# Adiabatic evolution of resonances in far from equilibrium systems

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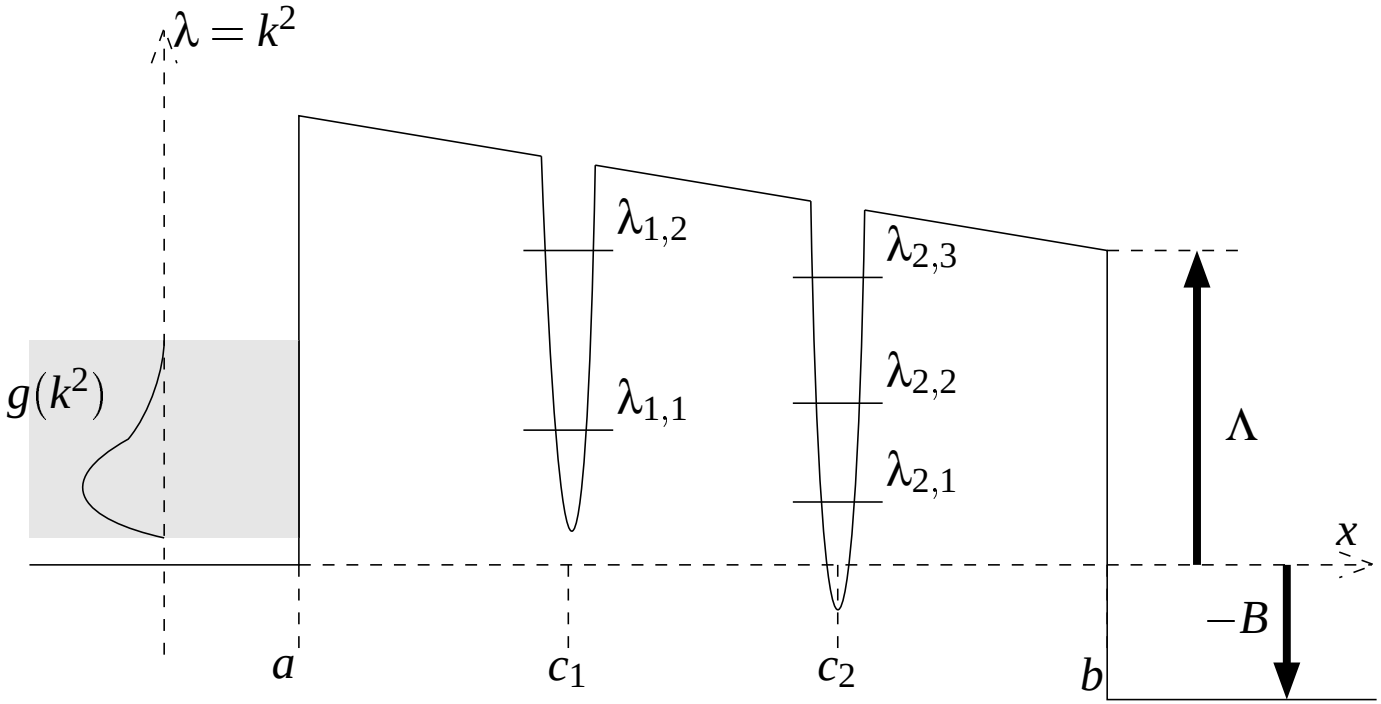
Joint work with A. Faraj and A. Mantile

(V. Bonnaillie, Y. Patel)

# Outline

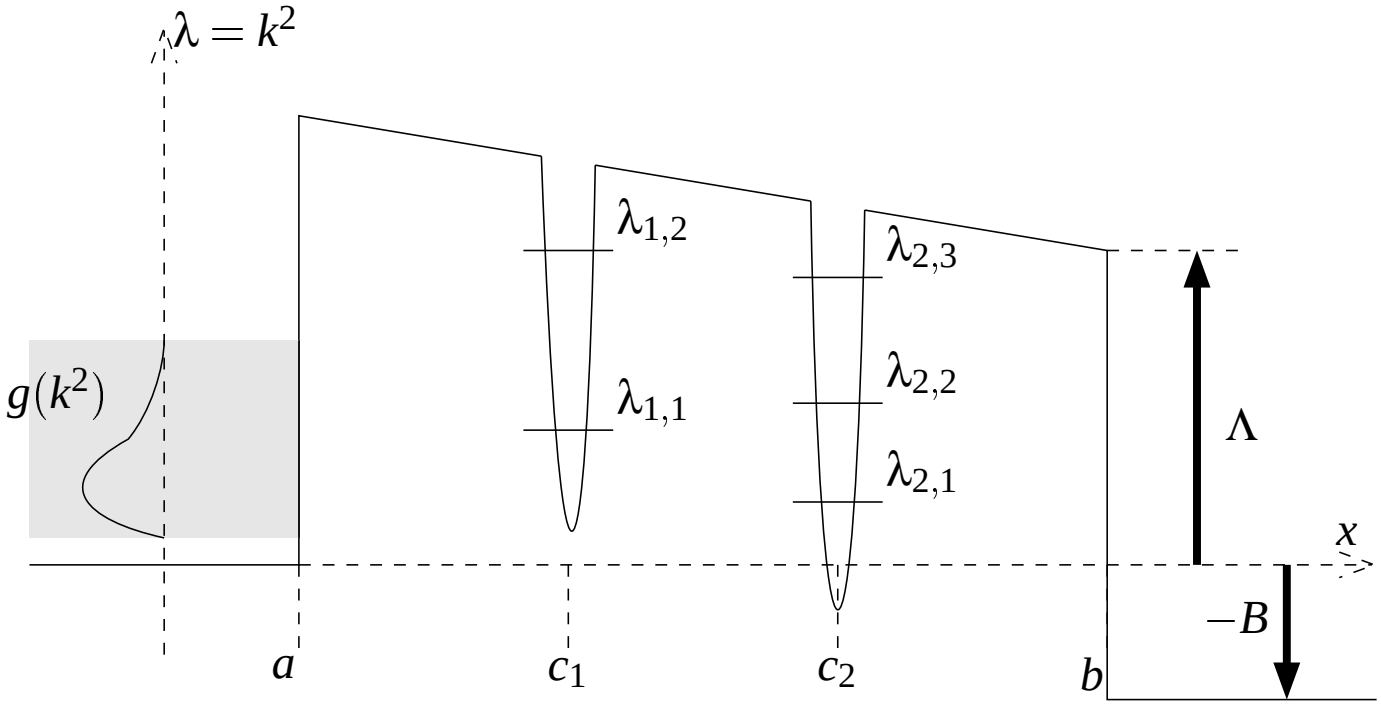
- RTD. Quantum inflow boundary conditions
- Asymptotic analysis
  - Introducing a small parameter
  - Asymptotic stationary model
  - Applications
- Adiabatic evolution of resonances
  - Outside complex deformation
  - Adiabatic problem
  - Artificial interface conditions
  - Comparison results
  - Adiabatic dynamics
  - Application

