Long time adiabatic evolution and resonances

joint project with Michael Hitrik and Andrea Mantile

Johannes Sjöstrand
IMB, Université de Bourgogne

Conference in memory of Louis Boutet de Monvel,
ENS, Paris, 20–24.06.2016

Introduction: Dedication

This talk is dedicated Louis Boutet de Monvel, a great mathematician from whom I have had a lot of inspiration through his works, through discussions, seminar talks and through a fruitful collaboration.
He was a kind and generous person who largely contributed to make me feel welcome in Paris more than 40 years ago.

Introduction: Background and goals

With C. Presilla [PrSj96] (following a work with Presilla and G. Jona-Lasinio) we considered a non-linear evolution problem for a mesoscopic semi-conductor device and did some *heuristic* work. On $\mathbf{R}$, we consider "metallic conductors" at $]-\infty, a]$, $[b, c]$ and $[d, +\infty[$ where $a < b < c < d$. Here a, b, d are fixed and $c = b + h$, $h \to 0$. $[a, b]$ and $[c, d]$ represent semi-conductors. Let V_1 be an exterior voltage applied between the two infinite conductors.

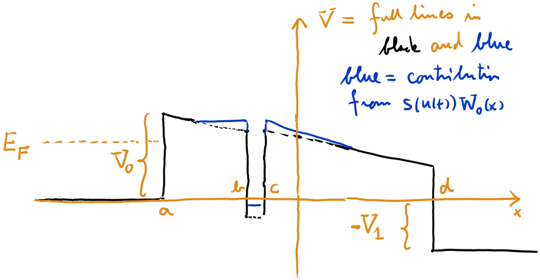
Incoming charged particles from the left of energy $E \geq 0$ with the distribution $g(E)dE$, supported on $[0, E_F]$, where $E_F < V_0$ is the Fermi energy. We assume that they interact only inside the device (i.e. on $[a, d]$) through a modification of the common potential due to charge accumulation there.

This leads to a Schrödinger equation, writing $D_* = -i\partial/\partial *$, $* = t, x$,

$$\left(hD_t + (hD_x)^2 + V(x, s(u(t,\cdot)))\right) u(t,x,E) = 0, \qquad (1)$$

where

$$V(x,s) = V(x,0) + sW_0(x),$$



$$s(u(t,\cdot)) = \int \int_{(a+b)/2}^{(c+d)/2} |u(t,x,E)|^2 g(E) dx dE, \qquad (2)$$

is the accumulated charge inside the device and $W_0(x) \geq 0$ is a fixed "profile" with support in $]a, d[$. We ([PrSj96]) used the 1-mode approximation

$$u(t, x, E) \approx e^{-iEt/h} z(t, E) e(x, s(u(t, \cdot))), \tag{3}$$

where $e = e(x, s(u(t, \cdot)))$ is a *resonant state* ($\notin L^2$) corresponding to a *resonance* $\lambda(s(u(t, \cdot)))$ in the lower half-plane. We derived a simpler evolution equation

$$\begin{aligned} h\partial_t z(t, E) &= i(E - \lambda(s)) z(t, E) + \mathcal{B}(t, s, E), \\ s = s(t) &\sim \int |z(t, E)|^2 g(E) dE. \end{aligned} \tag{4}$$

Related to an even simpler differential equation for $s(t)$. We could describe *fixed points* of the vector field in (4), and *hysteresis phenomena* under slow variations of the exterior bias $V_1 = V_1(t)$.

The mathematical treatment of the model (1) is a very vast program.

Some rigorous works:

- Bonnaillie-Nier-Patel [BoNiPa08, BoNiPa09], the stationary problem: fixed points,
- Faraj-Mantile-Nier [FaMaNi11].

We seem to need a strong adiabatic theorem with adiabatic parameter ε satisfying $\ln \varepsilon \asymp -1/h$.

