t,v,I) \log(f(t,v,I,)I^{-\alpha}) \,\mathrm{d}I \mathrm{d}v \leq 0.$$

ii. The three following properties are equivalent

(1) $\mathcal{D}(f) = 0$,
(2) $Q(f,f) = 0$ for all $(v,I) \in \mathbb{R}^{4+}$,
(3) There exists $n \geq 0, U \in \mathbb{R}^3$, and $T > 0$, such that the unit mass renormalized Maxwellian equilibrium for polyatomic gases is

$$M_{eq}(v,I) = \frac{n}{Z(T)} \left(\frac{m}{2\pi k_B T} \right)^{3/2} I^{\alpha} \; e^{-\frac{1}{kT}\left(\frac{m}{2}|v-U|^2 + I\right)},$$

where $Z(T)$ is a partition (normalization) function

$$Z(T) = \int_{[0,\infty)} I^{\alpha} e^{-\frac{I}{kT}} \,\mathrm{d}I = (kT)^{\alpha+1}\Gamma(\alpha+1),$$

with Γ as gamma function.

Space homogeneous problem

Cauchy problem

$$\begin{cases} \partial_t f(t,v,I) = Q(f,f)(v,I), \\ f(0,v,I) = f_0(v,I), \end{cases}$$

Functional spaces

- Lebesgue brackets for $v \in \mathbb{R}^3$ and $I \geq 0$,

$$\langle v, I \rangle = \sqrt{1 + \frac{1}{2}|v|^2 + \frac{1}{m} I}$$

- Polynomially weighted L^p spaces, $1 \leq p < \infty$, of the order $k \geq 0$,

$$L^p_k = \left\{ \chi(v,I) : \int_{(v,I)} \left(|\chi(v,I)| \langle v, I \rangle^k \right)^p = \| \chi \langle \cdot \rangle^k \|^p_{L^p} =: \|\chi\|^p_{L^p_k} < \infty \right\},$$

and for $p = \infty$,

$$L^\infty_k = \left\{ \chi(v,I) : \operatorname{ess\,sup} |\chi(v,I)| \langle v, I \rangle^k =: \|\chi\|_{L^\infty_k} < \infty \right\}.$$

- Moments associated to f

$$\mathfrak{m}_k[f](t) = \int_{(v,I)} f(t,v,I) \, \langle v, I \rangle^k$$

  - $\mathfrak{m}_0 =$ mass
  - $\mathfrak{m}_2 =$ mass + energy

Assumption on the collision kernel

- notation $u = \frac{u}{|u|}$, $u = v - v_*$, $E = \frac{m}{4}|u|^2 + I + I_*$

Assumption on the collision kernel (A)

$$\tilde{b}^{lb}(r,R)\, b(\hat{u}\cdot\sigma)\, \tilde{\mathcal{B}}(|u|, I, I_*) \le \mathcal{B}(v, v_*, I, I_*, R, r, \sigma) \le \tilde{b}^{ub}(r,R)\, b(\hat{u}\cdot\sigma)\, \tilde{\mathcal{B}}(|u|, I, I_*),$$

$\tilde{\mathcal{B}}(|u|, I, I_*) = E^{\gamma/2}$, $\gamma \in (0, 2]$ hard potentials-like

$b(\hat{u}\cdot\sigma) \in L^1(\mathbb{S}^2; \mathrm{d}\sigma)$, cut-off

$\tilde{b}^{lb}(r,R), \tilde{b}^{ub}(r,R) \in L^1([0,1]^2; d_\alpha(r,R)\mathrm{d}R)$

- for the simplicity of presentation, we will take $\tilde{b}^{lb}(r,R) = \tilde{b}^{ub}(r,R) = 1$, so

$$\mathcal{B}(v, v_*, I, I_*, R, r, \sigma) = b(\hat{u}\cdot\sigma)E^{\gamma/2}$$

Theorem 1. (Generation and propagation of polynomial moments)

Let f be a solution of the Boltzmann equation,

(i) (Polynomial moments generation estimate.) Then for any $k > 2$,

$$\mathfrak{m}_k[f](t) \lesssim C_k(f_0)\left(1 + t^{-\frac{k-2}{\gamma}}\right), \qquad \forall t > 0.$$

(ii) (Polynomial moments propagation estimate.) Moreover, if $\mathfrak{m}_k[f](0) < \infty$, $k > 2$, then

$$\mathfrak{m}_k[f](t) \lesssim \max\left\{\mathfrak{m}_k[f_0], C_k(f_0)\right\}, \qquad \forall t \geq 0.$$

Theorem 2. (Existence and Uniqueness)

Let the collision kernel satisfy assumption (A). Assume

$$f_0 \in \tilde{\Omega} = \left\{ f \in L^1_2 : f \geq 0\,, 0 < \mathfrak{m}_0[f] < \infty,\ \mathfrak{m}_{2^+}[f] < \infty \right\} \subset L^1_2.$$

Then the Cauchy problem has a unique solution in $\mathcal{C}([0,\infty),\tilde{\Omega}) \cap \mathcal{C}^1((0,\infty), L^1_2)$.

