# Rigorous derivation of the Fick cross-diffusion system from the multi-species Boltzmann equation in the diffusive scaling

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*Recent contributions in kinetic theory and applications*
*LJLL, March 6th, 2023*

# Outline of the talk

# Context of the study

- Non-reactive mixture of $p$ monoatomic gases
- Isothermal setting $T > 0$ uniform and constant
- Two different scales for the description of the mixture
  - mesoscopic scale (kinetic model): species $i$ described by its distribution function $f_i(t, x, v)$
  - macroscopic scale: species $i$ described by the physical observables
    - number density $n_i(t, x)$
    - velocity $u_i(t, x)$

  $\rightsquigarrow$ flux of species $i$ : $J_i(t, x) = n_i(t, x)u_i(t, x)$

  $\rightsquigarrow$ vectorial quantities $\mathbf{n} = \begin{bmatrix} n_1 \\ \vdots \\ n_p \end{bmatrix}$, $\mathbf{J} = \begin{bmatrix} J_1 \\ \vdots \\ J_p \end{bmatrix}$
- Link between the two scales in the diffusive scaling
  - Formal and theoretical convergence

# Diffusion models for mixtures: Maxwell-Stefan/Fick

Mass conservation:

$$\partial_t \mathbf{n} + \nabla \cdot \mathbf{J} = 0$$

Diffusion process (link between $\mathbf{J}$ and $\nabla \mathbf{n}$):

**Fick equations**

$$\boxed{\mathbf{J} = A(\mathbf{n}) \nabla \mathbf{n}}$$

**Maxwell-Stefan equations**

$$\boxed{\nabla \mathbf{n} = B(\mathbf{n}) \mathbf{J}}$$

- $A(\mathbf{n})$ and $B(\mathbf{n})$ are not invertible (rank $p-1$)
- Using pseudo-inverse: structural similarity [Giovangigli '91, '99]
- Equimolar diffusion setting [Bothe], [Jüngel, Stelzer]

Formal analogy of the two systems,
different ways of obtaining Fick and Maxwell-Stefan equations

# Mesoscopic point of view

## Hydrodynamic limit

- Obtention of these two equations from the kinetic description?
- Obtention of closure relations?

## Moment method (Maxwell-Stefan)

- [Levermore], [Müller, Ruggieri]
- Ansatz that the distribution functions are at local Maxwellian states
- Assumption: different species have different macroscopic velocities on macroscopic time scales
- Rigorous convergence [Bondesan, Briant]

## Perturbative method (Fick)

- [Bardos, Golse, Levermore], [Bisi, Desvillettes]
- Based on the Chapman-Enskog expansion
- Formal and rigorous convergence [Briant, G.]

# Outline of the talk

# Kinetic setting

- Boltzmann equations for mixtures on $\mathbb{R}_+ \times \mathbb{T}^d \times \mathbb{R}^d$

$$\varepsilon \partial_t f_i + v \cdot \nabla_x f_i = \frac{1}{\varepsilon} \sum_{j=1}^{p} Q_{ij}(f_i, f_j), \qquad 1 \leq i \leq p$$

[Desvillettes, Monaco, Salvarani, '05]

- Diffusive scaling: small mean free path and Mach number: Kn $\sim$ Ma $\sim \varepsilon$
- Boltzmann collision operator, for $v \in \mathbb{R}^d$

$$Q_{ij}(f_i, f_j)(v) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} \mathcal{B}_{ij}(v, v_*, \sigma) \Big[ f_i(v') f_j(v'_*) - f_i(v) f_j(v_*) \Big] \mathrm{d}\sigma \mathrm{d}v_*$$

- Elastic collision rules, for $\sigma \in \mathbb{S}^{d-1}$

$$\begin{cases} v' = (m_i v + m_j v_* + m_j |v - v_*| \sigma)/(m_i + m_j) \\ v'_* = (m_i v + m_j v_* - m_i |v - v_*| \sigma)/(m_i + m_j) \end{cases}$$

- Cross sections $\mathcal{B}_{ij} = \mathcal{B}_{ji} > 0$ (hard or Maxwell potentials with Grad's cutoff assumption)