- There are many works (E. Skibsted [Sk89], C. Gérard-I.M. Sigal [GeSi92], A. Soffer-M.I. Weinstein [SoWe98], G. Perelman [Pe00], S. Nakamura-P. Stefanov-M. Zworski [NaStZw03]) on time evolution in relation with resonances.
- We are interested in exact solutions of (1), (10) and their approximation with the formal ones. Adiabatic theorems have been obtained by G. Nenciu [Ne81], [Ne93], A. Joye, C.E. Pfister [JoPf97], Joye [Jo07]. Galina Perelman [Pe00] has an adiabatic theorem in the L^2-setting. She got adiabatic approximation over time intervals of length $\varepsilon^{-\delta}$ for some fixed $\delta > 0$.

To improve this result, we work in adapted Hilbert spaces that contain the relevant resonant states, with the goal of having an adiabatic approximation to all orders in ε, over time intervals of length ε^{-N} for any fixed $N \geq 0$. Then the evolution is no longer unitary and our main result so far says that we can arrange so that the generator of our evolution has an imaginary part which is $\leq \varepsilon^N$ for any N. We will describe this result and give an outline of the remaining work that should lead to the adiabatic goal.

Resonances for the Schrödinger operator

Let $P = -h^2\Delta + V(x)$ on $\mathbf{R}^n$, where $0 < h \leq 1$ and $V \in C^\infty(\mathbf{R}^n; \mathbf{R})$ has a holomorphic extension to a truncated sector, $\{x \in \mathbf{C}^n;\ |\Re x| > C,\ |\Im x| < |\Re x|/C\}$, where it tends to 0 as $x \to \infty$. The resonances of P are the poles of the meromorphic extension of $(z-P)^{-1} : L^2_{\mathrm{comp}}(\mathbf{R}^n) \to H^2_{\mathrm{loc}}(\mathbf{R}^n)$ from the open upper half-plane across $]0, +\infty[$ to a sector $\{z \in \mathbf{C} \setminus \{0\};\ -\theta_0 < \arg(z) \leq 0\}$, where $\theta_0 > 0$. They can also be viewed as poles of a meromorphic extension of the scattering matrix, when V is sufficiently short range.

P is self-adjoint in $L^2(\mathbf{R})$ and hence has real spectrum, nevertheless a standard approach to resonances is to find a suitable Hilbert space $\mathcal{H}$ containing the Hermite functions as a dense subspace and such that P acts on $\mathcal{H}$ as a closed unbounded operator with no spectrum in the open upper half-plane and discrete spectrum in the intersection of the lower half-plane with a disc $D(E_0, r_0)$, $E_0 > 0$, $r_0 > 0$.

Eigenfunctions in $\mathcal{H}$ = Resonant states.

The classical method of complex distorsions: Aguilar–Combes, Balslev–Combes, Simon, Hunziker, ... We replace $\mathbf{R}^n$ by a smooth manifold $\Gamma \subset \mathbf{C}^n$ of real dimension n, naturally diffeomorphic to $\mathbf{R}^n$, containing the ball $B_{\mathbf{R}^n}(0, C)$, and contained in the union of $\mathbf{R}^n$ and the truncated sector above. Typically we choose Γ so that Γ coincides with $e^{i\theta}\mathbf{R}^n$ far away, where $\theta > 0$ is small enough. Then $\mathcal{H} := L^2(\Gamma)$. ([SjZw91]).

A more intuitive approach with microlocal analysis, was developed by Helffer and the speaker [HeSj86]: Use of phase space weights and suitable FBI-transforms. Roughly, if $G(x, \xi)$ is such a weight and $s > 0$ small, we put

$$\mathcal{H} = H(\Lambda_{sG}, 1) = e^{(s/h)G(x, hD_x)} L^2(\mathbf{R}^n).$$

Here $\Lambda_{sG} = \{\rho + isH_G(\rho);\ \rho \in \mathbf{R}^{2n}\}$ is a *deformation of the real phase space*. Choose G with support in

$$\{(x,\xi) \in \mathbf{R}^{2n};\ |x| \geq C,\ |\xi| \leq \mathcal{O}(1)\}$$

in the class $S(\langle x \rangle)$, meaning that $\partial_x^\alpha \partial_\xi^\beta G = \mathcal{O}(\langle x \rangle^{1-|\alpha|} \langle \xi \rangle^{1-|\beta|})$. Then $P : \mathcal{H} \to \mathcal{H}$ is an h-pseudodifferential operator with leading symbol

$$p_{|_{\Lambda_{sG}}} = p(\rho + isH_G(\rho)) = p(\rho) - isH_p G(\rho) + \mathcal{O}(s^2),$$
$$\text{where } p(x,\xi) = \xi^2 + V(x).$$

