

**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 $L^2(\mathbf{R}^d)$.

Non degenerate case :

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

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

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

Remarks

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

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

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

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

- **(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)** $f(x) \rightarrow +\infty$ as $|x| \rightarrow +\infty$

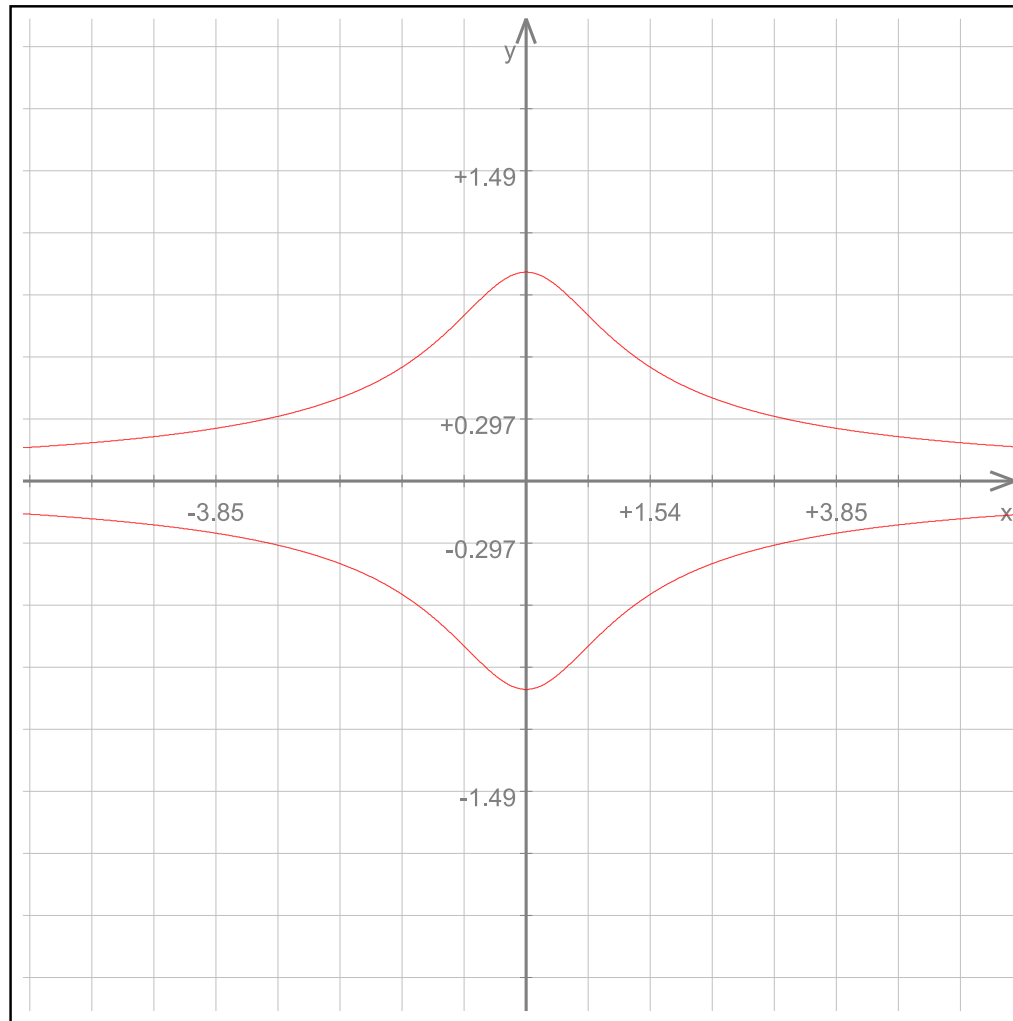
so $H_h = -h^2 \Delta + V$ has a compact resolvent.

- **(H3)** (local uniform regularity for f) :

$\exists b, c > 0$ s.t. $c^{-1} \leq f(x)$ and

$|f(x) - f(x')| \leq c f(x) |x - x'|^b$, 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 $h^{-n} (2\pi)^{-n} v_n n_{h,f}(\lambda)$,

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

- If moreover $f^{-m/a} \in L^1(\mathbf{R}^n)$ and $g \in C^1(\mathbf{R}^m \setminus \{0\})$, then the formula (1) holds.
- If there is some information on the growth of f , then the asymptotics can be computed in terms of power of h :

If $\frac{1}{C}|x|^k \leq f(x) \leq C|x|^k$ for $|x| > 1$, then

$$\text{if } k > a \quad N(\lambda, H_h) \approx h^{-d}$$

$$\text{if } k = a \quad N(\lambda, H_h) \approx h^{-d} \ln \frac{1}{h}$$

$$\text{if } k < a \quad N(\lambda, H_h) \approx h^{-n - \frac{ma}{k}}$$

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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 :

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

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

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

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

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

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

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 : $\lambda_j(x) = \mu_j f^{2/(2+a)}(x)$.

