Spectral scheme for the linearized Boltzmann BGK equation

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Contents

Linearized Boltzmann BGK equation

The equation

$$\begin{cases} \partial_t f + v\partial_x f - \partial_x \phi \partial_v f &= L(f) \quad \forall (t,x,v) \in \mathbb{R}^{+*} \times \mathbb{R} \times \mathbb{R} \\ f(0,.,.) &= f_0 \quad \in L^2(\mathcal{M}). \end{cases} \tag{1}$$

$$L(f) = -\left(f - \left(C_0 - C_1 v - C_2 \frac{v^2-1}{\sqrt{2}} \right) \right) \tag{2}$$

It is a linear evolution problem in the weighted space $L^2(\mathcal{M})$.

- $\phi =$ fixed, steady, confining potential;
- $\mu(v) =$ Gaussian density;
- $\rho(x) = e^{-\phi(x)}$;
- $\mathcal{M}(x,v) = \mu(v)\rho(x)$ (the Maxwellian);
- $C_0 = \int_{\mathbb{R}} f\mu(v)dv$, $C_1 = \int_{\mathbb{R}} vf\mu(v)dv$, $C_0 = \int_{\mathbb{R}} \frac{v^2-1}{\sqrt{2}} f\mu(v)dv$.

Assumptions and notations

- We assume that ϕ **is a polynomial**.
- We can assume w.l.o.g that $\int_{\mathbb{R}} \rho dx = 1; \int_{\mathbb{R}} x\rho dx = 0$.
- The space $L^2(\rho)$ is endowed with its canonical norm $\|.\|$ and scalar product $< ., . >$.
- The space $L^2(\mathcal{M})$ is endowed with its canonical norm $\|.\|_{L^2(\mathcal{M})}$ and scalar product $< ., . >_{L^2(\mathcal{M})}$.

Energy estimates

- The transport operator $\mathcal{T} := v\partial_x - \partial_x\phi\partial_v$ is skew-symetric in $L^2(\mathcal{M})$.
- An easy consequence is that $< \mathcal{T}f, f >_{L^2(\mathcal{M})} = 0$.
- Energy estimates : the $L^2(\mathcal{M})$-norm is nonincreasing in time.

$$\frac{1}{2}\frac{d}{dt}\|f\|^2_{L^2(\mathcal{M})} = - < \mathcal{T}f, f >_{L^2(\mathcal{M})} + < Lf, f >_{L^2(\mathcal{M})} \leq -\|f - \Pi_{Ker(L)}f\|^2_{L^2(\mathcal{M})}$$

Consequence

Steady states must belong to $Ker(L) = Span\{1, v, \frac{v^2-1}{\sqrt{2}}\}$.

Steady states

Steady states are then of the form $f(t,x,v) = a(t,x) + b(t,x)v + c(t,x)\frac{v^2-1}{\sqrt{2}}$. They form a finite dimensonal space $\mathcal{C}$ and are solutions of

$$\partial_t f + v\partial_x f - \partial_x \phi \partial_v f = 0 \tag{3}$$

For general potential ϕ :

- 1
- $E(x,v) = \frac{v^2-1}{2} + \phi(x) - <\phi>$

When $\phi(x) = \frac{1}{2}(x^2 + \ln(2\pi))$:

- $f_+(t,x,v) = x\cos(t) + v\sin(t)$
- $f_-(t,x,v) = v\cos(t) - x\sin(t)$
- $g_+(t,x,v) = xv\cos(2t) + \frac{1}{2}(x^2 - v^2)\sin(2t)$
- $g_-(t,x,v) = \frac{1}{2}(x^2 - v^2)\cos(2t) - xv\sin(2t)$

Steady states

Notation : $h = f - \Pi_{\mathcal{C}} f$.

