Quantum kinetic models of open quantum systems in semiconductor theory

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29 Aprile 2005

Outlook

1- Motivation

2- Quantum kinetic formulation

3- Analytical difficulties

4- Open quantum systems: two examples

5- The three well-posedness results

6- New tools and perspectives

7- Final considerations

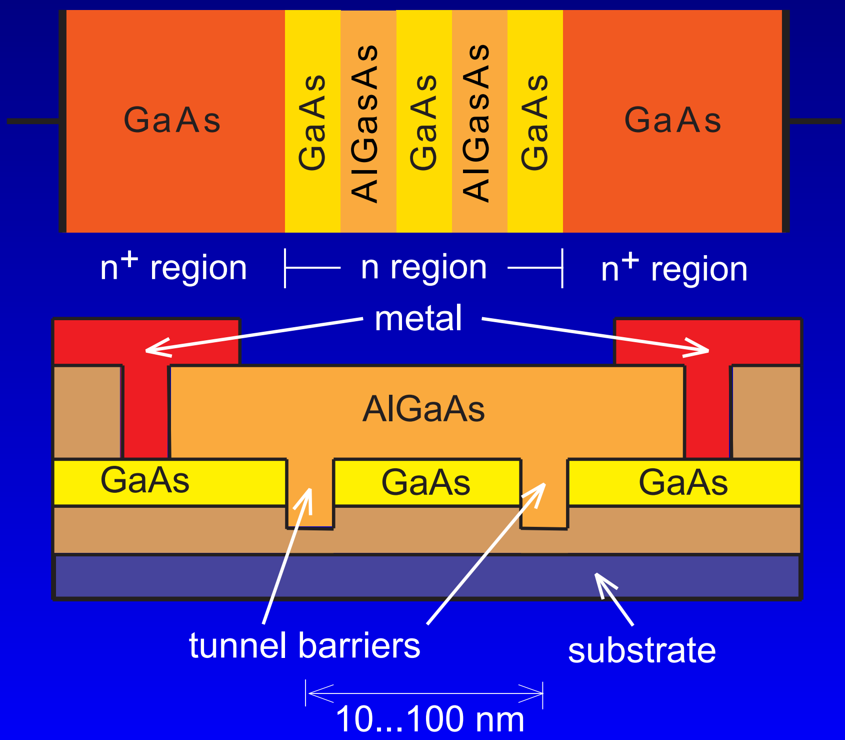
1- Motivation

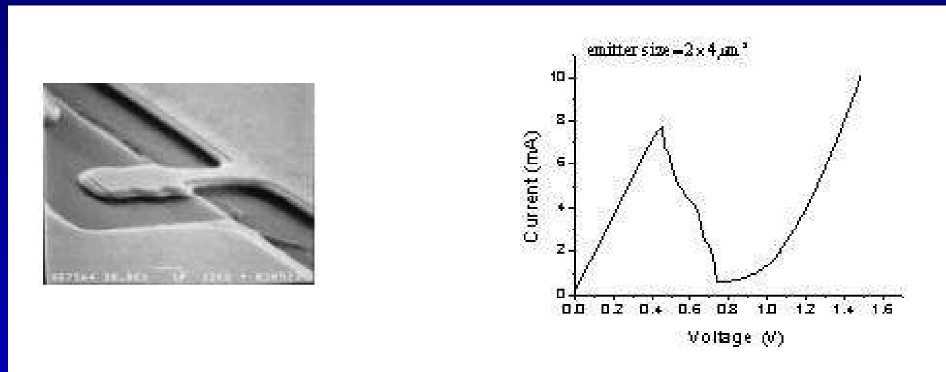
Trend in semiconductor technology: miniaturization

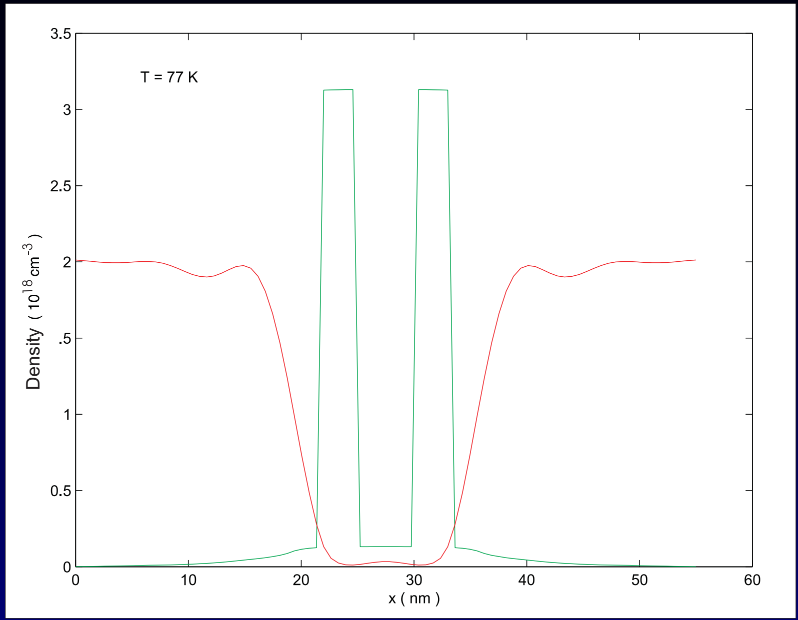
$\Longrightarrow$ Challenge: simulation tools

