

Fredholm Property of the Linearized Boltzmann Operator Mixture of Polyatomic Gases

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Reentry of a shuttle: complexity of the physics

A realistic modeling:

- Mixtures (O_2 and N_2)
- Monoatomic and Polyatomic (N and N_2)
- Different masses (N and N_2)



Polyatomic Gases

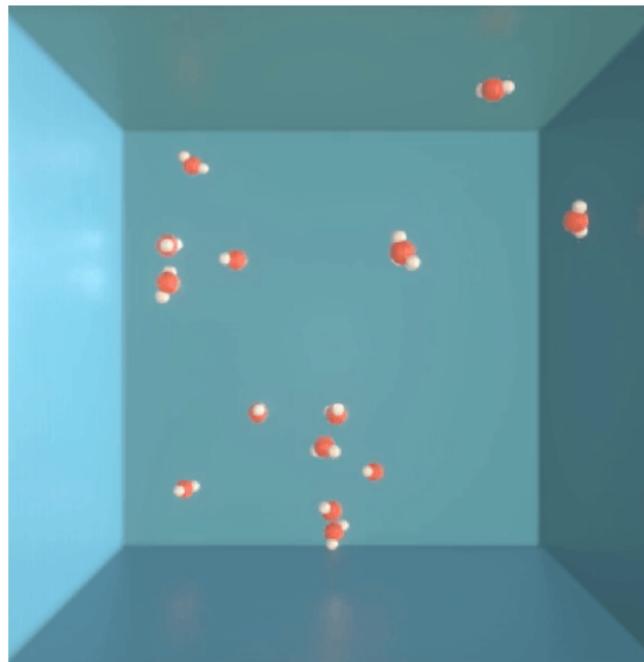


Figure: Polyatomic rarefied gas confined in a box

Kinetic Theory of Gases

- Distribution function

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$$\begin{cases} t \geq 0 & \text{time variable,} \\ x \in \mathbb{R}^3 & \text{position,} \\ v \in \mathbb{R}^3 & \text{microscopic velocity, and} \\ I \geq 0 & \text{continuous internal energy} \end{cases}$$

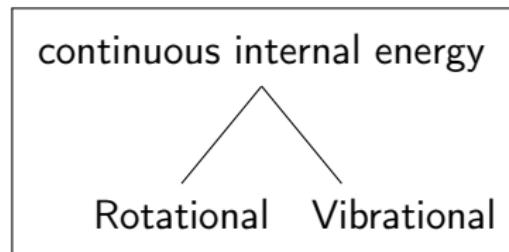
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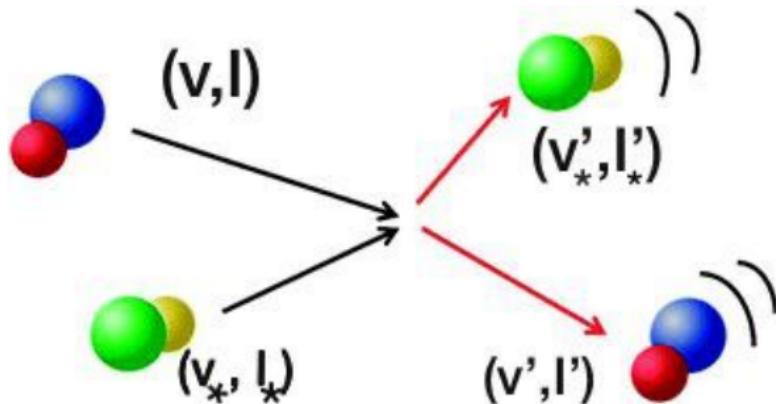


Internal Energy

References

- Continuous internal energy
 - ① Borgnakke, Larsen (1975).
 - ② Bourgat, Desvillettes, Le Tallec, Perthame (1994)
 - ③ Desvillettes, Monaco, Salvarani (2005)
 - ④ Baranger, Bisi, Brull, Desvillettes (2018)
 - ⑤ Andries, Le Tallec, Perlat, Perthame (2000)
 - ⑥ Brull, Schneider (2009)
- Discrete internal energy
 - ① Giovangigli, Multicomponent Flow Modeling (1999)
 - ② Bisi, Cáceres (2016)
 - ③ Bernhoff (2018)
- Undifferentiated
 - Bisi, Borsoni, Groppi (2022)