Theorem 3. (Propagation of integrability)

Let f be a solution of BE with initial data $\|f_0\|_{L^p_k} < \infty$ and $\|f_0\|_{L^1_{k+\gamma+1}} < \infty$. Then

$$\text{for } p \in (1,\infty), \quad \|f\|^p_{L^p_k}(t) \leq \max\left\{\|f_0\|^p_{L^p_k}, C_k(f_0)\right\}, \quad \text{for } t \geq 0.$$

$$\text{When } p = \infty, \quad \|f\|_{L^\infty_k}(t) \leq \max\left\{\|f_0\|_{L^\infty_k}, C_k(f_0)\right\}, \quad \text{for } t \geq 0.$$

Where all constants are explicitly computed !

Strategy of the proof

- Strategy based on a differential inequality approach

$$\partial_t f = Q(f,f) \qquad \text{(BE)}$$

L^1 theory $\quad /\langle v, I\rangle^k \,/ \int_{(v,I)}$

$$\Rightarrow \partial_t \mathfrak{m}_k[f] = \int_{(v,I)} Q(f,f)\,\langle v, I\rangle^k = \mathfrak{m}_k[Q(f,f)] \quad \begin{array}{l} \lesssim -A_\star \mathfrak{m}_k[f]^{1+\frac{\gamma}{k-2}} + B_k, \quad k \geq \bar{k}_* \\ \lesssim D_k\, \mathfrak{m}_k[f], \quad 2 < k < \bar{k}_*. \end{array}$$

L^p theory, $p \in (1,\infty)$ $\quad / f^{p-1} \langle v, I\rangle^{kp} \,/ \int_{(v,I)}$

$$\Rightarrow \partial_t \|f\|^p_{L^p_k} = p \int_{(v,I)} Q(f,f)\, f^{p-1}\, \langle v, I\rangle^{k\,p} =: p\, \mathcal{Q}[f,f] \lesssim \; -A\, \|f\|^p_{L^p_k} + B$$

L^∞ theory follows from the limit $p \to \infty$

Proof of Theorem 1 (Generation and propagation of polynomial moments)

$$\partial_t \mathfrak{m}_k[f] = \int_{(v,I)} Q(f,f)\,\langle v,I\rangle^k = \mathfrak{m}_k[Q(f,f)] \quad \begin{array}{l} \lesssim -A_\star \mathfrak{m}_k[f]^{1+\frac{\gamma}{k-2}} + B_k, \quad k \geq \bar{k}_* \\ \lesssim D_k\, \mathfrak{m}_k[f], \quad 2 < k < \bar{k}_*. \end{array}$$

For $k \geq \bar{k}_*$,

- Comparison principle of ODE

$$\begin{cases} y'(t) = -A_\star\; y(t)^{1+c} + B_k, & c := \gamma/(k-2), \\ y(0) = \mathfrak{m}_k(0), \end{cases}$$

- E_k is the equilibrium solution $E_k = \left(\frac{B_k}{A_\star}\right)^{1/(1+c)}$
- if $m_k(0) < \infty \;\Rightarrow\; \mathfrak{m}_k(t) \leq y(t) \leq \max\{E_k, \mathfrak{m}_k(0)\}$, $\forall t \geq 0$ $\blacksquare_{\text{(propagation)}}$
- $y(t) \leq z(t) := E_k\left(1 + t^{-1/c}\right)$, $t > 0$ $\blacksquare_{\text{(generation)}}$

For $2 < k < \bar{k}_*$,

- interpolation $\mathfrak{m}_k \leq \mathfrak{m}_2^{\tau_k}\; \mathfrak{m}_{\bar{k}_*+1}^{1-\tau_k}$, $\tau_k \geq 0$,
- on $\mathfrak{m}_{\bar{k}_*+1}$ apply generation and since $1-\tau_k \leq 1$ & $(1-\tau_k)\frac{1}{c} = \frac{k-2}{\gamma} \;\Rightarrow$

