4th WORKSHOP on

Mathematical Models for Transport in Macroscopic and Mesoscopic Systems

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The effect of time-dependent coupling on non-equilibrium steady states

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What do we like to study?

1. **Two leads coupled through a quantum well: spectral analysis.**
2. **What is a NESS?**
3. **Time-dependent Liouville equation for density matrices.**
4. **Current formulae (Landau-Lifschitz, Landauer-Büttiker).**

The model I

• In $\mathfrak{H} := L^2(\mathbb{R})$ we consider the self-adjoint Schrödinger operator (Buslaev-Fomin '62)

$$(Hf)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx}f(x) + V(x)f(x), \qquad x \in \mathbb{R},$$

with domain

$$\mathrm{dom}(H) := \{f \in W^{1,2}(\mathbb{R}) : \frac{1}{M}f' \in W^{1,2}(\mathbb{R})\}.$$

• **CONDITIONS:** **(a)** The *effective* mass $M(x) > 0$ and the real potential $V(x)$ admit decompositions of the form (with $v_a \geq v_b$) :

$$M(x) := \begin{cases} m_a & x \in (-\infty, a] \\ m(x) & x \in (a,b) \\ m_b & x \in [b, \infty) \end{cases} \quad V(x) := \begin{cases} v_a & x \in (-\infty, a] \\ v(x) & x \in (a,b) \\ v_b & x \in [b, \infty) \end{cases}$$

The model II

(b) The function

$$m(x) + \frac{1}{m_{a(b)}} \in L^\infty((a,b)),$$

and the *quantum well potential* : $v \in L^\infty((a,b))$.

The **quantum well** is identified with the *interval* (a,b), (or physically, with the three-dimensional *layer* $(a,b) \times \mathbb{R}^2$).

The regions $(-\infty, a)$ and (b, ∞) (or physically $(-\infty, a) \times \mathbb{R}^2$ and $(b, \infty) \times \mathbb{R}^2$), are the **reservoirs**.

The model III

• Besides its mathematical attraction, the model can be also interesting for:

1. Quantum well lasers.
2. Resonant tunneling diodes.
3. Nanotransistors.

Kirkner, D.; Lent, C.: The quantum transmitting boundary method, *J. Appl. Phys.* **67** (1990), 6353-6359.

Vinter, B.; Weisbuch, C.: *Quantum Semiconductor Structures: Fundamentals and Applications.* Academic Press, Boston, 1991.

What is (*our*) NESS? I

Definition 0.1. *We call a bounded, self-adjoint, non-negative operator* ϱ *in* $L^2(\mathbb{R})$ *density-matrix operator or state, if the product* $\varrho M(\chi_{(a,b)})$ *is a trace-class operator. Here* $M(\chi_{(a,b)})$ *is the multiplication operator induced in* $L^2(\mathbb{R})$ *by the characteristic function* $\chi_{(a,b)}$ *of any finite interval* (a, b)*.*

Definition 0.2. *We call operator* ϱ *a steady state for Hamilonian* H*, if it commutes with* H*, i.e. if* ϱ *belongs to the commutant* $\mathfrak{A}'(H)$ *of the algebra* $\mathfrak{A}(H)$ *generated by the functional calculus associated to* H*. A steady state is called an equilibrium state, if it belongs to the bi-commutant* $\mathfrak{A}''(H)$ *of this algebra.*

What is (*our*) NESS? II

Proposition 0.3. [RMP'04] *Since* $v_a \geq v_b$, *the operator* H *is* *unitarily equivalent* *to the multiplication* M *induced by the independent variable* λ *in the* *direct integral* *of the spaces* $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu) \simeq \oplus_{j=1}^{N} \mathbb{C} \oplus L^2([v_a, v_b], \mathbb{C}) \oplus L^2((v_a, \infty), \mathbb{C}^2)$ *where:*

$$\mathfrak{h}(\lambda) := \begin{cases} \mathbb{C}, & \lambda \in (-\infty, v_a] \\ \mathbb{C}^2, & \lambda \in (v_a, \infty) \end{cases},$$

and the measure:

$$d\nu(\lambda) = \sum_{j=1}^{N} \delta(\lambda - \lambda_j) d\lambda + \chi_{[v_b, \infty)}(\lambda) d\lambda, \quad \lambda \in \mathbb{R},$$

where $\{\lambda_j\}_{j=1}^{N}$ *denote the finite number of simple eigenvalues of* H, *which are all situated below the* *threshold* v_b.

