BORN-OPPENHEIMER-TYPE APPROXIMATIONS FOR A DEGENERATE POTENTIAL

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Summary

- Introduction
- Degenerate potentials and Weyl formula
- Accurate estimates on eigenvalues
- An application

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Introduction

- Let V be a nonnegative, real and continuous potential on $\mathbf{R}^d$, and h a small parameter.
- Study the spectral asymptotics of the operator $H_h = -h^2\Delta + V$ on $L^2(\mathbf{R}^d)$.

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Assume $V(x) \to +\infty$ as $|x| \to +\infty$. Then H_h is essentially selfadjoint with compact resolvent , and the following semiclassical asymptotics hold, as $h \to 0$:

$$N(\lambda, H_h) \sim h^{-d}(2\pi)^{-d} v_d \int_{\mathbf{R}^d} (\lambda - V(x))_+^{d/2} dx \ .$$

- $N(\lambda, H_h)$: number of eigenvalues less than a fixed energy λ. v_d : volume of the unit ball .

Remarks

$$N(\lambda, H_h) \sim h^{-d}(2\pi)^{-d} v_d \int_{\mathbf{R}^d} (\lambda - V(x))_+^{d/2} dx \ .$$

The classical asymptotics are also given by the formula , provided we let $h = 1$ and $\lambda \to +\infty$.

Remarks

$$N(\lambda, H_h) \sim h^{-d}(2\pi)^{-d} v_d \int_{\mathbf{R}^d} (\lambda - V(x))_+^{d/2} dx \ .$$

In both cases : asymptotic correspondance between :

- the number of eigenstates with energy less than λ and
- the volume in phase space of the set $S_\lambda = \{(x,\xi), \sigma(x,\xi) \leq \lambda\}$,

where $\sigma(x,\xi) = \xi^2 + V(x)$ is the principal symbol of H_h.

What about the degenerate case ?

If the potential V does not tend to infinity with $|x|$, the volume in phase space of S_λ may be infinite.

Degenerate potentials and Weyl formula

$X = (x, y) \in \mathbf{R}^n \times \mathbf{R}^m = \mathbf{R}^d$, $d \geq 2$

$V(X) = f(x)g(y)$, $f \in C(\mathbf{R}^n; \mathbf{R}_+^*)$, $g \in C(\mathbf{R}^m; \mathbf{R}_+)$,

- (H1) for any $t > 0$ $g(ty) = t^a g(y)$ ($a > 0$) and $g(y) > 0$ for $y \neq 0$.
  The spectrum of the operator $-\Delta_y + g(y)$ in $L^2(\mathbf{R}^m)$ is discrete and positive. Denote by μ_j its eigenvalues.