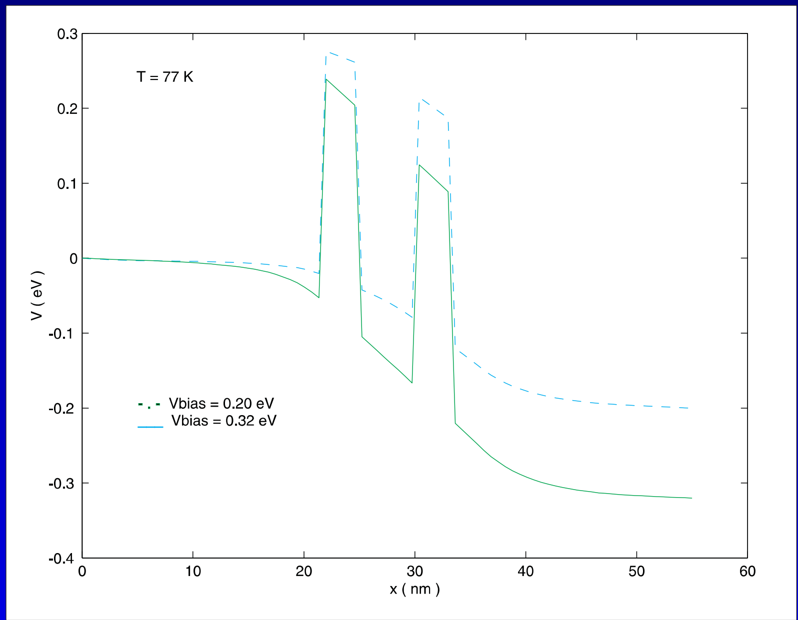
Features of novel devices $\Longrightarrow$ Quantum effects

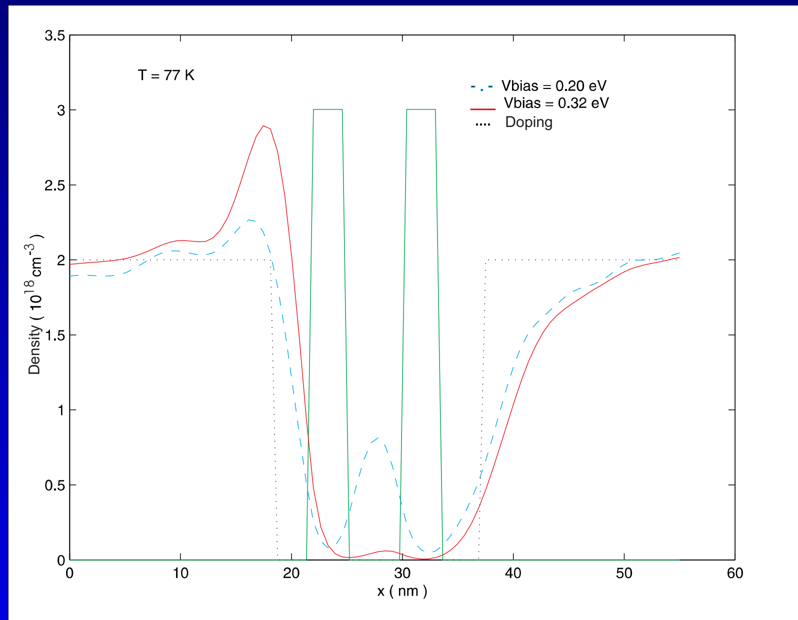
Prototype: Resonant Tunneling Diode






T = 77 K
Density (10^18 cm^-3)
x (nm)


T = 77 K
V (eV)
x (nm)
Vbias = 0.20 eV
Vbias = 0.32 eV


T = 77 K
Vbias = 0.20 eV
Vbias = 0.32 eV
Doping
Density (10^18 cm^-3)
x (nm)

Quantum description

QS Quantum System with d degrees of freedom:

- a pure state of QS $\leftrightarrow$ $\psi \in L^2(\mathbb{R}^d;\mathbb{C})$,
- a physical state of QS $\leftrightarrow$ $\hat\rho$ "density matrix" on $L^2(\mathbb{R}^d;\mathbb{C})$, i.e. $\rho(x,y) \in L^2(\mathbb{R}^{2d};\mathbb{C})$ kernel

$$\rho(x,y) = \sum_{j\in\mathbb{N}} \lambda_j \underbrace{\psi_j(x)\overline{\psi_j}(y)}_{\text{pure state}},$$

$\{\psi_j\}_j$ complete orthonormal set, $\lambda_j \geq 0$, $\sum_j \lambda_j = 1$.

The position density:

$$n(x) = \sum_j \lambda_j |\psi_j|^2(x) \in L^1(\mathbb{R}^d;\mathbb{R}^+) \Leftrightarrow \text{ finite mass.}$$

Quantum Evolution: reversible dynamics

$$\begin{cases} i\frac{d}{dt}\psi_j = -\frac{1}{2}\Delta_x\psi_j + V\psi_j,\ j\in\mathbb{N},\, x\in\mathbb{R}^d \\ -\Delta V(x,t) = n(x,t) = \sum_j \lambda_j|\psi_j|^2(x,t) \end{cases}$$

$$\rho(x,y,t) = \sum_{j\in\mathbb{N}} \lambda_j\psi_j(x,t)\overline{\psi_j}(y,t)\,,\ \{\psi_j(t)\}_j \subset L^2(\mathbb{R}^d;\mathbb{C})$$

