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Quantum Fokker-Planck models: global solutions, steady states & large-time behavior

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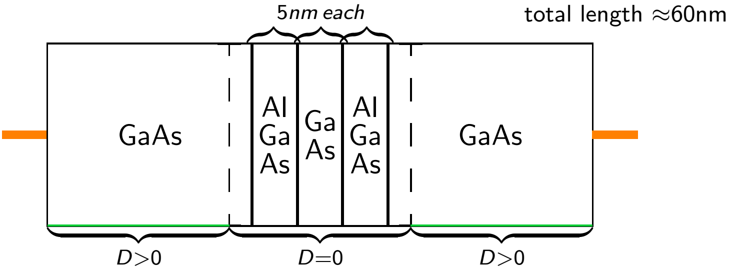
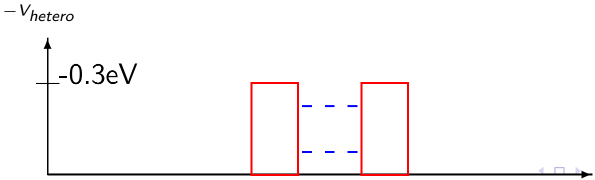
Guanajuato, September 2007

application: electron transport in nano-semiconductors

- resonant tunneling diode $\rightarrow$ for high frequency oscillators:



- $D(x) \geq 0 \ldots$ concentration of donor ions, „doping profile“
- **goal:** numerical simulation of electron transport
- potential barrier for electrons $\rightarrow$ resonant tunneling:



simulation model: Wigner functions, 1-particle approxim.

- Wigner Fokker-Planck equ. (augmented Caldeira-Leggett model)
- evolution for Wigner function $w(x, v, t) \in \mathbb{R}$:

$$\begin{cases} w_t + v \cdot \nabla_x w + \Theta[V]w = Qw, \quad x, v \in \mathbb{R}^d, \; t > 0 \\ w(x, v, t = 0) = w_0(x, v) \\ Qw = \underbrace{\sigma \Delta_v w}_{\text{class. diffusion}} + \underbrace{\beta \, \mathrm{div}_v(vw)}_{\text{friction}} + \underbrace{\alpha \Delta_x w + 2\gamma \, \mathrm{div}_x(\nabla_v w)}_{\text{quantum diffusion}} \end{cases}$$

- Fokker-Planck term Q models interaction of electrons with phonon heat bath $\rightarrow$ diffusive effects, open quantum system

- $V(x, t)$ ... electrostatic potential:

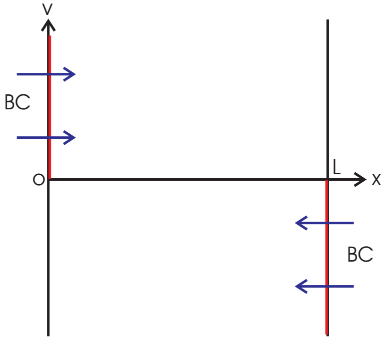
$$\Theta[V]w(x, v) = i(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} [V(x + \frac{\eta}{2}) - V(x - \frac{\eta}{2})] \hat{w}(x, \eta) e^{i\eta \cdot v} d\eta$$

- $n(x, t) = \int_{\mathbb{R}^d} w(x, v, t) \, dv$ ... particle density

- nonlinear mean-field model: selfconsistent Hartree potential $V(x,t)$:

$$-\Delta V = n(x,t) - D(x) = \int_{\mathbb{R}^d} w(x,v,t)dv - D(x)$$

- for RTD: $d=1$; inflow boundary conditions for w at $x=0$, $x=L$ (due to characteristics of free transport equation):



Outline:

1. nonlinear quantum Fokker-Planck-Poisson model
   - density matrix formulation
   - existence of global-in-time solution
2. linear quantum FP model in confinement potential
   - unique steady state (Wigner function)
   - large-time convergence (with exponential rate)

density matrix formulation

$w(x,v,t) = \int_{\mathbb{R}^d} \rho\left(x+\frac{\eta}{2}, x-\frac{\eta}{2}, t\right) e^{-i\eta\cdot v} d\eta$ ... Wigner-Weyl transformation