$\mathfrak{m}_k \leq \mathfrak{m}_2^{\tau_k} E_{\bar{k}_*+1}^{1-\tau_k}\left(1 + t^{-\frac{k-2}{\gamma}}\right) \lesssim C_k(f_0)\left(1 + t^{-\frac{k-2}{\gamma}}\right)$, $t > 0$ $\blacksquare_{\text{(generation)}}$

- for short time use ODI $\mathfrak{m}_k(t) \leq e\,\mathfrak{m}_k(0)$, $0 < t \leq \frac{1}{D_k}$
- for $t > \frac{1}{D_k}$, use generation $\mathfrak{m}_k \leq C_k(f_0)\left(1 + D_k^{\frac{k-2}{\gamma}}\right)$
- take the maximum of the two constants $\blacksquare_{\text{(propagation)}}$

Proof of Theorem 2 (Existence and Uniqueness)

- Method inspired by Bressan
- fix constants $C_0, C_2, C_\star > 0$, with $C_\star \geq E_{k_*} + B_{k_*} =: \mathfrak{h}_{k_*}$, with $k_* = \max\{2+2\gamma, \bar{k_*}\}$,

$$\Omega = \left\{ f \in L^1_2 : \; f \geq 0, \; \mathfrak{m}_0[f] = C_0, \; \mathfrak{m}_2[f] = C_2, \; \mathfrak{m}_{k_*}[f] \leq C_\star \right\} \subset L^1_2.$$

- Apply general ODE theory $\Rightarrow$ study collision operator Q as mapping $Q : \Omega \to L^1_2$ and show
  (i) Hölder continuity condition
  (ii) Sub-tangent condition
  (iii) One-sided Lipschitz condition to get

Theorem

Let the collision kernel satisfy assumption (A). Assume that $f_0 \in \Omega$. Then the Cauchy problem has a unique solution in $\mathcal{C}([0,\infty), \Omega) \cap \mathcal{C}^1((0,\infty), L^1_2)$.

- Boltzmann operator is one-sided Lipschitz assuming only 2^+ moments and thus, an approximate sequence of solutions can de drawn from previous Theorem and pass to the limit to find solutions in the bigger space

$$\Omega \subset \tilde{\Omega} = \left\{ f \in L^1_2 : f \geq 0\,, 0 < \mathfrak{m}_0[f] < \infty, \; \mathfrak{m}_{2^+}[f] < \infty \right\} \subset L^1_2.$$

Theorem 2

Let the collision kernel satisfy assumption (A). Assume that $f_0 \in \tilde{\Omega}$. Then the Cauchy problem has a unique solution in $\mathcal{C}([0,\infty), \tilde{\Omega}) \cap \mathcal{C}^1((0,\infty), L^1_2)$.

(i) Hölder continuity condition

$$\|Q(f,f) - Q(g,g)\|_{L^1_1} \leq C_H \|f - g\|_{L^1_1}^{1/2},$$

(ii) Sub-tangent condition

$$\lim_{h\to 0+} \frac{\text{dist}\,(f + hQ(f,f), \Omega)}{h} = 0,$$

where

$$\text{dist}\,(h, \Omega) = \inf_{\omega\in\Omega} \|h - \omega\|_{L^1_1},$$

(iii) One-sided Lipschitz condition

$$[Q(f,f) - Q(g,g), f - g] \leq C_L \|f - g\|_{L^1_1},$$

where brackets $[\cdot,\cdot]$ become

$$[Q(f,f) - Q(g,g), f - g]$$
$$\leq \int_{\mathbb{R}^3\times[0,\infty)} (Q(f,f)(v,I) - Q(g,g)(v,I))\,\text{sign}\,(f(v,I) - g(v,I))\,\langle v, I\rangle^2\,\mathrm{d}I\,\mathrm{d}v.$$

Proof of Theorem 3 (Propagation of L^p norms)

- for $p \in (1, \infty)$,

$$\partial_t \|f\|^p_{L^p_k} = p \int_{(v,I)} Q(f,f)\, f^{p-1} \langle v, I\rangle^{k\,p} =: p\, \mathcal{Q}[f,f] \lesssim -A\, \|f\|^p_{L^p_k} + B$$

- initial data $\|f_0\|_{L^p_k} < \infty$ and $\|f_0\|_{L^1_{k+\gamma+1}} < \infty$
- direct integration implies propagation

$$\|f\|_{L^p_k}(t) \leq \max\left\{ \|f_0\|_{L^p_k}, \left(\frac{B}{A}\right)^{1/p} \right\}, \quad \text{for } t \geq 0.$$

