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Quantum Fokker-Planck models: kinetic & operator theory approaches

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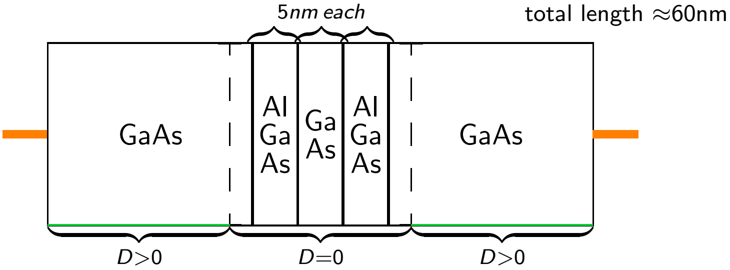
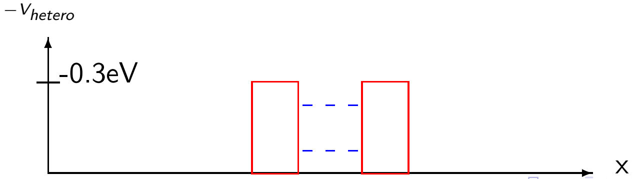
application: electron transport in nano-semiconductors

- resonant tunneling diode → 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 → resonant tunneling:



simulation model: Wigner functions, 1-particle approxim.

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

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

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

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

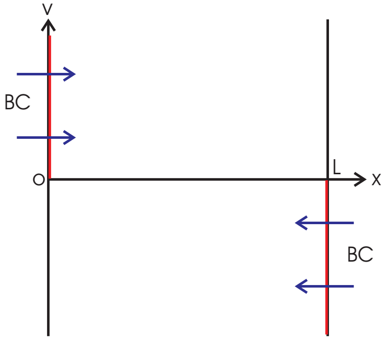
$$\Theta[V]w(x,v) = i(2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} [V(x+\frac{\eta}{2}) - V(x-\frac{\eta}{2})]\hat{w}(x,\eta)e^{i\eta\cdot v}\, d\eta$$

- $n(x,t) = \int_{\mathbb{R}^d} w(x,v,t)\, dv \geq 0$ ... 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):



Refs:

- let $x \in \mathbb{R}^d$, $V = \frac{|x|^2}{2} \;\Rightarrow\; \theta[V] = -x\nabla_v\, w$.
  Sparber-Carrillo-Dolbeault-Markovich [SCDM'04]:

$$\exists!\text{ normalized steady state } w_\infty;\text{ Gaussian (explicit comp.)}$$
$$w(t) \overset{t\to\infty}{\longrightarrow} w_\infty \text{ exponentially (entropy method)}$$

- (bounded) perturb. of V: difficult on Wigner level $\rightarrow$ work in progress

Outline

1. density matrix, Lindblad equation
2. evolution: global solution
3. main results
4. steady state proof
5. $t \longrightarrow \infty$ convergence

1) density matrix formulation

- Wigner-Weyl transformation:

$$
\begin{aligned}
w(x,v,t) &= \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \rho\left(x+\tfrac{\eta}{2}, x-\tfrac{\eta}{2}, t\right) e^{-i\eta\cdot v}\, d\eta \\
w \in \mathbb{R} &\leftrightarrow \rho(x,y) = \overline{\rho(y,x)} \\
n(x,t) &= \rho(x,x,t) \geq 0 \text{ ... particle density}
\end{aligned}
$$

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\end{aligned}
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- 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:

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

- evolution by Lindblad equation:

$$\partial_t \varrho = \underbrace{-i\,[H,\varrho]}_{\text{Hamiltonian}} + \sum_{l=1,2} \underbrace{L_l\,\varrho L_l^* - \frac{1}{2}(L_l^* L_l\,\varrho + \varrho L_l^* L_l)}_{\text{dissipative}} =: \underbrace{\mathcal{L}_*}_{\text{generator}}(\varrho)$$

$$H = -\frac{1}{2}\,\partial_{xx} + \underbrace{\frac{\omega^2}{2}\,x^2}_{\substack{\text{confinement}\\ \text{potential}}} + \underbrace{V(x)}_{\substack{\text{subquadrat.}\\ \text{perturb. pot.}}} - i\,\frac{\gamma}{2}\,\{x,\partial_x\}$$ ... (adjusted) Hamiltonian

