An explicit model for the adiabatic evolution of quantum observables driven by 1D shape resonances. Theory and numerics

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Joint work with A. Faraj and A. Mantile

Outline

- Adiabatic evolution of 1D resonant states
- A specific model for resonant tunneling diodes
- Numerics

Adiabatic evolution of resonances

Quantum system

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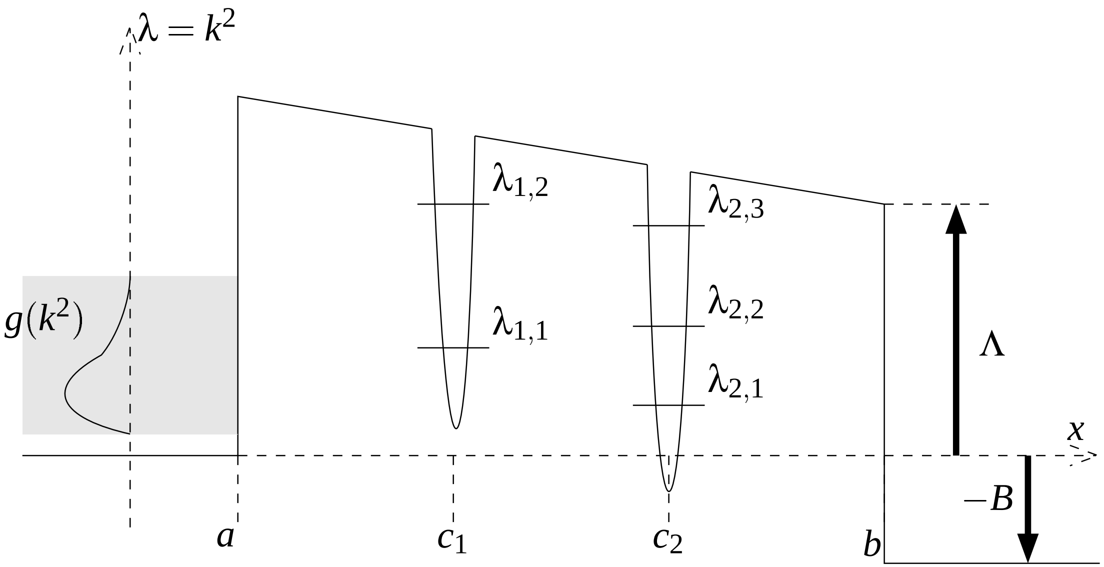


$$H^h = -h^2\Delta + V_0 1_{[a,b]} - \sum_{j=1}^{N} W_j\left(\frac{x-c_j}{h}\right).$$

Resonances require a complex deformation

Adiabatic evolution of resonances

Outside deformation

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

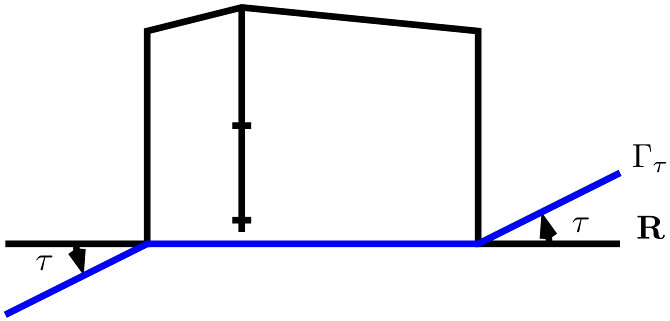
U_θ unitary when $\theta \in \mathbb{R}$

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

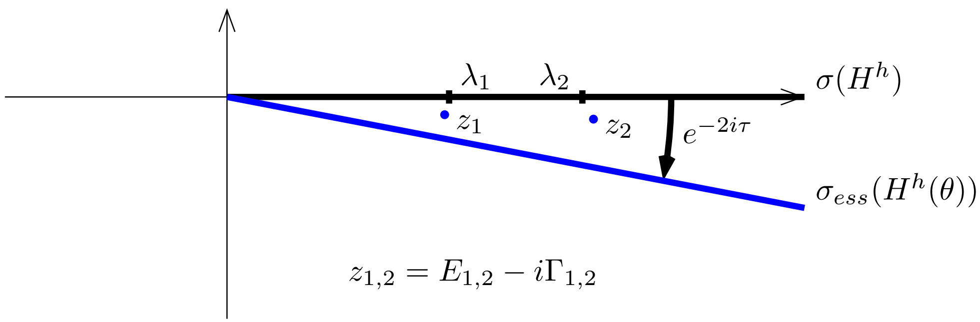
$$D(H^h(\theta)) = \left\{ u \in H^2(\mathbb{R} \setminus \{a,b\})\,, \begin{array}{l} e^{-\frac{\theta}{2}} u(b^+) = u(b^-)\,, \\ e^{-\frac{3\theta}{2}} u'(b^+) = u'(b^-)\,, \\ e^{-\frac{\theta}{2}} u(a^-) = u(a^+)\,, \\ e^{-\frac{3\theta}{2}} u'(a^-) = u'(a^+)\,, \end{array} \right\}.$$

Adiabatic evolution of resonances

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



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



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

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 :

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

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Life time of resonances $\frac{1}{\Gamma_{res}} \simeq he^{\frac{2S}{h}}$ exponentially large
We are concerned with time-dependent (non linear) problems which are governed by resonant states.

Life time of resonances $\varepsilon^{-1} = e^{\frac{C}{h}} -> $ adiabatic evolution in the time scale ε^{-1} .