# Properties of the collision operator

- Equilibrium: Maxwellian with same bulk velocity and temperature

$$n_i(t,x)\left(\frac{m_i}{2\pi k_B T}\right)^{d/2}\exp\left(-\frac{m_i|v-u(t,x)|^2}{2k_B T}\right)$$

- Conservation properties of the collision operator for $1 \leq i,j \leq p$

$$\int_{\mathbb{R}^d} Q_{ij}(f_i,f_j)(v)\,\mathrm{d}v = 0$$

$$\int_{\mathbb{R}^d}\Big(m_i Q_{ij}(f_i,f_j)(v) + m_j Q_{ji}(f_j,f_i)(v)\Big)v\,\mathrm{d}v = 0$$

In the following, bold notation for vectors: $\mathbf{f} = (f_i)_i$, $\mathbf{m} = (m_i)_i$

# Linearized Boltzmann operator

- Expansion around the global Maxwellian with zero bulk velocity (equilibrium) with number density $n_i$

$$f_i = M_i + \varepsilon g_i = n_i \mu_i + \varepsilon g_i$$

$$\mu_i = (m_i/2\pi k_B T)^{d/2} e^{-m_i|v|^2/2k_B T}$$

- Linearization of the collision operator, for $\mathbf{g} = (g_i)_i$

$$\mathcal{L}_i(\mathbf{g}) = \sum_j Q_{ij}(n_i\mu_i, g_j) + Q_{ji}(g_i, n_j\mu_j)$$

$\rightsquigarrow$ defines the linearized Boltzmann operator $\mathbf{L} = (\mathcal{L}_i)_i$ around $\mathbf{M} = \mathbf{n}\boldsymbol{\mu}$

- $\operatorname{Ker} \mathbf{L}$ is spanned by $p + d + 1$ explicit functions ($\sim M_k/\sqrt{n_k}\mathbf{e}_k$, $v_k\mathbf{mM}$, $|v|^2\mathbf{mM}$)
- Denote by $\pi_{\mathbf{L}}(\cdot)$ the projection on $\operatorname{Ker} \mathbf{L}$

$\mathbf{L}$ is a closed, self-adjoint operator in $L^2_v(\mathbf{M}^{-1/2})$, which is bounded and displays a spectral gap (with a gain of weight). [Briant, Daus]

# Definition of $\mathbf{L}^{-1}$

$\mathbf{L}^{-1}$ is a self-adjoint operator on $(\mathrm{Ker}\,\mathbf{L})^{\perp}$ which

- is bounded

$$\|\mathbf{L}^{-1}\mathbf{g}\|_{\mathbf{M}} \leq K\|\mathbf{g}\|_{\mathbf{M}}$$

- displays a spectral gap

$$\langle \mathbf{g}, \mathbf{L}^{-1}\mathbf{g}\rangle_{\mathbf{M}} \leq -\lambda\|\mathbf{g}\|_{\mathbf{M}}$$

with the shortcut $\|\cdot\|_{\mathbf{M}} = \|\cdot\|_{L^2_v(\mathbf{M}^{-1/2})}$.

## Remark

*Since $\mathbf{M} = \mathbf{n}\boldsymbol{\mu}$ depends on $\mathbf{n}$, the linearized operator $\mathbf{L}$, and thus $\mathbf{L}^{-1}$, also do: the constants $K$, $\lambda$ depend on $\mathbf{n}$.*

$\rightsquigarrow$ *track explicit computations of $K$, $\lambda$* [Baranger, Mouhot], [Briant, Daus]

# Outline of the talk

# Formal obtention of the diffusion equations

$$\boxed{\varepsilon\partial_t f_i^\varepsilon + v\cdot\nabla_x f_i^\varepsilon = \frac{1}{\varepsilon}\sum_{j=1}^{p} Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)}$$

## Moments of the distribution functions

- Number density of species $i$

$$n_i^\varepsilon(t,x) = \int_{\mathbb{R}^d} f_i^\varepsilon(t,x,v)\mathrm{d}v$$

- Flux of species $i$

$$J_i^\varepsilon(t,x) = n_i^\varepsilon(t,x)\, u_i^\varepsilon(t,x) = \frac{1}{\varepsilon}\int_{\mathbb{R}^d} v\, f_i^\varepsilon(t,x,v)\mathrm{d}v$$