- for $p = \infty$,
- properties of the constants $\lim_{p\to\infty} A^{1/p} = 1$ and $\lim_{p\to\infty} B^{1/p} = \tilde{B}$
- sending $p \to \infty$ in the last equation it follows $f(t) \in L^\infty_k$ and

$$\|f\|_{L^\infty_k}(t) \leq \max\left\{ \|f_0\|_{L^\infty_k}, \tilde{B} \right\}, \quad \text{for } t \geq 0.$$

Let's dig into the details...

$$\partial_t f = Q(f,f) \qquad \text{(BE)}$$

L^1 theory $\quad /\langle v, I\rangle^k \; / \int_{(v,I)}$

$$\Rightarrow \partial_t \mathfrak{m}_k[f] = \int_{(v,I)} Q(f,f)\, \langle v, I\rangle^k = \mathfrak{m}_k[Q(f,f)] \quad \begin{array}{l} \lesssim -A_\star \mathfrak{m}_k[f]^{1+\frac{\gamma}{k-2}} + B_k, \quad k \geq \bar{k}_* \\ \lesssim D_k\, \mathfrak{m}_k[f], \quad 2 < k < \bar{k}_*. \end{array}$$

L^p theory, $p \in (1, \infty)$ $\quad / f^{p-1} \langle v, I\rangle^{kp} \; / \int_{(v,I)}$

$$\Rightarrow \partial_t \|f\|^p_{L^p_k} = p \int_{(v,I)} Q(f,f)\, f^{p-1}\, \langle v, I\rangle^{k\,p} =: p\, \mathcal{Q}[f,f] \lesssim -A\, \|f\|^p_{L^p_k} + B$$

L^∞ theory follows from the limit $p \to \infty$

L^1 theory – strategy

▶ Our first task: find a suitable Banach space
/ or /
knowing molecular dynamics, find a proper moment definition to show *dissipation* in the model

$$\mathfrak{m}_k[Q(f,f)] = \int_{(v,I)} \underbrace{Q(f,f)(v,I)}_{Q^+ - Q^-} \langle v, I\rangle^k = \mathfrak{m}_k[Q^+(f,f)] - \mathfrak{m}_k[Q^-(f,f)]$$

$$\langle v, I\rangle = \sqrt{1 + \frac{1}{2}|v|^2 + \frac{I}{m}}$$

Conservation for (*i*) $k = 0$ mass, (*iii*) $k = 2$ mass + energy
(?) what about $k > 2$

▶ the goal is to show that $\mathfrak{m}_k[Q^+(f,f)]$ has decaying properties with respect to k and becomes dominated by $\mathfrak{m}_k[Q^-(f,f)]$

- Energy Identity Lemma
- Averaging Lemma

- Total energy in the Lebesgue brackets form

$$E^{\langle\rangle} := \langle v, I\rangle^2 + \langle v_*, I_*\rangle^2 = \langle v', I'\rangle^2 + \langle v'_*, I'_*\rangle^2 = 2 + |V|^2 + \frac{E}{m}$$

Lemma. (Energy Identity)

There exist $p = p(v, v_*, I, I_*, R, r) \in [0,1]$ and $\lambda = \lambda(v, v_*, I, I_*, R) \geq 0$ such that

$$\langle v', I'\rangle^2 = E^{\langle\rangle}\left(p + \lambda \hat{V}\cdot\sigma\right) \quad \& \quad \langle v'_*, I'_*\rangle^2 = E^{\langle\rangle}\left((1-p) - \lambda\hat{V}\cdot\sigma\right)$$

- $p = \frac{s}{2} + r(1-s), \quad s(v, v_*, I, I_*, R)$

Lemma. (Averaging over (σ, r, R))

$$\int_{(\sigma,r,R)} \left(\left(p + \lambda\hat{V}\cdot\sigma\right)^k + \left((1-p) - \lambda\hat{V}\cdot\sigma\right)^k\right) b(\hat{u}\cdot\sigma) d_\alpha(r,R) \leq \mathcal{C}_k$$

with

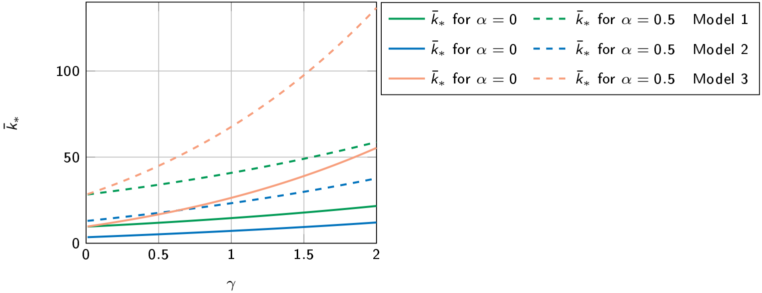
$$\mathcal{C}_k \to 0, \qquad k \to \infty,$$

and moreover there exists $\bar{k}_*$ such that

$$\mathcal{C}_k \leq \kappa^{lb}, \qquad k \geq \bar{k}_*.$$

$b(\hat{u}\cdot\sigma) \in L^\infty$

- $\mathcal{C}_k \sim \dfrac{1}{k}$
- compute $\bar{k}_*$ such that $\mathcal{C}_k < \kappa^{lb}$, $k > \bar{k}_*$, depending on $\alpha \geq 0$ and $\gamma \in (0,2]$