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

$$\begin{aligned} H^h_{\theta_0}(\theta) &= U_\theta H^h_{\theta_0} U_{-\theta} \\ &= -h^2 e^{-2\theta\times 1_{\mathbb{R}\setminus[a,b]}} \Delta_{\theta_0} + V - W^h \\ D(H^h_{\theta_0}(\theta)) &= \left\{ u \in H^2(\mathbb{R}\setminus\{a,b\}) \,, \begin{array}{l} e^{-\frac{\theta_0+\theta}{2}} u(b^+) = u(b^-)\,, \\ e^{-\frac{3\theta_0+3\theta}{2}} u'(b^+) = u'(b^-)\,, \\ e^{-\frac{\theta_0+\theta}{2}} u(a^-) = u(a^+)\,, \\ e^{-\frac{3\theta_0+3\theta}{2}} u'(a^-) = u'(a^+)\,, \end{array} \right\} \end{aligned}$$

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

Artificial interface conditions

With this modified boundary conditions, all the important quantities of the model, the dynamics (proved for $e^{it(\Delta)}$ and $e^{it\Delta_{\theta_0}}$) the generalized eigenfunctions, the imaginary parts of resonances (exponentially small), the terms of the Fermi golden rule..., are changed with a relative error of order $\mathcal{O}(\frac{\theta_0}{h^{5+\delta}})$ while θ_0 can be chosen such tat

$$e^{-\frac{c}{h}} \leq |\theta_0| \leq h^{5+\delta}\,.$$

Artificial interface conditions

Adiabatic result: 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 a cluster of resonances $z_{1,\theta_0}(t) \dots z_{K,\theta_0}(t)$ around $\lambda_0(t)$.
Let $\Phi_0(t,s)$ denote the parallel transport

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

The solutions to

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

and

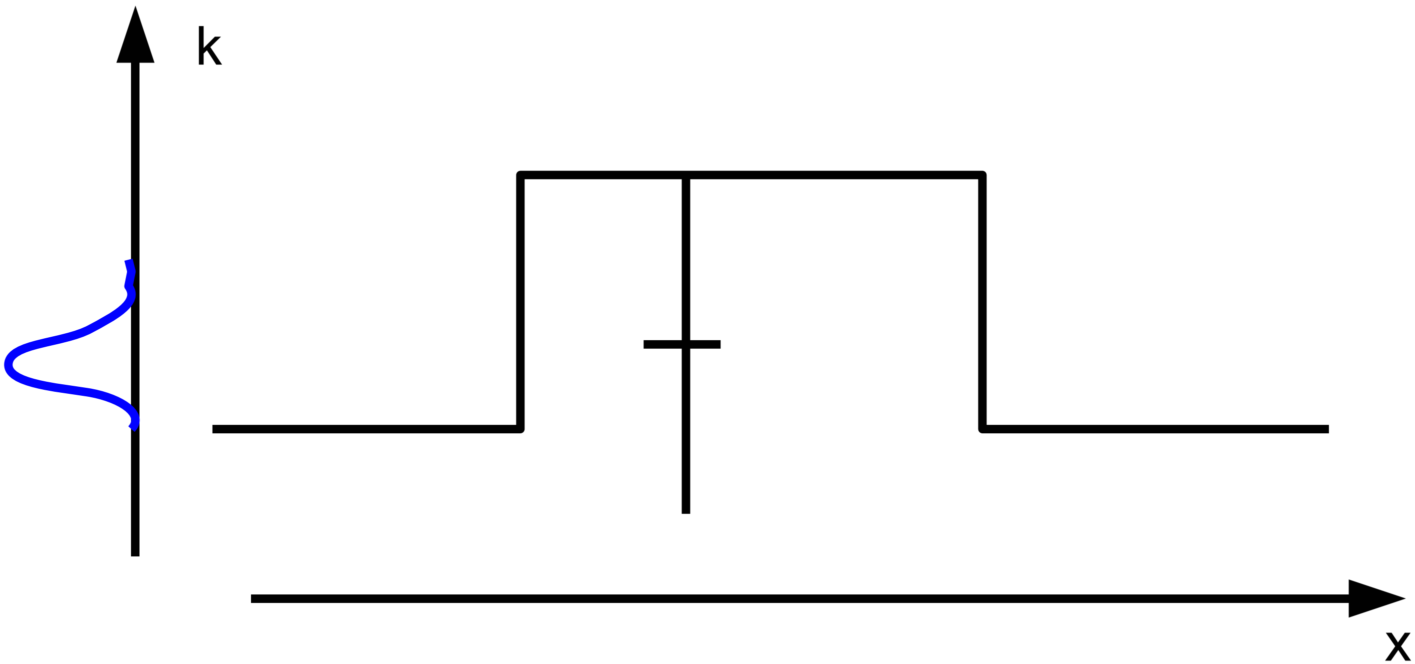
$$i\varepsilon\partial_t w = \Phi_0(0,t)P_0(t)H^h_{\theta_0}(\theta,t)P_0(t)\Phi_0(t,0)w\,,$$

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

satisfy

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

Explicit adiabatically driven system



Explicit adiabatically driven system

- Hamiltonian : $H^h_{\theta_0}(t) = -h^2\Delta_{\theta_0} + V_0 1_{[a,b]}(x) - h\alpha(t,h)\delta_c$, $c \in (a,b)$.
- Assumptions on $\alpha(t,h)$:, $\mathcal{C}^\infty$, $\partial_t\alpha = \mathcal{O}(h)$ and there exist J, N such that $\max_{j\leq J}|\partial_t^j\alpha(t)| \geq h$ for all t .
- Initial state : $\varrho_0(x,y) = \int_0^{+\infty} g(k)\psi_{\theta_0,-}(k,x)\overline{\psi_{\theta_0,-}(k,y)}\ \frac{dy}{2\pi h}$ $\psi_{\theta_0,-}(k,.)$ incoming generalized eigenfunction for $H^h_{\theta_0}(0)$.
  $\operatorname{supp} g \subset \left\{|k^2-\lambda_0| \leq Ch\right\}$.
- Dynamics : $i\varepsilon\partial_t\varrho = [H_{\theta_0}(t),\varrho]$
- Observable : $A_{\theta_0}(t) = \ \mathrm{Tr}\ [\chi(x)\varrho(t)]$ with $\operatorname{supp}\chi \subset (a,b)$, $\chi \equiv 1$ around c .