E.g. evolution of an electron ensemble with d d.o.f., ballistic regime, mean-field approximation

Quantum Evolution: reversible dynamics

$$\begin{cases} i\frac{d}{dt}\psi_j = -\frac{1}{2}\Delta_x\psi_j + V\psi_j,\ j\in\mathbb{N},\ x\in\mathbb{R}^d \\ -\Delta V(x,t) = n(x,t) = \sum_j \lambda_j|\psi_j|^2(x,t) \end{cases}$$

$$w(x,v) = \mathcal{F}_{\eta\to v}\sum_{j\in\mathbb{N}}\lambda_j\psi_j(x+\frac{\eta}{2})\overline{\psi_j(x-\frac{\eta}{2})}$$

Quantum Liouville equation: Wigner-Poisson

$$\begin{cases} w_t + v\cdot\nabla_x w - \Theta[V]w = 0 \\ -\Delta_x V(x,t) = n[w](x,t) = \int w(x,v,t)\,dv \end{cases}$$

$$\mathcal{F}_{\eta\to v}\{\Theta[V]w\}(x,v) := i\,[V(x+\eta/2) - V(x-\eta/2)]\mathcal{F}_{v\to\eta}w(x,\eta)$$

2- Quantum Kinetic description

A physical state of QS $\longleftrightarrow$ a *quasiprobability* on the phase space, $w : (x,v) \in \mathbb{R}^{2d} \mapsto \mathbb{R} \quad \Longrightarrow$

$$w(x,v) := \mathcal{F}_{\eta \to v}\rho\left(x + \frac{\eta}{2}, x - \frac{\eta}{2}\right) \in L^2(\mathbb{R}^{2d};\mathbb{R})$$

w is the **Wigner** function for the physical state of QS

The position density

$$n[w](x,t) := \int w(x,v,t)\,dv$$

$w \in L^2(\mathbb{R}^{2d};\mathbb{R}) \not\Rightarrow n[w]$ well-defined, non-negative

3- Analytical difficulties

- $w \in L^2(\mathbb{R}^{2d};\mathbb{R})$ NOT $\Rightarrow$ $n[w]$ well-defined

$$w(x,v,t) \gtrless 0 \;\Rightarrow\; n[w](x,t) := \int w(x,v,t)\,dv \gtrless 0$$

Quantum counterpart :

$\{\psi_j(t)\}_j \subset L^2(\mathbb{R}^d;\mathbb{C}),\ \lambda_j \geq 0,\ \sum_j \lambda_j = 1$

$\Rightarrow n(t) = \sum_j \lambda_j |\psi_j|^2(t),\ \|n(t)\|_{L^1} < \infty\,,\ \forall\, t$

$$\Rightarrow \text{ (mass cons.)} \quad \|\psi_j(t)\|^2_{L^2} = \text{const.}$$

First a-priori estimate for Schr.-Poisson systems

3- Analytical difficulties

- $w \in L^2(\mathbb{R}^{2d};\mathbb{R})$ NOT $\Rightarrow$ $n[w]$ well-defined
- $e_{\text{kin}}(x,t) := \frac{1}{2}\int |v|^2 w(x,v,t)\,dv$:

$$w(x,v,t) \gtrless 0 \;\Rightarrow\; e_{\text{kin}}(x,t) \gtrless 0$$

Quantum cp. : $E_{\text{kin}}(t) := \frac{1}{2}\sum_j \lambda_j \|\nabla\psi_j(t)\|_{L^2}$

$$\frac{1}{2}\sum_j \lambda_j \|\nabla\psi_j(t)\|^2_{L^2} + \underbrace{\frac{1}{2}\|\nabla V(t)\|^2_{L^2}}_{E^2_{\text{pot}}(t)} = \text{const.}$$

(energy cons.) $\Rightarrow$ $\|\nabla\psi_j(t)\|^2_{L^2} =$ const.

$\Longrightarrow$ can NOT apply physical cons. laws

Advantages

- $w \in L^2(\mathbb{R}^{2d};\mathbb{R})$ is *necessary* for a physical state of QS
- L^2-setting is suitable for numerical approximation (cf.[Arnold. . . 96])
- pseudo-differential operator

$$\|\Theta[V]w\|_{L^2_{x,v}} = \|\,[V(x+\eta/2)-V(x-\eta/2)]\mathcal{F}_{v\to\eta}w\|_{L^2_{x,\eta}}$$

$$<\Theta[V]w, w>_{L^2_v} = 0 \quad \text{(skew-simmetry)}$$

$$w_t + v\cdot\nabla_x w - \Theta[V]w = 0$$

$$\Longrightarrow \|w(t)\|_{L^2_{x,v}} = \text{const.}$$

4- Open QS: irreversible dynamics

Motivation for quantum kinetic approach

Two examples:

• electron ensemble with d d.o.f. in RTD

[Frensley90]: Time-dependent boundary conditions (b.c.) for w model ideal reservoir

$\Rightarrow$ Boundary-value problem for Wigner-Poisson:

• inflow time-dependent b.c. for w
• mixed Dirichlet-Neumann b.c. for V

Remark: Reformulation with $\{\psi_j\}_j$ impossible:

λ_j NOT const.