Colliding Particles



Conservation Equations:

$$m_i v + m_j v_* = m_i v' + m_j v'_*$$
$$\frac{m_i}{2} v^2 + \frac{m_j}{2} v_*^2 + I + I_* = \frac{m_i}{2} v'^2 + \frac{m_j}{2} v'^2_* + I'_* + I'$$

Borgnakke-Larsen Model

The Borgnakke-Larsen Procedure¹

- Equivalent Formulation of Conservation Equations

$$m_i v + m_j v_* = m_i v' + m_j v'_*$$

$$\frac{\mu_{ij}}{2}(v - v_*)^2 + I + I_* = \frac{\mu_{ij}}{2}(v' - v'_*)^2 + I'_* + I' = E$$

- Partition of total energy by the variable R

$$\frac{\mu_{ij}}{2}(v' - v'_*)^2 = RE$$

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

- Partition of internal energy by the variable r

$$I' = r(1 - R)E$$

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

¹Borgnakke, Larsen (1975)

Borgnakke-Larsen Model

- Post collisional velocities

$$v' = \frac{m_i v + m_j v_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} \sqrt{\frac{2RE}{\mu_{ij}}} \sigma$$

$$v'_* = \frac{m_i v + m_j v_*}{m_i + m_j} - \frac{m_i}{m_i + m_j} \sqrt{\frac{2RE}{\mu_{ij}}} \sigma,$$

with $\sigma \in S^2$

- $\omega - \sigma$ notation

$$\sigma = T_\omega \left[\frac{v - v_*}{|v - v_*|} \right]$$

- $T_\omega(z) = z - 2(z \cdot \omega)\omega$, and $d\omega = \frac{d\sigma}{2 \left| \sigma - \frac{v - v_*}{|v - v_*|} \right|}$

The Boltzmann Equation (Mixtures)

- Boltzmann equation:

$$\boxed{\partial_t f_i + \nu \cdot \nabla_x f_i = \sum_{j=1}^n Q_{ij}(f_i, f_j), \quad 1 \leq i \leq n,}$$

$Q_{ij}(f, f)$: quadratic Boltzmann operator

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- Collision Operator:

$$Q_{ij}(f_i, f_j)(\nu, I) = \int_{\mathbb{R}^3 \times \mathbb{R}_+ \times S^2 \times (0,1)^2} \left(\frac{f'_i f'_{j*}}{I'^{\alpha_i} I_*'^{\alpha_j}} - \frac{f_i f_{j*}}{I^{\alpha_i} I_*^{\alpha_j}} \right) \times \mathcal{B}_{ij} \times r^{\alpha_i} (1-r)^{\alpha_j} (1-R)^{\alpha_i + \alpha_j} I^{\alpha_i} I_*^{\alpha_j} (1-R) R^{1/2} \, dR dr d\omega dI_* \, dv_*,$$

The Boltzmann Equation (Mixtures)

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- $f_{j*} = f_j(v_*, I_*)$, $f'_i = f_i(v', I')$, and $f'_{j*} = f_j(v'_*, I'_*)$

The Boltzmann Equation (Monospecies)

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- Collision Operator²:

$$Q(f, f)(v, I) = \int_{\Delta} \left(\frac{f' f'_*}{(I' I'_*)^{\alpha}} - \frac{f f_*}{(I I_*)^{\alpha}} \right) \tilde{\mathcal{B}}(v, v_*, I, I_*, r, R, \sigma) dR dr d\omega dI_* dv_*,$$

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where $\Delta = \mathbb{R}^3 \times \mathbb{R}_+ \times S^2 \times (0, 1)^2$ and

$$\tilde{\mathcal{B}} = (r(1-r))^{\alpha} (1-R)^{2\alpha} (1-R) R^{1/2} I^{\alpha} I_*^{\alpha} \mathcal{B}$$

²Bourgat, Desvillettes, Le Tallec, Perthame (1994)

The Parameter α

	Translation and rotation		Translation, rotation and vibration
	Linear molecule	Non- linear molecule	
Degrees of freedom	5	6	$3N$
α	0	$\frac{1}{2}$	$\frac{1}{2}(3N - 5)$



The Collision Cross-Section

- Micro-reversibility conditions:

$$\mathcal{B}(v, v_*, I, I_*, r, R, \omega) = \mathcal{B}(v_*, v, I_*, I, 1 - r, R, \omega)$$

$$\mathcal{B}(v, v_*, I, I_*, r, R, \omega) = \mathcal{B}(v', v'_*, I', I'_*, r', R', \omega),$$