- (H2) $f(x) \to +\infty$ as $|x| \to +\infty$
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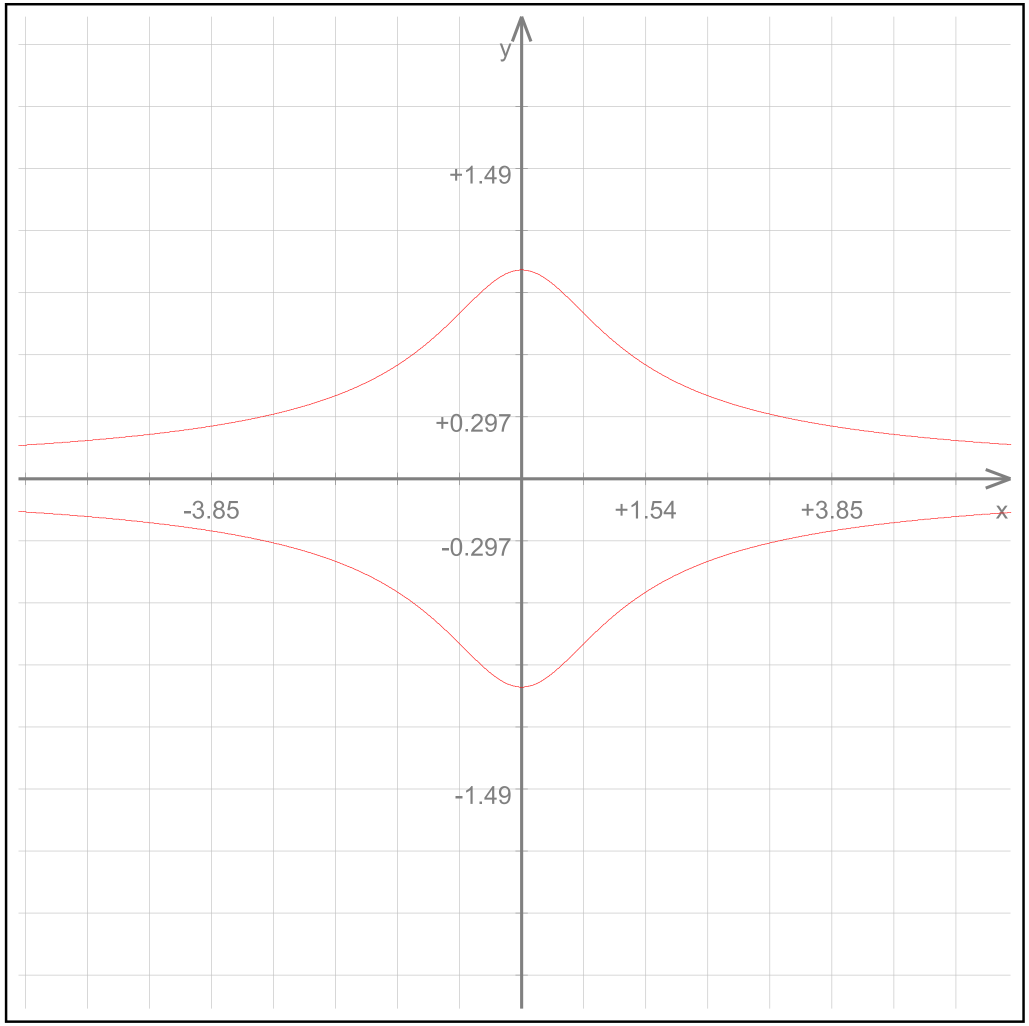
- (H3) (local uniform regularity for f) :
  $\exists\, b, c > 0$ s.t. $c^{-1} \leq f(x)$ and
  $|f(x) - f(x')| \leq cf(x)|x - x'|^b$, if $|x - x'| \leq 1$.

Level curve



Theorem

Let us assume the previous conditions on f and g. Then $N(\lambda; H_h)$ "behaves" like $h^{-n}(2\pi)^{-n} v_n n_{h,f}(\lambda)$,

$n_{h,f}(\lambda) = \int_{\mathbf{R}^n} \Sigma_{j\in\mathbf{N}} [\lambda - h^{2a/(2+a)} f^{2/(2+a)}(x)\mu_j]_+^{n/2} dx$.

- If moreover $f^{-m/a} \in L^1(\mathbf{R}^n)$ and $g \in C^1(\mathbf{R}^m \backslash \{0\})$, then the formula (1) holds.
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If $\frac{1}{C}|x|^k \leq f(x) \leq C|x|^k$ for $|x| > 1$, then

$$\begin{array}{ll} \text{if } k > a & N(\lambda, H_h) \approx h^{-d} \\ \text{if } k = a & N(\lambda, H_h) \approx h^{-d} \ln \frac{1}{h} \\ \text{if } k < a & N(\lambda, H_h) \approx h^{-n-\frac{ma}{k}} \end{array}$$

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- Accurate estimates on eigenvalues
- An application

Accurate estimates on eigenvalues

- Homogeneity
- Born-Oppenheimer approximation
- Improving Born-Oppenheimer approximation
- Refinement for $a \geq 2$

Accurate estimates on eigenvalues

$$\widehat{H}_h = h^2 D_x^2 + h^2 D_y^2 + f(x)g(y)$$

with $g \in C^\infty(\mathbf{R}^m \setminus \{0\})$ homogeneous of degree $a > 0$,

We replace assumptions (H2-H3) by :

$f \in C^\infty(\mathbf{R}^n),\ \forall \alpha \in \mathbb{N}^n,\ (|f(x)| + 1)^{-1} \partial_x^\alpha f(x) \in L^\infty(\mathbf{R}^n)$

$0 < f(0) = \inf_{x \in \mathbf{R}^n} f(x)$

$f(0) < \liminf_{|x| \to \infty} f(x) = f(\infty)\ , \partial^2 f(0) > 0$

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Homogeneity :

Define : $\hbar = h^{2/(2+a)}$.