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- WFP representable as Lindblad equ. if: (set $D_{pq} = 0$ here)

Lindblad cond: $\Delta := D_{pp}\,D_{qq} - \frac{\gamma^2}{4} \geq 0$ (diffusion dominates friction)

hence: $\varrho_0 \geq 0 \quad \Rightarrow \quad \varrho(t) \geq 0 \quad \forall\, t \geq 0$

$$L_1 = \frac{i\gamma}{\sqrt{2\,D_{pp}}}\underbrace{p}_{-i\,\partial_x} + \sqrt{2\,D_{pp}}\,\underbrace{q}_{x}, \quad L_2 = \frac{2\sqrt{\Delta}}{\sqrt{2\,D_{pp}}}\,p \quad \text{... Lindblad op.}$$

- linearly independent for $\Delta > 0 \;\Rightarrow\;$ span $(L_1, L_2) =$ span (p, q)

2) global in time solution for Quantum Fokker-Planck

Theorem ([AA-Sparber'04]: quadratic pot. $+ V \in L^\infty$)

1. *lin. QFP; let* $\varrho_0 \in \mathcal{J}_1(L_2(\mathbb{R}^d))$

$$\Rightarrow \ \exists! \ \textit{global, sol.} \ \varrho \in C([0,\infty); \mathcal{J}_1), \quad \varrho(t) \geq 0, \ tr\,\varrho(t) = tr\,\varrho_0$$

2. *QFP – Poisson* $(-\Delta V(t) = n(t) = \rho(x,x,t),$ *in* $\mathbb{R}^3)$
let $\varrho_0 \in \mathcal{E}$ $\left(\textit{i.e.}\ \varrho_0 \in \mathcal{J}_1,\ E_{kin} := -\frac{1}{2}\, tr(\Delta \varrho_0) < \infty\right)$

$$\Rightarrow \ \exists! \ \textit{global, trace preserving solution} \ \varrho \in C([0,\infty); \mathcal{E})$$

Proof (by semigroup theory).

- construction of linear evolution semigroup in $\mathcal{J}_1, \mathcal{E}$ (for $V = 0$)
- nonlinearity is locally Lipschitz + a-priori estimates in $\mathcal{E}$

□

construction of linear evolution semigroup in $\mathcal{J}_1, \mathcal{E}$-details:
(for $V = 0$)

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

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

$A(\varrho)$ ... dissipative / Lindblad terms

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

possible problems:

- semigroup not unique
- $\mathcal{D}(\mathcal{L}_*)$ "too small"
- not conservative: $\mathrm{tr}\,(\varrho(t)) \le \mathrm{tr}\ \varrho_0$

$\Rightarrow$ 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,* $\mathcal{D}(P) := C_0^\infty(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$.

$$\Rightarrow \quad \bar{P} \text{ is the "maximum extension" of } P,$$
$$\text{i.e. } \mathcal{D}(\bar{P}) = \{f \in L^2 \mid Pf \in L^2\}$$

Proof.

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

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

□

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.).

$$\Rightarrow \overline{\mathcal{L}_*|_{D_\infty}} \text{ is the "maximum extension" in } \mathcal{J}_1$$

$D_\infty \subset \mathcal{J}_1$ ... 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

3) main results

Theorem ([AA-Fagnola-Neumann '08])

Let $|V'(x)| \leq c\,(1+x^2)^{\frac{\alpha}{2}}$ *for some* $0 \leq \alpha < 1$ *(subquadratic)* $\Rightarrow$