Explicit adiabatically driven system

Result: Set $\lambda_t = V_0 - \frac{\alpha(t)^2}{4}$ and assume $\lambda_t^{1/2} \in \operatorname{supp} g \subset (0, V_0^{1/2})$ for all t and fix $\varepsilon = e^{\frac{-|\alpha_0| d(c,\{a,b\})}{h}}$. Then

- For all t, $H_{\theta_0}(t)$ has a single resonance $E(t) = E_R(t) - i\Gamma(t)$ such that $E_R(t)^{1/2} \operatorname{supp} g$ with

$$E_R(t) = \lambda_t + \mathcal{O}(e^{-\frac{|\alpha(t)| d(c,\{a,b\})}{h}}), \quad \Gamma(t) = \mathcal{O}(e^{-\frac{|\alpha(t)| d(c,\{a,b\})}{h}}) = \mathcal{O}(\varepsilon).$$

- There exists $\tau_{J,\chi} > 0$ such that

$$A_{\theta_0}(t) = a(t) + \mathcal{J}(t) + \mathcal{O}(\frac{\theta_0}{h^2}) + \mathcal{O}(e^{-\frac{\tau_{J,\chi}}{h}}).$$

Explicit adiabatically driven system

Result : $\lambda_t = V_0 - \frac{\alpha(t)^2}{4}$.

- There exists $\tau_{J,\chi} > 0$ such that

$$A_{\theta_0}(t) = a(t) + \mathcal{J}(t) + \mathcal{O}(\frac{\theta_0}{h^{N_0}}) + \mathcal{O}(e^{-\frac{\tau_{J,\chi}}{h}}) .$$

- When $d(c, \{a, b\}) = d(c, a)$,

$$\begin{cases} \partial_t a = -\frac{2\Gamma(t)}{\varepsilon} \left(a(t) - \frac{|\alpha(t)|^3}{|\alpha(0)|^3} g(\lambda_t^{1/2}) \right) \\ a(t = 0) = g(\lambda_0^{1/2}) . \end{cases}$$

- $\mathcal{J}(t) = \mathcal{J}_1(t) + \mathcal{J}_2(t)$ with $\mathcal{J}_2(t) = \mathcal{O}(|\lambda_t - \lambda_0|^{1/2} \varepsilon^{1/2})$ and

$$\mathcal{J}_1(t) = \left| 1 - \left| \frac{\alpha(t)}{\alpha(0)} \right|^{3/2} \right|^2 g(\lambda_t^{1/2}) = \mathcal{O}(h^2) .$$

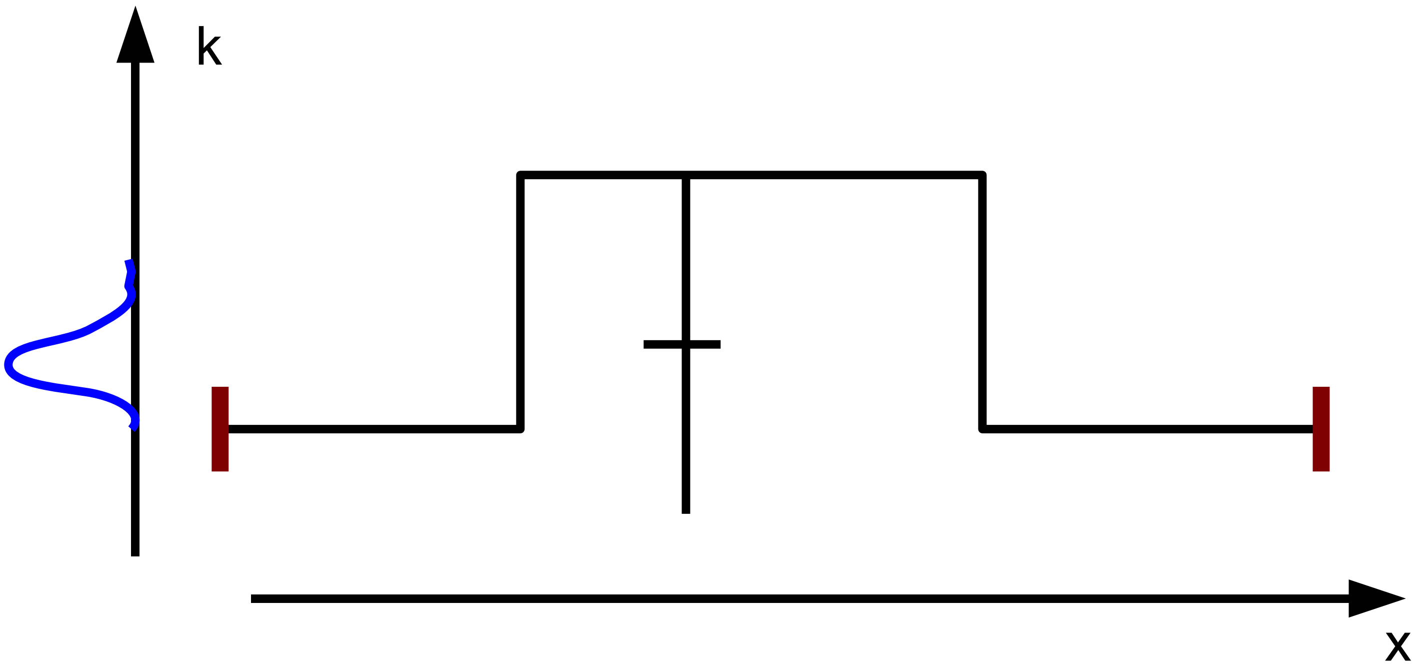
Explicit adiabatically driven system

Idea of the complete calculation :