$w \in \mathbb{R} \quad \leftrightarrow \quad \rho(x,y) = \overline{\rho(y,x)}$

- density matrix operator on $L^2(\mathbb{R}^d)$:

$$(\varrho f)(x) = \int_{\mathbb{R}^d} \rho(x,y) f(y) dy \qquad \text{... self-adjoint}$$

- physical quantum states:

$$\varrho \geq 0,\ \varrho \in \mathcal{J}_1(L^2(\mathbb{R}^d)),\ \mathrm{Tr}\varrho = 1 \qquad \text{... positive trace class operator}$$

- definition of particle density → for Poisson coupling $-\Delta V = n$:

$$n(x,t) := \rho(x,x,t) \quad \dots \text{ rigorous for } \varrho \in \mathcal{J}_1 \ :$$

$$\|n(t)\|_{L^1(\mathbb{R}^d)} \le \|\varrho(t)\|_{\mathcal{J}_1} \overset{\varrho\ge 0}{=} \mathrm{Tr}\varrho(t) = const$$

- kinetic energy:

$$E_{\text{kin}}(\varrho) := -\frac{1}{2}\mathrm{Tr}\,(\Delta\varrho) \ge 0 \text{ for } \varrho \ge 0$$

- kinetic energy space, energy norm:

$$\mathcal{E} := \{\varrho \in \mathcal{J}_1 | E_{\text{kin}}(\varrho) < \infty\}, \qquad \|\varrho\|_{\mathcal{E}} := \|\sqrt{1-\Delta}\varrho\sqrt{1-\Delta}\|_{\mathcal{J}_1}$$

Lemma ([Lions-Paul '93], [A.A., CPDE '96])

$$\|n[\varrho]\|_{L^q(\mathbb{R}^d)} \le C_q\|\varrho\|_{\mathcal{E}}, \qquad 1 \le q \le \frac{d}{d-2}$$

generalized Lieb-Thirring inequality (i.e. collective Sobolev inequality)

time evolution of density matrix

$$w_t + v \cdot \nabla_x w + \Theta[V]w = \alpha \Delta_x w + 2\gamma \, \mathrm{div}_x(\nabla_v w) + \sigma \Delta_v w + \beta \, \mathrm{div}_v(vw)$$

- Wigner-Fokker-Planck equivalent to Lindblad form iff $\alpha\,\sigma - \gamma^2 \geq \frac{\beta^2}{16}$
  $\rightarrow$ classical FP-term (Caldeira-Leggett) not OK

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- evolution of density matrix function $\rho(x, y, t)$ in $L^2(\mathbb{R}^{2d})$:

$$\begin{aligned} \rho_t &= -i(H_x - H_y)\rho - \frac{\beta}{2}(x-y)\cdot(\nabla_x - \nabla_y)\rho \\ &+ \left[\alpha|\nabla_x + \nabla_y|^2 + 2i\gamma(x-y)\cdot(\nabla_x + \nabla_y) - \sigma|x-y|^2\right]\rho \end{aligned}$$

$$H_x = -\frac{1}{2}\Delta_x + V(x,t)$$

time evolution of density matrix

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$$H_x = -\frac{1}{2}\Delta_x + V(x,t)$$

- evolution of density matrix operator $\varrho(t)$ in $\mathcal{J}_1$ (Schrödinger picture):

$$\frac{d}{dt}\varrho = \underbrace{-i[\tilde{H},\varrho]}_{\text{Hamiltonian}} + \sum_k \underbrace{L_k \varrho L_k^* - \frac{1}{2}(L_k^* L_k \varrho + \varrho L_k^* L_k)}_{\text{dissipative}}$$

$$\tilde{H} = -\frac{1}{2}\Delta_x + V(x,t) - i\frac{\beta}{4}\{x,\nabla\}$$

unbounded Lindblad operators L_k

- Lindblad equation:

$$\frac{d}{dt}\varrho(t) = -i[\tilde{H}, \varrho] + \sum_k \underbrace{L_k \varrho L_k^* - \frac{1}{2}(L_k^* L_k \varrho + \varrho L_k^* L_k)}_{=:A(\varrho)}$$

- correspondence: Lindblad operator $\leftrightarrow$ Wigner collision operator:
  1. $L_1 = x \qquad \Rightarrow Qw = \frac{1}{2}\Delta_v w$
  2. $L_1 = \nabla_x \qquad \Rightarrow Qw = \frac{1}{2}\Delta_x w$
  3. $Q = QFP \qquad \Rightarrow L_k = \alpha_k \cdot x + \beta_k \cdot \nabla_x\,; \quad k = 1, ..., 2d$