1. Mass conservation : moment of order 0 of the equation

$$\varepsilon\frac{\partial}{\partial t}\left(\int_{\mathbb{R}^3} f_i^\varepsilon(v)\,\mathrm{d}v\right) + \nabla_x\cdot\left(\int_{\mathbb{R}^3} v\, f_i^\varepsilon(v)\,\mathrm{d}v\right) = \varepsilon\Big(\partial_t n_i^\varepsilon + \nabla_x\cdot J_i^\varepsilon\Big) = 0,$$

where the collision term vanishes (conservation property).

# Momentum equation (Maxwell-Stefan/Fick)

## Moment method: moment of order 1 of the equation

- Use of an ansatz that $f_i$ are local Maxwellians
- (Explicit) computations depending on $\mathcal{B}_{ij}$
- Maxwell-Stefan cross-diffusion equations at the limit $\varepsilon \to 0$
- Possible expression of the diffusion coefficients involving $\mathbf{L}$
- Closure relation obtained from the moment of order 2 of the equation
- [Boudin, G., Salvarani], [Boudin, G., Pavan]

## Perturbative method

Inject expansion $\mathbf{f}^\varepsilon = \mathbf{n}^\varepsilon \boldsymbol{\mu} + \varepsilon \mathbf{g}^\varepsilon$ in the Boltzmann equation, at leading order ($\varepsilon^0$)

$$\mu_i v \cdot \nabla_x n_i^\varepsilon = \mathcal{L}_i(\mathbf{g}^\varepsilon)$$

and $J_i^\varepsilon = \dfrac{1}{\varepsilon} \displaystyle\int v\, f_i^\varepsilon \mathrm{d}v = \int v\, g_i^\varepsilon \mathrm{d}v$.

*Let us drop superscript $\varepsilon$ for the time being.*

- In a vectorial form, defining $W_i = \mu_i v \cdot \nabla_x n_i$ and $\mathbf{W} = (W_i)_i$

$$\mathbf{W} = \mathbf{L}(\mathbf{g}) \quad \underset{(\star)}{\rightsquigarrow} \quad \mathbf{g} = \mathbf{L}^{-1}\mathbf{W}$$

- Inject this expression for $g_i$ in the definition of $J_i$

$$J_i = \int v[\mathbf{L}^{-1}\mathbf{W}]_i \mathrm{d}v = \int n_i \mu_i v[\mathbf{L}^{-1}\mathbf{W}]_i M_i^{-1} \mathrm{d}v$$

- With $\mathbf{C}_i = (\mu_i v \delta_{ij})_j$, we get

$$J_i = n_i \langle \mathbf{C}, \mathbf{L}^{-1}\mathbf{W} \rangle_{\mathbf{M}}$$

- $\mathbf{L}^{-1}$ is self-adjoint on $(\mathrm{Ker}\,\mathbf{L})^{\perp}$. Let $\mathbf{\Gamma} = \pi_{\mathbf{L}}(\mathbf{C})$. Thus

$$J_i = n_i \sum_j \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_j, W_j \rangle_{\mathbf{M}}$$

- Since $W_j = \mu_j v \cdot \nabla_x n_j =$ "$\mathbf{C}_j \cdot \nabla_x n_j$"

$$J_i = \sum_j \underbrace{n_i \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_j, \mathbf{C}_j \rangle_{\mathbf{M}}}_{a_{ij}(n_i)} \nabla_x n_j$$

$\rightsquigarrow$ Fick equation: $\mathbf{J} = A(\mathbf{n}) \nabla_x \mathbf{n}$

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$$J_i = \sum_j \underbrace{n_i \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_j, \mathbf{C}_j \rangle_{\mathbf{M}}}_{a_{ij}(n_i)} \nabla_x n_j$$