What is (*our*) NESS? III

• If ϱ_{st} is a *steady state* for H, then there exists a ν-measurable function

$$\mathbb{R} \ni \lambda \mapsto \tilde{\rho}_{st}(\lambda) \in B(\mathfrak{h}(\lambda))$$

of non-negative bounded operators on $\mathfrak{h}(\lambda)$ such that $\nu - \sup_{\lambda \in \mathbb{R}} \|\tilde{\rho}_{st}(\lambda)\|_{\mathfrak{B}(\mathfrak{h}(\lambda))} < \infty$ and ϱ_{st} is unitarily equivalent to the multiplication operator $M(\tilde{\rho})$ induced by $\tilde{\rho}$ via a generalized Fourier transform Φ which makes H diagonal:

$$\varrho_{st} = \Phi^{-1} M(\tilde{\rho}) \Phi.$$

• If ϱ_{eq} is an *equilibrium state* for H, then the corresponding $\tilde{\rho}_{eq}(\lambda)$ is proportional to the *identity matrix*: $\tilde{\rho}_{eq}(\lambda) = \alpha(\lambda) \cdot \mathbb{I}$, hence one gets $\varrho_{eq} = \mathfrak{D}(H)$.

Decoupled system I

- We start with a completely decoupled system:

$$\mathfrak{H}_a := L^2((-\infty, a]), \quad \mathfrak{H}_{\mathcal{I}} := L^2(\mathcal{I}), \quad \mathfrak{H}_b := L^2([b, \infty))$$

isolated quantum well $\mathcal{I} = (a, b)$. Then the total Hilbert space is direct sum:

$$\mathfrak{H} = \mathfrak{H}_a \oplus \mathfrak{H}_{\mathcal{I}} \oplus \mathfrak{H}_b \, .$$

- With the subspace $\mathfrak{H}_a$ we associate the Hamiltonian H_a:

$$\begin{aligned} (H_a f)(x) &:= -\frac{1}{2m_a}\frac{d^2}{dx^2} f(x) + v_a f(x), \\ f \in \mathrm{dom}(H_a) &:= \{f \in W^{2,2}((-\infty, a)) : f(a) = 0\}. \end{aligned}$$

Decoupled system II

- With $\mathfrak{H}_{\mathcal{I}}$ we associate the Hamiltonian of isolated quantum well $H_{\mathcal{I}}$:

$$
\begin{aligned}
(H_{\mathcal{I}} f)(x) &:= -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}f(x) + v(x)f(x), \\
f \in \mathrm{dom}(H_{\mathcal{I}}) &:= \left\{ f \in W^{1,2}(\mathcal{I}) : \begin{array}{l} \frac{1}{m}f' \in W^{1,2}(\mathcal{I}) \\ f(a) = f(b) = 0 \end{array} \right\}
\end{aligned}
$$

- With $\mathfrak{H}_b$ we associate the Hamiltonian H_b:

$$
\begin{aligned}
(H_b f)(x) &:= -\frac{1}{2m_b}\frac{d^2}{dx^2}f(x) + v_b f(x), \\
f \in \mathrm{dom}(H_b) &:= \{f \in W^{2,2}((b,\infty) : f(b) = 0\}.
\end{aligned}
$$

Decoupled system III

• Hence in the space $\mathfrak{H}$ we have three isolated subsystems:

$$H_D := H_a \oplus H_{\mathcal{I}} \oplus H_b$$

• The quantum subsystems $\{\mathfrak{H}_a, H_a\}$ and $\{\mathfrak{H}_b, H_b\}$ are called left- and right-hand reservoirs. The middle system $\{\mathfrak{H}_{\mathcal{I}}, H_{\mathcal{I}}\}$ is identified with a closed quantum well.