Let G be an *escape function* in the sense that

$$H_p G \geq 1/C,\ \text{when } |x| \geq C,\ p(x,\xi) = E_0$$

for some fixed energy $E_0 > 0$. Then $p(\Lambda_{sG} \setminus \text{a compact set})$ avoids a region $[E_0 - 1/C, E_0 + 1/C] + i[-s/C, +\infty[$ and $P : \mathcal{H} \to \mathcal{H}$ has discrete spectrum there, confined to the lower half-plane.

A semiboundedness result

We have chosen to study the time evolution in a space $\mathcal{H}$ that contains the relevant resonant states. Then we loose the unitarity and the very first problem is to avoid a too strong exponential growth in time. Our main result so far in the project with A. Mantile and M. Hitrik is:

Theorem

There is an escape function $G = G_\epsilon(x,\xi)$, $0 < \epsilon \ll 1$ *which vanishes when* $|x| \le 1/\epsilon$ *and when* $|p(x,\xi) - E_0| \ge 1/C$, *such that if* $\mathcal{H} = H(\Lambda_{sG_\epsilon})$, $0 < s \le 1$, *then*

$$P : \mathcal{H} \to \mathcal{H} \tag{5}$$

fulfills the bounds

$$\Im P \le s C_N h^N \epsilon^N, \tag{6}$$

for every $N \ge 1$. *Moreover,* G_ϵ *form a bounded family in* $S(\langle x \rangle)$.
P *in (5) has discrete spectrum in*
$]E_0 - 1/C, E_0 + 1/C[+i] - s/C, +\infty[$.

The use of spaces of [HeSj86] seems essential. A. Faraj, Mantile and F. Nier [FaMaNi11] have used complex distorsions and achieved $\Im P \le 0$ by modifying a transmission condition. This however changes the resonances and the problem under study.

Corollary

Let I be an interval. If $\ni t \to u(t)$ is of class $C^0(I;\mathcal{D}(P)) \cap C^1(I;\mathcal{H})$ and solves $(D_t + P)u(t,x) = 0$, then

$$\|u(t_2)\|_{\mathcal{H}} \leq e^{sC_N h^N \epsilon^N (t_2 - t_1)} \|u(t_1)\|_{\mathcal{H}}, \tag{7}$$

for $t_1 \leq t_2$, $t_1, t_2 \in I$.

The proof of the corollary is standard:

$$\partial_t \|u(t)\|^2 = 2\Im(Pu|u) \leq 2C_N s(h\epsilon)^N \|u(t)\|^2$$

which leads to the estimate (7).

Outline of the proof. Applying results and ideas from [HeSj86] and C. Gérard–Sj [GéSj87] we first construct an escape function G vanishing for $|x| \le 1$ such that $H_p G \ge (1/\mathcal{O}(1))\|H_G\|_g$ in $p^{-1}([E_0 - 1/C, E_0 + 1/C])$, where $g = (dx/\langle x\rangle)^2 + (d\xi/\langle \xi\rangle)^2$. Let $0 \le \chi \in C_0^\infty(]E_0 - 1/C_0, E_0 + 1/C_0[)$, be equal to one on a slightly smaller interval and put $G_0 = \chi(p)G$. Then G_0 is an escape function with