# Quantum inflow boundary conditions




Resonant tunneling diodes

# Quantum inflow boundary conditions




Resonant tunneling diodes

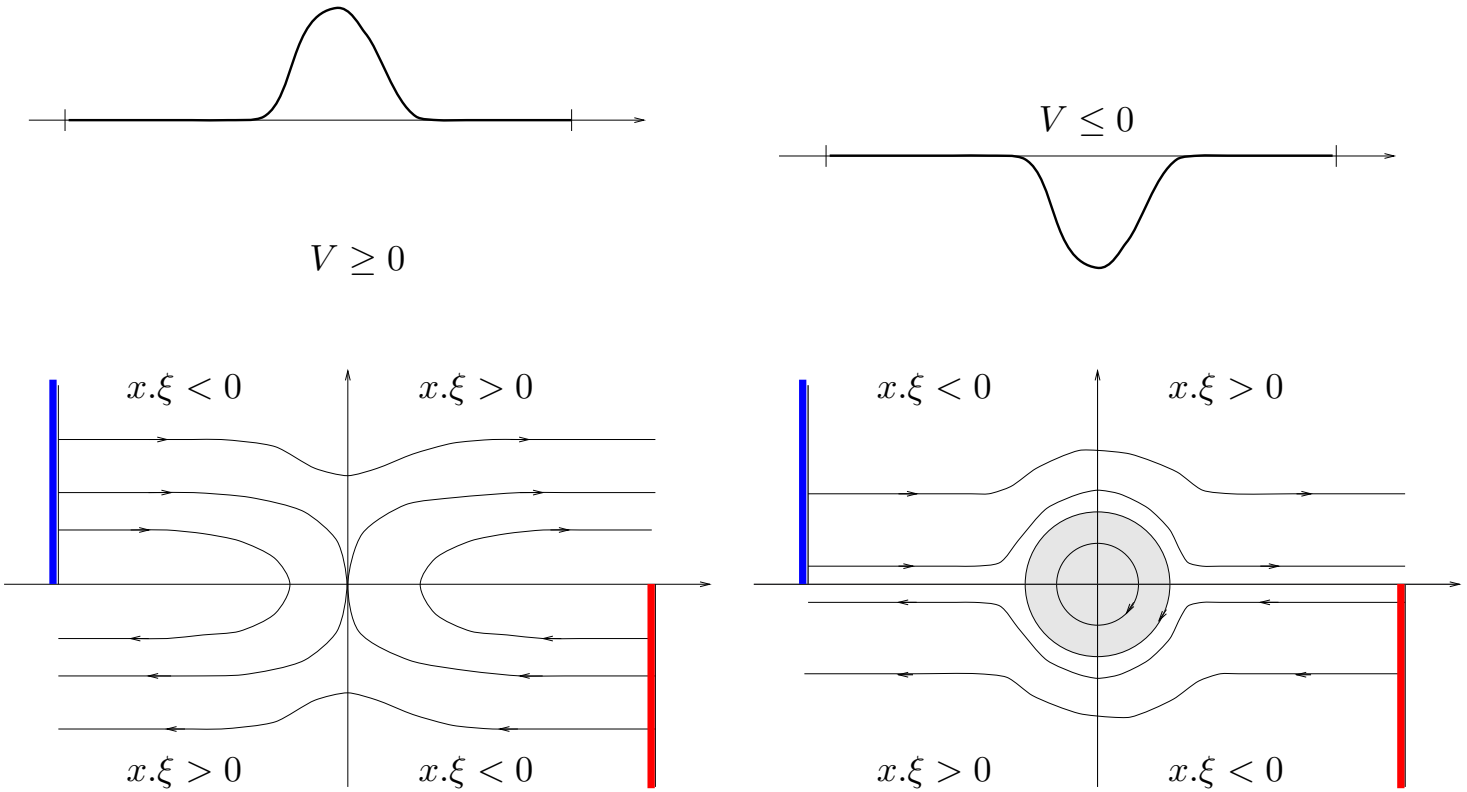
= Far from equilibrium quantum system

+ resonances and tunnel effect

+ nonlinearities

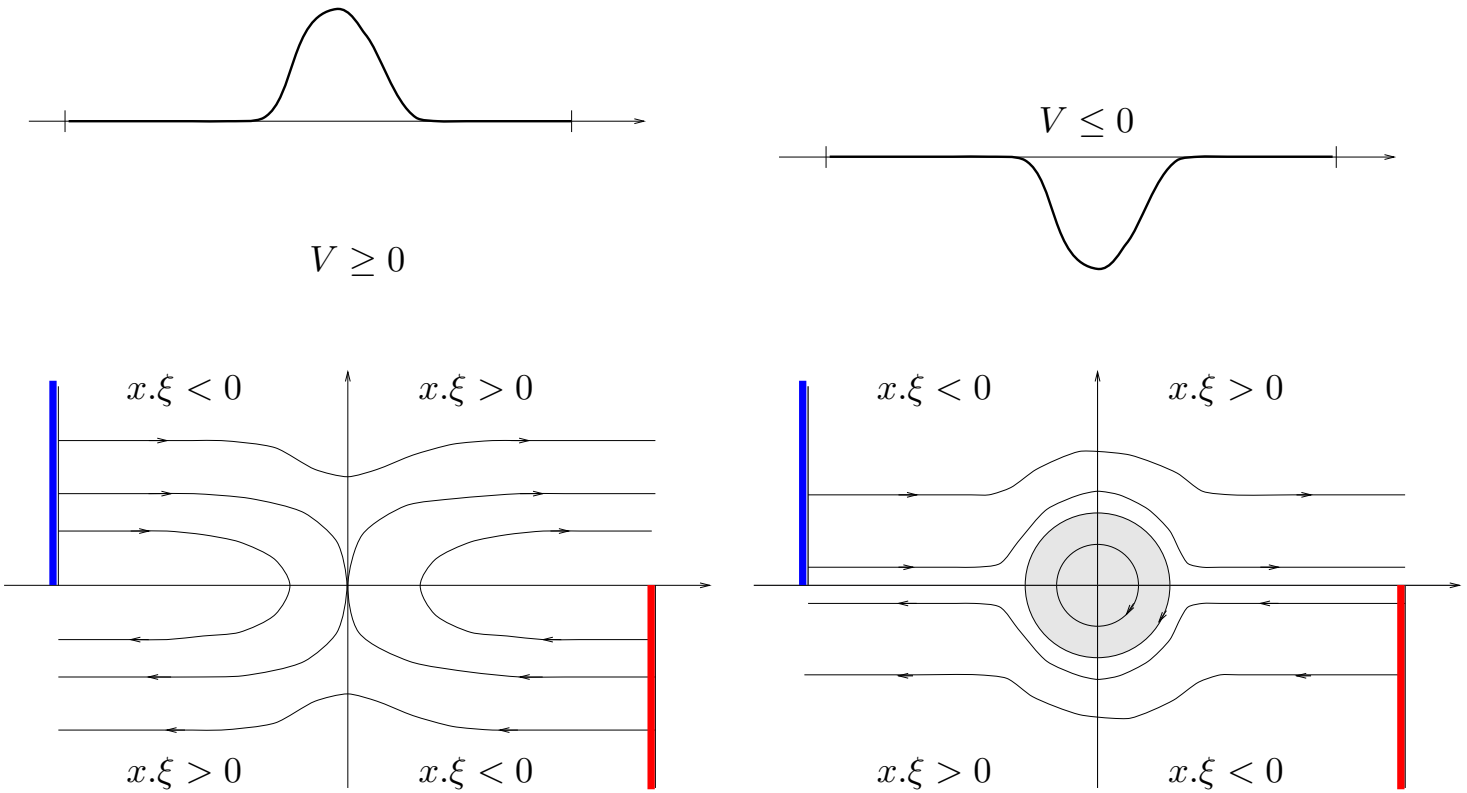
# Quantum inflow boundary conditions

Classical inflow BC for $\{h, f\} = 0$ or $\partial_t f + \{h, f\} = 0$



# Quantum inflow boundary conditions

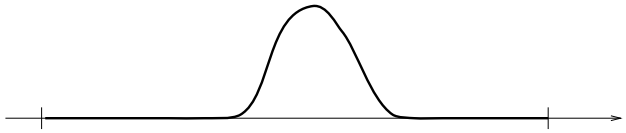
## Classical inflow BC



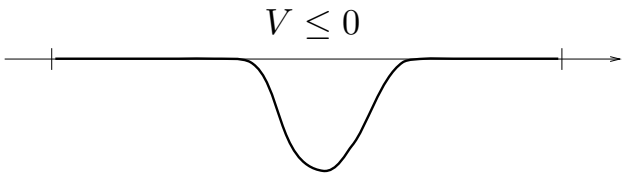

Inflow BC determines stationary solutions up to bound states

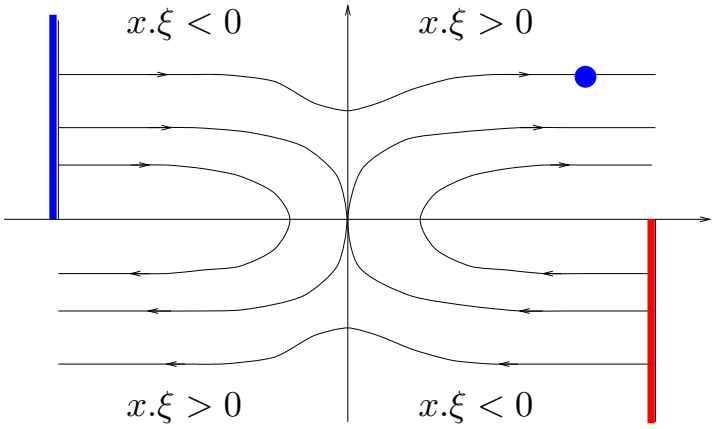
# Quantum inflow boundary conditions

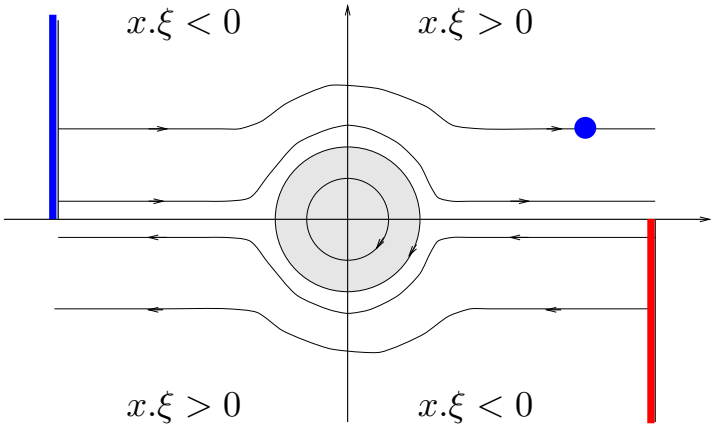
## Classical inflow BC



$V \geq 0$



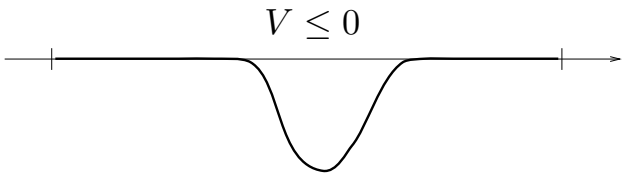



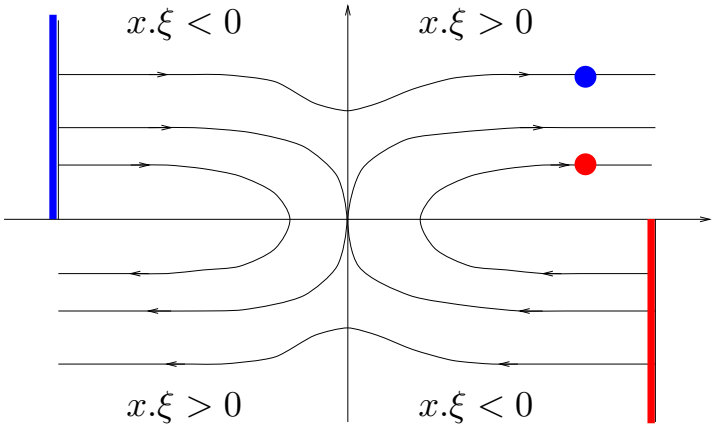

Non homegeneous BC: Work in an affine space

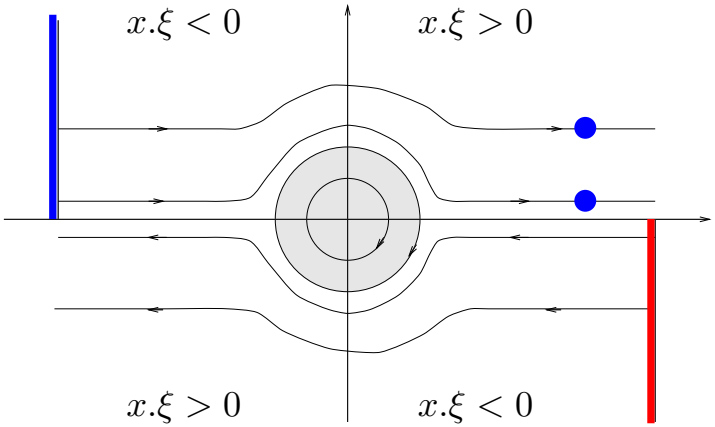
# Quantum inflow boundary conditions

## Classical inflow BC

$V \geq 0$




Variation of stationary solutions w.r.t $V$: Small in $x.\xi < 0$ large in $x.\xi > 0$.

# Quantum inflow boundary conditions

Quantum inflow BC for $[H, \varrho] = 0$ or $i\partial_t \varrho = [H, \varrho]$

- Reference Hamiltonian ,ex: $H_0 = -\Delta$ .
- Reference steady state $[H_0, \varrho_0] = 0$ , ex: $\varrho_0 = f(-i\nabla)$ .
- Conjugate operator (Mourre) $[H_0, iA] \geq 0$ ,
  ex: $A = (x.\xi)^W = \frac{1}{2}(x.D_x + D_x.x)$ .
- Weight function $F_\mu(a) = 1$ is $a \leq -1 \quad F_\mu(a) \sim a^{-\mu}$ ,