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- Lower bound⁴

$$C_1 \Phi(r, R) \left| \omega \cdot \frac{(v - v_*)}{|v - v_*|} \right| \left(|v - v_*|^{\gamma} + I^{\frac{\gamma}{2}} + I_*^{\frac{\gamma}{2}} \right) \leq \mathcal{B}(v, v_*, I, I_*, r, R, \omega)$$

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- Upper Bound³

$$\mathcal{B}(v, v_*, I, I_*, r, R, \omega) \leq C_2 \Psi(r, R) \left| \omega \cdot \frac{(v - v_*)}{|v - v_*|} \right| \left(|v - v_*|^\gamma + I^{\frac{\gamma}{2}} + I_*^{\frac{\gamma}{2}} \right)$$

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Properties of the Cross-section

- **Positivity**

- Φ_γ, Ψ , are positive functions such that

$$\Phi_\gamma \leq \Psi$$

- **Symmetry**

- $\Phi(r, R) = \Phi(1 - r, R)$
- $\Psi(r, R) = \Psi(1 - r, R)$

- **Boundedness**

- $\Psi^2(r, R)(r(1 - r))^{\min\{2\alpha - 1 - \gamma, \alpha - 1\}} R(1 - R)^{3\alpha - \gamma} \in L^1((0, 1)^2).$

Models

For $\gamma < 2\alpha$, the following models satisfy the required assumptions:

- Model 1

$$\mathcal{B}(v, v_*, I, I_*, r, R, \omega) = c \left| \omega \cdot \frac{v - v_*}{|v - v_*|} \right| (|v - v_*|^\gamma + I^{\gamma/2} + I_*^{\gamma/2})$$

- Model 2

$$\begin{aligned} \mathcal{B}(v, v_*, I, I_*, r, R, \omega) = c \left| \omega \cdot \frac{v - v_*}{|v - v_*|} \right| \\ \left(R^{\frac{\gamma}{2}} |v - v_*|^\gamma + (r(1-R)I)^{\frac{\gamma}{2}} + ((1-r)(1-R)I_*)^{\frac{\gamma}{2}} \right) \end{aligned}$$

Linearization

- Global Maxwellian function: $M(v, I) = \frac{I^\alpha}{(2\pi)^{\frac{3}{2}} \Gamma(\alpha+1)} e^{-(\frac{1}{2}v^2 + I)}$

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- Define g as $f = M + M^{\frac{1}{2}}g$
- Linearized Boltzmann operator:

$$\mathcal{L}g = M^{-\frac{1}{2}} [Q(M, M^{\frac{1}{2}}g) + Q(M^{\frac{1}{2}}g, M)].$$

Linearized Boltzmann Operator

- Linearized Boltzmann Operator:

$$\left. \begin{aligned} \mathcal{L}(g) = & - \int_{\Delta} \frac{M^{\frac{1}{2}}}{I^{\frac{\alpha}{2}}} \frac{M_*^{\frac{1}{2}}}{I_*^{\frac{\alpha}{2}}} g(v_*, I_*) \tilde{\mathcal{B}}(v, v_*, I, I_*, r, R, \omega) dr dR d\omega dI_* dv_* \\ & + \int_{\Delta} \frac{M_*^{\frac{1}{2}}}{I_*^{\frac{\alpha}{2}}} \frac{M'^{\frac{1}{2}}}{I'^{\frac{\alpha}{2}}} g(v', I') \tilde{\mathcal{B}}(v, v_*, I, I_*, r, R, \omega) dr dR d\omega dI_* dv_* \\ & + \int_{\Delta} \frac{M_*^{\frac{1}{2}}}{I_*^{\frac{\alpha}{2}}} \frac{M'^{\frac{1}{2}}}{I'^{\frac{\alpha}{2}}} g(v', I') \tilde{\mathcal{B}}(v, v_*, I, I_*, r, R, \omega) dr dR d\omega dI_* dv_* \\ & - \int_{\Delta} \frac{M_*}{I_*^{\alpha}} g(v, I) \tilde{\mathcal{B}}(v, v_*, I, I_*, r, R, \omega) dr dR d\omega dI_* dv_* \end{aligned} \right\} = \mathcal{K} = \nu$$

- Write

$$\mathcal{L}g(v, I) = \underbrace{\mathcal{K}}_{\text{Perturbation operator}} g(v, I) + \underbrace{\nu(v, I)}_{\text{Collision Frequency}} g(v, I)$$