4- Open QS: irreversible dynamics

Motivation for quantum kinetic approach

Two examples:

- electron ensemble with d d.o.f. in RTD
- electron ensemble with d d.o.f. in GaAs: electron-phonon interaction

Semiclassical cp. : Boltzmann for semiconductors

Density-matrix form. : NOT suitable for boundary-value problems

Open QS: irreversible dynamics

$$w_t + v \cdot \nabla_x w - \Theta[V]w = Qw$$

- $Qw = \frac{1}{\tau}(w - \mathcal{M}_\rho) \Rightarrow$ [Degond,. . .03] QDD,QET

Open QS: irreversible dynamics

$$w_t + v \cdot \nabla_x w - \Theta[V]w = Qw$$

- $Qw = \frac{1}{\tau}(w - \mathcal{M}_\rho)$ $\Rightarrow$ [Degond,. . .03] QDD,QET
- Boltzmann-like collision operator [Demeio,. . .04] $\Rightarrow$ simulation

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- Boltzmann-like collision operator [Demeio,. . .04] $\Rightarrow$ simulation
- scattering term for electron-phonon interaction [Fromlet,. . .99]

Open QS: irreversible dynamics

$$w_t + v \cdot \nabla_x w - \Theta[V]w = Qw$$

- $Qw = \frac{1}{\tau}(w - \mathcal{M}_\rho) \Rightarrow$ [Degond,. . .03] QDD,QET
- Boltzmann-like collision operator [Demeio,. . .04] $\Rightarrow$ simulation
- scattering term for electron-phonon interaction [Fromlet,. . .99]
- quantum Fokker-Planck term [Castella,. . .00] $\Rightarrow$ [Jüngel,. . .05] QHD

  Classical cp. :Vlasov-Fokker-Planck

Quantum Fokker-Planck term

$$Qw = \beta \mathrm{div}_v(vw) + \sigma \Delta_v w + 2\gamma \mathrm{div}_v(\nabla_x w) + \alpha \Delta_x w \qquad \text{(QFP)}$$

with $\alpha, \beta, \gamma \geq 0,\ \sigma > 0$.

[Caldeira. . .83]: QS={electrons+reservoir}

$\beta \sim \xi$ coupling, $\sigma \sim T$ temp., $\gamma, \alpha \sim \frac{1}{T}$, $\epsilon \sim \frac{\xi}{T}$

Lindblad condition: $\alpha\,\sigma \geq \gamma^2 + \beta^2/16$

Model	Term	Accuracy	Lindblad
Classical	$\beta\, \mathrm{div}_v(vw) + \sigma\Delta_v w$	$\mathcal{O}(\epsilon^2)$	NOT ok
Frictionless	$\sigma\Delta_v w$	$\mathcal{O}(\epsilon)$	ok
Quantum	(QFP)	$\mathcal{O}(\epsilon^3)$	ok

5- Three well-posedness results

- WP system with inflow, time-dependent b.c. :
  - $d = 1$, global-in-time well-p. [M,Barletti04]
  - $d = 3$, local-in-time well-p. [M05]

- WPFP system, $d = 3$ [Arnold,Dhamo,M05]:
  - global-in-time well-p., NEW a-priori estimates

    $\Rightarrow$ NEW strategy for well-p. of WP(FP)

Common feature: L^2-setting, ONLY kinetic tools

WP system with inflow b.c. $d = 1, 3$

$$\begin{cases} \{\partial_t + v \cdot \nabla_x - \Theta[V(t) + V_e(t)]\}\, w(t) = 0,\ t \geq 0, \\ \underline{-\Delta_x V(x,t) = n[w](x,t) = \int w(x,v,t)\, dv} \end{cases}$$

$(x, v) \in \Omega \times \mathbb{R}^d,\ \Omega \subset \mathbb{R}^d$ open, bounded, convex,
$V_e \equiv V_e(x,t),\ (x,t) \in \mathbb{R}^d \times \mathbb{R}^+$

$$\begin{cases} w(s,v,t) = \gamma(s,v,t),\ (s,v) \in \Phi_{\text{in}}, t \geq 0, \\ \underline{V(x,t) = 0,\ x \in \partial\Omega, t \geq 0}, \\ w(x,v,0) = w_0(x,v) \end{cases}$$

$$\Phi_{\text{in}} := \left\{(s,v) \in \partial\Omega \times \mathbb{R}^d \middle|\, v \cdot n(s) > 0\right\}$$

Easy: non homogeneous Dirichlet/Neumann b.c.

- Weighted space:

$$X_k := L^2(\Omega \times \mathbb{R}^d; (1 + |v|^{2k})dxdv), \; d = 1,3 \Rightarrow k = 1,2$$

cf. [Markowich,…89,Arnold,…96]

Prop. : $\quad d = 3, \; w \in X_2 \Rightarrow \|n[w]\|_{L^2} \leq C\|w\|_{X_2}$

- Weighted space:

$X_k := L^2(\Omega \times \mathbb{R}^d; (1+|v|^{2k})dxdv), \; d=1,3 \Rightarrow k=1,2$

cf. [Markowich,...89,Arnold,...96]

Prop. : $\quad d=3, \; w \in X_2 \Rightarrow \|n[w]\|_{L^2} \leq C\|w\|_{X_2}$

$\Longrightarrow V$ solution of Poisson pb. with $n[w] \in L^2(\Omega)$:

$V \in W_0^{1,2}(\Omega) \cap W^{2,2}(\Omega), \; \|V\|_{W^{2,2}} \leq C\|n[w]\|_{L^2}$

