Compressed asymptotic analysis of a quantum transport equation

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Wigner-BGK equation

$$\partial_t w + v\cdot\nabla_x w - \Theta[V]w \;=\; -\nu(w - w_{\rm eq}),\;\; x, v \in \mathbb{R}^d,\; t>0 \tag{1}$$

- $w(x,v,t) \in \mathbb{R}$ quasi-distribution function, $w(t=0)=w_0$,
- V external potential enters via

$$\Theta[V]w(x,v) \;=\; \frac{i}{\hbar(2\pi)^{\frac{d}{2}}}\int \delta V(x,\hbar\eta)\mathcal{F}_v w(x,\eta)e^{i\eta v}d\eta$$

with $\delta V(x,\hbar\eta) := V(x+\hbar\eta/2) - V(x-\hbar\eta/2)$, $\mathcal{F}_v$ Fourier tr.

- interaction with the environment: after a time $1/\nu$ the system will relax to $w_{\rm eq}$ (quantum corrected thermal eq.)

$$w_{\rm eq}(x,v) := \left(\frac{m}{2\pi\hbar}\right)^d e^{-\beta H}\left\{1+\hbar^2\left[-\frac{\beta^2}{8m}\sum_{r=1}^d\frac{\partial^2 V}{\partial x_r^2} + \frac{\beta^3}{24m}\sum_{r=1}^d\left(\frac{\partial V}{\partial x_r}\right)^2 + \frac{\beta^3}{24}\sum_{r,s=1}^d v_r v_s\frac{\partial^2 V}{\partial x_r\partial x_s}\right] + O(\hbar^4)\right\}$$

where $H(x,v) := mv^2/2 + V(x)$ is the Hamiltonian, $\beta \equiv 1/kT$, with T (constant) temperature and k Boltzmann constant.

Formulation of the problem

- Parametrize ([Gardner 94]) the equilibrium function via

$$n(x,t) \equiv n[w](x,t) := \int w(x,v,t)\,dv \approx \int w_{\rm eq}(x,v)\,dv \tag{2}$$

then the Wigner thermal equilibrium function reads

$$w_{\rm eq}(x,v) = n(x,t)\left\{F(v) + \hbar^2 F^{(2)}(x,v)\right\} + O(\hbar^4),$$

with $F(v) = (\beta m/2\pi)^{d/2}e^{-\beta m v^2/2}$ and $F^{(2)}$ $O(\hbar^2)$-correction.

- Rescale (1) such that $\frac{t_V}{t_0} \approx \frac{t_C}{t_0} \approx \epsilon$, with t_V, t_C, t_0 potential, collision and system characteristic times. Thus,

$$\epsilon\,\partial_t w + \epsilon\, v\cdot\nabla_x w - \Theta[V]w \;=\; -\nu\,(w - w_{\rm eq}), \tag{3}$$

- Let $X_k := L^2(\mathbb{R}^{2d}, (1+|v|^{2k})dx\,dv; \mathbb{R})$, $X_k^v := L^2(\mathbb{R}^d, (1+|v|^{2k})dv; \mathbb{R})$. Eq. (3) in abstract form reads

$$\epsilon\,\partial_t w = \epsilon\, Sw + \mathcal{A}w + \mathcal{C}w, \qquad \lim_{t\to 0^+}\|w(t) - w_0\|_{X_k} = 0 \tag{4}$$

with $Su := -v\cdot\nabla_x$, $\mathcal{A}w := \Theta[V]w$, $\mathcal{C}w := -(\nu\, w - \Omega\, w)$,

$$\Omega w(x,v) = \nu n[w](x)\left[F(v) + \hbar^2 F^{(2)}(x,v)\right].$$

Preliminary result ((4) with $\epsilon = 0$)

If $V \in W^{k,\infty}$ with $2k > d$, $\mathcal{A}+\mathcal{C} \in \mathcal{B}(X_k)$ (resp.ly, $\mathcal{B}(X_k^v)$).

$\forall x \in \mathbb{R}^d$ fixed, $\ker(\mathcal{A}+\mathcal{C}) := \{cM(v), c \in \mathbb{R}\} \subset X_k^v$ with

$$M(x,v) := \nu\mathcal{F}^{-1}\left\{\frac{\mathcal{F}_v F(\eta)}{\nu - i\delta V(x,\eta)}\left(1 - \frac{\beta\hbar^2}{24m^2}\sum_{r,s=1}^d \eta_r\eta_s\frac{\partial^2 V(x)}{\partial x_s x_s}\right)\right\}$$