• We assume that all three subsystems are at (*internal*) thermal equilibrium. Then according our Definitions, the corresponding sub-states must be functions of their corresponding sub-Hamiltonians.

• The total (non-equilibrium) state is direct sum of these three sub-states: $\varrho_D := \varrho_a \oplus \varrho_{\mathcal{I}} \oplus \varrho_b$.

The initial state

• According our Definitions 0.1 ,0.2 the thermal equilibrium sub-states ϱ_a, $\varrho_{\mathcal{I}}$ and ϱ_b are the functions of corresponding Hamiltonians :

$$\varrho_a := \mathfrak{f}_a(H_a - \mu_a), \quad \varrho_{\mathcal{I}} := \mathfrak{f}_{\mathcal{I}}(H_{\mathcal{I}} - \mu_{\mathcal{I}}), \quad \varrho_b := \mathfrak{f}_b(H_b - \mu_b).$$

• Physical examples for fermions with chemical potentials $\mu_a, \mu_{\mathcal{I}}, \mu_b$ one can take from: Frensley, W. R.: Boundary conditions for open quantum systems driven far from equilibrium, Rev. Modern Phys. **62** (1990), 745-791, proposes

$$\mathfrak{f}_j(\lambda) := c_j \ln(1 + e^{-\beta\lambda}), \quad j \in \{a, \mathcal{I}, b\}$$

$\lambda \in \mathbb{R}$, $\beta := 1/T$. The constants are given by $c_j := m_j^*/\hbar^2\pi\,\beta$, where the m_j^*'s are one dimensional effective masses. The initial state is:

$$\varrho_D := \varrho_a \oplus \varrho_{\mathcal{I}} \oplus \varrho_b.$$

NESS via time-dependent coupling

• The main question: can we construct a NESS for $\{\mathfrak{H}, H\}$ starting from ϱ_D?

• Let $\varrho_D = \varrho_a \oplus \varrho_{\mathcal{I}} \oplus \varrho_b$ be the state of the the quantum system

$$\{\mathfrak{H}, H_D = H_a \oplus H_{\mathcal{I}} \oplus H_b\}$$

at $t = -\infty$. By **Definitions** 0.1,0.2 it is a NESS (and even an "ES"):

$$[H_D, \varrho_D] = 0 \, .$$

• The systems are isolated at $t = -\infty$ and then we connect them in a time dependent manner the left- and right-hand reservoirs to the closed quantum well $\{\mathfrak{H}_{\mathcal{I}}, H_{\mathcal{I}}\}$.

• We assume that the connection process is described by the time-dependent Hamiltonian

$$H_\alpha(t) := H + e^{-\alpha t}\delta(x-a) + e^{-\alpha t}\delta(x-b), \quad t \in \mathbb{R}, \quad \alpha > 0.$$

Time-dependent coupling I

- The operator $H_\alpha(t)$ is defined by

$$(H_\alpha(t)f)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx}f(x)+V(x)f(x), f \in \mathrm{dom}(H_\alpha(t))\,.$$

- The domain $\mathrm{dom}(H_\alpha(t))$ is given by

$$\mathrm{dom}(H_\alpha(t)) :=$$

$$\left\{ f \in W^{1,2}(\mathbb{R}) : \begin{array}{c} \frac{1}{M}f' \in W^{1,2}(\mathbb{R}) \\ (\frac{1}{2M}f')(a+0) - (\frac{1}{2M}f')(a-0) = e^{-\alpha t}f(a) \\ (\frac{1}{2M}f')(b+0) - (\frac{1}{2M}f')(b-0) = e^{-\alpha t}f(b) \end{array} \right.$$

Time-dependent coupling II

THEOREM: One gets the following *operator-norm* convergence of resolvents:

$$\|\cdot\| - \lim_{t\to-\infty} (H_\alpha(t) - z)^{-1} = (H_D - z)^{-1}$$

and

$$\|\cdot\| - \lim_{t\to+\infty} (H_\alpha(t) - z)^{-1} = (H - z)^{-1} \quad ,$$

for any $z \in \mathbb{C} \setminus \mathbb{R}$.