Define $P : X_2 \longrightarrow W^{2,2}(\mathbb{R}^3)$

$P : w \in X_2 \longmapsto V \longmapsto Pw \equiv V$ a.e. Ω, $Pw = 0$ outside Σ

with Σ open, $\overline{\Omega} \subset \Sigma$ and $\boxed{\|Pw\|_{W^{2,2}(\mathbb{R}^3)} \leq C\|w\|_{X_2}}$

WP system with inflow b.c. in X_2

$$\begin{cases} w_t + v \cdot \nabla_x w - \boxed{\Theta[Pw]w} = 0, \ t \geq 0, \\ w(s,v,t) = \gamma(s,v,t), \ (s,v) \in \Phi_{\text{in}}, t \geq 0, \\ w(x,v,0) = w_0(x,v) \in X_2 \end{cases}$$

- for all $u \in X_2$, $\|\Theta[U]u\|_{X_2}$: contains $\|v_i^2 \Theta[U]u\|_{L^2}$

$$\mathcal{F}_{\eta \to v}\{v_i^2 \Theta[U]u\} = \partial_{\eta_i}^2 \{ \ [U(x+\eta/2) - U(x-\eta/2)]\mathcal{F}_{v \to \eta} u\}$$

contains ∂_{η_i}, $\partial_{x_i}^2 U$ and v_i, $v_i^2 u$

WP system with inflow b.c. in X_2

$$\begin{cases} w_t + v\cdot\nabla_x w - \boxed{\Theta[Pw]w} = 0,\ t\geq 0, \\ w(s,v,t) = \gamma(s,v,t),\ (s,v)\in\Phi_{\text{in}}, t\geq 0, \\ w(x,v,0) = w_0(x,v) \in X_2 \end{cases}$$

- for all $u\in X_2$, $\|\Theta[U]u\|_{X_2}$: contains $\|v_i^2\Theta[U]u\|_{L^2}$

$$\mathcal{F}_{\eta\to v}\{v_i^2\Theta[U]u\} = \partial_{\eta_i}^2\,\{\ [U(x+\eta/2) - U(x-\eta/2)]\mathcal{F}_{v\to\eta}u\}$$

$$\textbf{Prop.}:\quad \|\Theta[U]u\|_{X_2} \leq C\|U\|_{W^{2,2}(\mathbb{R}^3)}\|u\|_{X_2}$$

$$\Rightarrow \|\Theta[Pw]w\|_{X_2} \leq C\|Pw\|_{W^{2,2}(\mathbb{R}^3)}\|w\|_{X_2} \leq C\|w\|_{X_2}^2$$

WP system with inflow b.c. in X_2

$$\begin{cases} \{\partial_t - T_{\gamma(t)} - \Theta[Pw](t)\}\, w(t) = 0, \; t \geq 0, \\ w(x, v, 0) = w_0(x, v) \in X_2 \end{cases}$$

$$w(t) \in \mathcal{D}(T_{\gamma(t)}) := \{u \in X_2 \,|\, v \cdot \nabla_x u \in X_2, u|_{\Phi_{\text{in}}} = \gamma(t)\}$$

Remark $\forall u_1, u_2 \in \mathcal{D}(T_{\gamma(t)}) \Rightarrow u_1 - u_2 \in \mathcal{D}(T_0)$

$$\forall\, p : [0, +\infty) \to X_2, \text{ s.t. } p(t) \in \mathcal{D}(T_{\gamma(t)}), \forall t \geq 0$$

$$\Rightarrow \; \mathcal{D}(T_{\gamma(t)}) = p(t) + \mathcal{D}(T_0)$$

(cf.[Barletti00])

WP system with inflow b.c. in X_2

$$\begin{cases} \{\partial_t - T_{\gamma(t)} - \Theta[Pw](t)\}\, w(t) = 0, \ t \geq 0, \\ w(x,v,0) = w_0(x,v) \in X_2 \end{cases}$$

$\forall\, w : [0,+\infty) \to X_2$, s.t. $w(t) \in \mathcal{D}(T_{\gamma(t)})$, $\forall t \geq 0$

$w(t) = p(t) + u(t)$, with $u : [0,+\infty) \to \mathcal{D}(T_0)$

$$\begin{cases} \{\partial_t - T_0 - L_p(t) - \Theta[Pu](t)\}\, u(t) = Q_p(t) \\ u(x,v,0) = w_0(x,v) - p(x,v,0) \ \in \mathcal{D}(T_0) \end{cases}$$

$$L_p(t)u(t) := \Theta[Pp](t)u(t) + \Theta[Pu](t)p(t)$$

$$Q_p(t) := -\{\partial_t - T_{\gamma(t)} - \Theta[Pp](t)\}\, p(t)$$

Choose p s.t. $Q_p \in \mathcal{C}[0,+\infty), Q_p' \in L^1(0,T], \forall T$ (1)

WP system with inflow b.c. in X_2: local-in-t solution

$$\begin{cases} \{\partial_t - T_{\gamma(t)} - \Theta[Pw](t)\}\, w(t) = 0, \ t \geq 0, \\ w(x,v,0) = w_0(x,v) \in X_2 \end{cases}$$

Theorem

$\boxed{\forall\, \gamma \text{ s.t. } \exists\, p \text{ as in } (1)}$, $\forall\, w_0 \in \mathcal{D}(T_{\gamma(0)})$, $\exists t_{\max} \leq \infty$ s.t.
$\exists!$ classical solution $w(t), \forall\, t \in [0, t_{\max})$.
If $t_{\max} < \infty$, then $\lim_{t \nearrow t_{\max}} \|w(t)\|_{X_2} = \infty$.