$\leadsto$ Fick equation: $\mathbf{J} = A(\mathbf{n}) \nabla_x \mathbf{n}$

# Closure relation for Fick equations

- Summing over $i$ the equations ($A$ has rank $p-1$) implies that $\sum_i m_i J_i = 0$
- Mass conservation for each species implies (when summing with weights $m_i$)

$$0 = \frac{\mathrm{d}}{\mathrm{dt}} \int \sum_i m_i n_i \mathrm{d}x$$

- Inversion giving the perturbation $\mathbf{g}$ (relation $(\star)$) only valid if the RHS $W_i = \mu_i v \cdot \nabla_x n_i \in (\mathrm{Ker}\,\mathbf{L})^\perp$.
- $\mathrm{Ker}\,\mathbf{L}$ spanned by $M_k/\sqrt{n_k}\mathbf{e}_k$, $v_k \mathbf{mM}$, $|v|^2\mathbf{mM}$
- Orthogonality

$$0 = \langle \mu_i v \cdot \nabla_x n_i, m_i M_i v \rangle_{\mathbf{M}} = \sum_i \int \mu_i v \cdot \nabla_x n_i \, m_i v \mathrm{d}v \propto \nabla_x \sum_i m_i n_i$$

- $\rightsquigarrow$ Constant mass $\sum_i m_i n_i$
- Closure relation inherent to the perturbative setting

# Fick equation

- $A = (a_{ij})$ is not symmetric, denote $A(\mathbf{n}) = N(\mathbf{n})\bar{A}(\mathbf{n})$, with $N(\mathbf{n}) = (n_i \delta_{ij})$.

## Properties of $\bar{A}(\mathbf{n})$

- $\bar{A}(\mathbf{n})$ is symmetric
- $\mathrm{Ker}\, \bar{A}(\mathbf{n}) = \mathrm{Span}(\mathbf{nm})$
- Denote $\pi_{\bar{A}}$ the projection on $\mathrm{Ker}\, \bar{A}$, $\pi_{\bar{A}}^{\perp}$ on $(\mathrm{Ker}\, \bar{A})^{\perp}$
- $\bar{A}(\mathbf{n})$ depends on $\mathbf{n}$ via $\mathbf{L}^{-1}$ and the weight $\mathbf{M}$
- coercivity of $\bar{A}(\mathbf{n})$ outside its kernel: $(p-1)$ non zero eigenvalues $\beta_i$ s. th.

$$\beta_i \leq -\beta_{\mathsf{max}} < 0,$$

where $\beta_{\mathsf{max}}$ depends on $\lambda$.

- Combine $\mathbf{J} = N(\mathbf{n})\bar{A}(\mathbf{n})\nabla_x \mathbf{n}$ with mass conservation + closure relation

$$\begin{cases} \partial_t \mathbf{n} + \nabla_x \cdot (N(\mathbf{n})\bar{A}(\mathbf{n})\nabla_x \mathbf{n}) = 0, \\ \langle \mathbf{m}, \mathbf{n} \rangle_{\mathbb{R}^p} = cst. \end{cases}$$

# Outline of the talk

# Perturbative Cauchy theory for the Fick equation

Fix a constant global equilibrium $\mathbf{n}_\infty > 0$, and write

$$\mathbf{n}(t,x) = \mathbf{n}_\infty + \tilde{\mathbf{n}}(t,x) \qquad (\bullet)$$

Fick equation

$$\begin{cases} \partial_t \tilde{\mathbf{n}} + \nabla_x \cdot \left(N(\mathbf{n}_\infty)\bar{A}(\mathbf{n}_\infty + \tilde{\mathbf{n}})\nabla_x \tilde{\mathbf{n}}\right) = -\nabla_x \cdot \left(N(\tilde{\mathbf{n}})\bar{A}(\mathbf{n}_\infty + \tilde{\mathbf{n}})\nabla_x \tilde{\mathbf{n}}\right), \\ \langle \mathbf{m}, \tilde{\mathbf{n}} \rangle = 0. \end{cases}$$

**Theorem**

*Let $s > d/2$. For $\|\tilde{\mathbf{n}}^{(\mathrm{in})}\|_{H^s_x}$ compatible and sufficiently small, there exists a unique solution of the form $(\bullet)$ to the Fick equation, and it satisfies*

$$\|\tilde{\mathbf{n}}\|_{H^s_x} \leq \|\tilde{\mathbf{n}}^{(\mathrm{in})}\|_{H^s_x} e^{-\lambda_s t}.$$