- First note that $A_{\theta_0}(t) = \mathrm{Tr}\,\left[U_{\theta_0,\theta_0}(t,0)\varrho_0 U_{\theta_0,\theta_0}(0,t)^*\chi(x)\right]$, where $U_{\theta_0,\theta_0}(t,s)$ is the complex deformation of $U_{\theta_0,0}(t,0)$ with $\theta=\theta_0$ (contraction).
- Decompose $\psi(k,.,t) = U_{\theta_0,\theta_0}(t,0)\psi_{-,\theta_0}(k,.)$ into $e^{-i\frac{tk^2}{\varepsilon}}\tilde{\psi}_{-,\theta_0}(k,t) + C(k,t)G(k^2,x,c)$ where $\tilde{\psi}_{-,\theta_0}$ and $G(k^2,x,y)$ the gen. eigen and the Green function of $-h^2\Delta_{\theta_0} + V_0 1[a,b]$.
- When k^2 is close to $E(t)$ then the Green function is close to the resonant state $G(E(t),x,c)$.
- Use the adiabatic result for the evolution of $U_{\theta_0,\theta_0}(t,s)G(E(s),x,c)$, the comparison results $\theta_0\neq 0$ with $\theta_0=0$, the Stone formula and contour integration to compute or estimate the four terms of

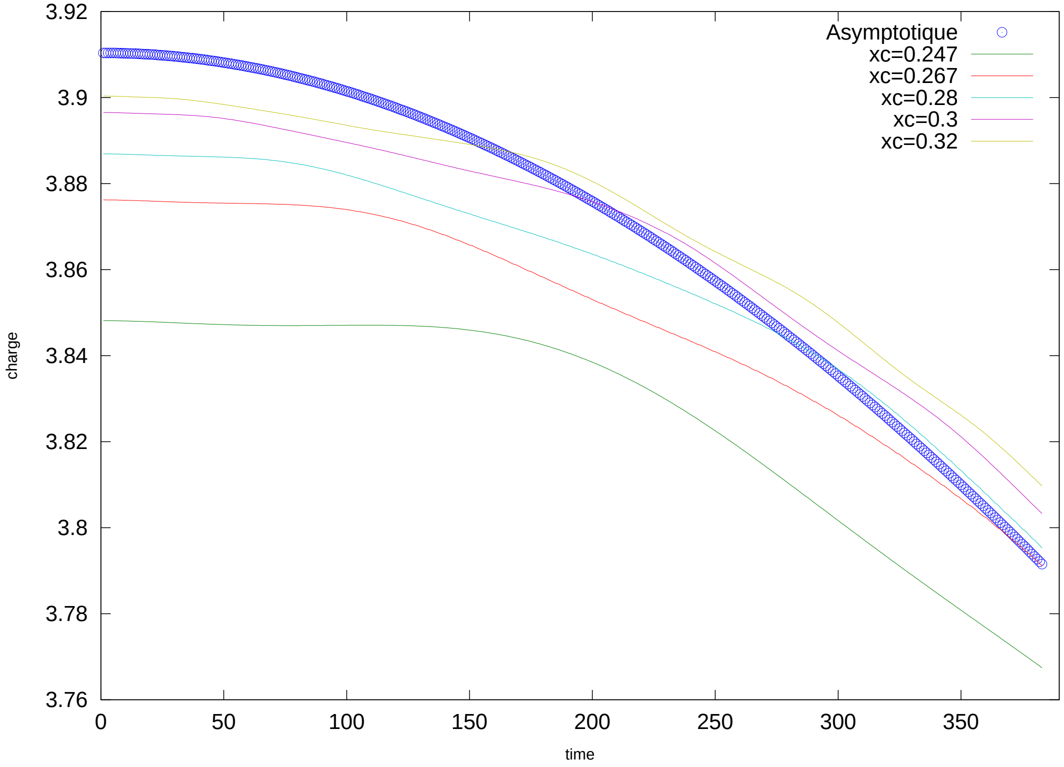
$$\int_{[c-\varepsilon,c+\varepsilon]}\int_0^{+\infty} g(k)|\psi(k,t)|^2\frac{dk}{2\pi h}\,dx\,.$$