Goal and Plan of Proof

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- Find the kernel form of each \mathcal{K}_i , $i = 1, \dots, 3$
- Prove that the kernel of each \mathcal{K}_i is L^2 integrable

Kernel of \mathcal{K}_1

$$\mathcal{K}_1 g(v, I) = \frac{1}{\Gamma(\alpha + 1)(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3 \times \mathbb{R}_+} dI_* dv_* g(v_*, I_*) \\ \left[\int_{S^2 \times (0,1)^2} e^{-\frac{1}{4}v_*^2 - \frac{1}{4}v^2 - \frac{1}{2}I_* - \frac{1}{2}I} (r(1-r))^\alpha (1-R)^{2\alpha+1} R^{1/2} I_*^{\frac{\alpha}{2}} \mathcal{B} dr dR d\omega \right]$$

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- Kernel of \mathcal{K}_1

$$k_1(v, I, v_*, I_*) = \frac{1}{\Gamma(\alpha + 1)(2\pi)^{\frac{3}{2}}} \\ \int_{S^2 \times (0,1)^2} e^{-\frac{1}{4}v_*^2 - \frac{1}{4}v^2 - \frac{1}{2}I_* - \frac{1}{2}I} (r(1-r))^\alpha (1-R)^{2\alpha+1} R^{1/2} I^{\frac{\alpha}{2}} I_*^{\frac{\alpha}{2}} \mathcal{B} dr dR d\omega$$

- Assumption on \mathcal{B} $\rightsquigarrow k_1$ is L^2 integrable

Kernel of \mathcal{K}_2

- Define the **change of variable**:

$$\mathbf{h} : \mathbb{R}^3 \times \mathbb{R}_+ \longrightarrow \mathbf{h}(\mathbb{R}^3 \times \mathbb{R}_+) \subset \mathbb{R}^3 \times \mathbb{R}_+$$

$$(v_*, I_*) \longmapsto (x, y) = \left(\frac{v + v_*}{2} - \sqrt{R\left(\frac{1}{4}(v - v_*)^2 + I + I_*\right)\sigma}, (1 - R)(1 - r)\left[\frac{1}{4}(v - v_*)^2 + I + I_*\right]\right)$$

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- Jacobian:

$$J = \left| \frac{\partial v_* \partial I_*}{\partial x \partial y} \right| = \frac{8}{(1 - r)(1 - R)}$$

Kernel of \mathcal{K}_2

$$\mathcal{K}_2 g(v, I) = \int_{\Delta} e^{-\frac{I_*}{2} - \frac{1}{2}r(1-R)\left(\frac{(v-v_*)^2}{4} + I + I_*\right) - \frac{1}{4}v_*^2 - \frac{1}{4}\left(\frac{v+v_*}{2} + \sqrt{R(\frac{1}{4}(v-v_*)^2 + I + I_*)}\sigma\right)^2}$$
$$g\left(\frac{v+v_*}{2} - \sqrt{R(\frac{1}{4}(v-v_*)^2 + I + I_*)}\sigma, (1-R)(1-r)\left[\frac{1}{4}(v-v_*)^2 + I + I_*\right]\right)$$
$$\frac{1}{\Gamma(\alpha+1)(2\pi)^{\frac{3}{2}}} \left| \sigma - \frac{v-v_*}{|v-v_*|} \right|^{-1} \tilde{\mathcal{B}} \quad I_*'^{-\frac{\alpha}{2}} dr dR d\sigma dI_* dv_*.$$

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$$g\left(\frac{v+v_*}{2} - \sqrt{R(\frac{1}{4}(v-v_*)^2 + I + I_*)}\sigma, (1-R)(1-r)\left[\frac{1}{4}(v-v_*)^2 + I + I_*\right]\right)$$

$$\frac{1}{\Gamma(\alpha+1)(2\pi)^{\frac{3}{2}}} \left| \sigma - \frac{v-v_*}{|v-v_*|} \right|^{-1} \tilde{\mathcal{B}} \, I_*'^{-\frac{\alpha}{2}} dr dR d\sigma dI_* dv_*.$$