Model 1: $\mathcal{B} = b(\hat{u}\cdot\sigma)\left(\frac{m}{4}|v-v_*|^2 + I + I_*\right)^{\gamma/2}$

Model 2: $\mathcal{B} = b(\hat{u}\cdot\sigma)\left(R^{\gamma/2}|v-v_*|^\gamma + (1-R)^{\gamma/2}\left(\frac{I+I_*}{m}\right)^{\gamma/2}\right)$

Model 3: $\mathcal{B} = b(\hat{u}\cdot\sigma)\left(R^{\gamma/2}|v-v_*|^\gamma + \left(r(1-R)\frac{I}{m}\right)^{\gamma/2} + \left((1-r)(1-R)\frac{I_*}{m}\right)^{\gamma/2}\right)$

$$\mathfrak{m}_k[Q^+(f,f)] \approx \int_{(v,I),(v_*,I_*)} \int_{(\sigma,r,R)} ff_* \left(\langle v', I' \rangle^k + \langle v'_*, I'_* \rangle^k \right) \mathcal{B}\, d_\alpha(r,R)$$

assumption on the collision kernel

$$\lesssim \int_{(v,I),(v_*,I_*)} f\, f_*\, E^{\gamma/2} \int_{(\sigma,r,R)} \left(\langle v', I' \rangle^k + \langle v'_*, I'_* \rangle^k \right) b(\hat{u}\cdot\sigma)\, d_\alpha(r,R)$$

Energy Identity Lemma

$$\lesssim \int_{(v,I),(v_*,I_*)} f\, f_*\, E^{\gamma/2}\, (E^{\langle\rangle})^{k/2} \int_{(\sigma,r,R)} F^k\, b(\hat{u}\cdot\sigma)\, d_\alpha(r,R)$$

Averaging Lemma

$$\lesssim \mathcal{C}_k \int_{(v,I),(v_*,I_*)} f\, f_*\, E^{\gamma/2}\, (E^{\langle\rangle})^{k/2}, \quad \mathcal{C}_k \to 0,\, k \to \infty \;\&\; \mathcal{C}_k \lesssim 1,\, k \geq \bar{k}_*$$

$$\mathfrak{m}_k[Q(f,f)] \lesssim \int_{(v,I),(v_*,I_*)} f\, f_* \left(\mathcal{C}_k \left(\langle v, I \rangle^2 + \langle v_*, I_* \rangle^2 \right)^{k/2} - \left(\langle v, I \rangle^k + \langle v_*, I_* \rangle^k \right) \right) E^{\gamma/2}$$

$p-$Binomial inequality $(x+y)^p \leq x^p + y^p + 2^{p+1} \left(x y^{p-1}\, 1_{y \geq x} + x^{p-1} y\, 1_{x \geq y} \right)$, $p > 1$, $x, y > 0$

Bounds on collision kernel $L_\gamma \langle v, I \rangle^\gamma - \langle v_*, I_* \rangle^\gamma \leq E^{\gamma/2} \leq \langle v, I \rangle^\gamma + \langle v_*, I_* \rangle^\gamma$

$$\lesssim \int_{(v,I),(v_*,I_*)} f\, f_* \Big(- \underbrace{(1 - \mathcal{C}_k)}_{>0,\ k > \bar{k}_*} \left(\langle v, I \rangle^{k+\gamma} + \langle v_*, I_* \rangle^{k+\gamma} \right) + L.O.T. \Big) \lesssim -A_\star \mathfrak{m}_{k+\gamma} + \underbrace{L.O.T.}_{(\mathfrak{m}_k \mathfrak{m}_\gamma,\, \mathfrak{m}_2 \mathfrak{m}_{k-2+\gamma})}$$

Moment interpolation $\mathfrak{m}_\lambda = \mathfrak{m}_{\lambda_1}^\tau \mathfrak{m}_{\lambda_2}^{1-\tau}$, $0 \leq \lambda_1 \leq \lambda \leq \lambda_2$, $0 < \tau < 1$, $\lambda = \tau \lambda_1 + (1-\tau)\lambda_2$
$\lambda \to (\lambda_1, \lambda_2)$ used for $k \to (2, k+\gamma)$, $k - 2 + \gamma \to (0, k+\gamma)$