Numerics



Numerics

Evolution of the charge for linear variations of $\alpha(t)$



Numerics

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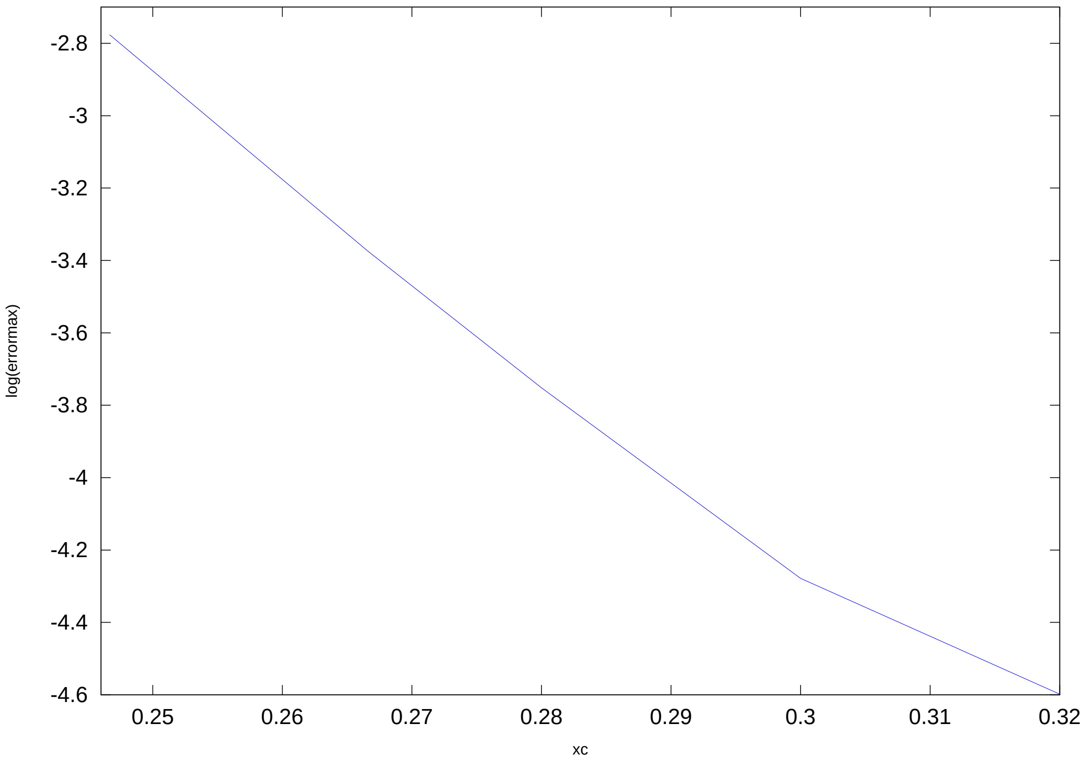
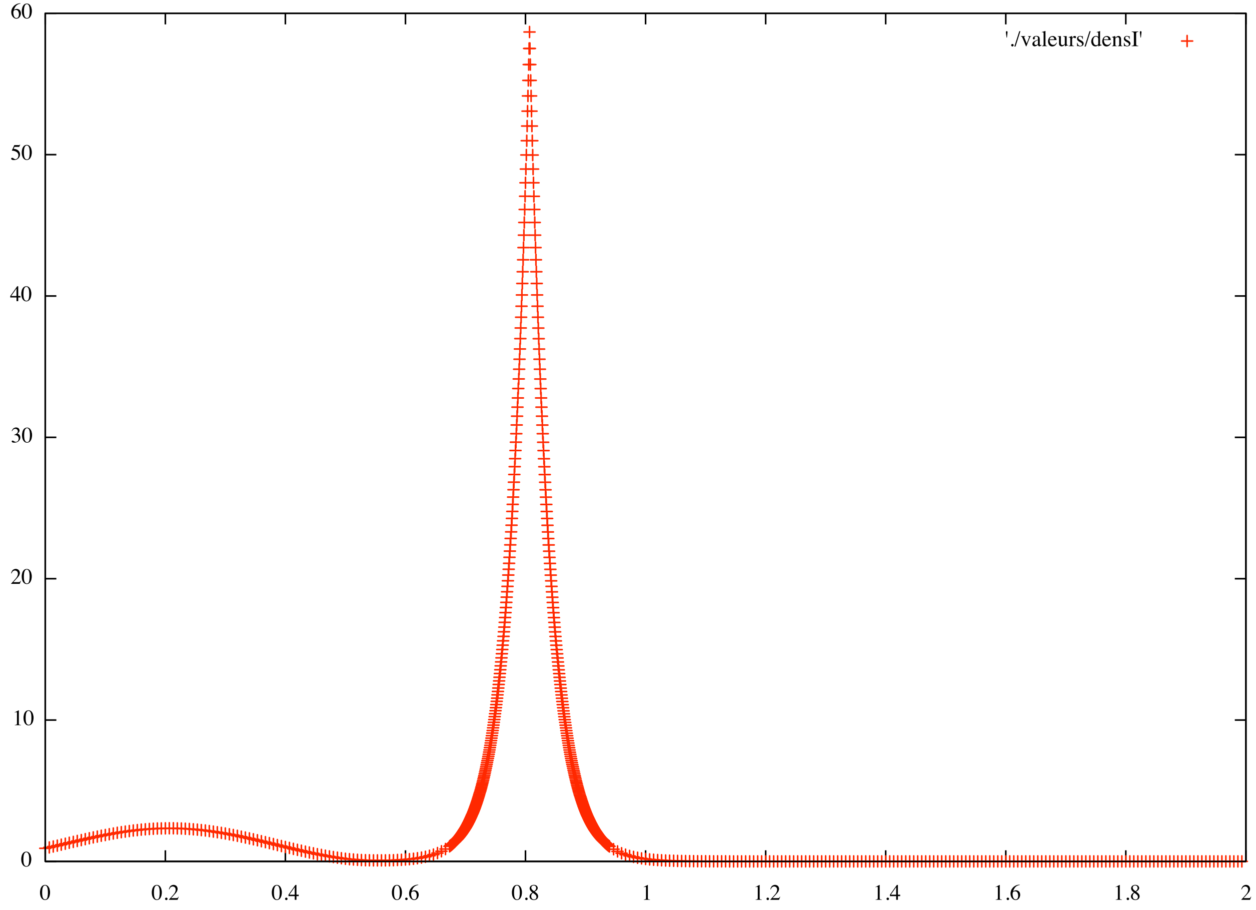