- If $-L$ was λ-coercive ($Ker(L) = 0$), then

$$\frac{1}{2}\frac{d}{dt}\|h\|^2_{L^2(\mathcal{M})} =< Lh, h >_{L^2(\mathcal{M})} \leq -\lambda\|h\|^2_{L^2(\mathcal{M})}$$

  By Gronwall, $\|h\|_{L^2(\mathcal{M})} \leq e^{-\lambda t}\|h(t=0)\|_{L^2(\mathcal{M})}$

- Problem : is it possible to prove an estimation of the form

$$\forall t \geq 0, \quad \|h(t)\|_{L^2(\mathcal{M})} \leq Ce^{-\kappa t}\|h(t=0)\|_{L^2(\mathcal{M})}?$$

- Answer : yes, via hypocoercivity techniques.

Hypocoercivity and entropy method

- We describe here the entropy method.
- We find a hilbert norm $\|.\|_{eq}$ equivalent to the norm $\|.\|_{L^2(\mathcal{M})}$ in which $-\mathcal{T} - L$ is λ-coercive :

$$\|h(t)\|_{eq} \leq e^{-\lambda t}\|h(t=0)\|_{eq} \tag{4}$$

- We then conclude using the equivalence of norms :

$$\|h(t)\|_{L^2(\mathcal{M})} \leq \frac{M}{m} e^{-\lambda t}\|h(t=0)\|_{L^2(\mathcal{M})} \tag{5}$$

if $m\|h(t)\|_{L^2(\mathcal{M})} \leq \|h(t)\|_{eq} \leq M\|h(t)\|_{L^2(\mathcal{M})}$

Hypocoercivity for the linearized BGK equation

Theorem (Hypocoercivity for linearized BGK [1])

There exists two positive constants C, κ such that for any solution $f \in \mathcal{C}(\mathbb{R}^+, L^2(\mathcal{M}))$ of (1) with initial condition $f_0 \in L^2(\mathcal{M})$,

$$\forall t \geq 0, \quad \|h(t)\|_{L^2(\mathcal{M})} \leq Ce^{-\kappa t}\|h(t=0)\|_{L^2(\mathcal{M})}.$$

Our goal is to design a scheme that

- implementable in practice,
- preserves algebraic structures (invariants, symetric/skew-symetric parts)
- presents hypocoercivity.

Spectral scheme

Projection on Hermite polynomials in v

$h(t,x,.) \in L^2(\mu(v)dv) \implies h$ it can be decomposed in the Hermite polynomials basis $(\tilde{H}_k)_{k\in\mathbb{N}}$

$$h(t,x,v) = \sum_{k=0}^{\infty} C_k(t,x)\tilde{H}_k(v) \tag{6}$$

The kinetic equation is then projected on this basis to get the system

$$\partial_t C_k = \sqrt{k+1}\partial_x^* C_{k+1} - \sqrt{k}\partial_x C_{k-1} - \delta_{k\geq 3} C_k \quad (\mathbf{E_k}) \tag{7}$$

$\partial_x,\ \partial_x^* := \partial_x\phi - \partial_x$ are adjoint in $L^2(\rho)$.

Mass and energy conservation

Let us prove mass and energy conservation in this framework :

$$\frac{d}{dt} < C_0 >= 0; \quad \frac{d}{dt}\left(\frac{1}{\sqrt{2}} < C_2 > + < \phi C_0 >\right) = 0$$

Remember that

$$\partial_t C_0 = \partial_x^* C_1 \quad (\mathbf{E_0})$$

$(\mathbf{E_0}) \times \rho$ and integration :

$$\frac{d}{dt} < C_0 >=< \partial_x^* C_1, 1 >=< C_1, \partial_x 1 >= 0$$

Mass and energy conservation

$$\partial_t C_0 = \partial_x^* C_1 \quad (\mathbf{E_0})$$

$$\partial_t C_2 = \sqrt{3}\partial_x^* C_3 - \sqrt{2}\partial_x C_1 \quad (\mathbf{E_2})$$

$(\mathbf{E_2}) \times \rho$ and integration :

$$\begin{aligned} \frac{d}{dt} < C_2 > &= \sqrt{3} < \partial_x^* C_3, 1 > - \sqrt{2} < \partial_x C_1, 1 > \\ &= -\sqrt{2} < \partial_x C_1, 1 > \\ &= -\sqrt{2} < C_1 \partial_x \phi > \;\; (\partial_x^* 1 = \partial_x \phi) \end{aligned}$$