Young's inequality $|a\, b| \leq \frac{1}{p\, \varepsilon^{p/p'}} |a|^p + \frac{\varepsilon}{p'} |b|^{p'}$, for $\varepsilon > 0$ and $\frac{1}{p} + \frac{1}{p'} = 1$,

$L.O.T.(\mathfrak{m}_k \mathfrak{m}_\gamma, \mathfrak{m}_2 \mathfrak{m}_{k-2+\gamma}) \to B(k, \gamma, \mathfrak{m}_0, \mathfrak{m}_2) + \varepsilon \mathfrak{m}_{k+\gamma}$

- $\mathfrak{m}_k[Q(f,f)] \lesssim -A_\star \mathfrak{m}_{k+\gamma} + B_k \lesssim -A_\star \mathfrak{m}_k[f]^{1+\frac{\gamma}{k-2}} + B_k$, $\quad k \geq \bar{k}_*$
- $\mathfrak{m}_k[Q(f,f)] \lesssim D_k\, \mathfrak{m}_k[f]$, $\quad k > 2$

L^p theory – strategy

$$\mathcal{Q}[f,g] = \int_{(v,I)} Q(f,g)\, f^{p-1} \, \langle v, I\rangle^{k\,p} = \underbrace{\int_{(v,I)} Q^+(f,g)\, f^{p-1}\, \langle v, I\rangle^{kp}}_{\mathcal{Q}^+[f,g]} - \underbrace{\int_{(v,I)} \nu[g](v,I)\, f^p\, \langle v, I\rangle^{kp}}_{\mathcal{Q}^-[f,g]}$$

upper bound on gain part

lower bound on collision frequency

- upper bound on the gain part
  - the goal is to find a suitable representation of Q^+ which will allow absorption

$$\int_{(v,I)} Q^+(f,g)\, \chi(v,I) \lesssim \int_{(v,I)} \int_{(v_*,I_*)} f \langle v, I\rangle^{\gamma/p}\, g_* \langle v_*, I_*\rangle^{\gamma}\, \mathcal{S}(\chi\langle\cdot\rangle^{\gamma/q})(v, I, v_*, I_*)$$

  - averaging operator

$$\mathcal{S}(\chi)(v,I,v_*,I_*) = \int_{(\sigma,r,R)} \chi(v', I')\, b(\hat{u}\cdot\sigma)\, r^{-\frac{\gamma}{2q}}\, d_\alpha(r,R)$$

- lower bound on the collision frequency
  - entropy based estimate

Lower bound on the collision frequency

- entropy-based estimate, requiring

$$H[g] = \int_{(v,I)} g(v,I)\, |\log g(v,I)| < \infty$$

- quantity related to the entropy $\mathcal{H}(f) = \int_{(v,I)} f(v,I) \log f(v,I)$ of the solution $f \geq 0$,

$$H[f] \lesssim \mathcal{H}(f_0) + \|f\|_{L^1_2}^{3/4}$$

$\Rightarrow$ Thus, solution f with finite initial entropy satisfies $\sup_{t \geq 0} H[f] < \infty$ with bound depending only on the naturally propagated quantities of mass, energy and entropy.

Lower Bound Lemma. $g \in L^1_\gamma$ and $H[g] < \infty$, there exists $c_g > 0$,

$$\int_{(v_*, I_*)} g(v_*, I_*)\, \tilde{B} \geq c_g \langle v, I \rangle^\gamma, \tag{1}$$

and consequently,

$$\nu[g](v,I) = \int_{(v_*, I_*)} \int_{(r,R,\sigma)} g(v_*, I_*)\, \mathcal{B}\, d_\alpha(r,R) \geq \|b\|_{L^1}\, c_g \langle v, I \rangle^\gamma$$

- leads to the lower bound on the loss form

$$\mathcal{Q}^-[f,g] = \int_{(v,I)} \nu[g](v,I)\, f^p \langle v, I \rangle^{kp} \geq \|b\|_{L^1} \|f\|^p_{L^p_{\gamma/p+k}}$$

Toward the upper bound on the gain part – Averaging operator

- for q such that the following constant ρ is finite

$$\rho(q) = \int_{(r,R)} r^{-\left(1+\frac{\gamma}{2}\right)\frac{1}{q}} (1-R)^{-\frac{1}{q}}\, d_\alpha(r,R) < \infty$$

- define averaging operator, for $\hat{u}\cdot\sigma \geq 0$,

$$\mathcal{S}(\chi)(v, I, v_*, I_*) = \int_{(\sigma,r,R)} \chi(v', I')\, b(\hat{u}\cdot\sigma)\, r^{-\frac{\gamma}{2q}}\, d_\alpha(r,R)$$

Lemma.