$$H_p G_0 = \chi(p) H_p G \ge \|H_{G_0}\|_g^2.$$

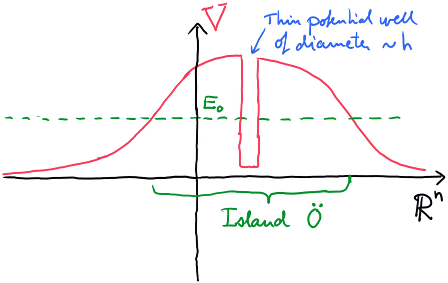
If $\mathcal{H} = H(\Lambda_{sG_0})$, we get $\Im P \le \mathcal{O}(1)sh$ and microlocally $\le s\mathcal{O}(h^\infty)$ away from $\mathrm{supp}\, G_0$. Successive improvements lead to $\widetilde{G} \sim G_0 + hG_1 + h^2 G_2 + \dots$ such that

$$\Im P \le s\mathcal{O}(h^\infty)$$

for P acting in $H(\Lambda_{s\widetilde{G}})$. Here $H_p G_1 \gg 1/C$ near $\mathrm{supp}\, G_0$, ...
To gain powers of ϵ, work in a region $|x| \ge 1/\epsilon$ and use that there is an effective Planck's constant $\widetilde{h} = h/\langle x\rangle$ which is $\le h/\epsilon$ for $|x| \ge 1/\epsilon$. □

Adiabatic evolution and shape resonances

Consider a potential V with a thin potential well in an island $\ddot{\mathrm{O}}$ (defined to be open)



Assume that V is analytic near the sea $\mathbf{R}^n \setminus \ddot{\mathrm{O}}$, and that $p = \xi^2 + V$ has no trapped classical trajectories at energy E_0 over the sea.

Then for $h > 0$ small enough, $P = -h^2\Delta + V$ has finitely many resonances $\lambda_j(h) = \lambda_{j,0} + \mathcal{O}(h)$ in a fixed neighborhood of E_0 with $\Im\lambda_j = \mathcal{O}(e^{-1/Ch})$.
We often have a full asymptotic expansion for λ_j and its imaginary part (with exponential prefactor) [HeSj86]. Pick one of these resonances λ_0 and assume to fix the ideas that $\Re\lambda_{0,0} = E_0$, that λ_0 is simple and separated from the other resonances by some fixed distance.
Now let $V = V_t = V_0 + W_t$, be smoothly time dependent for t in some interval I, and assume that $\mathrm{supp}\, W_t$ is contained in a fixed compact subset of the island. Also assume that W_t is small. Then, $P_t = -h^2\Delta + V_t$ has a simple resonance $\lambda_0(t)$, separated from the other ones by some fixed distance. Let G be an adapted escape function ([HeSj86]) and consider $P = P_t : \mathcal{D} \to \mathcal{H}$, $\mathcal{H} = H(\Lambda_{sG})$, $\mathcal{D} = H(\Lambda_{sG}, \langle\xi\rangle^2)$ (an associated Sobolev space).

Formal adiabatic solutions. We are interested in the evolution $(D_\tau + P(\varepsilon\tau))u = 0$ where $\varepsilon > 0$ is very small (actually exponentially small in h) or equivalently, in $(\varepsilon D_t + P(t))u = 0$ with $t = \varepsilon\tau \in I$. The formal adiabatic construction is well known ([Ne81, Ne93]):

Proposition

There exist two asymptotic series independent of the particular choice of $\mathcal{H}$,

$$\nu(t,\varepsilon) \sim \nu_0(t) + \varepsilon\nu_1(t) + \dots, \text{ in } C^\infty(I;\mathcal{D}),$$
$$\lambda(t,\varepsilon) \sim \lambda_0(t) + \varepsilon\lambda_1(t) + \dots, \text{ in } C^\infty(I),$$

where $\nu_0(t)$ is a non-vanishing resonant state of $P(t)$: $(P - \lambda_0(t))\nu_0(t) = 0$, such that

$$(\varepsilon D_t + P(t) - \lambda(t,\epsilon))\nu(t,\varepsilon) \sim 0 \text{ in } C^\infty(I;\mathcal{H}). \tag{8}$$

Proof.