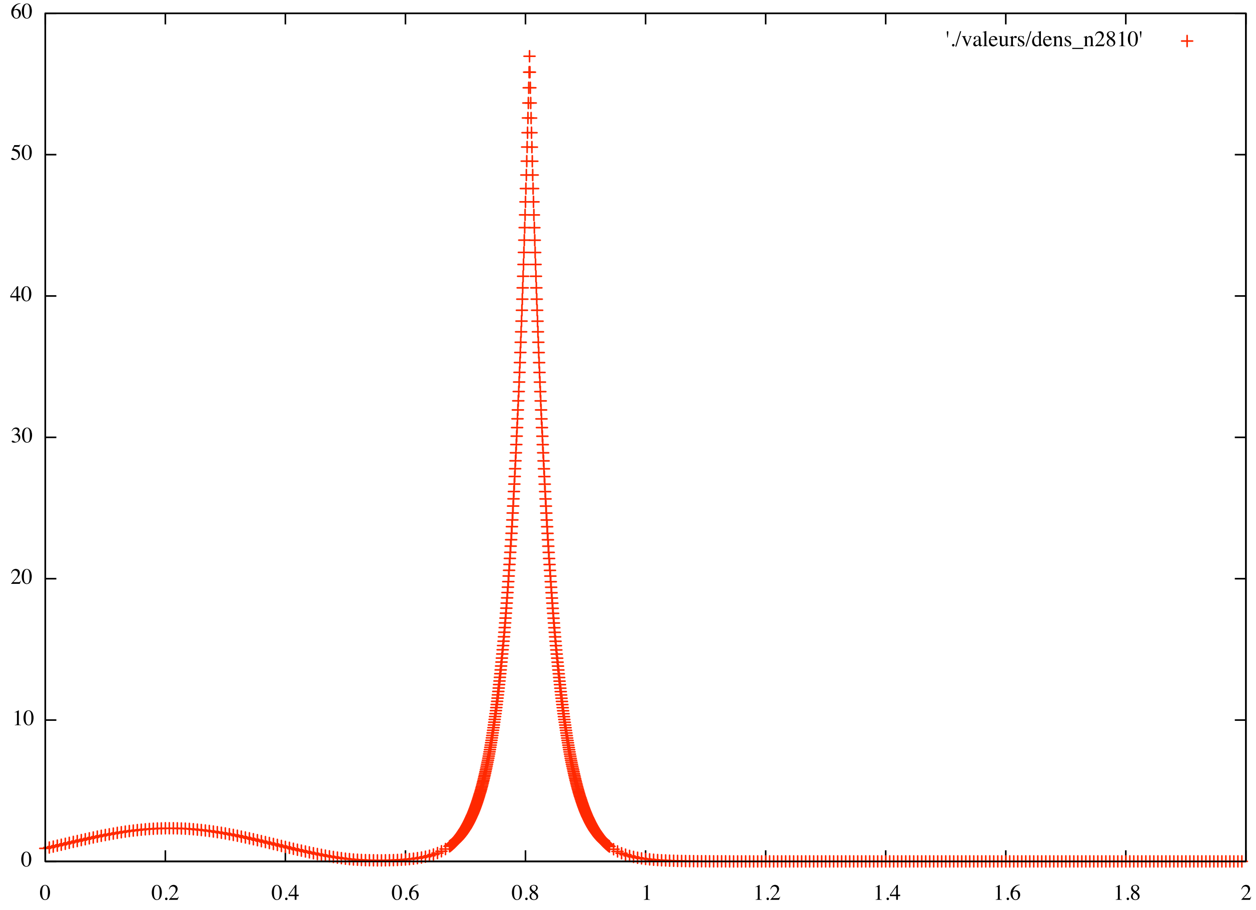
Numerics

The density at $t = 0$



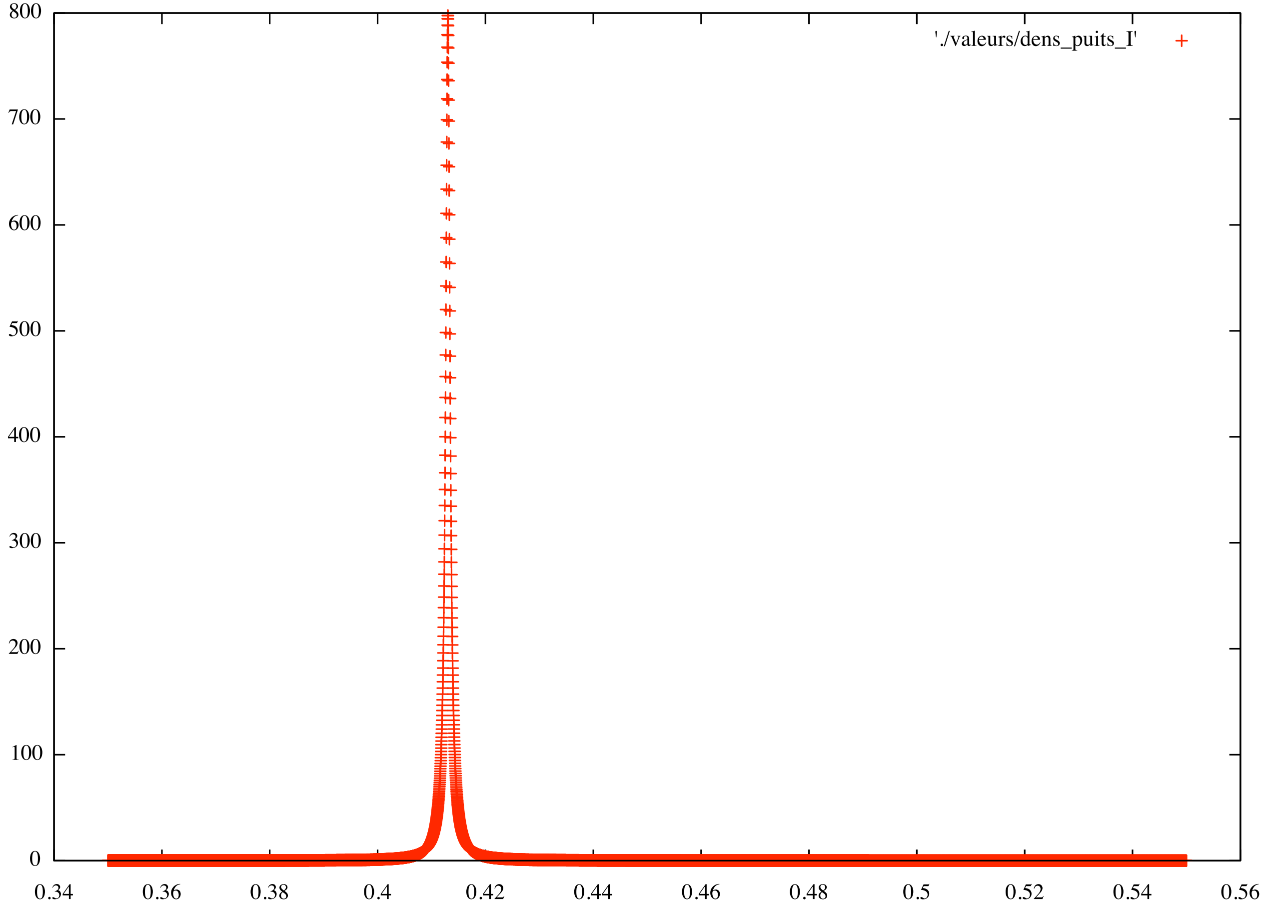
Numerics

The density at $t = T_{end}$



Numerics

The "density of states", $\int \chi(x)|\psi(k,t)|^2 \, dx$ w.r.t $E = k^2$, at $t = 0$



