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

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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[1]
- Cross sections[2]

[1] for $\sigma \in \mathbb{S}^{d-1}$

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

[2] $\mathcal{B}_{ij} = \mathcal{B}_{ji} > 0$ (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 property of the collision operator for $1 \leq i,j \leq p$

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

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:

$$\sim M_k \mathbf{e}_k, \; v_\ell \mathbf{m}\mathbf{M}, \; |v|^2 \mathbf{m}\mathbf{M}$$

- Denote by $\pi_{\mathbf{L}}(\cdot)$ the projection on $\operatorname{Ker} \mathbf{L}$

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

$\mathbf{L}$ 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]

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

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

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.
$\rightsquigarrow$ *track explicit computations of boundedness and spectral gap constants w.r.t. $\mathbf{n}$*
[Baranger, Mouhot], [Briant, Daus]

Outline of the talk

Formal obtention of the diffusion equations

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

Moments of the distribution functions

- Number density of species i

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

- Flux of species i

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

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

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

where the collision term vanishes (conservation property).

Momentum equation

Perturbative method

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

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

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

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

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

Inversion $(\star)$ only valid if the LHS $W_i = \mu_i v \cdot \nabla_x n_i \in (\mathrm{Ker}\, \mathbf{L})^{\perp}$

- Inject $g_i = [\mathbf{L}^{-1}\mathbf{W}]_i$ in the definition of $J_i = \int v\, g_i^\varepsilon \mathrm{d}v$

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

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

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

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

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

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

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

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

Fick equation

- $A = (a_{ij})$ is not symmetric. Introduce $N(\mathbf{n}) = (n_i \delta_{ij})$, so that

$$A(\mathbf{n}) = N(\mathbf{n})\bar{A}(\mathbf{n}).$$

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

- $\bar{A}(\mathbf{n})$ is symmetric
- $\bar{A}(\mathbf{n})$ depends on $\mathbf{n}$ via $\mathbf{L}^{-1}$ and the weight $\mathbf{M}$
- $\operatorname{Ker} \bar{A}(\mathbf{n}) = \mathrm{Span}(\mathbf{nm})$
- Denote $\pi_{\bar{A}}$ the projection on $\operatorname{Ker} \bar{A}$, $\pi_{\bar{A}}^{\perp}$ on $(\operatorname{Ker} \bar{A})^{\perp}$
- Coercivity of $\bar{A}(\mathbf{n})$ outside its kernel

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

$$\partial_t \mathbf{n} + \nabla_x \cdot (N(\mathbf{n})\bar{A}(\mathbf{n})\nabla_x \mathbf{n}) = 0;$$

Closure relation for Fick equations

- Integrating the equation gives $\frac{\mathrm{d}}{\mathrm{dt}} \int \sum_i m_i n_i \mathrm{d}x = 0$

- Inversion $(\star)$: $W_i = \mu_i v \cdot \nabla_x n_i \in (\mathrm{Ker}\, \mathbf{L})^\perp$.
- $\mathrm{Ker}\, \mathbf{L}$ spanned by $M_k \mathbf{e}_k$, $v_k \mathbf{mM}$, $|v|^2 \mathbf{mM}$
- 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

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

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

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

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 $N(\mathbf{n}_\infty)^{-1/2}$

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

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

Rescaling in time and space

$$\boxed{\tilde{\eta}_i(t,x) = \tilde{n}_i(n^a_{\infty\,i}t, n^b_{\infty\,i}x)}$$

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

- Choice $a=-1 \rightsquigarrow$ use the coercivity of $\bar{A}$

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

$$\leq -C\left\|\pi^\perp_{\bar{A}}\left[\nabla_x\left(\frac{\tilde{\eta}}{\mathbf{n}^b_\infty}\right)\right]\right\|^2_{L^2_x} + \left\langle\dots\right\rangle$$

- Control of the kernel part: $\pi_{\bar{A}}\left[\nabla_x\left(\frac{\tilde{\eta}}{\mathbf{n}^b_\infty}\right)\right]$ colinear to

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

- Choice $b=1 \rightsquigarrow$ use of the closure relation

Rescaling in time and space

$$\boxed{\tilde{\eta}_i(t,x) = \tilde{n}_i(n^a_{\infty\,i}t, n^b_{\infty\,i}x)}$$

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

- Choice $a = -1 \rightsquigarrow$ use the coercivity of $\bar{A}$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{\boldsymbol{\eta}}\|^2_{L^2_x} = \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}^b_\infty}\right), \nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}^b_\infty}\right) \right\rangle + \left\langle \bar{A}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}^b_\infty}\right), \tilde{\boldsymbol{\eta}}\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}^{b+1}_\infty}\right) \right\rangle$$
$$\leq -C \left\| \pi^\perp_{\bar{A}} \left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}^b_\infty}\right)\right] \right\|^2_{L^2_x} + \langle \dots \rangle$$

- Control of the kernel part: $\pi_{\bar{A}}\left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}^b_\infty}\right)\right]$ colinear to

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

- Choice $b = 1 \rightsquigarrow$ use of the closure relation

Rescaling in time and space

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

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

- Choice $a = -1 \rightsquigarrow$ use the coercivity of $\bar{A}$

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

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

- Control of the kernel part: $\pi_{\bar{A}}\left[\nabla_x\left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^b}\right)\right]$ colinear to

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

- Choice $b = 1 \rightsquigarrow$ use of the closure relation

Rescaling in time and space

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

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

- Choice $a = -1 \rightsquigarrow$ use the coercivity of $\bar{A}$

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

- Control of the kernel part: $\pi_{\bar{A}} \left[\nabla_x \left(\frac{\tilde{\boldsymbol{\eta}}}{\mathbf{n}_\infty^b} \right) \right]$ colinear to

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

- Choice $b = 1 \rightsquigarrow$ use of the closure relation

End of the proof

- 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 $\bar{A}(\tilde{\boldsymbol{\eta}})$

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

- A priori estimate in H^s_x, with some polynomial P^s such that $P^s(0) = 0$

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

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

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_{ij}
- possibility to get rid of the fluxes and have a parabolic setting

Main ingredients

- 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]
- Spectral gap on $\mathbf{L} \rightsquigarrow$ control of the microscopic part of $\mathbf{g}^\varepsilon$ (in $(\mathrm{Ker}\,\mathbf{L})^\perp$)
- Control of the fluid part with a hypocoercive norm depending on ε (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]:

- Perturbative framework
- 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 $\varepsilon\|\partial_t \tilde{\mathbf{n}}\|_{H^s} + \|\nabla_x \tilde{\mathbf{n}}\|_{H^s}$: Cauchy theory for $\tilde{\mathbf{n}}$ and estimates on $A(\mathbf{n})$ via P^s

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?
- Other mixtures: non isothermal, polyatomic gases
- AP numerical scheme
- Compare 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 $\bar{v}$
- Use that $\mathbf{\Gamma} \in (\mathrm{Ker}\, \mathbf{L})$

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