- Ex. :

$\gamma \in \mathcal{C}^1([0,\infty); L^2(\partial\Omega \times \mathbb{R}^d; (v \cdot n(s))(1 + |v|^4) ds dv))$

- A priori estimates are needed for global-in-t result

WPFP system, $d = 3$

$$\begin{cases} \{\partial_t + v \cdot \nabla_x - \Theta[V(t)]\}\, w(t) = Qw(t) \\ -\Delta_x V(x,t) = n[w](x,t) \\ w(x,v,t=0) = w_0(x,v) \end{cases}$$

$w \equiv w(x,v,t),\ (x,v,t) \in \mathbb{R}^{2d} \times [0,\infty)$

$Qw = \beta \mathrm{div}_v(vw) + \sigma \Delta_v w + 2\gamma \mathrm{div}(\nabla_x w) + \alpha \Delta_x w$

Assume $\alpha\, \sigma > \gamma^2 \ \Rightarrow\ Q$ uniformly elliptic in x and v.

- Classical cp. : Vlasov-PFP with
  - non-linear term: $\nabla_x V \cdot \nabla_v w$,
  - FP term: $\beta\, \mathrm{div}_v(vw) + \sigma \Delta_v w$.
- Frictionless FP term: $\sigma \Delta_v w$ hypoelliptic case.

Existing results

- "density matrix" $\hat{\rho}$: [Arnold,. . .03]
  global-in-t solution, by conservation laws.

- Quantum Kinetic: L^1-analysis [Cañizo,. . .04]
  global-in-t solution, by $\hat{\rho}(t) \geq 0$, cons. laws:

$$w(t) \in L^1(\mathbb{R}^{2d};\mathbb{R}) \;\Rightarrow\; n[w](t) \in L^1(\mathbb{R}^d)$$

$$\text{(mass cons.)} \Rightarrow \|n[w](t)\|_{L^1} = \text{const.}$$

$$e_{\text{kin}}[w](x,t) > -\infty \Rightarrow e_{\text{kin}}[w](x,t) < \infty$$

INSTEAD keep to L^2-setting, purely kinetic analysis

- Weighted space: $X_2 := L^2(\mathbb{R}^6; (1+|v|^4)dxdv)$

Prop. : $w \in X_2 \Rightarrow \|n[w]\|_{L^2} \le C\|w\|_{X_2}$

$$\Longrightarrow V(x) := \frac{1}{4\pi|x|} * n[w](x), \quad x \in \mathbb{R}^3 :$$

- $V \notin L^p,\ \forall p,\ \nabla V = -\frac{x}{4\pi|x|^3} * n[w] \in L^6.$

$$\mathcal{F}_v\Theta[V]z(x,\eta) = i\underbrace{\left(V\left(x+\eta/2\right) - V\left(x-\eta/2\right)\right)}_{=:\delta V(x,\eta)}\mathcal{F}_v z(x,\eta)$$

For η fixed, $\|\delta V(.\,,\eta)\|_{L^\infty} \le C|\eta|^{\frac{1}{2}}\|n[w]\|_{L^2}$

- $\|\Theta[V]z\|_{L^2} \le C\|n[w]\|_{L^2}\||\eta|^{\frac{1}{2}}\mathcal{F}_v z\|_{L^2}$

- Weighted space: $X_2 := L^2(\mathbb{R}^6; (1+|v|^4)dxdv)$
  - $V \notin L^p,\ \forall p,\ \nabla V = -\dfrac{x}{4\pi|x|^3} * n[w] \in L^6.$
    - $\|\Theta[V]z\|_{L^2} \le C\|n[w]\|_{L^2}\||\eta|^{\frac{1}{2}}\mathcal{F}_v z\|_{L^2}$

Prop. : $w, z, \nabla_v z \in X_2 \Rightarrow$

$$\|\Theta[V]z\|_{X_2} \le C\{\|z\|_{X_2} + \|\nabla_v z\|_{X_2}\}\|w\|_{X_2}$$

$\Rightarrow$ parabolic reguralization is needed

The linear equation

$$w_t = \overline{A} w(t),\ t > 0,\ \ Aw := -v \cdot \nabla_x w + Qw$$
$$w(t=0) = w_0 \in X_2\,,$$

- $\{e^{t\overline{A}}, t \geq 0\}$ C_0–semigroup on X_2 (cf. [Arnold,. . .02])

$$\Rightarrow \quad \|w(t)\|_{L^2} \leq e^{\frac{3}{2}\beta t} \|w_0\|_{L^2}, \quad t \geq 0$$

- $w(x,v,t) = G(x,v,t) * w_0$ (cf. [Sparber,. . .03]) $\Rightarrow$

$$\|\nabla_v w(t)\|_{X_2} \leq B\, t^{-1/2}\, e^{\kappa t} \|w_0\|_{X_2}, \quad 0 < t \leq T_0$$

(cf. classical cp. VPFP [Carpio98])

The non-linear equation

$\forall\, T \in (0,\infty)$ fixed

$$w_t = \overline{A}w(t) + (\Theta[V]w)(t), \quad t \in [0,T],\ w(t=0) = w_0,$$

$$Y_T := \{z \in \mathcal{C}([0,T];X_2) \mid \nabla_v z \in \mathcal{C}((0,T];X_2),$$
$$t^{1/2}\|\nabla_v z(t)\|_{X_2} \leq C_T\ \forall t \in (0,T)\}.$$

$\forall\, T < T_0$, the map $w \in Y_T \longmapsto \widetilde{w}$ s. t.

$$\widetilde{w}(t) = \mathrm{e}^{t\overline{A}}w_0 + \int_0^t \mathrm{e}^{(t-s)\overline{A}}(\Theta[\widetilde{V}]w)(s)\,ds,\ t \in [0,T]$$

is a strict contraction on some ball of Y_τ with $\tau(\|w_0\|_{X_2})$.