Change y in $y\hbar$ and get :

$$sp\,(\widehat{H}_h) = \hbar^a\ sp\,(\widehat{H}^\hbar)\ ,$$

with $\widehat{H}^\hbar = \hbar^2 D_x^2 + D_y^2 + f(x)g(y)$.

Homogeneity

$$\widehat{H}^\hbar = \hbar^2 D_x^2 + Q(x, y, D_y) :$$

$$Q(x, y, D_y) = D_y^2 + f(x)g(y) .$$

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$$\widehat{H}^{\hbar} = \hbar^2 D_x^2 + Q(x, y, D_y) :$$

$$Q(x, y, D_y) = D_y^2 + f(x)g(y) .$$

Denote the eigenvalues of $D_y^2 + g(y)$ by $(\mu_j)_{j>0}$.

By homogeneity the eigenvalues of $Q_x(y, D_y)$, for a fixed x, are given by the $(\lambda_j(x))_{j>0}$, where : $\lambda_j(x) = \mu_j \, f^{2/(2+a)}(x)$.

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So we get :

$$\widehat{H}^{\hbar} \geq \left[\hbar^2 D_x^2 + \mu_1 f^{2/(2+a)}(x) \right] \, .$$

$$\inf \; sp_{ess}(\widehat{H}^{\hbar}) \geq \mu_1 f^{2/(2+a)}(\infty) \, .$$

Born-Oppenheimer approximation

- "Effective " potential : $\lambda_1(x) = \mu_1 \, f^{2/(2+a)}(x)$.
- Assumptions on $f \Longrightarrow$ existence of a unique and non degenerate well $U = \{0\}$, with minimal value : μ_1 .
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Theorem

For any $C > 0$, $\exists \; h_0 > 0$ s. t.
for any $0 < \hbar < h_0$, the operator $(\widehat{H}^{\hbar})$ admits a finite number of eigenvalues $E_k(\hbar)$ in $[\mu_1, \mu_1 + C\hbar]$,

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$$E_k(\hbar) = \lambda_k\left(\hbar^2 D_x^2 + \mu_1 f^{2/(2+a)}(x)\right) + \mathbf{O}(\hbar^2)\ .$$

More precisely

$$E_k(\hbar) = \mu_1 + \hbar\lambda_k\left(D_x^2 + \tfrac{\mu_1}{2+a} < \partial^2 f(0)\, x, x >\right) + \mathbf{O}(\hbar^{3/2})\ .$$

Improving Born-Oppenheimer approximation

- Change of variables : $(x,\ y)\ \rightarrow\ (x,\ f^{1/(2+a)}(x)y)$.
- Change of test functions : $u\ \rightarrow\ f^{-m/(4+2a)}(x)u$,

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Thus we obtain :

$$sp\ (\widehat{H}^{\hbar})\ =\ sp\ (\widetilde{H}^{\hbar})$$

$$\widetilde{H}^{\hbar}\ =\ \hbar^2 D_x^2\ +\ f^{2/(2+a)}(x)\left(D_y^2 + g(y)\right)$$

$$...+\hbar^2\frac{2}{(2+a)f(x)}(\nabla f(x)D_x)(yD_y)$$

$$...+i\hbar^2\frac{1}{(2+a)f^2(x)}\left(|\nabla f(x)|^2 - f(x)\Delta f(x)\right)[(yD_y) - i\frac{m}{2}]$$

$$...+\ \hbar^2\frac{1}{(2+a)^2 f^2(x)}|\nabla f(x)|^2[(yD_y)^2\ +\ \frac{m^2}{4}]$$

Eigenfunctions for $\widetilde{H}_1^\hbar$:

$$\widetilde{H}_1^\hbar \;=\; \hbar^2 D_x^2 \;+\; f^{2/(2+a)}(x)\left(D_y^2 + g(y)\right) .$$

- $\nu_{j,k}^\hbar$: the eigenvalues of $\hbar^2 D_x^2 \;+\; \mu_j f^{2/(2+a)}(x)$,
- $\psi_{j,k}^\hbar$: the associated normalized eigenfunctions .