$(\mathbf{E_0}) \times \phi\rho$ and integration :

$$\frac{d}{dt} < C_0 \phi > = < \partial_x^* C_1, \phi > = < C_1, \partial_x \phi > = < C_1 \partial_x \phi >$$

Expansion in the x variable

Let $(\tilde{P}_n)_{n\in\mathbb{N}}$ be the sequence of orthonormal polynomials in $L^2(\rho)$.
Define $C_{k,n}(t) =< C_k, \tilde{P}_n >$, and notice that :

$$C_k(t,x) := \sum_{n=0}^{\infty} C_{k,n}(t)\tilde{P}_n(x); \quad h(t,x,v) := \sum_{k=0}^{\infty} C_k(t,x)\tilde{H}_k(v) \tag{8}$$

Projecting $(\mathbf{E_k})$ on $\tilde{P}_n$ gives :

$$\begin{aligned} \frac{d}{dt}C_{k,n}(t) &= \sqrt{k+1}\sum_{r=0}^{\infty} < \tilde{P}_r, \partial_x \tilde{P}_n > C_{k+1,r}(t) \\ &- \sqrt{k}\sum_{r=0}^{\infty} < \tilde{P}_n, \partial_x \tilde{P}_r > C_{k-1,r}(t) - \delta_{k\geq 3}C_{k,n}(t) \end{aligned} \tag{9}$$

The scheme

Now, choose $K, N \in \mathbb{N}$ ($\mathbf{N} \geq \mathbf{deg}(\boldsymbol{\phi})$). Define an approximation of C_k and h:

$$\tilde{C}_k(t,x) := \sum_{n=0}^{N} \tilde{C}_{k,n}(t)\tilde{P}_n(x); \quad \tilde{C}_{K+1} = \tilde{C}_{-1} = 0, \quad \tilde{h}(t,x,v) := \sum_{k=0}^{K} \tilde{C}_k(t,x)\tilde{H}_k(v) \tag{10}$$

$$\begin{aligned} \frac{d}{dt}\tilde{C}_{k,n}(t) &= \sqrt{k+1}\sum_{r=0}^{N} < \tilde{P}_r, \partial_x \tilde{P}_n > \tilde{C}_{k+1,r}(t) \\ &- \sqrt{k}\sum_{r=0}^{N} < \tilde{P}_n, \partial_x \tilde{P}_r > \tilde{C}_{k-1,r}(t) - \delta_{k\geq 3}\tilde{C}_{k,n}(t) \end{aligned} \tag{11}$$

We can write more compactly:

$$\partial_t \tilde{C}_k = \sqrt{k+1}\Pi_{\mathbb{P}_N}\partial_x^* \tilde{C}_{k+1} - \sqrt{k}\partial_x \tilde{C}_{k-1} - \delta_{k\geq 3}\tilde{C}_k(\tilde{\mathbf{E}}_{\mathbf{k}}) \tag{12}$$

Conserved quantities for the scheme

We can try to prove the mass and energy conservation on the scheme.

$$\frac{d}{dt} < \tilde{C}_0 >= 0; \quad \frac{d}{dt}\left(\frac{1}{\sqrt{2}} < \tilde{C}_2 > + < \phi \tilde{C}_0 >\right) = 0$$

Remember that

$$\partial_t \tilde{C}_0 = \Pi_{\mathbb{P}_N} \partial_x^* \tilde{C}_1 \quad (\tilde{\mathbf{E}}_\mathbf{0})$$

$(\tilde{\mathbf{E}}_\mathbf{0}) \times \rho$ and integration :

$$\frac{d}{dt} < \tilde{C}_0 >=< \Pi_{\mathbb{P}_N} \partial_x^* \tilde{C}_1, 1 >=< \tilde{C}_1, \partial_x \Pi_{\mathbb{P}_N} 1 >= 0$$

since $\Pi_{\mathbb{P}_N} 1 = 1 \in \mathbb{P}_N$.