The non-linear equation

$\forall\, T \in (0,\infty)$ fixed

$$w_t = \overline{A}w(t) + (\Theta[V]w)(t), \quad t \in [0,T],\ w(t=0) = w_0,$$

$$Y_T := \{z \in \mathcal{C}([0,T];X_2) \mid \nabla_v z \in \mathcal{C}((0,T];X_2),$$
$$t^{1/2}\|\nabla_v z(t)\|_{X_2} \le C_T\ \forall t \in (0,T)\}.$$

Existence and Uniqueness Theorem

$\forall\, w_0 \in X_2, \exists\, t_{\max} \le \infty$ s.t. $\exists\,!$ *mild* solution $w \in Y_T,\ \forall\, T < t_{\max}$. If $t_{\max} < \infty$, then

$\lim_{t \nearrow t_{\max}} \|w(t)\|_{X_2} = \infty.$

Global-in-t well-posedness

A priori estimates

- $\|w(t)\|_2 \leq e^{\frac{3}{2}\beta t}\|w_0\|_2,\ t \geq 0,$
- for $\||v|^2 w(t)\|_2 < \infty \quad 0 \leq t \leq T,$

  some L^p-bounds for $\nabla_x V(t)$ are needed

$\Rightarrow$**Idea**: get bounds for $\nabla_x V(t)$ depending on $\|w(t)\|_2$

Strategy: exploit dispersive effects of the free-str. (cf. [Perthame96]) $\Longrightarrow$

estimate(define) $\nabla_x V$ via integral equation

$\Rightarrow$ definition of $n[w]$ is by-passed

Anticipation: global-in-t well-posedness WITHOUT WEIGHTS

A priori estimate for electric field: WP case

$$E(x,t) = -\nabla V(x,t) = -\frac{1}{4\pi}\frac{x}{|x|^3} * n(x,t)$$

$$\int_{\mathbb{R}_v^3} w(x,v,t)\,dv = \int_{\mathbb{R}_v^3} w_0(x-vt,v)\,dv + \int_{\mathbb{R}_v^3}\int_0^t (\Theta[V]w)(x-vs,v,t-s)\,ds\,dv$$

Correspondingly E into

$$E_0(x,t) = -\frac{1}{4\pi}\frac{x}{|x|^3} *_x \int_{\mathbb{R}_v^3} w_0(x-vt,v)\,dv$$

$$E_1(x,t) = -\frac{1}{4\pi}\frac{x}{|x|^3} *_x \int_{\mathbb{R}_v^3}\int_0^t (\Theta[V]w)(x-vs,v,t-s)\,ds$$

A priori estimate for electric field: WP, E_1

$$n_1(x,t) = \int \int_0^t (\Theta[V]w)(x - vs, v, t-s)\, ds\, dv$$

Classical cp. : Vlasov-Poisson [Perthame96]

$$n_1(x,t) = \int_{\mathbb{R}^3_v} \int_0^t \boxed{E \cdot \nabla_v w}(x - vs, v, t-s)\, ds\, dv$$

$$= \mathrm{div}_x \int_{\mathbb{R}^3_v} \int_0^t s(E\, w)(x - vs, v, t-s)\, ds\, dv$$

- $\Theta[V]w = \mathcal{F}_\eta^{-1}(\delta V \widehat{w}) = \mathcal{F}_\eta^{-1}\left(\boxed{W[E] \cdot \widehat{\nabla_v w}}\right)$

since $\quad \delta V(x,\eta) = V(x + \frac{\eta}{2}) - V(x - \frac{\eta}{2})$

$$= \eta \cdot \int_{-\frac{1}{2}}^{\frac{1}{2}} E(x - r\eta) dr =: \boxed{W[E](x,\eta) \cdot \eta}$$

A priori estimate for electric field: WP, E_1

$$n_1(x,t) = \int\int_0^t (\Theta[V]w)(x - vs, v, t-s)\, ds\, dv$$

- $\Theta[V]w = \mathcal{F}_\eta^{-1}(\delta V \widehat{w}) = \mathcal{F}_\eta^{-1}\left(\boxed{W[E]\cdot \widehat{\nabla_v w}}\right)$

since $\quad \delta V(x,\eta) = V(x + \frac{\eta}{2}) - V(x - \frac{\eta}{2})$

$$= \eta \cdot \int_{-\frac{1}{2}}^{\frac{1}{2}} E(x - r\eta) dr =: \boxed{W[E](x,\eta)\cdot \eta}$$

$$n_1(x,t) \;=\; \int_{\mathbb{R}_v^3}\int_0^t \mathcal{F}_\eta^{-1}\left(\boxed{W[E]\cdot \widehat{\nabla_v w}}\right)(x - vs, v, t-s)\, ds$$

$$= \mathrm{div}_x \int_{\mathbb{R}_v^3}\int_0^t s\, \mathcal{F}_\eta^{-1}(W[E]\widehat{w})(x - vs, v, t-s) ds$$