L_k is NOT uniquely defined by Q

quantum Fokker-Planck-Poisson system in $\mathbb{R}^3$

$$\begin{cases} \frac{d}{dt}\varrho(t) = -i[\tilde{H}, \varrho] + A(\varrho), \quad t > 0 \\ \tilde{H} = -\frac{1}{2}\Delta_x + V(x,t) - i\frac{\beta}{4}\{x, \nabla\} \\ -\Delta V(x,t) = n(x,t) = \rho(x,x,t) \\ \varrho(0) = \varrho_0 \end{cases}$$

$[V[\varrho], \varrho]$ ... quadratically nonlinear

Theorem (AA-Sparber, CMP '04)

Let $\varrho_0 \in \mathcal{E}$, $\varrho_0 \geq 0$.
$\Rightarrow$ $\exists!$ *global-in-time, trace preserving, finite energy solution of QFPP:*

$$\hat{\rho} \in C(0, \infty; \mathcal{E}), \quad \varrho(t) \geq 0, \quad Tr\,\varrho(t) = Tr\,\varrho_0$$

Proof.

(a) construction of linear evolution semigroup in $\mathcal{J}_1$ and in $\mathcal{E}$
(b) nonlinear perturbation $[V[\varrho], \varrho] \rightarrow$ local sol. (PDE-semigroup theory)
(c) a-priori estimates $\rightarrow$ global-in-time solution □

(a) construction of linear evolution semigroup in $\mathcal{J}_1$

- dissipative open quantum system (linear — V given):

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{dt}}\varrho(t) &= \mathcal{L}(\varrho) := -i[\tilde{H},\varrho] + A(\varrho), \quad t>0 \\ \varrho(t=0) &= \varrho_0 \end{cases}$$

$A(\hat{\rho})$ ... dissipative / Lindblad terms

[E. Davies '77]: $\exists$ a linear C_0-semigroup on $\mathcal{J}_1$ ("minimal solution")

possible problems:

- semigroup not unique
- $\mathcal{D}(\mathcal{L})$ "too small"
- not conservative: $\mathrm{Tr}\,(\varrho(t)) \leq \mathrm{Tr}\ \varrho_0$

$\Rightarrow$ need to prove: $\mathcal{D}(\overline{\mathcal{L}})$ is "big enough"

Lemma ([AA-Carrillo-Dhamo '02], [AA-Sparber '04])

Let operator $P = p_2(x, -i\nabla)$ *be a quadratic polynomial,*
$\mathcal{D}(P) := C_0^\infty(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$.
$\Rightarrow$ $\bar{P}$ *is the "maximum extension" of* P,
i.e. $\mathcal{D}(\bar{P}) = \{f \in L^2 | Pf \in L^2\}$

Proof.

for $f \in \mathcal{D}(\bar{P})$:

$$f_n(x) := \underbrace{\chi_n(x)}_{C_0^\infty\text{-cutoff}} \cdot (f * \underbrace{\varphi_n}_{C_0^\infty\text{-mollifier}})(x) \stackrel{n\to\infty}{\longrightarrow} f \qquad \text{in graph norm } \|.\|_P$$

□

application/limitation of lemma:

Example 1: $P = -\Delta - |x|^2$, $\mathcal{D}(P) = C_0^\infty(\mathbb{R}^d)$
$\Rightarrow$ P is essentially selfadjoint on $C_0^\infty(\mathbb{R}^d)$

Example 2: $P = -\partial_x^2 - x^4$ not essentially selfadjoint on $C_0^\infty(\mathbb{R}^d)$
[Reed-Simon]
$\Rightarrow$ lemma can't be extended to all $P = p_4(x, -i\nabla)$

prove: $\mathcal{D}(\overline{\mathcal{L}})$ is "big enough"

Lemma (AA-Sparber, CMP '04)

Let generator $\mathcal{L}(\varrho)$ be quadratic in x and ∇_x (QFP, e.g.).
$\Rightarrow \overline{\mathcal{L}|_{D_\infty}}$ *is the "maximum extension" in* $\mathcal{J}_1$
$D_\infty \subset \mathcal{J}_1$ *... dense subset with* C_0^∞*-kernels*

Proof.