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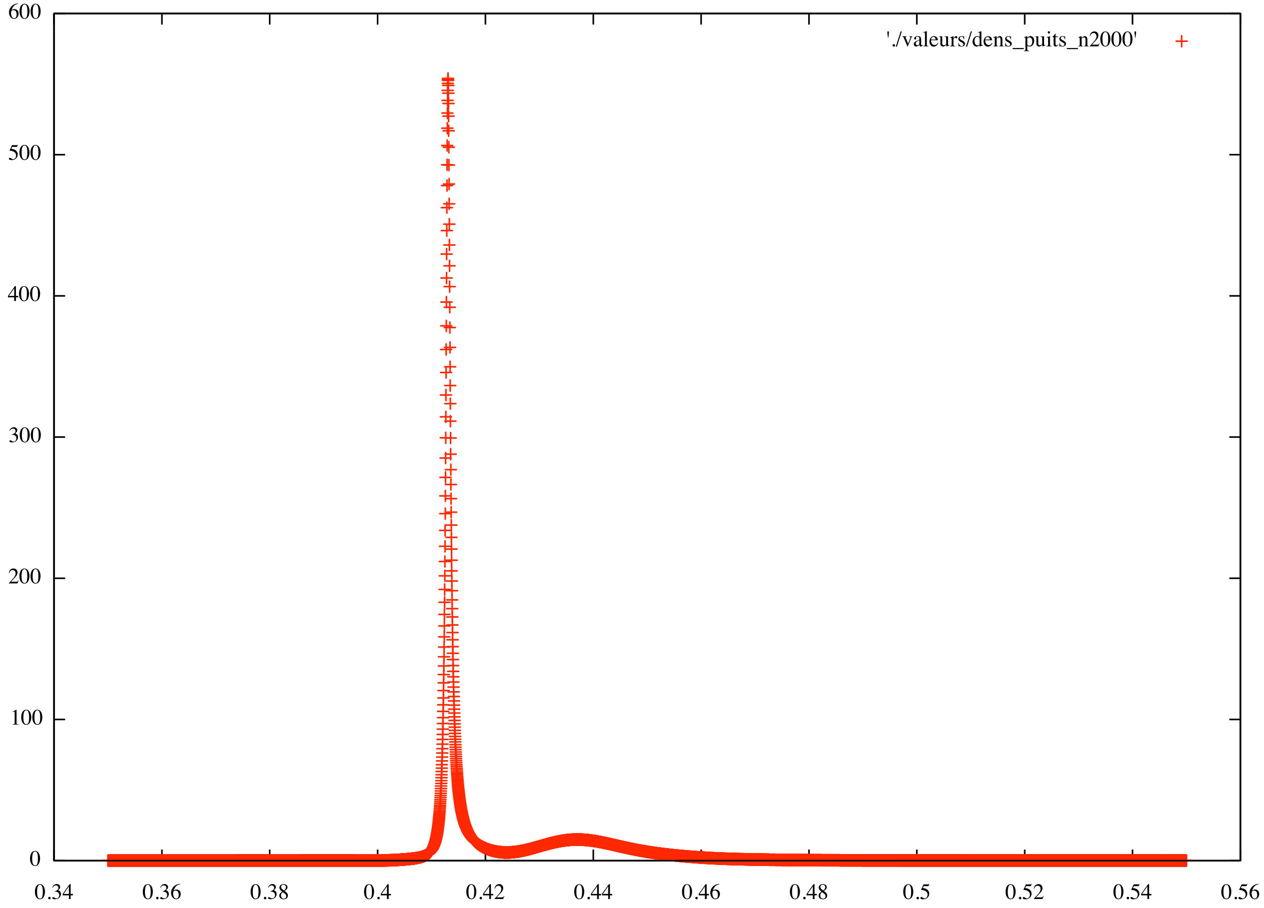
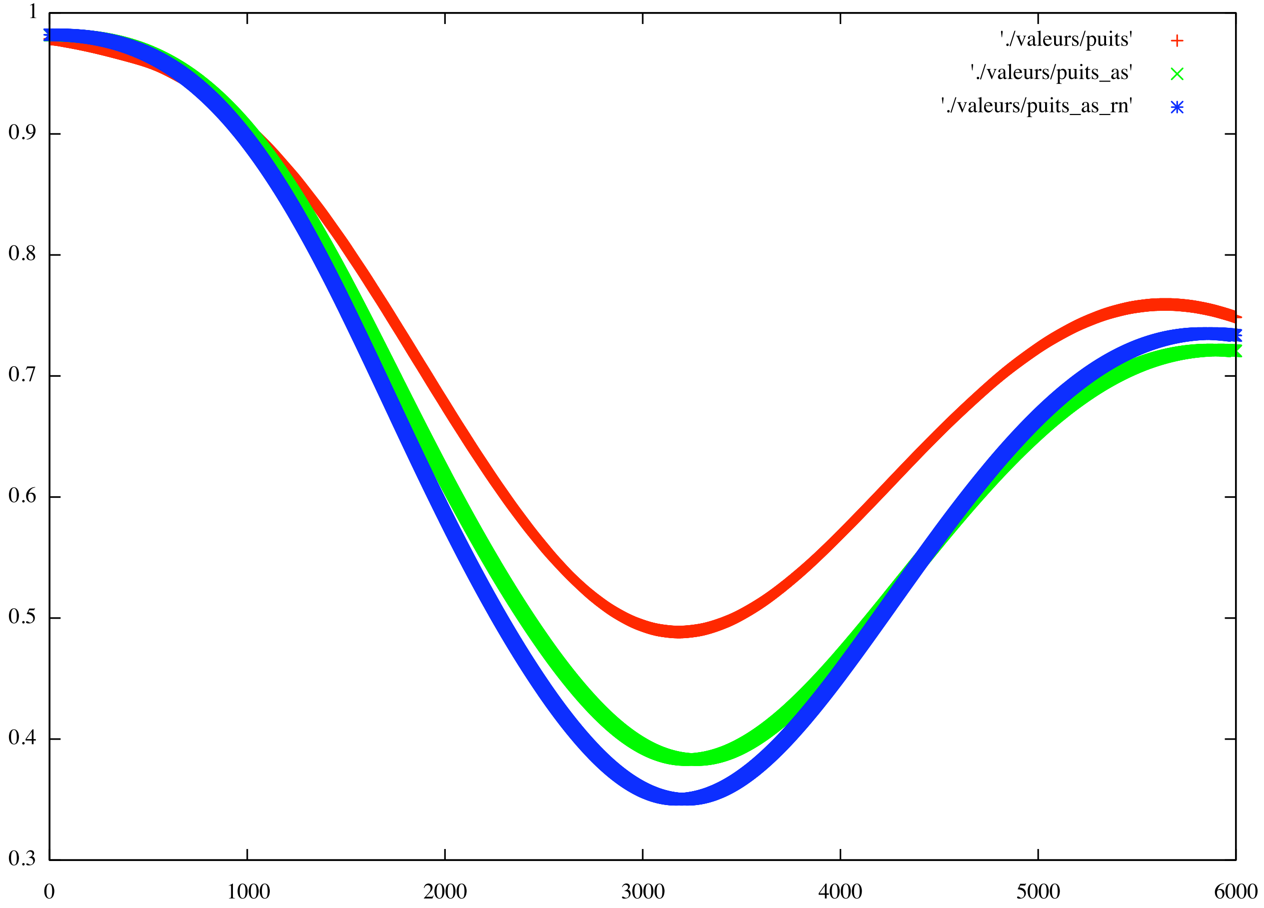