  $\mu > 1$ , if $a > 1$ .
- Admissible state $F_\mu(A)(\varrho - \varrho_0)F_\mu(A)$ trace-class.
  Affine space $\varrho \in \mathcal{E}_{\varrho_0, A, \mu}$.
- Admissible potentials. ex: $V \in L^\infty(\mathbb{R})$, $\operatorname{supp} V$ compact.
  $H = H_0 + V$.

# Quantum inflow boundary conditions

Functional Analysis results

Ex: $H_0 = -\Delta$ on $\mathbb{R}$, $\varrho_0 = f(-i\nabla)$, $V = \underset{\geq 0}{V_0} + V_{NL}(\varrho)$

$-\Delta V_{NL} = n_\varrho(x)$ for $a < x < b$, $\qquad V_{NL}(a) = V_{NL}(b) = 0$.

- $\varrho \in \mathcal{E}_{\varrho_0, A, \mu}$ and $[H, \varrho] = 0$ implies

$$\varrho(x,y) = \int_{\mathbb{R}} f(k)\psi_-(k,x)\overline{\psi_-(k,y)}\,\frac{dk}{2\pi} + (no\ bound\ state)$$

  $\psi_-(k,x)$ incoming scattering state for $H = -\Delta + V(x)$.

- The nonlinear Cauchy problem

$$i\partial_t \varrho = [H(\varrho(t)), \varrho] \quad \varrho_{t=0} = \varrho_{ini}$$

  is well posed globally in time in $\mathcal{E}_{\varrho_0, A, \mu}$.

# Quantum inflow boundary conditions

Functional Analysis results

Ex: $H_0 = -\Delta$ on $\mathbb{R}$, $\varrho_0 = f(-i\nabla)$, $V = \underset{\geq 0}{V_0} + V_{NL}(\varrho)$

$-\Delta V_{NL} = n_\varrho(x)$ for $a < x < b$, $\qquad V_{NL}(a) = V_{NL}(b) = 0$.

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  $\psi_-(k,x)$ incoming scattering state for $H = -\Delta + V(x)$.

- The nonlinear stationary problem $[H, \varrho] = 0$ with $H = H_0 + V_0 + V_{NL}(\varrho)$ admits solutions in $\mathcal{E}_{\varrho_0, A, \mu}$ .