- \mathcal{K}_2 becomes

$$\mathcal{K}_2 g = \frac{1}{\Gamma(\alpha+1)(2\pi)^{\frac{3}{2}}} \int_{(0,1)^2 \times S^2} \int_{\mathbf{h}(\mathbb{R}^3 \times \mathbb{R}_+)} g(x, y) J \mathcal{B} \left| \sigma - \frac{v-x-\sqrt{Ray}\sigma}{|v-x-\sqrt{Ray}\sigma|} \right|^{-1}$$

$$e^{-\frac{ay-I-(x-v+\sqrt{Ray}\sigma)^2}{2} - \frac{r}{2(1-r)}y - \frac{1}{4}(2x+2\sqrt{Ray}\sigma-v)^2 - \frac{1}{4}(x+2\sqrt{Ray}\sigma)^2}$$

$$(r(1-r))^{\alpha} (1-R)^{2\alpha+1} R^{1/2} I_*^{\alpha} dy dx d\sigma dr dR$$

Kernel of \mathcal{K}_2

- Extracting the kernel

$$\mathcal{K}_2 g(v, I) = \frac{1}{\Gamma(\alpha + 1)(2\pi)^{\frac{3}{2}}} \int_{\mathbb{R}^3 \times \mathbb{R}_+} \left[\int_{H_{x,y}^{v,I}} y^{-1} J \mathcal{B} \left| \sigma - \frac{v - x - \sqrt{Ray}\sigma}{|v - x - \sqrt{Ray}\sigma|} \right|^{-1} e^{-\frac{ay - I - (x - v + \sqrt{Ray}\sigma)^2}{2}} - \frac{r}{2(1-r)} y - \frac{1}{4}(2x + 2\sqrt{Ray}\sigma - v)^2 - \frac{1}{4}(x + 2\sqrt{Ray}\sigma)^2 \right. \right. \\ \left. \left. (r(1-r))^\alpha (1-R)^{2\alpha+1} R^{1/2} I_*^{\alpha/2} d\sigma dr dR \right] g(x, y) dy dx \right]$$

- Kernel of \mathcal{K}_2 in $L^2(\mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R}^3 \times \mathbb{R}_+)$?

L^2 integrability of kernel

$$\|k_2\|_{L^2}^2 = \frac{1}{\Gamma(\alpha+1)(2\pi)^{\frac{3}{2}}} \int_{(\mathbb{R}^3 \times \mathbb{R}_+)^2} \left[\int_{H_{x,y}^{v,I}} y^{-1} J\mathcal{B} \left| \sigma - \frac{v-x-\sqrt{Ray}\sigma}{|v-x-\sqrt{Ray}\sigma|} \right|^{-1} e^{-\frac{ay-I}{2} - \frac{1}{2}(x-v+\sqrt{Ray}\sigma)^2 - \frac{r}{2(1-r)}y - \frac{1}{4}(2x+2\sqrt{Ray}\sigma-v)^2 - \frac{1}{4}(x+2\sqrt{Ray}\sigma)^2} (r(1-r))^\alpha (1-R)^{2\alpha+1} R^{1/2} I_*^{\frac{\alpha}{2}} I_*^\alpha d\sigma dr dR \right]^2 dy dx dI dv$$

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Apply Cauchy-Schwarz:

$$\|k_2\|_{L^2}^2 \leq \frac{1}{\Gamma(\alpha+1)(2\pi)^{\frac{3}{2}}} \int_{(\mathbb{R}^3 \times \mathbb{R}_+)^2} \int_{H_{x,y}^{v,I}} y^{-2} J\mathcal{B}^2 \left| \sigma - \frac{v-x-\sqrt{Ray}\sigma}{|v-x-\sqrt{Ray}\sigma|} \right|^{-2} e^{-ay-I-(x-v+\sqrt{Ray}\sigma)^2 - \frac{r}{(1-r)}y - \frac{1}{2}(2x+2\sqrt{Ray}\sigma-v)^2 - \frac{1}{2}(x+2\sqrt{Ray}\sigma)^2} (r(1-r))^{2\alpha} (1-R)^{4\alpha+2} RI_*^{\alpha/2} d\sigma dr dR dy dx dI dv$$

L^2 integrability of kernel

Move backwards by h^{-1}

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$$\|k_2\|_{L^2}^2 \leq c \int_{\mathbb{R}^3} \int_{\mathbb{R}_+} \int_{\mathbb{R}^3} \int_{\mathbb{R}_+} \int_{(0,1)^2 \times S^2} J(r(1-r))^\alpha (1-R)^{2\alpha+1} R^{1/2} I_*^{\frac{\alpha}{2}} I_*^\alpha e^{-r(1-R)\left(\frac{(v-v_*)^2}{4} + I + I_*\right) - \frac{1}{4}\left(\frac{v+v_*}{2} - \sqrt{R(\frac{1}{4}(v-v_*)^2 + I + I_*)}\sigma\right)^2} e^{-I_* - \frac{1}{2}v_*^2} \mathcal{B}^2(v, v_*, I, I_*, r, R, \sigma) d\sigma dr dR dI_* dv_* dI dv$$