Without nonlinear terms, standard a priori estimate with the weight $N(\mathbf{n}_\infty)^{-1/2}$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\mathbf{n}}\|^2_{L^2_x(N(\mathbf{n}_\infty)^{-1/2})} = \langle \bar{A}\nabla_x \tilde{\mathbf{n}}, \nabla_x \tilde{\mathbf{n}} \rangle_{L^2_x} \leq \beta_{\max} \|\pi^\perp_{\bar{A}}(\nabla_x \tilde{\mathbf{n}})\|^2_{L^2_x}$$

No control of the kernel part $\pi_{\bar{A}}(\nabla_x \tilde{\mathbf{n}})$: $\langle \mathbf{n}\mathbf{m}, \nabla_x \tilde{\mathbf{n}} \rangle$ even at the main order

# Rescaling in time and space

$$\boxed{\tilde{\eta}_i(t,x) = \tilde{n}_i(n_{\infty\,i}^{\alpha} t, n_{\infty\,i}^{\beta} x)}$$

$$\begin{cases} \partial_t \tilde{\eta}_i + \nabla_x \cdot \left( \sum_j \frac{n_{\infty\,i}^{1+\alpha}}{n_{\infty\,j}^{2\beta}} \bar{a}_{ij}(\mathbf{n}_\infty + \tilde{\eta}) \nabla_x \tilde{\eta}_j \right) = -\nabla_x \cdot \left( \tilde{\eta}_i \sum_j \frac{n_{\infty\,i}^{\alpha}}{n_{\infty\,j}^{2\beta}} \bar{a}_{ij}(\mathbf{n}_\infty + \tilde{\eta}) \nabla_x \tilde{\eta}_j \right), \\ \langle \mathbf{m}, \tilde{\boldsymbol{\eta}} \rangle = 0. \end{cases}$$

- Choice $1 + \alpha = -2\beta \rightsquigarrow$ use of the coercivity of $\bar{A}$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{\eta}}\|_{L^2_x}^2 = \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right), \nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle + \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right), \tilde{\boldsymbol{\eta}}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle$$

$$\leq -\beta_{\max} \left\| \pi_{\bar{A}}^{\perp} \left[ \nabla_x \left( \frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}} \right) \right] \right\|_{L^2_x}^2 + \left\langle \dots \right\rangle$$

- Control of the kernel part & nonlinear terms (cf. next slide)
- A priori estimate in $H^s_x$, with $P^s(0) = 0$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{\eta}}\|_{H^s_x}^2 \leq -C\beta_{\max}\left(1 - CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H^s_x})\right)\|\nabla_x \tilde{\boldsymbol{\eta}}\|_{H^s_x}^2$$

- For small initial datum, $CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H^s_x}) \leq 1/2$ & Poincaré + Grönwall

# Rescaling in time and space

$$\boxed{\tilde{\eta}_i(t,x) = \tilde{n}_i(n_{\infty\,i}^{\alpha} t, n_{\infty\,i}^{\beta} x)}$$

$$\begin{cases} \partial_t \tilde{\eta}_i + \nabla_x \cdot \left( \frac{1}{n_{\infty\,i}^{2\beta}} \sum_j \bar{a}_{ij}(\mathbf{n}_\infty + \tilde{\eta}) \nabla_x \frac{\tilde{\eta}_j}{n_{\infty\,j}^{2\beta}} \right) = -\nabla_x \cdot \left( \frac{\tilde{\eta}_i}{n_{\infty\,i}^{2\beta}} \sum_j \bar{a}_{ij}(\mathbf{n}_\infty + \tilde{\eta}) \nabla_x \frac{\tilde{\eta}_j}{n_{\infty\,j}^{2\beta}} \right) \\ \langle \mathbf{m}, \tilde{\boldsymbol{\eta}} \rangle = 0. \end{cases}$$