# Asymptotic analysis

Limit $h \to 0 \to$ finite dimensional system:
"The phenomena are governed by a finite number of resonant states"
Quantum wells in a semiclassical island:

$$H^h = -h^2\Delta + V_0(x) + V_{NL}^h(x) - \sum_{j=1}^{N} W_j(\frac{x-c_j}{h})$$

$$H\psi_- = k^2\psi_- \qquad \psi(k>0,x) = \begin{cases} e^{i\frac{kx}{h}} + R(k)e^{-i\frac{ikx}{h}}, & x < a\,, \\ T(k)e^{i\frac{kx}{h}}, & x > b\,. \end{cases}$$

$$-\Delta V_{NL}^h(x) = n_\varrho(x) = \int g(k^2)1_{(0,+\infty)}(k)\left|\psi_-^h(k,x)\right|^2 \frac{dk}{2\pi h}$$

# Asymptotic analysis

Limit $h \to 0 \to$ finite dimensional system:
"The phenomena are governed by a finite number of resonant states"
Asymptotic model: The limit points of the family $\{V_{NL}^h\}$ as $h \to 0$ are piecewise affine potentials solutions to

$$-\Delta V_{NL} = \sum_{j=1}^{N} \sum_{e \in \mathcal{E}_j} t_{j,e} g(\lambda(e)) 1_{(0,+\infty)}(\lambda(e)) \delta_{c_j}(x) \,,$$

$$V_{NL}(a) = V_{NL}(b) = 0 \quad , \quad \lambda(e) = V_0(c_j) + V_{NL}(c_j) - e \,,$$

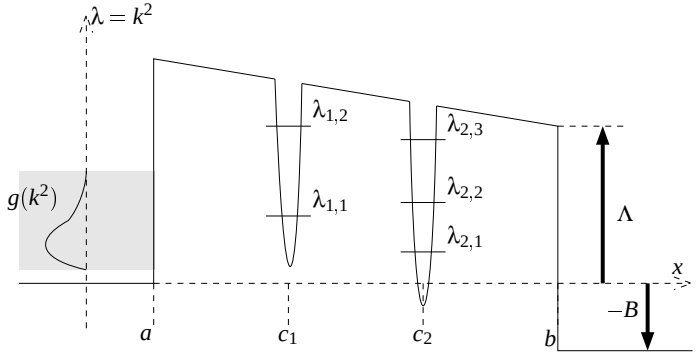
$$\mathcal{E}_j = \sigma(-\Delta - W_j) \cap (-\infty, 0) \,,$$

$$t_{j,e} = \begin{cases} 1 & \text{if } d_{Ag}(a, c_j; V, \lambda(e)) < d_{Ag}(c_j, b, V, \lambda(e)) \,, \\ 0 & \text{if } d_{Ag}(a, c_j; V, \lambda(e)) < d_{Ag}(c_j, b; V, \lambda(e)) \end{cases}$$

# Asymptotic analysis

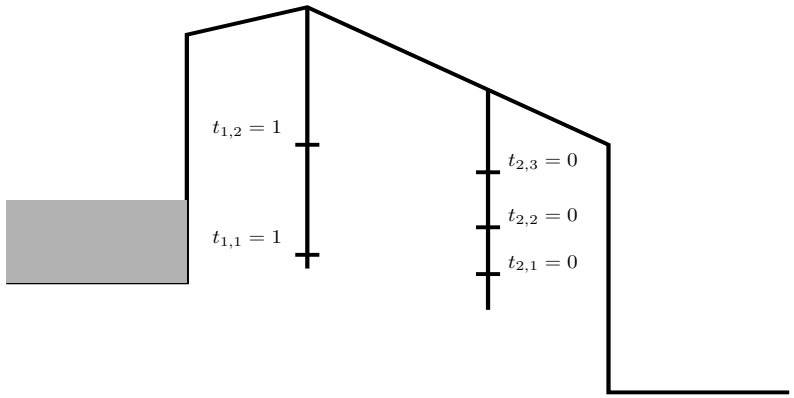
i

$h > 0$




(without $V_{NL}^h$)

$\lim_{h \to 0}$



# Asymptotic analysis

## Phase space aspect of the tunnel effect

The coefficients $t_{j,e}$ are the asymptotic branching ratio

$$
\begin{aligned}
t_{j,e} &= \lim_{h\to 0} \frac{|\langle W^h \tilde{\psi}_-(+k,x)\,,\ \Phi_j^h\rangle|^2}{4hk\Gamma_j^h} \\
\Gamma_j^h + o(\Gamma_j^h) &= \frac{|\langle W^h \tilde{\psi}_-(+k,x)\,,\ \Phi_j^h\rangle|^2 + |\langle W^h \tilde{\psi}_-(-k,x)\,,\ \Phi_j^h\rangle|^2}{4hk} \\
&\propto \frac{e^{-\frac{2S_0}{h}}}{h}\,.
\end{aligned}
$$

$\Phi_j^h$ Dirichlet eigenvector, $\tilde{\psi}_-$ gen eigenfunction associated with $W \equiv 0$ (exponential decay).

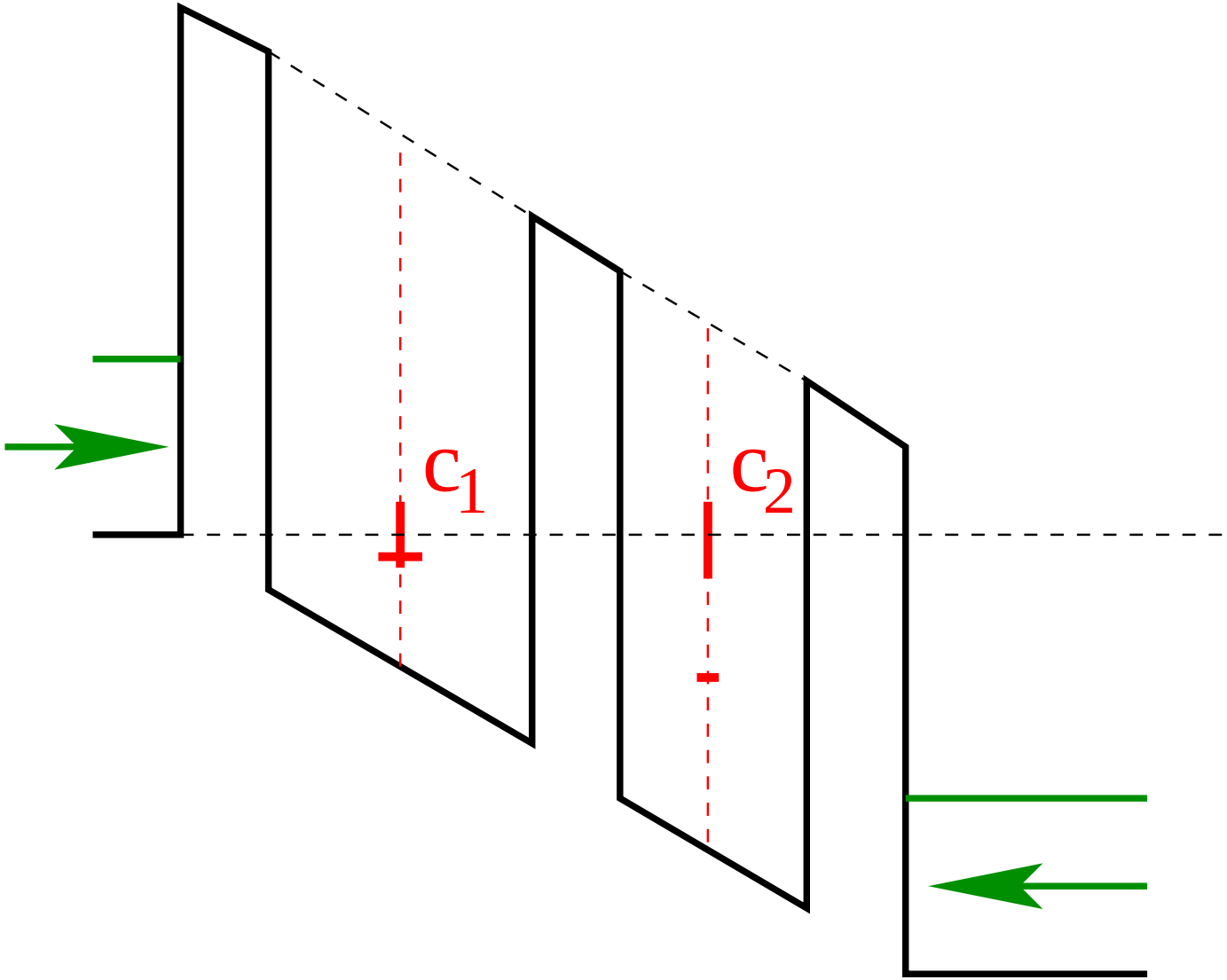
# Asymptotic analysis

## Applications

- Practical cases for GaAs-GaAlAs or Si-$SiO_2$ can be studied after a rescaling leading ot $h_{eff}$ between $0.1$ and $0.3$.
- For 1 well, the asymptotic model explains that hysteresis phenomena are possible when the second barrier is larger than the first one.
- For 2 wells the geometry can be adjusted so that 2 types of NL solutions coexist with a possible interaction of resonances. (Bifurcation diagram sensitive to a 1nm variation of the sizes of the barrier).

