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

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Topics

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 formulas (Landau-Lifschitz, Landauer-Büttiker).

The model

In $\mathfrak{H} := L^2(\mathbb{R})$ we consider the Schrödinger operator

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

with domain

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

It is assumed that the effective mass $M(x)$ and the real potential $V(x)$ admit decompositions of the form

$$M(x) := \begin{cases} m_a & x \in (-\infty, a] \\ m(x) & x \in (a, b) \\ m_b & x \in [b, \infty) \end{cases}, \tag{3}$$

The model

$0 < m_a, m_b < \infty$, $m(x) > 0$, $x \in (a,b)$, $m + \frac{1}{m_{a(b)}} \in L^\infty((a,b))$,

and

$$V(x) := \begin{cases} v_a & x \in (-\infty, a] \\ v(x) & x \in (a,b) \\ v_b & x \in [b, \infty) \end{cases}, \quad v_a \geq v_b, \tag{4}$$

$v_a, v_b \in \mathbb{R}$, $v \in L^\infty((a,b))$. The quantum well is identified with the interval (a,b), (or physically, with the three-dimensional region $(a,b) \times \mathbb{R}^2$). 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

Besides its mathematical beauty, the model is 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 a NESS?

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

Definition 0.2. *A state* ϱ *is called a steady state for* H *if* ϱ *commutes with* H*, i.e.* ϱ *belongs to the commutant of the algebra generated by the functional calculus associated to* H*. A steady state is an equilibrium state if it belongs to the bicommutant of this algebra.*

What is a NESS?

H is unitarily equivalent to the multiplication M induced by the independent variable λ in the direct integral $L^2(\mathbb{R}, \mathfrak{h}(\lambda), \nu)$,

$$\mathfrak{h}(\lambda) := \begin{cases} \mathbb{C}, & \lambda \in (-\infty, v_a] \\ \mathbb{C}^2, & \lambda \in (v_a, \infty) \end{cases}, \tag{5}$$

and (with the usual abuse of notation)

$$d\nu(\lambda) = \sum_{j=1}^{N} \delta(\lambda - \lambda_j)d\lambda + \chi_{[v_b,\infty)}(\lambda)d\lambda, \quad \lambda \in \mathbb{R}, \tag{6}$$

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

What is a NESS?

If ϱ is a steady state for H, then there exists a ν-measurable function

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

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

$$\varrho = \Phi^{-1} M(\tilde{\rho}) \Phi. \tag{7}$$

If ϱ is an equilibrium state for H, then $\tilde{\rho}(\lambda)$ is proportional to the identity matrix.

The decoupled system

We start with a completely decoupled system:

$$\mathfrak{H}_a := L^2((-\infty, a]), \quad \mathfrak{H}_{\mathcal{I}} := L^2(\mathcal{I}), \quad \mathfrak{H}_b := L^2([b, \infty)) \tag{8}$$

where $\mathcal{I} = (a, b)$. We note that

$$\mathfrak{H} = \mathfrak{H}_a \oplus \mathfrak{H}_{\mathcal{I}} \oplus \mathfrak{H}_b. \tag{9}$$

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

$$(H_a f)(x) := -\frac{1}{2m_a} \frac{d^2}{dx^2} f(x) + v_a f(x), \tag{10}$$

$$f \in \mathrm{Dom}\,(H_a) := \{f \in W^{2,2}((-\infty, a)) : f(a) = 0\} \tag{11}$$

The decoupled system

with $\mathfrak{H}_{\mathcal{I}}$ the Hamiltonian $H_{\mathcal{I}}$,

$$(H_{\mathcal{I}} f)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx} f(x) + v(x) f(x), \tag{12}$$

$$f \in \mathrm{Dom}\,(H_{\mathcal{I}}) := \left\{ f \in W^{1,2}(\mathcal{I}) : \begin{array}{l} \frac{1}{m} f' \in W^{1,2}(\mathcal{I}) \\ f(a) = f(b) = 0 \end{array} \right\} \tag{13}$$

and with $\mathfrak{H}_b$ the Hamiltonian H_b,

$$(H_b f)(x) := -\frac{1}{2m_b}\frac{d^2}{dx^2} f(x) + v_b f(x), \tag{14}$$

$$f \in \mathrm{Dom}\,(H_b) := \{ f \in W^{2,2}((b,\infty) : f(b) = 0 \}. \tag{15}$$

The decoupled system

In $\mathfrak{H}$ we set

$$H_D := H_a \oplus H_{\mathcal{I}} \oplus H_b \tag{16}$$

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 thermal equilibrium; according to Definition 0.2, the corresponding sub-states must be functions of their corresponding sub-Hamiltonians. The total state is the direct sum of the three sub-states.