1. $\exists!$ *global, trace preserving solution* $\varrho = \varrho(t)$ *of QFP*
2. $\exists$ *normal steady state of Quantum Fokker-Planck (QFP)*
3. *if* $\Delta = D_{pp}\,D_{pp} - \frac{\gamma^2}{4} > 0$:
   - $\exists!$ *normal steady state* ϱ_∞,
   - ϱ_∞ *is faithful (i.e.* $0 \notin \sigma(\varrho_\infty)$; *rank* $\varrho_\infty = \infty$*),*
   - $\varrho(t) \xrightarrow{t\to\infty} \varrho_\infty$ *in* $\mathcal{J}_1(L^2)$.

4) existence of steady state

2 results (by compactness): [Fagnola–Rebolledo 2001]:

notation:

$\mathcal{T}_{*t}$ ... QM–semigroup on $\varrho \in \mathcal{J}_1$; $t \geq 0$ (Schrödinger picture)
$\mathcal{T}_t$ ... dual QMS on (observables in) $\mathcal{B}(L^2)$ (Heisenberg picture)

$$\underbrace{Y}_{\text{s.a.}} \wedge \underbrace{r}_{\in \mathbb{R}} := \underbrace{Y\, E_r}_{\text{cut-off op.}} + r\, E_r^{\perp} \qquad E_r \text{ ... spectral proj. for } Y \text{ on } (-\infty, r]$$

Theorem ([Fagnola–Rebolledo 2001])

Let $\mathcal{T}$ be QMS.
assume: $\exists$ s.a. $X \geq 0$, $Y \geq -b \in \mathbb{R}$ (Y with finite dim. spectral proj. for bounded intervals) with

$$\int_0^t \langle u, \mathcal{T}_s \underbrace{(Y \wedge r)}_{\in \mathcal{B}(L^2)} u \rangle \, ds \leq \langle u, Xu \rangle \quad \forall\, t, r > 0,\ \forall\, u \in \mathcal{D}(X)$$

$\Rightarrow$ $\exists$ *normalized steady state for $\mathcal{T}$, $\mathcal{T}_*$.*

condition in Th: $$\int_0^t \langle u, \mathcal{T}_s(Y \wedge r)u\rangle \, ds \le \langle u, Xu\rangle \qquad (1)$$

Proof.

from (1) with $Y \wedge r \ge -(b+r)\, E_r + r\,\mathbf{1} : \forall \epsilon > 0 \;\; \exists\, t(\epsilon) > 0,\; r(\epsilon) > 0 :$

1. $\frac{1}{t}\int_0^t \operatorname{tr}\left(\mathcal{T}_{*s}\,\underbrace{(|u\rangle\langle u|)}_{\text{pure state}}\, E_{r(\epsilon)}\right) ds \ge 1-\epsilon, \quad t > t(\epsilon) \quad$ (= Prohorov cond.)

   $E_{r(\epsilon)}$ ... "compact support in spectrum" of Y, finite rank projector

   $$\text{i.e.} \quad \tilde\varrho(t) := \frac{1}{t}\int_0^t \mathcal{T}_{*s}(|u\rangle\langle u|)\, ds\,, \quad t > t(\epsilon) \text{ is tight} \qquad (2)$$

2. $\Rightarrow\; \exists\; \mathcal{J}_1$ - weakly convergent subsequence $\tilde\varrho(t_n)$, $t_n \nearrow \infty$

   $$\text{i.e.} \quad \operatorname{tr}(\tilde\varrho(t_n)\, A) \to \operatorname{tr}(\varrho\, A)\,, \quad \forall\, A \in \mathcal{B}(L^2)$$

3. such weak limits of (2) are normalized steady states of $\mathcal{T}_*$.

□

existence of steady state – simplified condition:

Theorem ([Fagnola–Rebolledo 2001])

Let $\exists$ *s.a.* $X \geq 0\,,\ \ Y \geq -b:$

$$\langle u, \mathcal{L}(X)\, u\rangle \leq -\langle u, Y\, u\rangle \quad \forall\, u \in \mathcal{D} \tag{3}$$

$+$ *technical assumption (on domains)*

$\Rightarrow\ \exists$ *normalized steady state*

Proof.