Density-matrix operator: time evolution

• We define a time-dependent density-matrix operator of the quantum system with Hamiltonian $H_\alpha(t)$ as an operator-valued family:

$$\mathbb{R} \ni t \mapsto \varrho_\alpha(t) \in B(W^{1,2}(\mathbb{R})),$$

(a) which is time-differentiable in the space $B(W^{1,2}(\mathbb{R}), W^{-1,2}(\mathbb{R}))$;
(b) which is (weak) solution of the quantum *Liouville* equation:

$$i\frac{\partial}{\partial t}\varrho_\alpha(t) = [H_\alpha(t), \varrho_\alpha(t)], \quad t \in \mathbb{R},$$

satisfying (for any fixed $\alpha > 0$) the initial (decoupling) condition

$$\text{s-}\lim_{t\to-\infty} \varrho_\alpha(t) = \varrho_D.$$

NESS for coupled system

Main strategy:

• Having found a solution $\varrho_\alpha(t)$ we are interested in the *ergodic* limit

$$\varrho_\alpha = \lim_{T \to +\infty} \frac{1}{T} \int_0^T dt \; \varrho_\alpha(t) \; .$$

• If we can verify that the limit ϱ_α exists and commutes with H, then we regard the state ϱ_α as the desired **NESS** of the fully coupled system $\{\mathfrak{H}, H\}$.

Digression: The unitary evolution I

- Let $\mathbb{R} \ni t \mapsto u(t) \in W^{1,2}(\mathbb{R})$ be weakly differentiable map.
- We are interested in the evolution equation

$$i\frac{\partial}{\partial t}u(t) = H_\alpha(t)u(t), \quad t \in \mathbb{R}, \quad \alpha > 0.$$

where $H_\alpha(t)$ is regarded as a *bounded* operator acting from $W^{1,2}(\mathbb{R})$ into $W^{-1,2}(\mathbb{R})$.

Digression: The unitary evolution II

THEOREM: There is a unique unitary solution operator, or *propagator* $\{U(t,s)\}_{(t,s)\in\mathbb{R}\times\mathbb{R}}$, leaving invariant the Hilbert space $W^{1,2}(\mathbb{R})$ and such that:

$$\frac{\partial}{\partial t}\langle U(t,s)x,y\rangle = -i\langle H_\alpha(t)U(t,s)x,y\rangle, \quad x,y\in W^{1,2}(\mathbb{R}),$$
$$\frac{\partial}{\partial s}\langle U(t,s)x,y\rangle = i\langle H_\alpha(s)x,U(s,t)y\rangle, \quad x,y\in W^{1,2}(\mathbb{R}),$$
$$U(s,s) = 1.$$

H.Neidhardt and V.A.Zagrebnov : *Linear non-autonomous Cauchy problems and evolution semigroups*. **JEE** (submitted)

Quantum Liouville equation

REMARKS:

- We note that relation:

$$\varrho_\alpha(t) := U(t,s)\varrho_\alpha(s)U(s,t), \quad t, s \in \mathbb{R},$$

can be seen as a map from $W^{1,2}(\mathbb{R})$ into $W^{-1,2}(\mathbb{R})$.

- Then it is differentiable.
- It solves the quantum *Liouville* equation satisfying the initial condition $\varrho_\alpha(t)|_{t=s} = \varrho_\alpha(s)$, provided $\varrho_\alpha(s)$ leaves $W^{1,2}(\mathbb{R})$ invariant.

Time-dependent scattering and the Liouville equation

PROPOSITION:

Let $U(t) := U(t, 0)$, $t \in \mathbb{R}$. Consider the wave operators

$$\Omega_- := \text{s-}\lim_{t \to -\infty} U(t)^* e^{-itH_D}$$

and

$$\Omega_+ := \text{s-}\lim_{t \to +\infty} U(t)^* e^{-itH}.$$

• Then the both exist, and Ω_+ is unitary.