# Asymptotic analysis

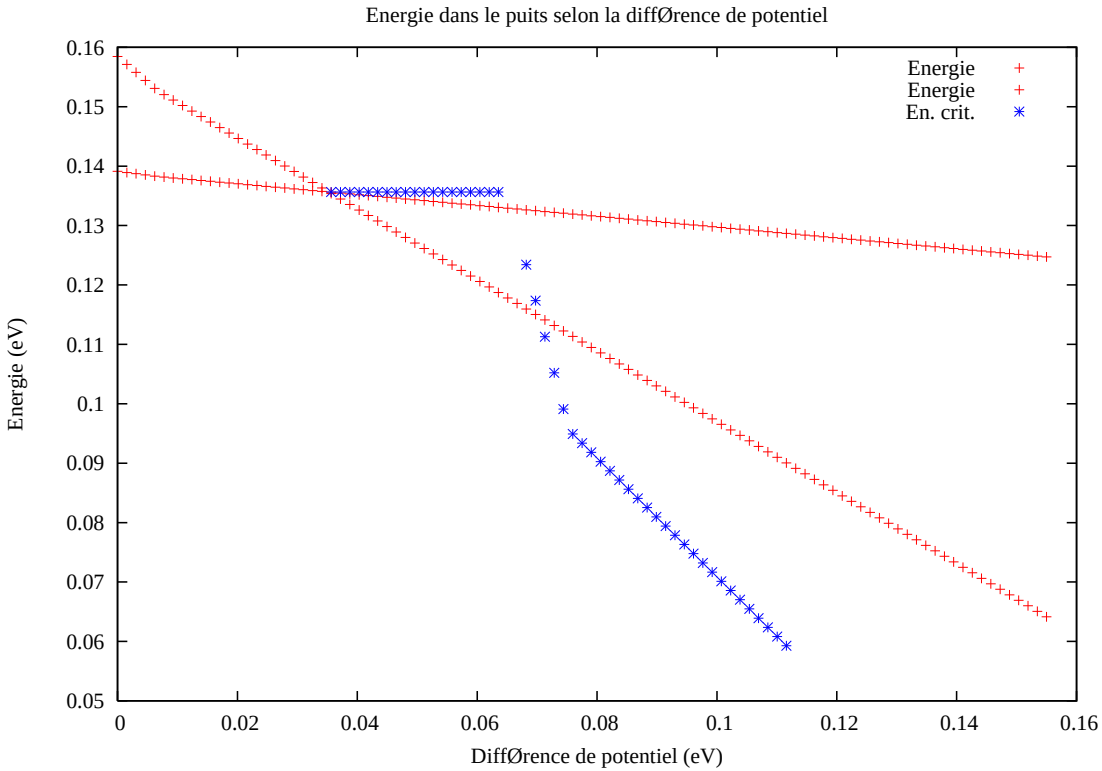
Applications : Possible nonlinear interaction of resonances



# Asymptotic analysis

Applications : Possible nonlinear interaction of resonances

Asymptotic model, $E_{res} - V$ curve



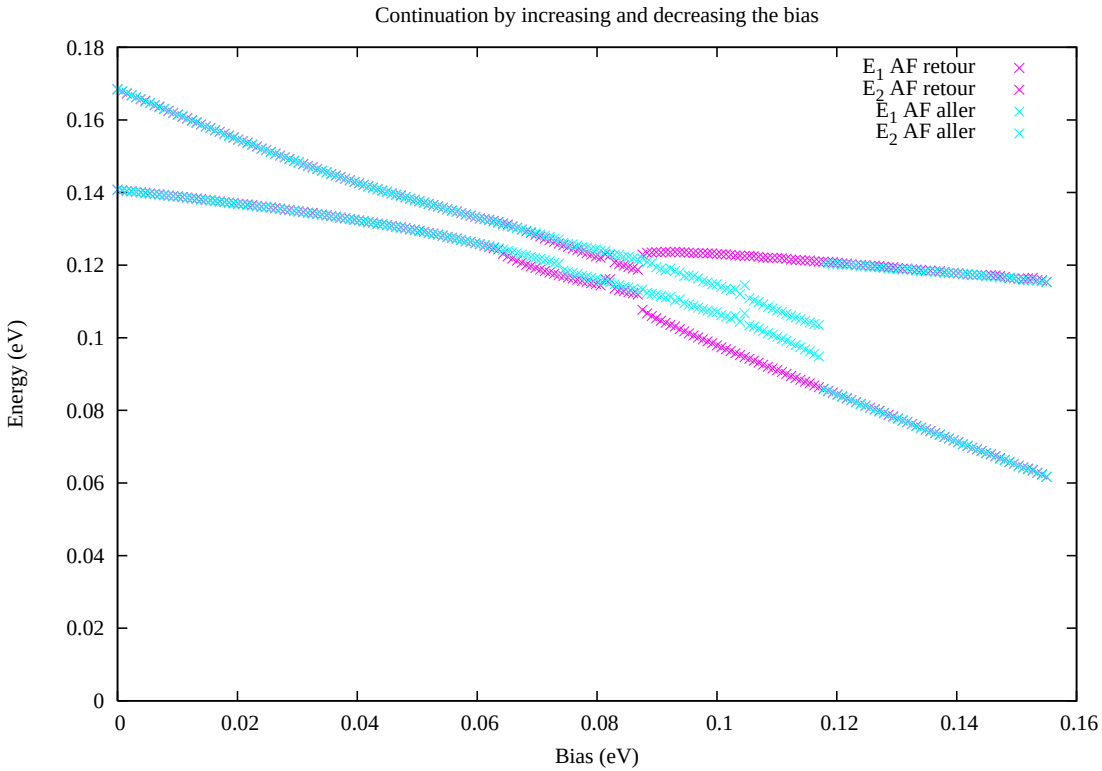

—: Energy crossing.

—: The resonant energies are equal.