Eigenfunctions for $\widetilde{H}_1^\hbar$:

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- $\nu_{j,k}^\hbar$: the eigenvalues of $\hbar^2 D_x^2 + \mu_j f^{2/(2+a)}(x)$,
- $\psi_{j,k}^\hbar$: the associated normalized eigenfunctions .
- Consider the test functions : $u_{j,k}^\hbar(x,y) = \psi_{j,k}^\hbar(x)\varphi_j(y)$,

$$(D_y^2 + g(y))\varphi_j(y) = \mu_j\varphi_j(y)) .$$

We have immediately :

$$\widetilde{H}_1^\hbar(u_{j,k}^\hbar(x,y)) = \nu_{j,k}^\hbar u_{j,k}^\hbar(x,y) .$$

Theorem

For any fixed integer $N > 0$, there exists $h_0(N) > 0$ verifying : for any $\hbar \in]0, h_0(N)[$, for any $k \leq N$ and any $j \leq N$ such that $\mu_j < \mu_1 f^{2/(2+a)}(\infty)$,

one can find an eigenvalue $\lambda_{jk} \in sp_d\,(\widehat{H}^{\hbar})$ such that

$$| \lambda_{jk} - \lambda_k \left(\hbar^2 D_x^2 + \mu_j f^{2/(2+a)}(x)\right) | \leq \hbar^2 C .$$

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Consequently, when $k = 1$, we have

$$| \lambda_{j1} - \left[\mu_j + \hbar(\mu_j)^{1/2} \frac{tr((\partial^2 f(0))^{1/2})}{(2+a)^{1/2}}\right] | \leq \hbar^2 C \,.$$

Outline of the proof

Prove that :

$$\|(\widehat{H}^{\hbar} - \widetilde{H}_1^{\hbar})(u_{j,k}^{\hbar}(x,y))\| = |(\widehat{H}^{\hbar} - \nu_{j,k}^{\hbar})u_{j,k}^{\hbar}(x,y)\| = \mathbf{O}(\hbar^2) .$$

Lemma :

For any integer N , there exists a positive constant $C = C(N)$ such that, for any $k \leq N$, the eigenfunction $\psi_{j,k}^{\hbar}$ satisfi es the following inequalities :

for any $\alpha \in \mathbb{N}^n$, $|\alpha| \leq 2$,

$$\|\hbar_j{}^{|\alpha|/2} |D_x^{\alpha} \psi_{j,k}^{\hbar}| \| < C$$

$$\| \left(\frac{\nabla f(x)}{f(x)}\right)^{\alpha} \psi_{j,k}^{\hbar} \| < \hbar_j{}^{|\alpha|/2} C$$

with $\hbar_j = \hbar \mu_j^{-1/2}$.

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- Middle energies

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Assume : $a \geq 2$ and $f(\infty) = \infty$, and $g \in C^{\infty}(\mathbf{R}^m)$.

Goal : get sharp localization near the μ_j's for much higher values of j's.

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Theorem

If j is such that $\mu_j \leq \hbar^{-2}$,

then for any integer N , there exists $C = C(N)$ such that, for any $k \leq N$, there exists an eigenvalue $\lambda_{jk} \in sp_d\,(\widehat{H}^\hbar)$ verifying :

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An application

We consider a Schrödinger operator on $L^2(\mathbf{R}^d_z)$ with $d \geq 2$,

$$P^h \;=\; -h^2\Delta \;+\; V(z)$$

- $V \;\in\; C^\infty(\mathbf{R}^d\;;\;[0,+\infty[)\;\;, \liminf_{|z|\to\infty} V(z) \;>\; 0$
- $\Gamma = V^{-1}(0)$ is a regular and connected hypersurface .