- Choice $1 + \alpha = -2\beta \rightsquigarrow$ use of the coercivity of $\bar{A}$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{\eta}}\|^2_{L^2_x} = \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right), \nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle + \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right), \tilde{\boldsymbol{\eta}}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle$$
$$\leq -\beta_{\max}\left\| \pi_{\bar{A}}^{\perp}\left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right]\right\|^2_{L^2_x} + \left\langle \dots \right\rangle$$

- Control of the kernel part & nonlinear terms (cf. next slide)
- A priori estimate in $H^s_x$, with $P^s(0) = 0$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{\eta}}\|^2_{H^s_x} \leq -C\beta_{\max}\left(1 - CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H^s_x})\right)\|\nabla_x \tilde{\boldsymbol{\eta}}\|^2_{H^s_x}$$

- For small initial datum, $CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H^s_x}) \leq 1/2$ & Poincaré + Grönwall

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- Choice $1 + \alpha = -2\beta \rightsquigarrow$ use of the coercivity of $\bar{A}$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{\eta}}\|_{L_x^2}^2 = \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right), \nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle + \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right), \tilde{\boldsymbol{\eta}}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle$$
$$\leq -\beta_{\max}\left\| \pi_{\bar{A}}^{\perp}\left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right]\right\|_{L_x^2}^2 + \left\langle \dots \right\rangle$$

- Control of the kernel part & nonlinear terms (cf. next slide)
- A priori estimate in $H_x^s$, with $P^s(0) = 0$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{\eta}}\|_{H_x^s}^2 \leq -C\beta_{\max}\left(1 - CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H_x^s})\right)\|\nabla_x\tilde{\boldsymbol{\eta}}\|_{H_x^s}^2$$

- For small initial datum, $CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H_x^s}) \leq 1/2$ & Poincaré + Grönwall

# Rescaling in time and space

$$\boxed{\tilde{\eta}_i(t,x) = \tilde{n}_i(n_{\infty\,i}^{\alpha} t, n_{\infty\,i}^{\beta} x)}$$

$$\begin{cases} \partial_t \tilde{\eta}_i + \nabla_x \cdot \left( \dfrac{1}{n_{\infty\,i}^{2\beta}} \sum_j \bar{a}_{ij}(\mathbf{n}_\infty + \tilde{\eta}) \nabla_x \dfrac{\tilde{\eta}_j}{n_{\infty\,j}^{2\beta}} \right) = -\nabla_x \cdot \left( \dfrac{\tilde{\eta}_i}{n_{\infty\,i}^{2\beta}} \sum_j \bar{a}_{ij}(\mathbf{n}_\infty + \tilde{\eta}) \nabla_x \dfrac{\tilde{\eta}_j}{n_{\infty\,j}^{2\beta}} \right) \\ \langle \mathbf{m}, \tilde{\boldsymbol{\eta}} \rangle = 0. \end{cases}$$

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$$\leq -\beta_{\max} \left\| \pi_{\bar{A}}^{\perp} \left[ \nabla_x \left( \frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}} \right) \right] \right\|_{L_x^2}^2 + \left\langle \dots \right\rangle$$

- Control of the kernel part & nonlinear terms (cf. next slide)
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- Control of the kernel part & nonlinear terms (cf. next slide)
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$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \|\tilde{\boldsymbol{\eta}}\|_{H_x^s}^2 \leq -C \beta_{\max} \left( 1 - C P^s(\|\tilde{\boldsymbol{\eta}}\|_{H_x^s}) \right) \|\nabla_x \tilde{\boldsymbol{\eta}}\|_{H_x^s}^2$$

- For small initial datum, $CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H_x^s}) \leq 1/2$ & Poincaré + Grönwall

# Control of the kernel part & nonlinear terms

- $\pi_{\bar{A}}\left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right]$ colinear to

$$\left\langle(\mathbf{n}_\infty+\tilde{\boldsymbol{\eta}})\mathbf{m},\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle=\left\langle\mathbf{n}_\infty\mathbf{m},\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle+\left\langle\tilde{\boldsymbol{\eta}}\mathbf{m},\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle$$