# Asymptotic analysis

Applications : Possible nonlinear interaction of resonances

Complete model, $E_{res} - V$ curve



# Adiabatic evolution of resonances

## Outside deformation

$$U_\theta u(x) = \begin{cases} e^{\frac{\theta}{2}} u(a + e^\theta (x-a)) & \text{if } x < a\,, \\ u(x) & \text{if} a < x < b\,, \\ e^{\frac{\theta}{2}} u(b + e^\theta (x-b)) & \text{if } x > b\,. \end{cases}$$

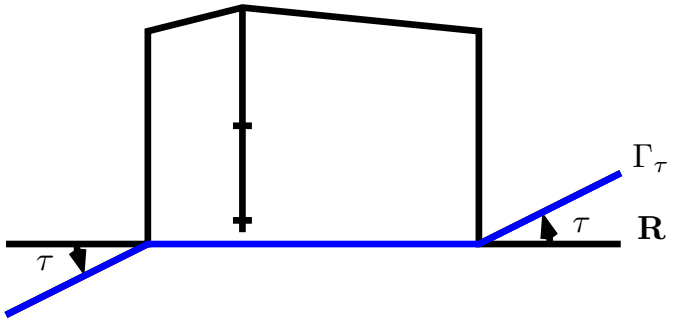
$U_\theta$ unitary when $\theta \in \mathbb{R}$

$$\begin{aligned} H^h(\theta) &= U_\theta H^h U_{-\theta} \\ &= -h^2 e^{-2\theta \times 1_{\mathbb{R}\setminus[a,b]}} \Delta + V - W^h \end{aligned}$$

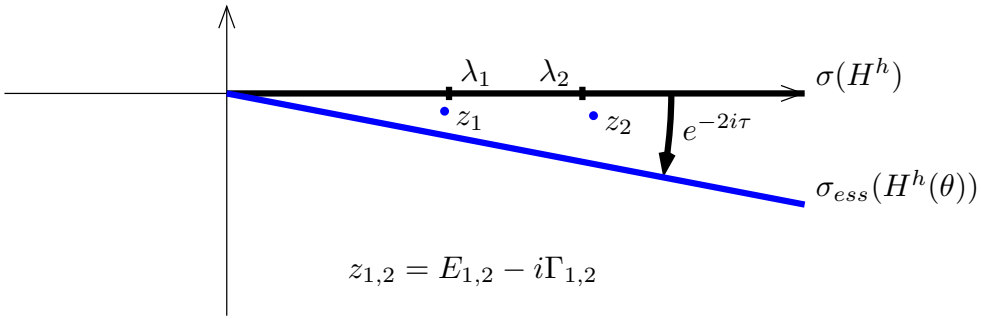
$$D(H^h(\theta)) = \left\{ u \in H^2(\mathbb{R} \setminus \{a,b\})\,, \begin{array}{l} e^{-\frac{\theta}{2}} u(b^+) = u(b^-)\,, \\ e^{-\frac{3\theta}{2}} u'(b^+) = u'(b^-)\,, \\ e^{-\frac{\theta}{2}} u(a^-) = u(a^+)\,, \\ e^{-\frac{3\theta}{2}} u'(a^-) = u'(a^+)\,, \end{array} \right\}.$$

# Adiabatic evolution of resonances

Outside complex deformation: $\theta = i\tau$




$H^h(i\tau)$ on $L^2(\mathbb{R}) \Leftrightarrow H^h$ on $L^2(\Gamma_\tau)$




$$z_i - \lambda_i = \tilde{\mathcal{O}}(e^{-\frac{2S_i}{h}}), \quad S_i = d_{Ag}(\operatorname{supp} W^h, \{a, b\}, V; \lambda_i).$$

# Adiabatic evolution of resonances

Time evolution :

- $e^{-itH^h(\theta)}\psi_{res} = e^{-t\Gamma_{res}}e^{-itE_{res}}\psi_{res} \quad , \theta = i\tau \, .$
- On the real space with $\psi_{qres} = \chi\psi_{res}$:

$$e^{-itH^h}\psi_{qres} = e^{-t\Gamma_{res}}e^{-itE_{res}}\psi_{qres} + \mathcal{R}(t,h) \, .$$

Life time of resonances $\frac{1}{\Gamma_{res}} \sim he^{\frac{2S}{h}}$ exponentially large

The remainder term is negligible only when $t = \mathcal{O}(1/\Gamma_{res})$.

# Adiabatic evolution of resonances

Time evolution :

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Life time of resonances $\frac{1}{\Gamma_{res}} \simeq he^{\frac{2S}{h}}$ exponentially large

"The phenomena are governed by a finite number of resonant states"

The nonlinearity can be assumed to evolve very slowly $-$ $>$

Adiabatic evolution.

# Adiabatic evolution of resonances

## Time evolution : Adiabatic dynamics

$$i\varepsilon\partial_t\psi = H^h(\theta;t)\psi \quad \psi_{t=0} = \psi_{res}(t=0)\,,$$

should be close to $e^{-\frac{i}{\varepsilon}\int_0^t z_{res}(s)\,ds}\psi_{res}(t)$ .

Two problems

- The exponential scale $\varepsilon^{-1} = \Gamma_j(t)^{-1} \simeq he^{\frac{2S_j(t)}{h}}$ may depend on $j$ and on time.
- $iH(\theta = i\tau;t)$ is not accretive

$$\mathrm{Re}\,\langle u\,, iH(\theta;t)u\rangle = \mathrm{Re}\,\left[ih^2(\bar{u}u')\Big|_{a^-}^{b^+}(e^{-2\theta} - e^{-\frac{\bar{\theta}+3\theta}{2}})\right] + h^2\sin(2\tau)\int_{\mathbb{R}\setminus[a,b]}|u'|^2\,dx\,.$$

# Adiabatic evolution of resonances

Time evolution : Adiabatic dynamics

$$i\varepsilon\partial_t\psi = H^h(\theta;t)\psi \quad \psi_{t=0} = \psi_{res}(t=0)\,,$$

should be close to $e^{-\frac{i}{\varepsilon}\int_0^t z_{res}(s)\ ds}\psi_{res}(t)$ .

Two problems

- The exponential scale $\Gamma_j(t)^{-1} \simeq e^{\frac{2S_j(t)}{h}}$ may depend on $j$ and on time.
- $iH(\theta = i\tau;t)$ is not accretive

  $\mathrm{Re}\ \left[ih^2(\bar{u}u'(b^+) - \bar{u}u'(a^-))(e^{-2\theta} - e^{-\frac{\bar{\theta}+3\theta}{2}})\right]$ has no sign.

  $\|e^{-\frac{itH^h(\theta)}{\varepsilon}}\|$ or $\|U^\varepsilon(t,0)\|$ behaves like $e^{\frac{Ct}{\varepsilon}}$!!!

# Artificial interface conditions

$$
\begin{aligned}
H^h(\theta) &= U_\theta H^h U_{-\theta} \\
&= -h^2 e^{-2\theta \times 1_{\mathbb{R}\setminus[a,b]}} \Delta + V - W^h \\
D(H^h(\theta)) &= \left\{ u \in H^2(\mathbb{R}\setminus\{a,b\}) \,, \begin{array}{l} e^{-\frac{\theta}{2}} u(b^+) = u(b^-) \,, \\ e^{-\frac{3\theta}{2}} u'(b^+) = u'(b^-) \,, \\ e^{-\frac{\theta}{2}} u(a^-) = u(a^+) \,, \\ e^{-\frac{3\theta}{2}} u'(a^-) = u'(a^+) \,, \end{array} \right\}
\end{aligned}
$$

Boundary term

$$
\mathrm{Re}\left[ i h^2 (\bar{u} u'(b^+) - \bar{u} u'(a^-)) \times (e^{-2\theta} - e^{-\frac{\bar{\theta}-3\theta}{2}}) \right]
$$

# Artificial interface conditions

$$
\begin{aligned}
H^h_{\theta_0}(\theta) &= U_\theta H^h_{\theta_0} U_{-\theta} \\
&= -h^2 e^{-2\theta \times 1_{\mathbb{R}\setminus[a,b]}} \Delta_{\theta_0} + V - W^h
\end{aligned}
$$

$$
D(H^h_{\theta_0}(\theta)) = \left\{ u \in H^2(\mathbb{R}\setminus\{a,b\}) \,,\ \begin{array}{l} e^{-\frac{\theta_0+\theta}{2}} u(b^+) = u(b^-) \,, \\ e^{-\frac{3\theta_0+3\theta}{2}} u'(b^+) = u'(b^-) \,, \\ e^{-\frac{\theta_0+\theta}{2}} u(a^-) = u(a^+) \,, \\ e^{-\frac{3\theta_0+3\theta}{2}} u'(a^-) = u'(a^+) \,, \end{array} \right\}
$$

Boundary term

$$
\mathrm{Re}\left[ ih^2(\bar{u}u'(b^+) - \bar{u}u'(a^-)) \times (e^{-2\theta} - e^{-\frac{\overline{\theta_0+\theta}+3\theta_0+3\theta}{2}}) \right]
$$

vanishes for $\theta_0 = \theta = i\tau$ .