(1) for $b \in L^1$, $\sup_{(v_*, I_*)} \|\mathcal{S}(\chi)\|_{L^q(\mathrm{d}v\,\mathrm{d}I)} \lesssim \rho(q)\, \|b\|_{L^1}\, \|\chi\|_{L^q}$

(2) for $b \in L^\infty$, $\sup_{(v,I)} \|\mathcal{S}(\chi)\|_{L^q(\mathrm{d}v_*\,\mathrm{d}I_*)} \lesssim \rho(q)\, \|b\|_{L^\infty}\, \|\chi\|_{L^q}$

Elements of proof.

- Apply Minkowski & Hölder inequality, Fubini's theorem...

$$\|\mathcal{S}(\chi)\|_{L^q(\mathrm{d}v\,\mathrm{d}I)} \leq \|b\|_{L^1}^{1/p} \int_{(r,R)} \left(\int_\sigma \int_{(v,I)} \left|\chi(v',I')\right|^q\, b(\hat{u}\cdot\sigma) \right)^{1/q} r^{-\frac{\gamma}{2q}}\, d_\alpha(r,R)$$

- for fixed (r,R,σ) change $(v,I) \mapsto (v',I')$

$$\left| \frac{\partial(v',I')}{\partial(v,I)} \right| = \frac{r\,(1-R)}{2^3}$$

! no singularity in $\hat{u}\cdot\sigma$, yet, problem with r.

- treat b, $\int_\sigma b(\star) = \ldots$(3d helps !)$\ldots \lesssim \|b\|_{L^1}$

Toward the upper bound on the gain form

Lemma. (Weight arrangement)

$$E^{\gamma/2} \lesssim r^{-\frac{\gamma}{2q}} \langle v', I' \rangle^{\frac{\gamma}{q}} \langle v_*, I_* \rangle^{\gamma} \langle v, I \rangle^{\frac{\gamma}{p}}$$

Elements of proof.

$$E^{\frac{\gamma}{2}\left(\frac{1}{p}+\frac{1}{q}\right)} \leq \left(\langle v, I\rangle \langle v_*, I_* \rangle\right)^{\frac{\gamma}{p}} \left(2\sqrt{2}\,\frac{1}{\sqrt{r}} \langle v', I' \rangle_i \langle v_*, I_* \rangle_j\right)^{\frac{\gamma}{q}}$$

Proposition.

(1) for $b \in L^1$,

$$\int_{(v,I)} Q^+(f,g)\,\chi\,\langle v, I\rangle^k \lesssim \|f\|_{L^p_{(k+\gamma)/p}} \|g\|_{L^1_{k/p+\gamma}}\, \rho(q)\, \|b\|_{L^1} \|\chi\|_{L^q_{(k+\gamma)/q}}$$

(2) for $b \in L^\infty$, (control by L^p norm of any of the two input functions, albeit with the different polynomial order),

$$\int_{(v,I)} Q^+(f,g)\,\chi\,\langle v, I\rangle^k \lesssim \|f\|_{L^1_{(k+\gamma)/p}} \|g\|_{L^p_{k/p+\gamma}}\, \rho(q)\, \|b\|_{L^\infty} \|\chi\|_{L^q_{(k+\gamma)/q}}$$

- $k=0$,

$$\int_{(v,I)} Q^+(f,g)\,\chi \approx \int_{(v,I),(v_*,I_*)} \int_{(\sigma,r,R)} f\, g_*\, \chi(v',I')\, E^{\gamma/2}\, b(\hat{u}\cdot\sigma)\, d_\alpha(r,R)$$

weight arrangement

$$\lesssim \int_{(v,I),(v_*,I_*)} \int_{(\sigma,r,R)} f\langle v,I\rangle^{\frac{\gamma}{p}}\, g_* \langle v_*,I_*\rangle^{\gamma}\, \chi(v',I')\langle v',I'\rangle^{\frac{\gamma}{q}}\, r^{-\frac{\gamma}{2q}}\, b(\hat{u}\cdot\sigma)\, d_\alpha(r,R)$$

$$\lesssim \int_{(v,I),(v_*,I_*)} f\langle v,I\rangle^{\frac{\gamma}{p}}\, g_* \langle v_*,I_*\rangle^{\gamma}\, \mathcal{S}(\chi\langle\cdot\rangle^{\frac{\gamma}{q}})(v,I,v_*,I_*)$$