for $\varrho \in \mathcal{D}(\mathcal{L}_{\max}) = \{\varrho \in \mathcal{J}_1 | \mathcal{L}(\varrho) \in \mathcal{J}_1\}$:

$$D_\infty \ni \vartheta_n \stackrel{n\to\infty}{\longrightarrow} \varrho \quad \text{in graph norm } \|.\|_{\mathcal{L}}$$

$$\theta_n(x,y) := \underbrace{\chi_n(x)}_{C_0^\infty\text{-cutoff}} \left[\varphi_n(x) *_x \rho(x,y) *_y \underbrace{\varphi_n(y)}_{C_0^\infty\text{-mollifier}} \right] \chi_n(y)$$

□

Theorem

QFP: C_0-semigroup $e^{\mathcal{L}t}$ of Davies is unique & trace preserving

(b) nonlinear perturbation for $d = 3$

- $e^{\mathcal{L}t}$ is C_0-semigroup in $\mathcal{E} := \{\varrho \in \mathcal{J}_1 | E_{\text{kin}}(\varrho) < \infty\}$ ... kinetic energy space
- Hartree-term $[V[\varrho], \varrho]$ ... local Lipschitz map in $\mathcal{E}$ (but *not* in $\mathcal{J}_1$ $\rightarrow$ reason for using $\mathcal{E}$)

Proof.

$$\begin{aligned} \|V[\varrho]\|_{L^p(\mathbb{R}^3)} \quad &\leq \quad C_q \|n[\varrho]\|_{L^q(\mathbb{R}^3)} \leq C_q \|\varrho\|_{\mathcal{E}} \\ & \quad\quad 3 < p \leq \infty, \ 1 \leq q \leq 3 \end{aligned}$$

□

- $\Rightarrow \exists$ local-in-t solution to QFP-Poisson (PDE-semigoup theory)

(c) a-priori estimate for total energy

$$E_{\mathrm{tot}}(\varrho) := E_{\mathrm{kin}}(\varrho) + \frac{1}{2}\|\nabla_x V[\varrho]\|_{L^2}^2$$

$$\frac{\mathrm{d}}{\mathrm{dt}} E_{\mathrm{tot}}(t) = 3\sigma \,\mathrm{Tr}\,\varrho_0 - \beta\, E_{\mathrm{kin}}(t) - \alpha\,\|n(t)\|_{L^2}^2$$

$\Rightarrow$ no finite-time-blow-up of $\|\varrho(t)\|_{\mathcal{E}} \overset{\varrho \geq 0}{=} \underbrace{\mathrm{Tr}\,\varrho(t)}_{=const} + 2E_{\mathrm{kin}}(t)$

$\Rightarrow$ QFP-Poisson solution $\varrho(t)$ is global-in-time □

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linear Wigner-Fokker-Planck in confinement potential

$V(x) := \frac{1}{2}|x|^2 + \lambda V_0(x)$ ... quadratic confinement + (small) perturbation

$$w_t + \lambda\Theta[V_0]w = \underbrace{-v\cdot\nabla_x w + x\cdot\nabla_v w + \Delta_v w + 2\,\mathrm{div}_v(vw) + \Delta_x w}_{=:Lw} \quad (1)$$

Theorem (Sparber-Carrillo-Dolbeault-Markowich '04)

Let $\lambda = 0$ (uniformly parabolic equation) $\Rightarrow$

(a) *WFP (1) has a unique Gaussian steady state $w_\infty(x,v) = e^{-A(x,v)}$, $A(x,v) = \frac{1}{4}[|x|^2 + 2x\cdot v + 3|v|^2] + const$*

(b) *$w(t) \stackrel{t\to\infty}{\longrightarrow} w_\infty$ in $L^1(\mathbb{R}^{2d})$ and in $\mathcal{H} := L^2(\mathbb{R}^{2d}, w_\infty^{-1}\,dxdv)$*

Proof of (b).