Conserved quantities for the scheme

$$\partial_t \tilde{C}_0 = \Pi_{\mathbb{P}_N} \partial_x^* \tilde{C}_1 \quad (\tilde{\mathbf{E}}_\mathbf{0})$$

$$\partial_t \tilde{C}_2 = \sqrt{3}\Pi_{\mathbb{P}_N} \partial_x^* \tilde{C}_3 - \sqrt{2}\partial_x \tilde{C}_1 \quad (\tilde{\mathbf{E}}_\mathbf{2})$$

$(\tilde{\mathbf{E}}_\mathbf{2}) \times \rho$ and integration :

$$\begin{aligned} \frac{d}{dt} < \tilde{C}_2 > &= \sqrt{3} < \Pi_{\mathbb{P}_N} \partial_x^* C_3, 1 > - \sqrt{2} < \partial_x \tilde{C}_1, 1 > \\ &= -\sqrt{2} < \partial_x \tilde{C}_1, 1 > \\ &= -\sqrt{2} < \tilde{C}_1 \partial_x \phi > \ (1 \in \mathbb{P}_N) \end{aligned}$$

$(\tilde{\mathbf{E}}_\mathbf{0}) \times \phi\rho$ and integration :

$$\frac{d}{dt} < \tilde{C}_0 \phi > = < \Pi_{\mathbb{P}_N} \partial_x^* \tilde{C}_1, \phi > = < \tilde{C}_1 \partial_x \Pi_{\mathbb{P}_N} \phi > = < \tilde{C}_1, \partial_x \phi >$$

since $\Pi_{\mathbb{P}_N} \phi = \phi \in \mathbb{P}_N$.

Hypocoercivity of the scheme

Theorem (Hypocoercivity of the scheme [3])

Let $\tilde{h}$ *be the solution of the scheme (11). There are two constants* $\omega_N, \lambda_N > 0$ *s.t.* $t \geq 0$*,*

$$\|\tilde{h}(t)\|_{L^2(\mathcal{M})} \leq \omega_N e^{-\lambda_N t} \|\tilde{h}(t=0)\|_{L^2(\mathcal{M})}$$

- It also uses the entropy method.
- Proof very similar to the original one for the PDE.
- The major difference is the presence of $\Pi_{\mathbb{P}_N}$ in the scheme.

Time discretization

We use the implicit Euler scheme since it preserves exponential decay.
Notations : $\Delta t > 0$ the time step, $t_i := i\Delta t$ for all i and $\alpha_{r,n} :=< \partial_x \tilde{P}_r, \tilde{P}_n >$.

The approximation $\tilde{C}^i_{k,n}$ of $\tilde{C}_{k,n}(t^i)$ satisfy the linear system : $\forall n \leq N, k \leq K, \forall i \in \mathbb{N}$,

$$\left\{ \begin{array}{ccl} \tilde{C}^0_{k,n} & = & \tilde{C}_{k,n}(0) \\ \frac{\tilde{C}^{i+1}_{k,n} - \tilde{C}^i_{k,n}}{\Delta t} & = & \sqrt{k+1} \sum_{r=0}^{N} \alpha_{r,n} \tilde{C}^{i+1}_{k+1,n} - \sqrt{k} \sum_{r=0}^{N} \alpha_{n,r} \tilde{C}^{i+1}_{k-1,r} - \delta_{k \geq 3} \tilde{C}^{i+1}_{k,n} \end{array} \right. \tag{13}$$

with initial conditions

$$\tilde{C}_{k,n}(0) = \int_{\mathbb{R}\times\mathbb{R}} h(0,x,v) \tilde{P}_n(x) \tilde{H}_k(v) \mathcal{M}(x,v) dx dv$$

Closure : $\tilde{C}_{-1,n} = \tilde{C}_{K+1,n} = 0$ for all $n \leq N$.

Implementation

Orthonormal polynomials satisfy a fundamental 3-terms recurrence relation :

$$\begin{cases} x\tilde{P}_n(x) & = & a_n\tilde{P}_{n+1}(x) + a_{n-1}\tilde{P}_{n-1}(x) \ \forall n \geq 0, \\ \tilde{P}_0 & = & 1 \\ \tilde{P}_{-1} & = & 0 \end{cases} \tag{14}$$

- They are characterized only by the coefficients a_k, which are positive and functions of the weight ρ.
- The question of their computation arises.