for $b\in L^1$, Hölder ineq in (v,I)

$$\lesssim \|f\langle\cdot\rangle^{\gamma/p}\|_{L^p} \int_{(v_*,I_*)} g(v_*,I_*)\,\langle v_*,I_*\rangle^{\gamma} \|\mathcal{S}^+(\chi\langle\cdot\rangle^{\gamma/q})\|_{L^q(\mathrm{d}v\,\mathrm{d}I)}$$

$$\lesssim \|f\|_{L^p_{\gamma/p}} \|g\|_{L^1_\gamma}\, \rho(q)\, \|b\|_{L^1} \|\chi\|_{L^q_{\gamma/q}}$$

for $b\in L^\infty$, Hölder ineq in (v_*,I_*)

$$\lesssim \|g\langle\cdot\rangle^{\gamma}\|_{L^p} \int_{(v,I)} f(v,I)\,\langle v,I\rangle^{\gamma/p} \|\mathcal{S}^+(\chi\langle\cdot\rangle^{\gamma/q})\|_{L^q(\mathrm{d}v_*\,\mathrm{d}I_*)}$$

$$\lesssim \|f\|_{L^1_{\gamma/p}} \|g\|_{L^p_\gamma}\, \rho(q)\, \|b\|_{L^\infty} \|\chi\|_{L^q_{\gamma/q}}$$

Upper bound on the gain form

- take $\chi = f^{p-1}$, so that $\|\chi\|_{L^q_{(k+\gamma)/q}} = \|f\|^{p-1}_{L^p_{\gamma/p+k}}$

$$\int_{(v,I)} Q^+(f,g)\, f^{p-1} \langle v, I\rangle^{kp} \lesssim \int_{(v,I)} \int_{(v_*,I_*)} f \langle v, I\rangle^{\gamma/p+k}\, g_* \langle v_*, I_*\rangle^{\gamma+k}\, \mathcal{S}(f^{p-1}\langle\cdot\rangle^{(\gamma+kp)/q})(v, I, v_*, I_*)$$

for $b \in L^1$,

$$\lesssim \|f\|^p_{L^p_{\gamma/p+k}} \|g\|_{L^1_{\gamma+k}}\, \rho(q)\, \|b\|_{L^1}$$

for $b \in L^\infty$,

$$\lesssim \|g\|_{L^p_{\gamma+k}} \|f\|_{L^1_{\gamma/p+k}}\, \rho(q)\, \|b\|_{L^\infty} \|f\|^{p-1}_{L^p_{\gamma/p+k}}$$

- Represent $b = b^1 + b^\infty$, $b^1 \in L^1$ with $\|b^1\|_{L^1} \le \varepsilon$ and $b^\infty \in L^\infty$

$$\mathcal{Q}^+[f,g] = \mathcal{Q}^+_{b^1}[f,g] + \mathcal{Q}^+_{b^\infty}[f, g(\mathbb{1}_{g\langle\cdot\rangle^\ell \le K} + \mathbb{1}_{g\langle\cdot\rangle^\ell \ge K})]$$

$$\lesssim \varepsilon\, \|f\|^p_{L^p_{\gamma/p+k}} + \begin{array}{c} K \|b^\infty\|_{L^\infty} \|f\|_{L^1_{\gamma/p+k}} \|f\|^{p-1}_{L^p_{\gamma/p+k}} \\ \lesssim \|b^\infty\|_{L^\infty} \left(\dfrac{K}{\tilde{\varepsilon}} \|f\|^p_{L^1_{\gamma/p+k}} + \tilde{\varepsilon} \|f\|^p_{L^p_{\gamma/p+k}} \right) \end{array} + \frac{\|b^\infty\|_{L^\infty}}{\log K} \|f\|^p_{L^p_{\gamma/p+k}}$$

$$\lesssim \epsilon\, \|f\|^p_{L^p_{\gamma/p+k}} + B$$

$$\Rightarrow \quad \mathcal{Q}[f,g] \lesssim \mathcal{Q}^+[f,g] - \|b\|_{L^1} \|f\|^p_{L^p_{\gamma/p+k}} \lesssim -A\, \|f\|^p_{L^p_{\gamma/p+k}} + B$$

Perspective

- Actually, we solved the Cauchy problem and proved integrability propagation for a gas mixture
- Theory can be refined to include
  - more complex collisions, for instance, inelastic
  - more general assumptions on the collision kernel, for instance, non cut-off
- Convergence to equilibrium

Thank you for your attention !