Oscillating variations of $\alpha(t)$

Total charge



Oscillating variations of $\alpha(t)$

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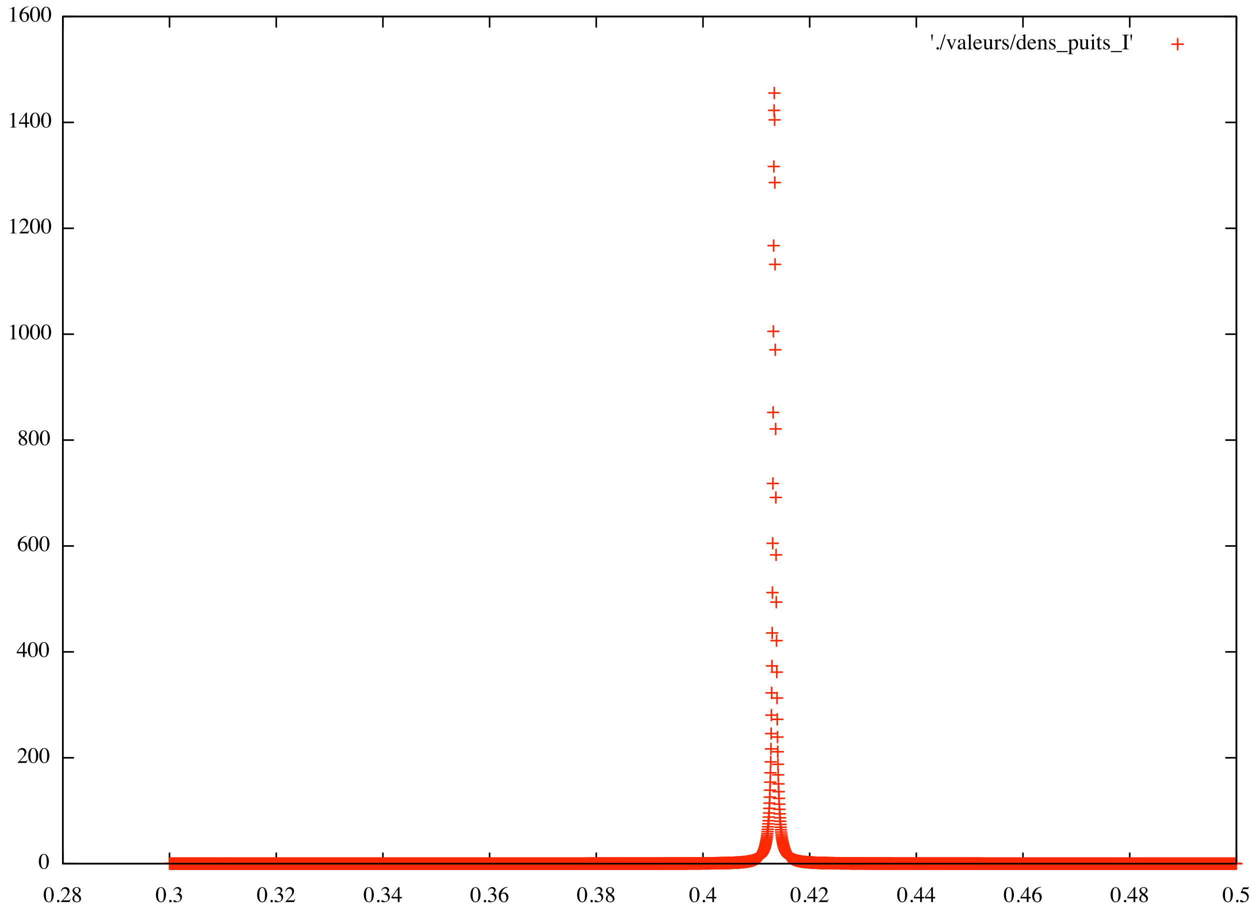

Oscillating variations of $\alpha(t)$

The "density of states", $\int \chi(x)|\psi(k,t)|^2\,dx$ w.r.t $E = k^2$, at $t = T_{end}$