The Chebychev algorithm

It is a moment based method.
If μ_k stands for the k-th moment of the measure $\rho(x)dx$, then for $n \in \mathbb{N}^*$ fixed, the algorithm requires the moments $(\mu_k)_{0 \leq k \leq 2n-1}$
It returns $((a_k)^2)_{0 \leq k \leq n-1}$

Main issues

- It is severly ill-conditionned [2];
- Moments can be hard to compute precisely;
- In the Hermite case $(\phi(x) = \frac{1}{2}(x^2 + \ln(2\pi))$,

$$\mu_{2k} = \frac{(2k)!}{2^k k!}.$$

Stirling's approximation states that $\mu_{2k} \sim \sqrt{2}\frac{k^k}{(2e)^k}$, hence they grow very fast.

Freud's equation

For conciseness, $\phi(x) = \gamma_4 x^4 + \gamma_2 x^2 + \gamma_0$ **in all the sequel.**
Using the 3-terms recurrence relation, we can express

$$\int_{\mathbb{R}} \tilde{P}_k \tilde{P}_{k+1} \partial_x \phi \rho dx = 2\gamma_2 a_k + 4\gamma_4 a_k (a_{k-1}^2 + a_k^2 + a_{k+1}^2) \ \forall k \geq 1 \tag{15}$$

Also, it is easy to see that the leading coefficient of $\tilde{P}_k$ is $\prod_{i=0}^{k-1} \frac{1}{a_i}$, hence

$$\begin{aligned} \int_{\mathbb{R}} \tilde{P}_k \tilde{P}_{k+1} \partial_x \phi \rho dx &= \int_{\mathbb{R}} (\tilde{P}_k' \tilde{P}_{k+1} + \tilde{P}_k \tilde{P}_{k+1}') \rho dx \\ &= (k+1) \prod_{i=0}^{k} \frac{1}{a_i} \int_{\mathbb{R}} \tilde{P}_k x^k \rho dx \\ &= \frac{k+1}{a_k} \int_{\mathbb{R}} \tilde{P}_k^2 \rho dx = \frac{k+1}{a_k} \ \forall k \in \mathbb{N} \end{aligned}$$

Freud's equation

Equaling the two expressions gives Freud's equation :

$$k + 1 = 2\gamma_2 a_k^2 + 4\gamma_4 a_k^2 (a_{k-1}^2 + a_k^2 + a_{k+1}^2) \ \forall k \geq 1 \tag{16}$$

Knowing a_0 and a_1, it permits to compute every coefficients. It is less costly than the Chebychev algorithm.

Main drawback

It is still ill-conditioned and diverges for large k.

Asymptotic expansion

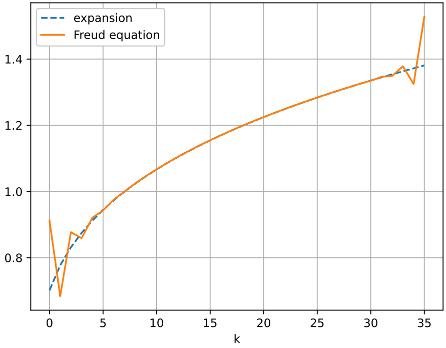
For large k, we can use the asymptotic exapnsion of a_k in powers of $k^{-\frac{1}{2m}}$. We know that there are explicit, real numbers $c^{(0)},^{(1)}, \ldots, c^{(4m)}$ such that

$$a_{k-1} = k^{\frac{1}{2m}} \sum_{l=0}^{4m} c^{(l)} k^{-\frac{l}{2m}} + O(k^{-2})$$

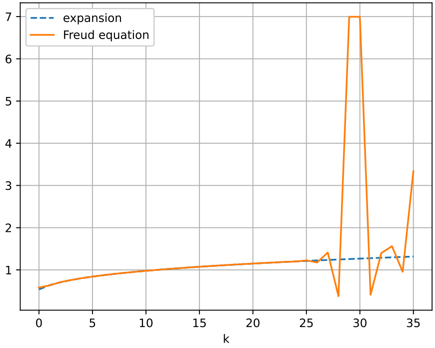
The coefficients can be computed explicitely by hand. It is asymptotically accurate, and does not diverges.