For all $h \in X_k^v$, $(\mathcal{A}+\mathcal{C})u = h$ has a solution if and only if

$$\int h(v)\,dv \;=\; 0\,.$$

Compressed expansion [Mika&Banasiak 95]

$$X_k = \{\alpha(x)M(x,v), \alpha \in X_k^x\} \oplus \left\{f \in X_k \,\middle|\, \int f(v)dv = 0\right\}$$

Define the projections $\mathcal{P}f = M\int f(v)dv$ and $\mathcal{Q} = \mathcal{I} - \mathcal{P}$.

$$w \;=\; \mathcal{P}w + \mathcal{Q}w \;=:\; \varphi + \psi \;\equiv\; Mn[w] + \psi$$

By operating formally with $\mathcal{P}$ and $\mathcal{Q}$ on both sides of (4),

$$\begin{aligned}\partial_t\varphi &= \mathcal{PSP}\varphi + \mathcal{PSQ}\psi \qquad (5)\\ \partial_t\psi &= \mathcal{QSP}\varphi + \mathcal{QSQ}\psi + (1/\epsilon)\,\mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}\psi\end{aligned}$$

with initial conditions $\varphi(0) = \varphi_0 = \mathcal{P}f_0, \psi(0) = \psi_0 = \mathcal{Q}f_0$. Split φ and ψ into the sums of "bulk" and initial layer parts

$$\varphi(t) = \bar\varphi(t) + \tilde\varphi\,(t/\epsilon)\,, \quad \psi(t) = \bar\psi(t) + \tilde\psi\,(t/\epsilon)\,.$$

Let $\bar\varphi$ *unexpanded* and expand $\tilde\varphi, \bar\psi, \tilde\psi$ as

$$\bar\psi(t) = \bar\psi_0(t) + \epsilon\bar\psi_1(t) + \epsilon^2\bar\psi_2(t) + \ldots$$

Eqs. (5) for the bulk part terms up to the order ϵ^2 become

$$\begin{aligned}\partial_t\bar\varphi &= \mathcal{PSP}\bar\varphi + \mathcal{PSQ}\bar\psi_0 + \epsilon\mathcal{PSQ}\bar\psi_1 \qquad (6)\\ 0 &= \mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}\bar\psi_0\\ 0 &= \mathcal{QSP}\bar\varphi + \mathcal{Q}(\mathcal{A}+\mathcal{C})\mathcal{Q}\bar\psi_1 \qquad (7)\end{aligned}$$

Auxiliary problems

- To solve (7) with unknown $\bar\psi_1$, solve

$$\begin{aligned}(\mathcal{A}+\mathcal{C})D_1 &= -v\cdot\nabla_x M + M\int v\cdot\nabla_x M\,dv\,,\\ (\mathcal{A}+\mathcal{C})D_2 &= M\left(-v + \int vM\,dv\right)\end{aligned}$$

with unknowns $D_1, (D_2)_i \in \ker\mathcal{P}$. Hence (6) becomes

$$\frac{\partial n}{\partial t} = -\nabla_x\cdot\left[n\int vMdv + \epsilon\left(\int v\otimes D_2\,dv\cdot\nabla_x n + n\int vD_1\,dv\right)\right]$$

- The initial value comes from the analysis of the initial layer.
- The coefficients can be expressed in terms of the *moments of* M $\int vM(x,v)\,dv\,,\;\int v\otimes vM(x,v)\,dv$

Quantum drift-diffusion equation (high-field)

$$\frac{\partial n}{\partial t} = \frac{1}{\nu m}\nabla\cdot(n\nabla V) + \frac{\epsilon}{\nu\beta m}\nabla\cdot\nabla n + \frac{\epsilon}{\nu^3 m^2}\nabla\cdot\left[\nabla V\otimes\nabla V\nabla n + n2\,(\nabla\otimes\nabla)\,V\nabla V + n\Delta V\nabla V\right] + \frac{\epsilon\beta\hbar^2}{12\nu m^2}\nabla\cdot\left[(\nabla\otimes\nabla)\,V\nabla n + n\nabla\cdot(\nabla\otimes\nabla)\,V\right]$$

(cf.[Poupaud 92]). By (2) $\nabla\log n \;=\; -\beta\nabla V + O(\hbar^2)$, thus

$$\frac{\partial n}{\partial t} - \frac{1}{\nu m}\nabla\cdot(n\nabla V) - \frac{\epsilon}{\nu\beta m}\nabla\cdot\nabla n - \frac{\epsilon}{\nu^3\beta^2 m^2}\nabla\cdot\left(\frac{(\nabla\otimes\nabla n)\nabla n}{n}\right) + \frac{\epsilon\hbar^2}{12\nu m^2}\left(\nabla^4 n - \nabla\otimes\nabla\frac{\nabla n\otimes\nabla n}{n}\right) = 0\,.$$

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