Establishing (8) in the sense of formal power series amounts to solving a sequence of equations,

$$\begin{aligned}
&(P(t)-\lambda_0(t))\nu_0(t)=0,\\
&(P(t)-\lambda_0(t))\nu_1(t)+(D_t-\lambda_1(t))\nu_0(t)=0,\\
&\qquad\qquad \cdots\cdots\cdots
\end{aligned} \tag{9}$$

Let first $\nu_0(t)$ be a resonant state depending smoothly on t. Then $\lambda_1(t)$ is uniquely determined by the requirement that $(D_t-\lambda_1(t))\nu_0(t)\in\mathcal{R}(P(t)-\lambda_0(t))=$ closed hyperplane transversal to $\nu_0(t)$. Iterate ... □

$u:=\nu\exp-(i/\varepsilon)\int^t\lambda(\widetilde{t},\varepsilon)d\widetilde{t}$ is a formal solution of

$$(\varepsilon D_t+P(t))u=0, \tag{10}$$

which in principle decays exponentially when t increases.

Let ν_{ad}, λ_{ad} denote asymptotic sums of ν, λ and define the corresponding function u_{ad}, so that

$$(\varepsilon D_t + P(t))u_{\mathrm{ad}} = r, \ \ r = \mathcal{O}(\varepsilon^{\infty}) \text{ in } \mathcal{H}. \tag{11}$$

Suppose that the conclusion of Theorem 3.1 were valid with a space $\mathcal{H}$ as above, *independent of* ε. Then, cf. Corollary 3.2 and T. Kato [Ka70], we have a forward fundamental matrix $E(t_2, t_1)$, $t_1 \leq t_2$, $t_j \in I$ for $\varepsilon D_t + P(t)$ such that $\|E(t_2, t_1)\|_{\mathcal{L}(\mathcal{H},\mathcal{H})} \leq \exp[\mathcal{O}_N(h^N \epsilon^N)(t_2 - t_1)]$ for every $N \geq 1$, and we have the exact solution of (10),

$$u = u_{\mathrm{ad}} - \varepsilon^{-1} \int_{t_0}^{t} E(t, \widetilde{t})r(\widetilde{t})d\widetilde{t},$$

defined on $I \cap [t_0, +\infty[$ for every $t_0 \in I$. Choosing $\epsilon = \varepsilon^{\delta}$ for some fixed small $\delta > 0$, we get $\|u - u_{\mathrm{ad}}\| = \mathcal{O}(\varepsilon^{\infty})$ on $[t_0, t_1] \subset I$, as long as $t_1 - t_0 \leq \mathcal{O}(\varepsilon^{-N_0})$ for some fixed $N_0 \geq 1$.

Now $\mathcal{H}$ does depend on ϵ and we need some uniform control on $(z - P(t))^{-1}$ for z not too close to $\lambda_0(t, \varepsilon)$. This seems to work in the following way: With $\varepsilon \geq e^{-C/h}/C$, we choose $\epsilon = \varepsilon^\delta$ for some small $\delta > 0$, so that $\lambda_0(t) \in]E_0 - 1/C, E_0 + 1/C[+i] - \epsilon/C, +\infty[$ as in Theorem 3.1.
Let $G_{\mathrm{sbd}} := \epsilon G_{\mathrm{Th.\,3.1}}$, where $G_{\mathrm{Th.\,3.1}}$ denotes the escape function of Theorem 3.1.

$$(z - P)^{-1} = \mathcal{O}(1/\epsilon^{N_0}) : \ H(\Lambda_{G_{\mathrm{sbd}}}) \to H(\Lambda_{G_{\mathrm{sbd}}}). \tag{12}$$

Returning to the adiabatic construction, we get (possibly with a new fixed N_0),

$$\nu_j = \mathcal{O}(\epsilon^{-N_0 j}) = \mathcal{O}(\varepsilon^{-N_0 \delta j}) \text{ in } H(\Lambda_{G_{\mathrm{sbd}}}),$$

so $\varepsilon^j \nu_j = \mathcal{O}(\varepsilon^{j(1-N_0\delta)})$ and $r = \mathcal{O}(\varepsilon^\infty)$ in $H(\Lambda_{G_{\mathrm{sbd}}})$, provided that δ is small enough.