- decompose in $\mathcal{H}$: $L = L^s + L^{as}$
- $L^s w = \mathrm{div}_{x,v}(\nabla_{x,v} w + w\nabla_{x,v} A)$ satisfies Bakry-Emery-condition: $\mathrm{Hess}A(x,v) \geq \lambda_1 \mathbb{I}$
  $\Rightarrow$ spectral gap $\lambda_1 = 1 - \frac{1}{\sqrt{2}}$, log. Sobolev inequality

□

WFP with perturbed confinement potential

$$w_t + \lambda\Theta[V_0]w = Lw \tag{2}$$

Theorem (AA-Gamba-Gualdani-Sparber '07)

Be $|\lambda|$ *small*, $w_0 \in \mathcal{H}$, $V_0 \in C^\infty(\mathbb{R}^d)$, ... $\Rightarrow$

(a) *WFP (2) has a unique normalized steady state* $\tilde{w}_\infty(x,v) \in \mathcal{H}$

(b)
$$\|w(t) - \tilde{w}_\infty\|_{\mathcal{H}} \le e^{-\varepsilon t}\|w_0 - \tilde{w}_\infty\|_{\mathcal{H}}, \quad t \ge 0,\ \varepsilon > 0$$

Proof.

(a) fixed point iteration for $L(w - w_\infty) = \lambda\Theta[V_0]w$ in $\mathcal{H}^\perp := \{w_\infty\}^\perp$

(b) $\|w(t) - \tilde{w}_\infty\|^2_{\mathcal{H}}$ is Lyapunov functional in $\mathcal{H}^\perp$ with exp. decay, spectral gap of L^s compensates perturbation $\lambda\Theta[V_0]$

□

linear QFP: exponential convergence of density matrix

analogous Lindblad equation:

$$\begin{cases} \frac{d}{dt}\varrho(t) = -i[\tilde{H}, \varrho] + A(\varrho), \quad t > 0 \\ \tilde{H} = -\frac{1}{2}\Delta_x + \frac{1}{2}|x|^2 + \lambda V_0(x) - \frac{i}{2}\{x, \nabla\} \\ \varrho(0) = \varrho_0 \in \mathcal{J}_1^+, \ \mathrm{Tr}\, \varrho_0 = 1 \end{cases} \tag{3}$$

Theorem (AA-Gamba-Gualdani-Sparber '07)

Be $|\lambda|$ small, $w_0 \in \mathcal{H}$, $V_0 \in C^\infty(\mathbb{R}^d)$, ... $\Rightarrow$

(a) *QFP (3) has a unique normalized positive steady state $\varrho_\infty \in \mathcal{J}_1(L^2)$*

(b)

$$\|\varrho(t) - \varrho_\infty\|_{\mathcal{J}_2} \le K e^{-\varepsilon t} \|\varrho_0 - \varrho_\infty\|_{\mathcal{J}_2}, \quad t \ge 0, \ \varepsilon > 0$$

(c)

$$\varrho(t) \overset{t\to\infty}{\longrightarrow} \varrho_\infty \quad \textit{in } \mathcal{J}_1(L^2) \quad \textit{(strongly !)}$$

Theorem (AA-Gamba-Gualdani-Sparber '07)

(a) *QFP has a unique normalized positive steady state* $\varrho_\infty \in \mathcal{J}_1(L^2)$

(b) $\|\varrho(t) - \varrho_\infty\|_{\mathcal{J}_2} \leq K e^{-\varepsilon t} \|\varrho_0 - \varrho_\infty\|_{\mathcal{J}_2}$

(c) $\varrho(t) \stackrel{t\to\infty}{\longrightarrow} \varrho_\infty$ *in* $\mathcal{J}_1(L^2)$ *(strongly !)*

Proof.

(b) $$\|\varrho\|_{\mathcal{J}_2} = \|\rho(.,.)\|_{L^2} = (2\pi)^{d/2} \|w(.,.)\|_{L^2} \leq K \|w(.,.)\|_{\mathcal{H}}$$

(a) QFP-solution satisfies:
$\varrho \in C([0,\infty); \mathcal{J}_1^+) \Rightarrow \varrho_\infty \geq 0$ (from (b)) ,
$\|\varrho(t)\|_{\mathcal{J}_1} = 1 \Rightarrow \varrho_\infty \in \mathcal{J}_1$ (by Alaoglu's theorem)

(c) from (b): convergence in strong operator topology;
and $\|\varrho(t)\|_{\mathcal{J}_1} = \|\varrho_\infty\|_{\mathcal{J}_1} = 1$
$\Rightarrow \mathcal{J}_1$–convergence to ϱ_∞ (by Grümm's theorem) □

Open problem: exponential convergence in $\mathcal{J}_1$