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- $V \in C^\infty(\mathbf{R}^d\,;\,[0,+\infty[)$, $\liminf_{|z|\to\infty} V(z) > 0$
- $\Gamma = V^{-1}(0)$ is a regular and connected hypersurface .
- (H1) $\exists\, m \in \mathbb{N}^\star$ and $C_0 > 0$ s.t.

$$C_0^{-1} d^{2m}(z,\,\Gamma) \leq V(z) \leq C_0\, d^{2m}(z,\,\Gamma)$$

$$\forall\, z\ ,\ d(z,\,\Gamma) < C_0^{-1}\ .$$

More assumptions :

Choose an orientation on Γ and then a unit normal vector $N(s)$ on each $s \in \Gamma$.

Defi ne the function on Γ : $f(s) = \frac{1}{(2m)!}\left(N(s)\frac{\partial}{\partial s}\right)^{2m} V(s)$

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- (H2) f achieves its minimum on Γ on a finite number of points:
  $\Sigma_0 = f^{-1}(\{\eta_0\}) = \{s_1, \ldots, s_{\ell_0}\}$,
  if $\eta_0 = \min_{s\in\Gamma} f(s)$.
- (H3) The hessian of f at each $s_l \in \Sigma_0$ is non degenerate.

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Thus $f(s) > 0$, $\forall\, s \in \Gamma$, and $Hess(f)_{s_l}$ has $d-1$ positive eigenvalues $\rho_1^2(s_l) \leq \ldots \leq \rho_{d-1}^2(s_l)$, $(\rho_j(s_l) > 0)$.

Theorem

For any $N \in \mathbb{N}^\star$, there exist $h_0 \in]0,1]$ and $C_0 > 0$ s.t.
if $\mu_j << h^{\frac{-4m}{(2m+3)(m+1)}}$, for any $0 < h < h_0$
and if $\alpha \in \mathbb{N}^{d-1}$ and $|\alpha| \leq N$,
then $\forall\, s_\ell \in \Sigma_0$, $\exists\, \lambda^h_{j\ell\alpha} \in sp_d(P^h)$ s.t.

$$\left| \lambda^h_{j\ell\alpha} - h^{\frac{2m}{m+1}} \left[\eta_0^{\frac{1}{m+1}} \mu_j + h^{\frac{1}{m+1}} \mu_j^{1/2} (\mathcal{A}_\ell) \right] \right| \leq h^2 \mu_j^{\frac{4m+3}{2m}} C_0 \,.$$

- $\mathcal{A}_\ell = C_m \left[2\alpha\, \rho(s_\ell) + Tr^+[Hess(f(s_\ell))] \right]$
- $\alpha\, \rho(s_\ell) = \alpha_1\, \rho_1(s_\ell) + \ldots \alpha_{d-1}\, \rho_{d-1}(s_\ell)$.

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- $\alpha\, \rho(s_\ell) = \alpha_1\, \rho_1(s_\ell) + \ldots \alpha_{d-1}\, \rho_{d-1}(s_\ell)$.
- $(\mu_j)_{j\geq 1}$: the increasing sequence of the eigenvalues of the operator $-\dfrac{d^2}{dt^2} + t^{2m}$ on $L^2(\mathbf{R})$.

Proof (1) :

- $\mathcal{O}_0 \subset \mathbb{R}^d$: open neighbourhood of $s_l \in \Sigma_0$, s.t.
  $\Gamma_0 = \Gamma \cap \mathcal{O}_0 = \{z \in \mathcal{O}_0 \, ; \, \phi(z) = 0\}$,
  $|\nabla \phi(z)| = 1 , \quad \forall \, z \in \mathcal{O}_0$.

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- find $\tau \in C^\infty(\mathcal{O}_0 \, ; \, \mathbb{R}^{d-1})$ s. t.
  $\nabla \tau_j(z).\nabla \phi(z) = 0 \, , \quad \forall j = 1, \ldots, d-1$
  $\mathrm{rank}\{\nabla \tau_1(\mathrm{z}), \ldots, \nabla \tau_{\mathrm{d-1}}(\mathrm{z})\} = \mathrm{d} - 1$.