(3) $\Rightarrow$ (1) □

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Proof.

$(3) \Rightarrow (1)$ □

application to Quantum Fokker-Planck [AA-Fagnola-Neumann]:

$$\text{choose:}\quad \begin{aligned} X \ &:= \ rp^2 + (pq + qp) + (\omega^2 r + 2\gamma)q^2 \geq 0 \quad \left(\text{for } r > \tfrac{1}{2\gamma}\right) \\ Y \ &:= \ \underbrace{C}_{>0}(p^2 + q^2) - \tilde{C} \end{aligned}$$

$\mathcal{L}(X)$ involves subquadratic perturbations (from $V(x)$)

$p\, V'(q)$ can be compensated by $-Y$

steady state ϱ_∞ is faithful [AA-F-N] (i.e. $0 \notin \sigma(\varrho_\infty)$):

let $\Delta > 0 \Rightarrow L_1, L_2$ linearly independent

$\Rightarrow$ QM semigroup $\mathcal{T}$ on $\mathcal{B}(L^2)$ is irreducible$^{\circledast}$,

i.e. $\nexists$ proper invariant subspaces of evolution (for any ϱ_0)

$\Rightarrow \varrho_\infty$ has full rank, i.e. faithful

Theorem ([Frigerio, 1977])

Let ϱ_∞ be faithful, then:

$\mathcal{T}$ is irreducible $\iff$ normal steady state ϱ_∞ is unique

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$\circledast$ Proof-Idea.

let χ be a subspace of L^2 with $L_l(\chi) \subset \chi$.

$$\text{span}\,(L_1, L_2) = \text{span}\,(p, q) = \text{span}\ \underbrace{(a, a^\dagger)}_{\text{creation/annihilation}}$$

proveable: $$e^{-\frac{t}{2}(p^2+q^2-1)}\chi \subseteq \chi \qquad \forall\, t \geq 0$$

$$\chi = \overline{\text{span}\,(e_j,\ j \in J \subset \mathbb{N})} \quad e_j \ldots \text{ eigenfct. of } N := \frac{1}{2}\,(p^2 + q^2 - 1)$$

$$a(\chi) \subset \chi,\ a^\dagger(\chi) \subset \chi \ \Rightarrow\ J = \mathbb{N}.$$

□

5) $t \to \infty$ convergence

Theorem ([Fagnola–Rebolledo '98])

Let $\mathcal{T}$ be QMS; let $\exists$ faithful normalized steady state ϱ_∞,
let commutant $\{L_l, L_l^*; l = 1, 2\}' = \{L_l, L_l^*, H\}'$ $\quad (\subseteq \{$ steady states $\})$
+ techn. assumpt. (on domains)

$$\Rightarrow \forall \varrho_0 \in \mathcal{J}_1, \ tr\, \varrho_0 = 1 : \varrho(t) \longrightarrow \varrho_\infty \text{ in } \mathcal{J}_1(L^2)$$

application to Quantum Fokker-Planck [AA-Fagnola-Neumann]:

$$\Delta := D_{pp} D_{qq} - \frac{\gamma^2}{4} > 0, \quad L_1 = \frac{i\gamma}{\sqrt{2 D_{pp}}} p + \sqrt{2 D_{pp}}\, q\,, \ L_2 = \frac{2\sqrt{\Delta}}{\sqrt{2 D_{pp}}} p$$

$$\Rightarrow \quad \{L_l, L_l^*\}' = \{p, q\}' = \{c\,\mathbf{1} \mid c \in \mathbb{C}\}$$

$$\Rightarrow \quad \{L_l, L_l^*\}' \overset{(\supseteq \text{trivial})}{=} \{L_l, L_l^*, H\}'$$

$\Rightarrow$ convergence of quantum Fokker-Planck solution to ϱ_∞