The initial state

The equilibrium sub-states are ϱ_a, $\varrho_{\mathcal{I}}$ and ϱ_b where:

$$\varrho_a := \mathfrak{f}_a(H_a - \mu_a), \quad \varrho_{\mathcal{I}} := \mathfrak{f}_{\mathcal{I}}(H_{\mathcal{I}} - \mu_{\mathcal{I}}), \quad \varrho_b := \mathfrak{f}_b(H_b - \mu_b). \quad (17)$$

A physical example 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 $c_j := \frac{q\, m_j^*}{\pi\, \beta}$, where the m_j^*'s are one dimensional effective masses. The initial state is:

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

Time-dependent coupling

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

Let us assume that at $t = -\infty$ the quantum system $\{\mathfrak{H}, H_D\}$ is described by the NESS ϱ_D. Then we connect 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

$$H_\alpha(t) := H + e^{-\alpha t}\delta(x-a) + e^{-\alpha t}\delta(x-b), \quad t \in \mathbb{R}, \quad \alpha > 0. \quad (18)$$

Time-dependent coupling

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

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

where the domain $\mathrm{Dom}\,(H_\alpha(t))$ is given by

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

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

Time-dependent coupling

One can prove the following operator norm convergence:

$$n - \lim_{t \to -\infty} (H_\alpha(t) - z)^{-1} = (H_D - z)^{-1} \tag{19}$$

and

$$n - \lim_{t \to +\infty} (H_\alpha(t) - z)^{-1} = (H - z)^{-1}, \tag{20}$$

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

Time-dependent coupling

Our density matrix will be given by a mapping

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

which is differentiable in the space $B(W^{1,2}(\mathbb{R}), W^{-1,2}(\mathbb{R}))$ and solves the (weak) quantum Liouville equation:

$$i\frac{\partial}{\partial t}\varrho_\alpha(t) = [H_\alpha(t), \varrho_\alpha(t)], \quad t \in \mathbb{R}, \tag{21}$$

for a fixed $\alpha > 0$ satisfying the initial condition

$$\text{s-}\lim_{t\to-\infty} \varrho_\alpha(t) = \varrho_D. \tag{22}$$

Time-dependent coupling

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

$$\varrho_\alpha = \lim_{T\to+\infty} \frac{1}{T}\int_0^T \varrho_\alpha(t)dt. \tag{23}$$

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

The unitary evolution

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

$$i\frac{\partial}{\partial t}u(t) = H_\alpha(t)u(t), \quad t \in \mathbb{R}, \quad \alpha > 0. \tag{24}$$

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

The unitary evolution

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:

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

Neidhardt, H.; Zagrebnov, V. A.: Linear non-autonomous Cauchy problems and evolution semigroups. To appear.

Quantum Liouville equation

We note that

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

seen as a map from $W^{1,2}(\mathbb{R})$ into $W^{-1,2}(\mathbb{R})$ is differentiable and 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

We set $U(t) := U(t,0)$, $t \in \mathbb{R}$ and consider the wave operators

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

and

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

Both exist, and Ω_+ is unitary.

The solution to the Liouville equation

...which also obeys the initial condition:

$$\varrho_\alpha(t) = U(t)\Omega_- \varrho_D \Omega_-^* U(t)^*, \quad t \in \mathbb{R}. \tag{25}$$

Incoming, stationary wave operator

We need to introduce the incoming wave operator

$$W_- := \text{s-}\lim_{t\to-\infty} e^{itH} e^{-itH_D} P^{ac}(H_D) \tag{26}$$

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

Theorem 0.3. *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*

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

$$= W_- \varrho_D W_-^* + \sum_{j=1}^N E_H(\{\lambda_j\}) S_\alpha \varrho_D S_\alpha^* E_H(\{\lambda_j\}) \qquad (27)$$

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

A comment

We stress once again 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 $\alpha > 0$, while the absolutely continuous part $\varrho_\alpha^{ac} := W_- \varrho_D W_-^*$ does not. Note that with respect to the decomposition $\mathfrak{H} = \mathfrak{H}^p(H) \oplus \mathfrak{H}^{ac}(H)$, one has $\varrho_\alpha = \varrho_\alpha^p \oplus \varrho_\alpha^{ac}$.

The result is stronger on $\mathfrak{H}^{ac}(H)$

Theorem 0.4. *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*

$$\text{s-}\lim_{t \to +\infty} \varrho_\alpha(t) P^{ac}(H) = W_- \varrho_D W_-^*. \tag{28}$$

A conjecture

The case $\alpha \searrow 0$ would correspond to the adiabatic limit. Inspired by the physical literature which seems to claim that the adiabatic limit would take care of the above mentioned oscillations, we *conjecture* the following result for the transient current:

Conjecture 0.5.

$$\lim_{\alpha \searrow 0} \limsup_{t \to \infty} \left| \mathrm{Tr}\{\varrho_\alpha(t) P^d(H) [H, \chi]\} \right| = 0,$$

where χ is any smoothed out characteristic function of one of the reservoirs.

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

The stationary current

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, let us assume that $H > 0$.

Definition 0.7. *The trace class operator*

$$j(\eta) := i[H(1+\eta H)^{-N}, \chi_b] \tag{29}$$

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

$$\mathfrak{I}_\alpha := \lim_{\eta \searrow 0} \mathrm{Tr}(\varrho_\alpha j(\eta)). \tag{30}$$

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

The Landau-Lifschitz formula

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

$$0 \leq \phi_c \leq 1, \quad \phi_c(x) = 1 \text{ if } x \geq c + 1, \quad \text{supp}(\phi_c) \subset (c - 1, \infty). \tag{31}$$

Then the stationary current is given by:

$$\mathfrak{I} =$$

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

$$= i\text{Tr}\left\{W_- \varrho_D W_-^* P^{ac}(H)[H, \phi_c]\right\}.$$

Compute the trace!

The Landau-Lifschitz formula

We compute 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 and get

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

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

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

The Landau-Lifschitz formula

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

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

where

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

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

The Landauer-Büttiker formula

... was obtained from Landau-Lifschitz 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. ”long-range” switching in time;
3. ”long-range” samples/quantum wells;
4. extensions to geometric scattering in hyperbolic manifolds;