• If the initial density-matrix condition is decoupled at $t = -\infty$, then one obtains:

$$\varrho_\alpha(t) = U(t)\Omega_- \varrho_D \Omega_-^* U(t)^*, \quad t \in \mathbb{R}.$$

Incoming (stationary) wave operator

Definition: We introduce the *incoming* wave operator by

$$W_- := \text{s-}\lim_{t \to -\infty} e^{itH} e^{-itH_D} P^{ac}(H_D)$$

where $P^{ac}(H_D)$ is the projection on the absolutely continuous subspace $\mathfrak{H}^{ac}(H_D)$ of H_D.

• Note that $\mathfrak{H}^{ac}(H_D) = L^2((-\infty, a]) \oplus L^2([b, \infty))$.

• The wave operator exists and is complete, that is, W_- is an isometric operator acting from $\mathfrak{H}^{ac}(H_D)$ onto $\mathfrak{H}^{ac}(H)$, where $\mathfrak{H}^{ac}(H)$ is the absolutely continuous subspace of H (the range of $P^{ac}(H)$).

The main result I

Theorem 0.4. *Let* $E_H(\cdot)$ *and* $\{\lambda_j\}_{j=1}^N$ *be the spectral measure and the eigenvalues of* H. *If* ϱ_D *is a steady state for the system* $\{\mathfrak{H}, H_D\}$ *such that the operator* $\widehat{\varrho}_D := (H_D + \tau)^4 \varrho_D$ *is bounded, then the limit*

$$\varrho_\alpha := \text{s-}\lim_{T\to+\infty} \frac{1}{T} \int_0^T dt \varrho_\alpha(t)$$

$$= W_- \varrho_D W_-^* + \sum_{j=1}^N E_H(\{\lambda_j\}) S_\alpha \varrho_D S_\alpha^* E_H(\{\lambda_j\})$$

exists and defines a steady state for the coupled system $\{\mathfrak{H}, H\}$ *,*
where $S_\alpha := \Omega_+^* \Omega_-$.

Comments

• We stress that only the part corresponding to the pure point spectrum $\varrho_\alpha^p := \sum_{j=1}^N E_H(\{\Lambda_j\}) S_\alpha \varrho_D S_\alpha^* E_H(\{\lambda_j\})$ of our NESS depends on the parameter $\alpha > 0$.

• The absolutely continuous part $\varrho_\alpha^{ac} := W_- \varrho_D W_-^*$ does not depend on the parameter on $\alpha > 0$.

• Note that with respect to the decomposition $\mathfrak{H} = \mathfrak{H}^p(H) \oplus \mathfrak{H}^{ac}(H)$, one has $\varrho_\alpha = \varrho_\alpha^p \oplus \varrho_\alpha^{ac}$.

More about the main result on $\mathfrak{H}^{ac}(H)$

- On $\mathfrak{H}^{ac}(H)$ we have a stronger result :

Theorem 0.5. *If ϱ_D is a steady state for the system $\{\mathfrak{H}, H_D\}$ such that the operator $\widehat{\varrho}_D := (H_D + \tau)^4 \varrho_D$ is bounded, then*

$$\text{s-}\lim_{t \to +\infty} \varrho_\alpha(t) P^{ac}(H) = W_- \varrho_D W_-^*.$$

Spectral representation

Corollary 0.6. *With respect to the spectral representation $\{L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu), M\}$ of H the distribution function $\{\tilde{\rho}_\alpha(\lambda)\}_{\lambda\in\mathbb{R}}$ of the steady state ϱ_α is given by*

$$\tilde{\rho}_\alpha(\lambda) := \begin{cases} 0, & \lambda \in \mathbb{R} \setminus \sigma(H) \\ \rho_{\alpha,j}, & \lambda = \lambda_j, \quad j = 1, \ldots, N \\ \mathfrak{f}_b(\lambda - \mu_b), & \lambda \in [v_b, v_a) \\ \begin{pmatrix} \mathfrak{f}_b(\lambda - \mu_b) & 0 \\ 0 & \mathfrak{f}_a(\lambda - \mu_a) \end{pmatrix}, & \lambda \in [v_a, \infty) \end{cases}$$

where $\rho_{\alpha,j} := \langle S_\alpha \phi_j, \phi_j \rangle$, $j = 1, 2, \ldots, N$, $v_a \geq v_b$.