- Choice $2\beta=1 \rightsquigarrow$ use of the closure relation
- Lower order term

$$\left\langle\tilde{\boldsymbol{\eta}}\mathbf{m},\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty}\right)\right\rangle\leq C\|\tilde{\boldsymbol{\eta}}\|_{L^2_x}\|\nabla_x\tilde{\boldsymbol{\eta}}\|_{L^2_x}$$

- Nonlinear terms: control on $\bar{A}(\tilde{\boldsymbol{\eta}})$

$$\|\bar{A}(\tilde{\boldsymbol{\eta}})\|_{H^s_x}\leq CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H^s_x})$$

# Control of the kernel part & nonlinear terms

- $\pi_{\bar{A}}\left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right]$ colinear to

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- Choice $2\beta=1\rightsquigarrow$ use of the closure relation
- Lower order term

$$\left\langle\tilde{\boldsymbol{\eta}}\mathbf{m},\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty}\right)\right\rangle\le C\|\tilde{\boldsymbol{\eta}}\|_{L^2_x}\|\nabla_x\tilde{\boldsymbol{\eta}}\|_{L^2_x}$$

- Nonlinear terms: control on $\bar{A}(\tilde{\boldsymbol{\eta}})$

$$\|\bar{A}(\tilde{\boldsymbol{\eta}})\|_{H^s_x}\le CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H^s_x})$$

# Control of the kernel part & nonlinear terms

- $\pi_{\bar{A}}\left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right]$ colinear to

$$\left\langle (\mathbf{n}_\infty + \tilde{\boldsymbol{\eta}})\mathbf{m}, \nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^{2\beta}}\right)\right\rangle = \underbrace{\langle \mathbf{m}, \nabla_x \tilde{\boldsymbol{\eta}}\rangle}_{=0} + \left\langle \tilde{\boldsymbol{\eta}}\mathbf{m}, \nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty}\right)\right\rangle$$

- Choice $2\beta = 1 \rightsquigarrow$ use of the closure relation
- Lower order term

$$\left\langle \tilde{\boldsymbol{\eta}}\mathbf{m}, \nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty}\right)\right\rangle \leq C\|\tilde{\boldsymbol{\eta}}\|_{L^2_x}\|\nabla_x\tilde{\boldsymbol{\eta}}\|_{L^2_x}$$

- Nonlinear terms: control on $\bar{A}(\tilde{\boldsymbol{\eta}})$

$$\|\bar{A}(\tilde{\boldsymbol{\eta}})\|_{H^s_x} \leq CP^s(\|\tilde{\boldsymbol{\eta}}\|_{H^s_x})$$

# Outline of the talk

# Rigorous convergence in a perturbative setting I

Expansion $\mathbf{f}^\varepsilon = \mathbf{M}^\varepsilon + \varepsilon \mathbf{g}^\varepsilon$ in the Boltzmann equation

## Use of the result (for Maxwell-Stefan) of [Bondesan, Briant]

Simpler setting since

- $\mathbf{M}^\varepsilon$ has equal velocities for all species $(= 0) \rightsquigarrow$ equilibrium of $Q$
- possibility to get rid of the fluxes and have a parabolic setting

## Main ingredients

- Spectral gap on $\mathbf{L} \rightsquigarrow$ control of the microscopic part of $\mathbf{g}^\varepsilon$ (in $(\mathrm{Ker}\,\mathbf{L})^\perp$)
- Choice of the Maxwellian $\mathbf{M}^\varepsilon(t,x,v) = (\mathbf{n}_\infty + \varepsilon \tilde{\mathbf{n}}(t,x))\boldsymbol{\mu}(v)$ [Caflisch], [De Masi, Esposito, Lebowitz]
- Control of the fluid part with a hypocoercive norm depending on $\varepsilon$ (via the commutator $[v \cdot \nabla_x, \nabla_v] = -\nabla_x$) [Mouhot, Neumann], [Briant]

$$\| \cdot \|^2_{\mathcal{H}^s_\varepsilon} \sim \sum_{|\ell| \le s} \|\partial_x^\ell \cdot \|_{L^2_{x,v}(\boldsymbol{\mu}^{-1/2})} + \varepsilon^2 \sum_{\substack{|\ell|+|j| \le s \\ |j| \ge 1}} \|\partial_x^\ell \partial_v^j \cdot \|_{L^2_{x,v}(\boldsymbol{\mu}^{-1/2})}$$