Main drawback

It may not be accurate for small k.



(a) $x^4 - 2x^2$



(b) x^4

Figure: Comparison of the sequeces given by the asymptotic expansion (dashed) and Freud's equation (solid) for different potentials ϕ.

Computation of the matrix

The computation of the numbers $\alpha_{r,n} = \int_{\mathbb{R}} \tilde{P}_r' \tilde{P}_n \rho dx$ is easy. Indeed,

$$\int_{\mathbb{R}} \tilde{P}_r' \tilde{P}_n \rho dx = -\int_{\mathbb{R}} \tilde{P}_r \tilde{P}_n' \rho dx + \int_{\mathbb{R}} \tilde{P}_r \tilde{P}_n \partial_x \phi \rho dx$$

- If $r \leq n$: $0 = -\int_{\mathbb{R}} \tilde{P}_r \tilde{P}_n' \rho dx + \int_{\mathbb{R}} \tilde{P}_r \tilde{P}_n \partial_x \phi \rho dx$
- If $r \geq n$: $\int_{\mathbb{R}} \tilde{P}_r' \tilde{P}_n \rho dx = \int_{\mathbb{R}} \tilde{P}_r \tilde{P}_n \partial_x \phi \rho dx$
- In any case, $\alpha_{r,n} = \int_{\mathbb{R}} \tilde{P}_r \tilde{P}_n \partial_x \phi \rho dx$.
- The vast majority of these integrals are zeros (if ϕ is of degree 4, then only $r = n \pm 1$ and $r = n \pm 3$ are nonzero).
- The matrix is thus very sparse. For $K = 20, N = 30$ and choosing a quartic potential, the sparsity index reaches 0.7%.

Experiments

Harmonic potential

$$h_0(x,v) = \tilde{H}_2(x)\tilde{H}_1(v) + \tilde{H}_1(x)\tilde{H}_2(v) + (\tilde{H}_0(x) + \tilde{H}_1(x))\tilde{H}_3(v);\ \phi(x) = \frac{1}{2}(x^2 + \ln(2\pi))$$

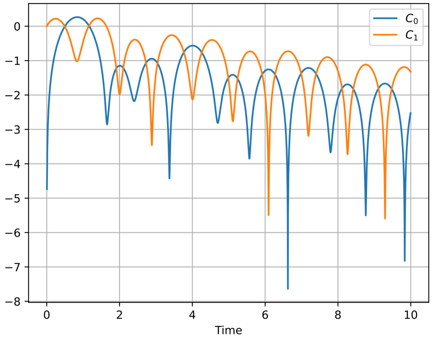
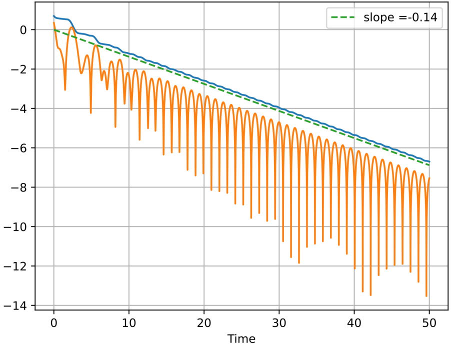
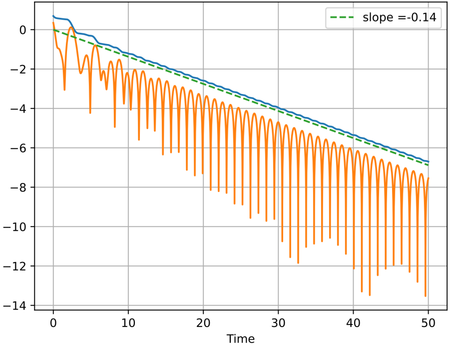


Figure: Evolution of the norms $\|\tilde{C}_0\|$ (blue) and $\|\tilde{C}_1\|$ (orange). The y-axis is in logscale.