The stationary current I

- Let $\eta > 0$, and choose an integer $N \geq 2$. Denote by χ_b the characteristic function of the interval (b, ∞) (the right reservoir).

- Without loss of generality, we assume that $H > 0$.

Definition 0.7. *The trace class operator*

$$j(\eta) := i[H(1 + \eta H)^{-N}, \chi_b]$$

is called the regularized current operator. The stationary current coming out of the right reservoir is defined by

$$\mathfrak{I}_\alpha := \lim_{\eta \searrow 0} \mathrm{Tr}(\varrho_\alpha j(\eta)).$$

Aschbacher, W., Jakšić, V., Pautrat, Y., Pillet, C.-A.: ”Transport properties of quasi-free fermions”, J. Math. Phys. **48**, 032101 (2007)

The stationary current II

- Let $c > b + 1$. Choose any function $\phi_c \in C^\infty(\mathbb{R})$ such that

$$0 \leq \phi_c \leq 1, \quad \phi_c(x) = 1 \text{ if } x \geq c + 1, \quad \operatorname{supp}(\phi_c) \subset (c - 1, \infty).$$

- Then the stationary current is given by:

$$\mathfrak{I} =$$
$$i\mathrm{Tr}\left\{W_- \varrho_D (1 + H_D)^3 W_-^* P^{ac}(H) (1 + H)^{-2} [H, \phi_c] (1 + H)^{-1}\right\}$$
$$= i\mathrm{Tr}\left\{W_- \varrho_D W_-^* P^{ac}(H) [H, \phi_c]\right\}.$$

- Problem : Compute the trace!

The Landau-Lifschitz formula I

- We have computed the *integral kernel* of

$$\mathcal{A} := iW_-\varrho_D W_-^* P^{ac}(H)\frac{1}{2m_b}\left(-\frac{d}{dx}\phi_c' - \phi_c'\frac{d}{dx}\right)$$

in the spectral representation of H.

- We obtain:

$$\mathcal{A}(\lambda, p; \lambda', p') =$$

$$= -\frac{i\tilde{\varrho}_D^{ac}(\lambda)_{pp}}{2m_b}\int_{\mathbb{R}} \overline{\tilde{\phi}_p(x,\lambda)}\left(\frac{d}{dx}\phi_c'(x) + \phi_c'(x)\frac{d}{dx}\right)\tilde{\phi}_{p'}(x,\lambda')dx$$

$$= -\frac{i\tilde{\varrho}_D^{ac}(\lambda)_{pp}}{2m_b}\int_{\mathbb{R}} \phi_c'(x)\{\overline{\tilde{\phi}_p(x,\lambda)}\tilde{\phi}_{p'}'(x,\lambda') - \overline{\tilde{\phi}_p'(x,\lambda)}\tilde{\phi}_{p'}(x,\lambda')\}dx.$$

Main result: The Landau-Lifschitz formula II

• In order to compute the trace, we put $\lambda = \lambda'$, $p = p'$, and integrate/sum over the variables.

• Then we obtain:

$$\mathfrak{I} = \int_{\mathbb{R}} \phi_c'(x) j(x) dx,$$

where

$$j(x) := \frac{1}{m_b} \int_{v_b}^{\infty} \sum_p \tilde{\varrho}_D^{ac}(\lambda)_{pp} \Im\{\overline{\tilde{\phi}_p(x,\lambda)} \tilde{\phi}_p'(x,\lambda)\} d\lambda.$$

• Density $j(x)$ is a constant, depending only on invariant, scattering quantities.

The Landauer-Büttiker formula

... was obtained from Landau-Lifschitz formula in

Baro, M.; Kaiser, H.-Chr.; Neidhardt, H.; Rehberg, J: A quantum transmitting Schrödinger-Poisson system, Rev. Math. Phys. **16** (2004), no. 3, 281–330.

Further questions ?

1. the multidimensional case
2. …

THANK YOU FOR YOUR ATTENTION !