# Comparison results

$$D(-\Delta_{\theta_0}) = \left\{ u \in H^2(\mathbb{R} \setminus \{a,b\}) \,, \quad \begin{array}{l} e^{-\frac{\theta_0}{2}} u(b^+) = u(b^-) \,, \\ e^{-\frac{3\theta_0}{2}} u'(b^+) = u'(b^-) \,, \\ e^{-\frac{\theta_0}{2}} u(a^-) = u(a^+) \,, \\ e^{-\frac{3\theta_0}{2}} u'(a^-) = u'(a^+) \,, \end{array} \right\}$$

$\Delta_{\theta_0}$ and $\Delta$ are conjugated

$$-\Delta_{\theta_0} = W_{\theta_0}(-\Delta)W_{\theta_0}^{-1}$$

with $\quad W_{\theta_0} = \mathrm{Id} + \mathcal{O}(\theta_0) \quad$ in $\mathcal{L}(L^2(\mathbb{R}))$ .

$W_{\theta_0}$ like a wave operator (non self-adjoint, cf Kato).

Application with $\theta_0 = \theta = ih^{N_0}$ .

# Comparison results

When $W^h = 0$, $H^h_{\theta_0} = -h^2\Delta_{\theta_0} + V$ with $V(x) \geq V_0 1_{[a,b]}(x)$.
The generalized eigenfunctions $\tilde{\psi}_{-,0}(k,.)$ for $\theta_0 = 0$ satisfy

$$|\tilde{\psi}_-(k,x)| \leq Ce^{-\frac{d_{Ag}(a,x,V,k^2)}{h}} \quad \text{for } 0 < k < \sqrt{V_0},\ a < x < v\,.$$

The comparison in given by

$$|\tilde{\psi}_{-,0}(k,x) - \tilde{\psi}_{-,\theta_0}(k,x)| \leq \frac{C|\theta_0|}{h^{3/2}} e^{-\frac{d_{Ag}(a,x,V,k^2)}{h}}\,.$$

# Comparison results

When $W^h \neq 0$ and $z_j = E_j - i\Gamma_j \in H^h(\theta)$, $\theta = i\tau = ih^{N_0}$ is a resonance with $\Gamma_j = \mathcal{O}(h^{-1}e^{-\frac{2S_j}{h}})$ then there is a resonance $z_{j,\theta_0} \in \sigma(H^h_{\theta_0}(\theta))$ with

$$|z_j - z_{j,\theta_0}| \leq \frac{C|\theta_0|}{h^4} e^{-\frac{2S_j}{h}} .$$

# Comparison results

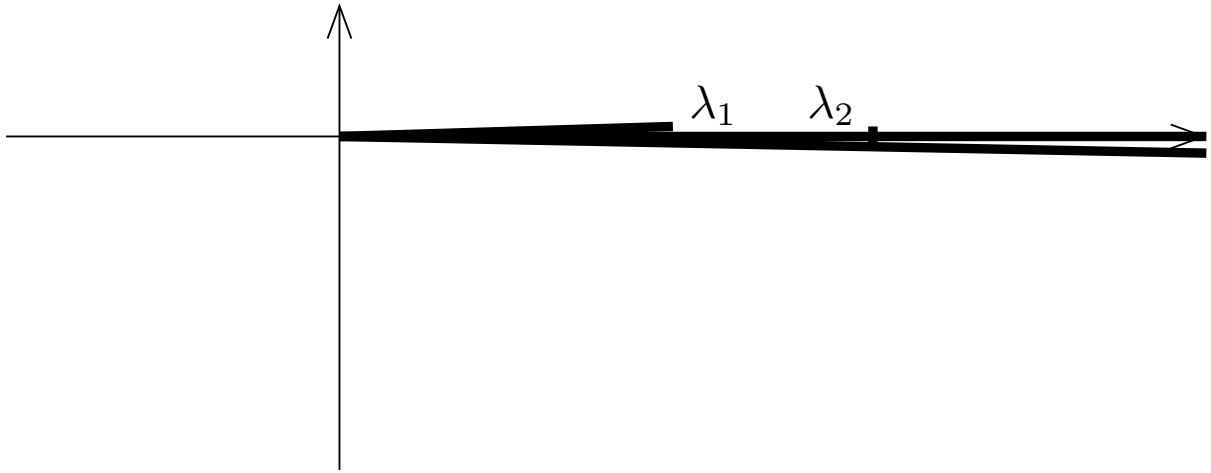
The Fermi Golden rule also holds when $|\theta_0| = h^{N_0}$, $N_0 > 5$ :

$$\Gamma^h_{j,\theta_0} + o(\Gamma^h_{j,\theta_0}) = \frac{|\langle W^h \tilde{\psi}_{-,\theta_0}(+k,x)\,,\ \Phi^h_j\rangle|^2 + |\langle W^h \tilde{\psi}_{-,\theta_0}(-k,x)\,,\ \Phi^h_j\rangle|^2}{4h}$$

Conclusion: All the important quantities are modified with a relatively small error when $\theta_0 = ih^{N_0}$, $N_0 > 5$ . When $\theta = \theta_0 = ih^{N_0}$, $H^h_{\theta_0}(\theta)$ is maximal accretive.

# Comparison results

Summary: $\theta_0 = \theta = ih^{N_0}$, $N_0 > 5$



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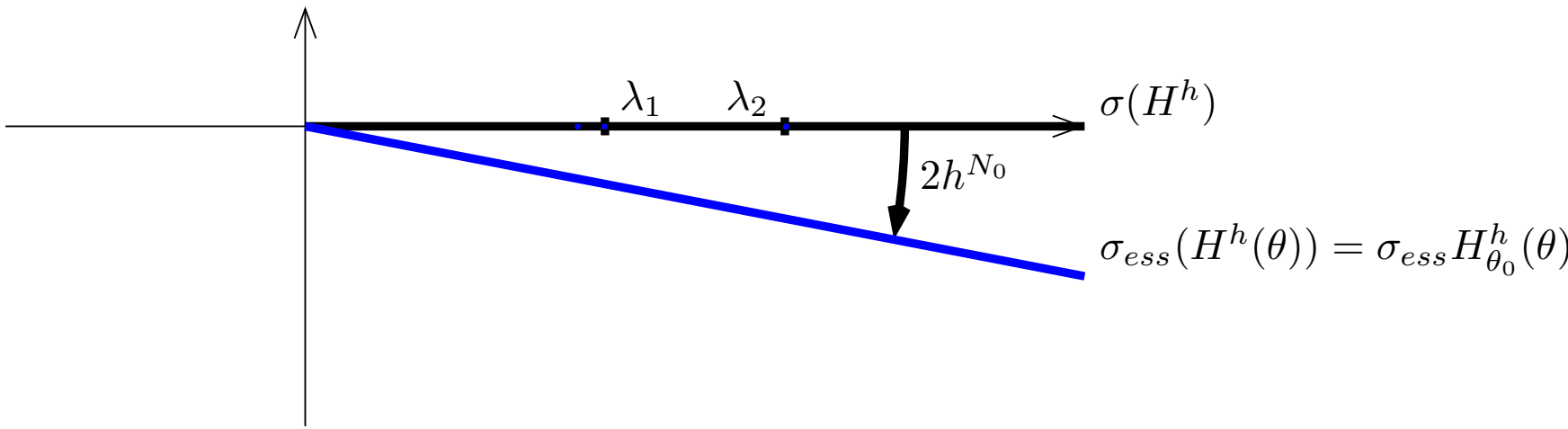