In conclusion, *it seems that we can justify the adiabatic approximation of exact solutions up to any power of ε over time intervals of length up to any fixed negative power of ε, for the case of a potential well in an island, with $\varepsilon \ge (1/C)e^{-C/h}$, $\forall$ fixed $C > 0$.*

Method of complex distorsions with small angles in similar contexts: Martinez, A. Lahmar-Benbernou, Martinez [LaMa02], Martinez, T. Ramond, Sj [MaRaSj09].

References I

- V. Bonnaillie-Noël, F. Nier, Y. Patel, *Far from equilibrium steady states of 1D-Schrödinger-Poisson systems with quantum wells. I,* Ann. Inst. H. Poincaré Anal. Non Linéaire, 25(2008), 937–968.
- V. Bonnaillie-Noël, F. Nier, Y. Patel, *Far from equilibrium steady states of 1D-Schrödinger-Poisson systems with quantum wells. II*, J. Math. Soc. Jpn., 61(2009), 65-106.
- L. Boutet de Monvel, P. Krée, *Pseudo-differential operators and Gevrey classes,* Ann. Inst. Fourier (Grenoble) 17(1)(1967), 295–323. *Singularités analytiques microlocales,* Astérisque, 95(1982).
- A. Faraj, A. Mantile, F. Nier, *Adiabatic evolution of 1D shape resonances: An artificial interface conditions approach,* Math. Models and Meth. in Appl. Sci., 21(3)(2011), 541–618.
- C. Gérard, I.M. Sigal, *Space-Time Picture of Semiclassical Resonances,* Comm. Math. Phys., 145(1992), 281-328.

References II

- C. Gérard, J. Sjöstrand, *Semiclassical resonances generated by a closed trajectory of hyperbolic type,* Comm. Math. Phys., 108(1987), 391-421.
- B. Helffer, J. Sjöstrand, *Résonances en limite semiclassique,* Bull. de la SMF 114(3), Mémoire 24/25(1986).
- A. Joye, C.E. Pfister, *Exponential estimates in adiabatic quantum evolution,* in XII Int. Congr. Mathematical Physics (ICMP '97) (Brisbane) (Int. Press, 1999), 309–315.
- A. Joye, *General adiabatic evolution with a gap condition,* Commun. Math. Phys., 275(2007), 139–162.
- T. Kato, *Linear evolution equations of "hyperbolic" type,* J. Fac. Sci. Univ. Tokyo Sect. I 17(1970), 241–258.
- A. Lahmar-Benbernou, A. Martinez, *On Helffer-Sjöstrand's theory of resonances,* Int. Math. Res. Not. 13(2002), 697–717.

References III

- A. Martinez, T. Ramond, J. Sjöstrand, *Resonances for non-analytic potentials,* Analysis and PDE, 2(1)(2009), 29–60. http://arxiv.org/abs/0805.1596
- S. Nakamura, P. Stefanov, M. Zworski, *Resonance expansions of propagators in the presence of potential barriers,* J. Funct. Anal. 205(1)(2003), 180–205.
- G. Nenciu, *Adiabatic theorem and spectral concentration. I. Arbitrary order spectral concentration for the Stark effect in atomic physics,* Comm. Math. Phys. 82(1)(1981), 121–135.
- G. Nenciu, *Linear adiabatic theory. Exponential estimates,* Comm. Math. Phys. 152(3)(1993), 479–496.
- G. Perelman, *Evolution of adiabatically perturbed resonant states,* Asymp. An., 22(2000), 177–203.
- C. Presilla, J. Sjöstrand, *Transport properties in resonant tunneling heterostructures,* J. Math. Phys., 37(10)(1996), 4816-4844.

References IV

- J. Sjöstrand, *Projecteurs adiabatiques du point de vue pseudodifférentiel,* CRAS t. 317, sér. I (1993), 217–220.
- J. Sjöstrand, M. Zworski, *Complex scaling and the distribution of scattering poles,* Journal of the AMS, 4(4)(1991), 729-769.
- E. Skibsted, *On the evolution of resonance states,* J. Math. An. Appl. 141(1989), 27–48.
- A. Soffer M.I. Weinstein, *Time dependent resonance theory,* Geom. Funct. Anal., 8(1998), 1086–1128.