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 $f \implies$ existence of a unique and non degenerate well $U = \{0\}$, with minimal value : μ_1 .
- Hence we can apply a theorem of A. Martinez and get :

Theorem

For any $C > 0$, $\exists h_0 > 0$ s. t.

for any $0 < \hbar < h_0$, the operator (\hat{H}^\hbar) admits a finite number of eigenvalues $E_k(\hbar)$ in $[\mu_1, \mu_1 + C\hbar]$,

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

More precisely

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

Improving Born-Oppenheimer approximation

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

Thus we obtain :

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

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

$$\dots + \hbar^2 \frac{2}{(2+a)f(x)} (\nabla f(x) D_x)(y D_y)$$

$$\dots + i\hbar^2 \frac{1}{(2+a)f^2(x)} (|\nabla f(x)|^2 - f(x)\Delta f(x)) [(y D_y) - i\frac{m}{2}]$$

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

Eigenfunctions for \tilde{H}_1^{\hbar} :

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

- $\nu_{j,k}^{\hbar}$: 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 :

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

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

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

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 $\psi_{j,k}^{\hbar}$ satisfies the following inequalities :

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

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

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

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

Accurate estimates on eigenvalues

- Homogeneity
- Born-Oppenheimer approximation
- Improving Born-Oppenheimer approximation
- Middle energies

Middle energies

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.

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 $\lambda_{jk} \in sp_d(\hat{H}^\hbar)$ verifying :

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

Consequently, when $k = 1$, we have

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

An application

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

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

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

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

- (H2) f achieves its minimum on Γ on a finite number of points:

$$\Sigma_0 = f^{-1}(\{\eta_0\}) = \{s_1, \dots, s_{\ell_0}\},$$

if $\eta_0 = \min_{s \in \Gamma} f(s)$.

- (H3) The hessian of f at each $s_l \in \Sigma_0$ is non degenerate.

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

Theorem

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

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

- $\mathcal{A}_\ell = C_m [2\alpha \rho(s_\ell) + Tr^+[Hess(f(s_\ell))]]$
- $\alpha \rho(s_\ell) = \alpha_1 \rho_1(s_\ell) + \dots + \alpha_{d-1} \rho_{d-1}(s_\ell)$.
- $(\mu_j)_{j \geq 1}$: the increasing sequence of the eigenvalues

of the operator $-\frac{d^2}{dt^2} + t^{2m}$ on $L^2(\mathbb{R})$.

Proof (1) :

- $\mathcal{O}_0 \subset \mathbb{R}^d$: open neighbourhood of $s_l \in \Sigma_0$, s.t.
 $\Gamma_0 = \Gamma \cap \mathcal{O}_0 = \{z \in \mathcal{O}_0 ; \phi(z) = 0\}$,
 $|\nabla\phi(z)| = 1, \quad \forall z \in \mathcal{O}_0$.
- find $\tau \in C^\infty(\mathcal{O}_0 ; \mathbb{R}^{d-1})$ s. t.
 $\nabla\tau_j(z) \cdot \nabla\phi(z) = 0, \quad \forall j = 1, \dots, d-1$
 $\text{rank}\{\nabla\tau_1(z), \dots, \nabla\tau_{d-1}(z)\} = d-1$.
- Then $(x, y) = (\tau_1, \dots, \tau_{d-1}, \phi)$ are local coordinates in \mathcal{O}_0 s. t.

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

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

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

Proof (2) :

$\tilde{g}^{ij}(x, y) = \tilde{g}^{ji}(x, y) \in C^\infty(\mathcal{V}_0; \mathbb{R})$, $|\tilde{g}|^{-1} = \det(\tilde{g}^{ij}(x, y)) > 0$.

$x = (x_1, \dots, x_{d-1})$ are local coordinates on Γ_0
and the metric $g = (g_{ij})$ on Γ_0 is given by

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

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

$$P^h w = \hat{P}^h u \quad \text{with}$$

$$u = |\tilde{g}|^{1/4} w \quad \text{and}$$

$$\hat{P}^h = -h^2 \sum_{1 \leq i, j \leq d-1} \partial_{x_i} (\tilde{g}^{ij} \partial_{x_j}) - h^2 \partial_y^2 + V + h^2 V_0, \quad (1)$$

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

Proof (3)

- Write :

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

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

- 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 : $\hat{P}^h u = \hat{Q}^h v$, where

$$\hat{Q}^h = Q_0^h + t^{2m+1} f_1^0(x) + h^2 R_0 + h^2 t R_1 + t^{2m+2} \tilde{f}_2^0$$

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

Proof (4)

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

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

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

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