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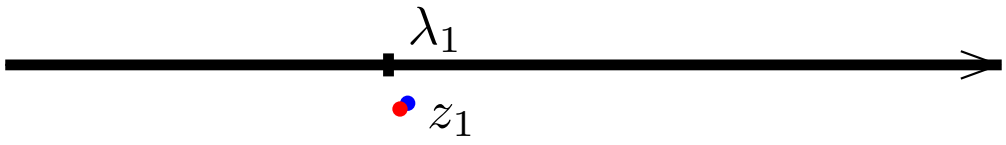


# Comparison results

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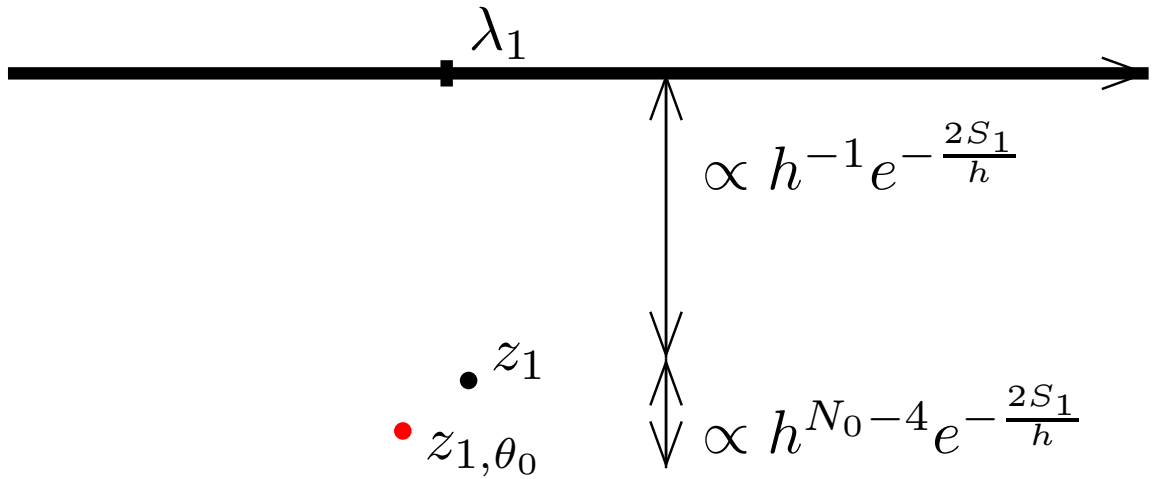



Adapt Helffer-Sjöstrand resonance analysis with low regularity.

# Adiabatic evolution, adapted from Nenciu

Take $\theta_0 = \theta = ih^{N_0}$, $N_0 > 5$, $\varepsilon = e^{-\frac{c}{h}}$ and let $P_0(t)$ be the spectral projector associated with $z_{1,\theta_0}(t) \dots z_{K,\theta_0}(t)$.
Let $\Phi_0(t,s)$ denote the parallel transport

$$\partial_t \Phi_0 + [P_0, \partial_t P_0]\, \Phi_0 = 0\,, \qquad \Phi_0(s,s) = \mathrm{Id}\,.$$

The solutions to

$$i\varepsilon \partial_t u = H^h_{\theta_0}(\theta,t) u\,,$$

and

$$i\varepsilon \partial_t w = \Phi_0(0,t) P_0(t) H^h_{\theta_0}(\theta,t) P_0(t) \Phi_0(t,0) w\,,$$

$$w(t=0) = u(t=0) = u_0, \qquad P_0(0) u_0 = u_0$$

satisfy

$$\|u(t) - \Phi_0(t,0) w(t)\| \le C_\delta \varepsilon^{1-\delta}\,.$$

# Application

Consider the time-dependent Hamiltonian

$$H^h = -h^2 \Delta_{\theta_0} + V_0 1_{[a,b]}(x) - h\alpha(t,h)\delta_c$$

with $\alpha(t) = \alpha_0 + h\alpha_1(t)$ and $\alpha_1'(0) \neq 0$ + some other non degeneracy assumptions.
Assume

$$\varrho^h(t=0,x,y) = \int_0^{+\infty} g(k)\psi_-^h(k,x,t=0)\overline{\psi_-^h(k,y,t=0)}\,\frac{dk}{2\pi h}$$

and compute

$$A^h(t) = \mathrm{Tr}\,\left[\varrho^h(t)1_{[a+\varepsilon,b-\varepsilon]}(x)\right]\,.$$

# Application

Then, for $d_{Ag}(a,c) < d_{Ag}(b,c)$ and $E_{res}(t) = \lambda(t) - i\Gamma(t)$,

$$A^h(t) = \mathrm{Tr}\left[\varrho^h(t) 1_{[a+\varepsilon, b-\varepsilon]}(x)\right] = a(t) + \mathcal{J}(t) + \mathcal{O}(\theta_0) + \mathcal{O}(\varepsilon^{1/\nu})$$

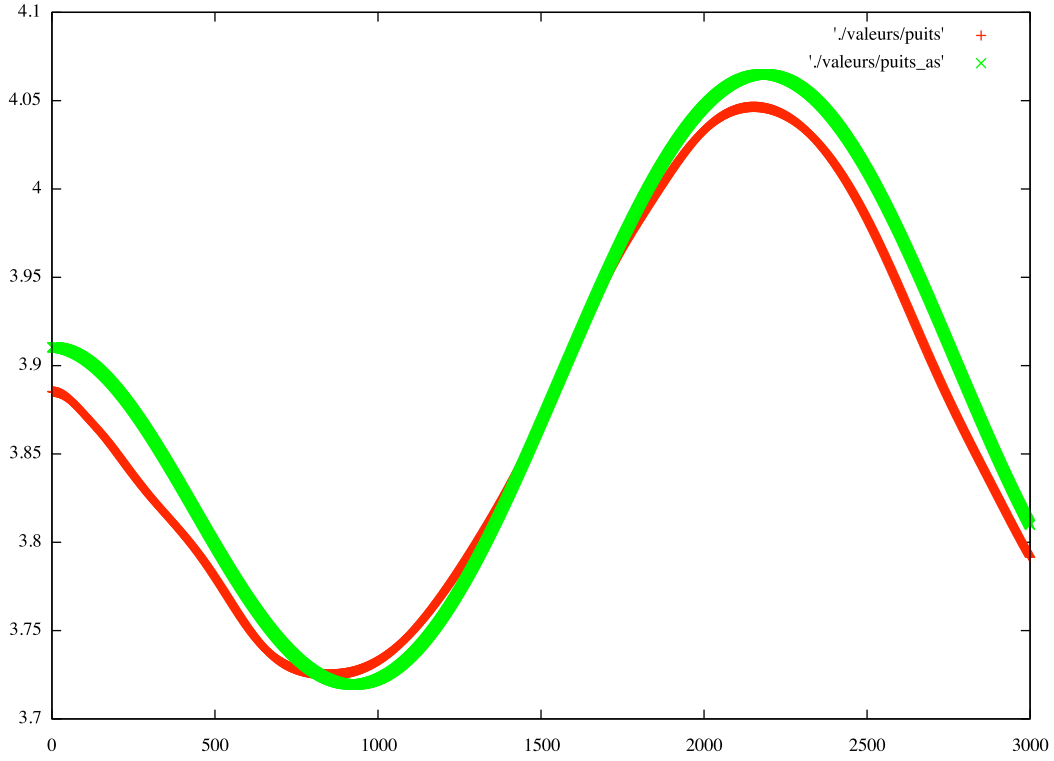
where $a(t)$ solves the Cauchy problem

$$\partial_t a = -\frac{\Gamma(t)}{2\varepsilon}\left(a(t) - |\frac{\alpha(t)}{\alpha(0)}|^3 g(\lambda(t)^{1/2})\right) \quad , \quad a(0) = g(\lambda(0)^{1/2})$$

$$\mathcal{J}(t) = \left|1 - \left|\frac{\alpha(t)}{\alpha(0)}\right|^{3/2}\right|^2 g(\lambda(t)^{1/2})\,.$$

# Application

Numerics




... small epsilon $\Rightarrow$ heavy numerical calculations...