Assumptions on \mathcal{B} : The following changes of variables

- $I \mapsto E = I + I_* + \frac{1}{4}|v - v_*|^2$ where $dI = dE$,
- $\tilde{V} \mapsto \frac{v}{2} + \frac{v_*}{2} + \sqrt{RE}\sigma$ where $d\tilde{V} = \frac{1}{2^3}dv_*$

L^2 integrability of kernel

Move backwards by h^{-1}

$$\|k_2\|_{L^2}^2 \leq c \int_{\mathbb{R}^3} \int_{\mathbb{R}_+} \int_{\mathbb{R}^3} \int_{\mathbb{R}_+} \int_{(0,1)^2 \times S^2} J(r(1-r))^\alpha (1-R)^{2\alpha+1} R^{1/2} I_*^{\frac{\alpha}{2}} \\ e^{-r(1-R)\left(\frac{(\nu-\nu_*)^2}{4} + I + I_*\right) - \frac{1}{4}\left(\frac{\nu+\nu_*}{2} - \sqrt{R(\frac{1}{4}(\nu-\nu_*)^2 + I + I_*)}\sigma\right)^2} \\ e^{-I_* - \frac{1}{2}\nu_*^2} \mathcal{B}^2(\nu, \nu_*, I, I_*, r, R, \sigma) d\sigma dr dR dI_* d\nu_* dI/d\nu$$

Assumptions on \mathcal{B} : The following changes of variables

- $I \mapsto E = I + I_* + \frac{1}{4}|v - v_*|^2$ where $dI = dE$,
- $\tilde{V} \mapsto \frac{\nu}{2} + \frac{\nu_*}{2} + \sqrt{RE}\sigma$ where $d\tilde{V} = \frac{1}{2^3}dv_*$

Finally imply

$$\|k_2\|_{L^2}^2 \leq c \int_{(0,1)^2} \Psi^2(r, R) r^{2\alpha-1-\gamma} (1-r)^{\alpha-1} R(1-R)^{3\alpha-\gamma} dr dR < \infty.$$

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- $-\mathcal{L}$ has a spectral gap

Comparison to the Mixtures?

- The pre-post collisional relations:
 - Post-collisional velocities

$$v' = \frac{m_i v + m_j v_*}{m_i + m_j} + \frac{m_j}{m_i + m_j} \sqrt{\frac{2RE}{\mu_{ij}}} T_\omega \left[\frac{v - v_*}{|v - v_*|} \right]$$
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- The change of variable map $\mathbf{h} : (v_*, I_*) \mapsto (x, y)$ has Jacobian:

$$J_{ij} = \left(\frac{m_i + m_j}{m_j} \right)^3 \frac{1}{(1 - r)(1 - R)}$$

State of Art

- Single monoatomic gas
 - Compactness of \mathcal{K} : **Grad (1963)**
 - Spectral gap estimate (Maxwell molecules) **Bobylev (1988)**
 - Spectral gap estimate (Hard potentials) **Mouhot , Baranger (2005)**

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- Mixture of monoatomic gases
 - Compactness of \mathcal{K} : **Boudin, Grec, Pavic, Salvarani (2014)**
 - Spectral gap estimate **Mouhot, Daus, Jungel, Zamponi (2015)**
 - Stability of spectral gap **Bonedesan, Briant, Boudin, Grec (2018)**
- Single polyatomic gas
 - Compactness of \mathcal{K} : **Bernhoff (2022)**
 - Compactness of \mathcal{K} : **Borsoni, Boudin, Salvarani(2022)(resonant model)**
- Mixture of polyatomic gases
 - Compactness of \mathcal{K} : **Brull, Shahine, Thieullen (2022): Continuous Internal Energy**
 - Compactness of \mathcal{K} : **Bernhoff (2022)Discrete Internal Energy**

Perspectives

- Perspectives

- Establish the same result for a mixture of monoatomic and polyatomic gases
- Spectral gap estimates of the linearized Boltzmann operator
- L^p compactness of \mathcal{K}

And Finally

Thanks for your ATTENTION!