# Rigorous convergence in a perturbative setting II

## Theorem (Briant, G.)

*With suitable assumptions on the cross sections, if* $\mathbf{g}^{(\mathrm{in})}$ *and* $\tilde{\mathbf{n}}^{(\mathrm{in})}$ *are small enough, the multispecies Boltzmann equation admits a unique global perturbative solution* $\mathbf{f}^\varepsilon(t,x,v) = \mathbf{M}^\varepsilon(t,x) + \varepsilon \mathbf{g}^\varepsilon(t,x,v) \geq 0$*, and*

$$\|\mathbf{f}^\varepsilon - \mathbf{M}^\varepsilon\|_{\mathcal{H}^s_\varepsilon}(t) \leq C\varepsilon.$$

Satisfy assumptions of the result in [Bondesan, Briant]:

- Smallness of the macroscopic perturbation: $\|\tilde{\mathbf{n}}\|_{L^\infty_t H^s_x} \leq \delta$ (Cauchy theory for $\tilde{\mathbf{n}}$)
- Control of $\mathbf{S}^\varepsilon = \frac{1}{\varepsilon}\partial_t \mathbf{M}^\varepsilon + \frac{1}{\varepsilon^2} v \cdot \nabla_x \mathbf{M}^\varepsilon$:

$$\pi_{\mathbf{L}}(\mathbf{S}^\varepsilon) = 0 \quad \text{and} \quad \pi_{\mathbf{L}}^\perp(\mathbf{S}^\varepsilon) \leq \frac{\delta}{\varepsilon}.$$

  The second estimate corresponds to the control of $\varepsilon\partial_t \tilde{\mathbf{n}} + v \cdot \nabla_x \tilde{\mathbf{n}}$ (Cauchy theory for $\tilde{\mathbf{n}}$ and estimates on $A(\mathbf{n})$ via $P^{s+2}$)

# Outline of the talk

# Conclusion and prospects

## Conclusions

- Derivation of Fick equations from the Boltzmann equation for mixtures in the diffusive regime in a perturbative setting
- Formal obtention of the diffusion coefficients and closure relation
- Cauchy theory in Sobolev spaces for the Fick sytem
- Stability of the Fick system in the Boltzmann equation

## Prospects

- Non perturbative setting
- Non isothermal setting
- Polyatomic gases
- Asymptotic Preserving numerical scheme
- Compare the experimental and theoretical relaxation times

Thank you for your attention!

# Fick diffusion coefficients

We had $a_{ij} = n_i \langle [\mathbf{L}^{-1}(\mathbf{C} - \mathbf{\Gamma})]_j, \mathbf{C}_j \rangle_{\mathbf{M}}$. More precisely

$$J_i^{(k)} = n_i \sum_{j=1}^{p} \sum_{\ell=1}^{d} \langle \mathbf{L}^{-1}(\mathbf{C}_i^{(k)} - \mathbf{\Gamma}_i^{(k)}), \mathbf{C}_j^{(\ell)} \rangle_{M_j} \partial_{x_\ell} n_j$$

## Properties of the term in red

- is zero if $k \neq \ell$
- is independent of $k = \ell$

Thus, it depends only on $i, j$ and allows to define the diffusion coefficients.

- Definition of $\mathbf{C}_i^{(k)} = (\mu_i v^{(k)} \delta_{ij})_j \rightsquigarrow$ choice of any velocity component
- Use that $\mathbf{\Gamma} \in (\mathrm{Ker}\, \mathbf{L})$

$$\boxed{a_{ij} = n_i \left\langle \mathbf{L}^{-1}\left(\pi_{\mathbf{L}}^{\perp}(\bar{v}\mu_i e_i)\right), \pi_{\mathbf{L}}^{\perp}(\bar{v}\mu_j e_j) \right\rangle_{\mathbf{M}}}$$

- $A = (a_{ij})$ is not symmetric, denote $A(\mathbf{n}) = N(\mathbf{n})\bar{A}(\mathbf{n})$, with $N(\mathbf{n}) = (n_i \delta_{ij})$.