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- Then $(x, y) = (\tau_1, \ldots, \tau_{d-1}, \phi)$ are local coordinates in $\mathcal{O}_0$ s. t.

$$\Delta = |\widetilde{g}|^{-1/2} \sum_{1 \leq i,j \leq d-1} \partial_{x_i} \left(|\widetilde{g}|^{1/2} \, \widetilde{g}^{ij} \partial_{x_j} \right) + |\widetilde{g}|^{-1/2} \partial_y \left(|\widetilde{g}|^{1/2} \partial_y \right)$$

$$V = y^{2m} \widetilde{f}(x, y) \quad \text{with} \quad \widetilde{f} \in C^\infty(\mathcal{V}_0)$$

$\mathcal{V}_0$ is an open neighbourhood of zero in $\mathbb{R}^d$.

Proof (2) :

$\widetilde{g}^{ij}(x,y) = \widetilde{g}^{ji}(x,y) \in C^\infty(\mathcal{V}_0;\ \mathbb{R})$, $|\widetilde{g}|^{-1} = det\left(\widetilde{g}^{ij}(x,y)\right) > 0$.
$x = (x_1, \ldots, x_{d-1})$ are local coordinates on Γ_0
and the metric $g = (g_{ij})$ on Γ_0 is given by

$$(g_{ij}(x))_{1\le i,j\le d-1} = G(x)\ , \quad \text{with} \quad (G(x))^{-1} = \left(\widetilde{g}^{ij}(x,0)\right)_{1\le i,j\le d-}$$

If $w \in C_0^2(\mathcal{O}_0)$ then

$$P^h w = \widehat{P}^h u \quad \text{with}$$
$$u = |\widetilde{g}|^{1/4} w \quad \text{and}$$
$$\widehat{P}^h = -h^2 \sum_{1\le i,j\le d-1} \partial_{x_i}\left(\widetilde{g}^{ij}\partial_{x_j}\right) - h^2\partial_y^2 + V + h^2 V_0\ , \tag{1}$$

for some $V_0 \in C^\infty(\mathcal{V}_0\ ;\ \mathbb{R})$.

Proof (3)

- Write :

$$V(x,y) = y^{2m} f(x) + y^{2m+1} f_1(x) + y^{2m+2} \widetilde{f}_2(x,y)$$

$f(x) = \widetilde{f}(x,0)$ and $\widetilde{f}_2 \in C^\infty(\mathcal{V}_0)$.

Proof (3)

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- perform the change of variable and the related unitary transformation :
$(x,y) \;\rightarrow\; (x,t) \;=\; (x, f^{1/2(m+1)}(x) y)$
$u \;\rightarrow\; v \;=\; f^{-1/4(m+1)}(x) u \;,$

- get that : $\widehat{P}^h u \;=\; \widehat{Q}^h v$, where
$\widehat{Q}^h \;=\; Q_0^h \;+\; t^{2m+1} f_1^0(x) \;+\; h^2 R_0 \;+\; + h^2 t R_1 \;+\; t^{2m+2} \widetilde{f}_2^0$

$$Q_0^h \;=\; -h^2 \sum_{1 \le k,\ell \le d-1} \partial_{x_k} \left(g^{k\ell} \partial_{x_\ell} \right) + f(x)^{1/(m+1)} \left(-h^2 \partial_t^2 \;+\; t^{2n} \right.$$

Proof (4)

$(\mu_j)_{j\geq 1}$: the increasing sequence of the eigenvalues of the operator $-\dfrac{d^2}{dt^2} + t^{2m}$ on $L^2(\mathbb{R})$.

Let us define $h_j = h^{1/(m+1)}/\mu_j^{1/2}$.

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Now work with the Dirichlet operator

$$H_0^{h_j} = -h_j^2 \sum_{1\leq k,\ell\leq d-1} \partial_{x_k}\left(g^{k\ell}\partial_{x_\ell}\right) + f^{1/(m+1)}(x)$$

instead of the preceding

$$Q_0^h = -h^2 \sum_{1\leq k,\ell\leq d-1} \partial_{x_k}\left(g^{k\ell}\partial_{x_\ell}\right) + f^{1/(m+1)}(x)\left(-h^2\partial_t^2 + t^{2m}\right) .$$