A priori estimate for electric field: WP, E_1

$$E_1(x,t) = -\frac{1}{4\pi}\frac{x}{|x|^3} * n_1(x,t) =$$

$$-\text{div}_x\left(\frac{1}{4\pi}\frac{x}{|x|^3}\right) * \int_0^t s \int \mathcal{F}_\eta^{-1}(W[E]\widehat{w})(x - vs, v, t-s)\,dv\,ds$$

Lemma : $\left\| \int \mathcal{F}_\eta^{-1}(W[E]\widehat{w})(x-vs, v, t-s)\,dv \right\|_{L^2_x}$

$$\leq s^{-3/2} \, \|E(t-s)\|_{L^2_x} \, \|w(t-s)\|_{L^2_{x,v}}$$

Quantum case: just in L^2.

Classical case: L^p-version.

A priori estimate for electric field: WP, E_1

$$E_1(x,t) = -\frac{1}{4\pi}\frac{x}{|x|^3} * n_1(x,t) =$$

$$-\mathrm{div}_x\left(\frac{1}{4\pi}\frac{x}{|x|^3}\right) * \int_0^t s \int \mathcal{F}_\eta^{-1}(W[E]\widehat{w})(x - vs, v, t-s)\,dv\,ds$$

Lemma : $\left\| \int \mathcal{F}_\eta^{-1}(W[E]\widehat{w})(x-vs, v, t-s)\,dv \right\|_{L^2_x}$

$$\leq s^{-3/2}\left(\|E_0(t-s)\|_{L^2} + \|E_1(t-s)\|_{L^2}\right)\|w(t-s)\|_{L^2}$$

Prop. : $\boxed{\|E_0(t)\|_{L^2} \leq C_T\, t^{-\omega}}$ with $\omega \in [0,1)$

$$\Rightarrow \|E_1(t)\|_{L^2} \leq C\left(T, \sup_{s\in[0,T]}\|w(s)\|_{L^2}\right) t^{1/2-\omega}.$$

NEW : $\boxed{w \in \mathcal{C}([0,T]; L^2_{x,v}) \mapsto E_1[w] \in L^1_t((0,T]; L^2_x)}$

A priori estimate for electric field: WP, E_0

$$E_0(x,t) = -\frac{1}{4\pi}\frac{x}{|x|^3} *_x \int w_0(x - vt, v)\, dv$$

Ex. Strichartz for free-str. [Castella-Perthame '96],

$$\left\| \int w_0(x - vt, v) dv \right\|_{L_x^{6/5}} \leq t^{-\frac{1}{2}} \|w_0\|_{L_x^1(L_v^{6/5})}, \quad t > 0.$$

Let $\forall\, t \in (0, T]$

$$\left\| \int w_0(x - vt, v) dv \right\|_{L_x^{6/5}} \leq C_T t^{-\omega}, \; \omega \in [0,1)$$

(HP1)

$$\Rightarrow \|E_0(t)\|_2 \leq C \left\| \int w_0(x - vt, v) dv \right\|_{L_x^{6/5}} \leq C C_T t^{-\omega}$$

WPFP: global-in-t, smooth solution

$$w(x,v,t) = G(t,x,v)*w_0 + \int_0^t G(s,x,v)*(\Theta[V]w)(t-s)\,ds$$

$E_1 \in L_t^1((0,T];L_x^{[2,6]})$ by parabolic reguralization.

Classical cp. : VPFP [Castella98]

Remark: $E(t) \in L^3$ is needed for bootstraping
$\|vw(t)\|_2,\ \||v|^2w(t)\|_2 \le C,\ 0 \le t \le T, \forall\, T.$

Theorem[Arnold,Dhamo,M05]
$\forall\, w_0 \in X_2$ s.t. (HP1) holds, $\exists! w$ *global* mild solution,
$w(t) \in \mathcal{C}^\infty(\mathbb{R}^6), \forall t > 0,$
$n(t), E(t) \in \mathcal{C}^\infty(\mathbb{R}^3), \forall t > 0.$

WPFP: global-in-t, smooth solution

$$w(x,v,t) = G(t,x,v)*w_0 + \int_0^t G(s,x,v)*(\Theta[V]w)(t-s)ds$$

$E_1 \in L_t^1((0,T];L_x^{[2,6]})$ by parabolic reguralization.

Remarks

- NOT used pseudo-conformal law (cf. classical cp.)
- $w \in \mathcal{C}([0,T];L^2_{x,v}) \mapsto E_1[w] \in L_t^1((0,T];L_x^{[2,6]}) \mapsto$ $V_1[w](x,t) := -\frac{1}{4\pi}\frac{x}{|x|^3} * E_1[w](x,t)$ $\Rightarrow\ V_1[w] \in L_t^1((0,T];L_x^{[6,\infty]}) \Rightarrow$ fixed-point-map for w

WPFP: global-in-t, smooth solution, without weights

7- Final considerations

- kinetic analysis, L^2-framework:
  - physically consistent,
  - suitable for real device simulation,
  - admissable parallelism with classical cp.
- by-pass the definition of the particle density

Perspectives

- WPFP: hypoelliptic case, WP $d = 3$, all-space case
- a priori estimates in the bounded domain case
- long-time-behaviour: decay $t \to \infty$ of $E(t), n(t)$

(cf. [Sparber,. . .04],[Perthame96])