Harmonic potential



(a) $N = 15, \quad K = 20.$



(b) $N = 30, \quad K = 20$

Figure: Exponential decay $\|\tilde{h}\|_{L^2(\mathcal{M})}$ (blue) and $\|(I - \Pi)\tilde{h}\|_{L^2(\mathcal{M})}$ (orange, jagged) for different parameters K and N (y-axis in logscale)

Double well potential

$h_0(x,v) = \tilde{P}_2(x)\tilde{H}_0(v) + \tilde{P}_0(x)\tilde{H}_1(v) - \sqrt{2} < \phi, \tilde{P}_2 > \tilde{P}_0(x)\tilde{H}_2(v) + \tilde{P}_1(x)\tilde{H}_3(v)$
$\phi(x) = (x-1)^2(x+1)^2$

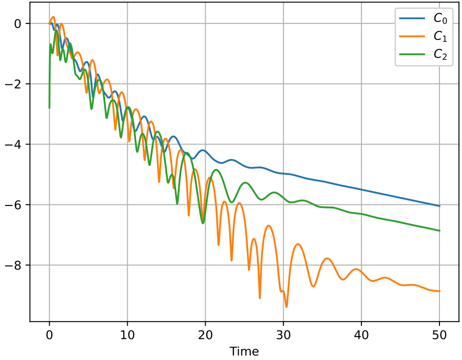
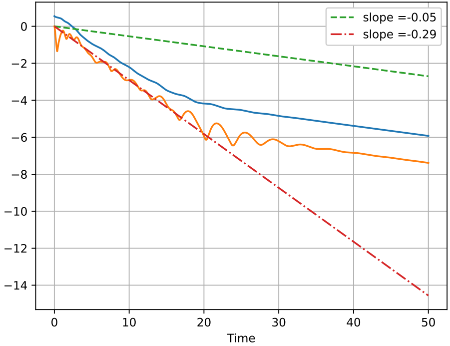
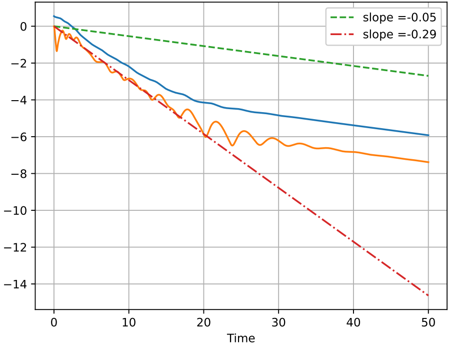


Figure: Evolution of the norms $\|\tilde{C}_0\|$ (blue), $\|\tilde{C}_1\|$ (orange), $\|\tilde{C}_2\|$ (green). The y-axis is in logscale.

Double well potential



(a) $N = 15, \quad K = 20.$



(b) $N = 30, \quad K = 20$

Figure: Exponential decay $\|\tilde{h}\|_{L^2(\mathcal{M})}$ (blue) and $\|(I - \Pi)\tilde{h}\|_{L^2(\mathcal{M})}$ (orange) for different parameters K and N (y-axis in logscale)

On the boundedness of the constants

$$\|\tilde{h}(t)\|_{L^2(\mathcal{M})} \leq \omega_N e^{-\lambda_N t} \|\tilde{h}(t=0)\|_{L^2(\mathcal{M})}$$

- Are the constants bounded w.r.t N ?
- It is sufficient to prove that $\|\partial_x \Pi_{\mathbb{P}_N}\|_{H^1(\rho)\to L^2(\rho)}$,$\|\partial_x \Pi_{\mathbb{P}_N}\|_{H^2(\rho)\to H^1(\rho)}$ are bounded w.r.t N.
- For ϕ of degree ≤ 4, it is easy to show.
- For ϕ of degree ≥ 6, we conjecture it is true.

Perspectives

- Apply this type of discretization on other kinetic equations;
- Study the approximation properties of the orthonormal polynomials;
- Investigate the 2-phases relaxation for the continuous model.

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