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Born-Oppenheimer-type approximations for degenerate potentials : recent results and a survey on the area

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Abstract

This paper is devoted to the asymptotics of eigenvalues for a Schrödinger operator $H_h = -h^2 \Delta + V$ on $L^2(\mathbf{R}^m)$, in the case when the potential V does not fulfill the non degeneracy condition : $V(x) \rightarrow +\infty$ as $|x| \rightarrow +\infty$. For such a model, the point is that the set defined in the phase space by : $H_h \leq \lambda$ may have an infinite volume, so that the Weyl formula which gives the behaviour of the counting function has to be revisited.

We recall various results in this area, in the classical context $(h = 1 \text{ and } \lambda \to +\infty)$, as well as in the semi-classical one $(h \to 0)$ and comment the different methods. In section 3, 4 we present our joint works with A Morame (*),where we consider a degenerate potential V(x) = f(y) g(z), where g is assumed to be a homogeneous positive function of m variables, smooth outside 0, and f is a smooth and strictly positive function of n variables, with a minimum in 0.

In the case where $f(y) \to +\infty$ as $|y| \to +\infty$, the operator has a compact resolvent and we give the asymptotic behaviour, for small values of h, of the number of eigenvalues less than a fixed energy.

Then, without assumptions on the limit of f, we give a sharp estimate of the low eigenvalues, using a Born Oppenheimer approximation. With a refined approach we localize also higher energies. In the case when the degree of homogeneity is not less than 2, we can even assume that the order of these energies is like the inverse power of the square of h.

Finally we apply the previous methods to a class of potentials in \mathbb{R}^d , $d \geq 2$, which vanish on a regular hypersurface.

1 Introduction

Let V be a nonnegative, real and continuous potential on \mathbf{R}^m , and h a parameter in]0, 1]. The spectral asymptotics of the operator $H_h = -h^2 \Delta + V$ on $L^2(\mathbf{R}^m)$ have been intensively studied. More precisely it is well known [16] that H_h is essentially selfadjoint with compact resolvent when $V(x) \to +\infty$ as $|x| \to +\infty$ (we shall say that V is non degenerate). Moreover, denoting by $N(\lambda, H_h)$ the number of eigenvalues less than a fixed energy λ , the following semiclassical asymptotics hold, as $h \to 0$:

$$N(\lambda, H_h) \sim h^{-m} (2\pi)^{-m} v_m \int_{\mathbf{R}^m} (\lambda - V(x))_+^{m/2} dx \ . \tag{1.1}$$

In this formula, v_m denotes the volume of the unit ball in \mathbb{R}^m , and the notation W_+ means the positive value of W.

Let us note that the classical asymptotics are also given by the formula (1.1), provided we let h = 1 and $\lambda \to +\infty$.

In both cases, the result points out the asymptotic correspondance between the number of eigenstates with energy less than λ and the volume in phase space of the set $\{(x,\xi), f(x,\xi) \leq \lambda\}$, where $f(x,\xi) = \xi^2 + V(x)$ is the principal symbol of H_h .

In this paper we propose a review of results concerning the degenerate case : the potential V does not tend to infinity with |x|, so that the volume in phase space of the previous set may be infinite.

2 The Tauberian approach

Let us explain how the problem of the degenerate case came from the non degenerate one.

In 1950 De Wet and Mandl ([3]) proved the formula (1.1) in its classical version, provided $V(x) \ge 1$ and two more conditions on V:

1) a smoothness condition : V differentiable and $|\nabla V| = o(V)$

2) a Tauberian type condition : let $\Phi(V, \lambda) = \int_{\mathbf{R}^m} (\lambda - V(x))_+^{m/2} dx$; it is assumed that there exists c and c' such that :

 $c\Phi(V,\lambda) \le \lambda\Phi'(V,\lambda) \le c'\Phi(V,\lambda).$

The first condition is local and the second is global. This last condition was needed to use a Tauberian technique, which consists on studying the asymptotic behavior of the Green's function of the operator H_1 and applying a Tauberian theorem.

Refinements were done by Titchmarsh, Levitan and Kostjucenko,([23], [11], [12]) and then Rosenbljum ([18]) proved that the formula (1.1) holds with "maximal" weakening conditions on V:

1) the smoothness condition is replaced by a condition on the " L^1 -modulus of continuity" on unit cubes and by the following assumption : $V(y) \leq C'V(x)$ if $|x - y| \leq 1$.

2) the Tauberian type condition becomes : $\sigma(2\lambda, V) \leq C\sigma(\lambda, V)$ (for large λ), where $\sigma(\lambda, V)$ denotes the volume of the set $\{x \in \mathbf{R}^m; V(x) < \lambda\}$.

Solomyak ([22]) makes the following remark :

Lemma 2.1 Let V be a positive a-homogeneous potential :

 $V(x) \ge 0; V(tx) = t^a V(x) \text{ for any } t \ge 0 \ (a > 0).$

If moreover V(x) is strictly positive $(V(x) \neq 0 \text{ if } x \neq 0)$ the spectrum of H_1 is discrete and the formula (1.1) takes the form :

$$N(\lambda, H_1) \sim \gamma_{m,a} \lambda^{\frac{2m+am}{2a}} \int_{S^{m-1}} (V(x))^{-m/a} dx$$

 $(\gamma_{m,a} \text{ is a constant depending only on the parameters } m \text{ and } a.)$

From that lemma comes out naturally the idea of investigating the spectrum whithout the condition of strict positivity (and thus in a case of degeneracy of the potential); the two main results are ([22]] :

Theorem 2.2 The formula of Lemma 2.1 still holds for a positive a-homogeneous potential such that $J(V) = \int_{S^{m-1}} (V(x))^{-m/a} dx$ is finite.

The second result deals with a case where J(V) is infinite :

let $V(x) = F(y, z), y \in \mathbf{R}^n, z \in \mathbf{R}^p, n + p = m, m \ge 2$, such that $F(sy, tz) = s^b t^{a-b} F(y, z)$ (with 0 < a < b) and F(y, z) > 0 for $|z||y| \neq 0$. Denote by $\lambda_j(y)$ the eigenvalues of the operator $-\Delta_z + F(y, z)$ in $L^2(\mathbf{R}^p)$ and let $s = \frac{2b}{2+a-b}$, then :

Theorem 2.3

$$If \ \frac{n}{b} > \frac{m}{a} \quad N(\lambda, H_1) \sim \gamma_{n,s} \lambda^{\frac{2m+am}{2b}} \int_{S^{m-1}} \Sigma(\lambda_j(y))^{-n/s} dx$$
$$if \ \frac{n}{b} = \frac{m}{a} \quad N(\lambda, H_1) \sim \frac{a(a+2)}{2b(a-b)} \gamma_{m,a} \lambda^{\frac{2m+am}{2b}} \ln \lambda \int_{S^{n-1}S^{p-1}} F(y,z)^{-m/a} dx.$$

The proof is based on variational techniques and spectral estimates proved in ([18]).But on a heuristic level the result can be understood in the framework of the theory of Schrödinger operators with operator potential.

This last approach can be found in ([17]) where D.Robert extended the theory of pseudodifferential operators in the form developped by Hörmander to pseudodifferential operators with operator symbols. It was thus possible to study cases where the operator has a compact resolvent but the condition $\lim_{\infty} V(x) = +\infty$ is not fulfilled. As an example it gives the asymptotics of $N(\lambda, H_1)$ for the 2-dimensional potential $V(y, z) = y^{2k}(1+z^2)^l$, where k et l are strictly positive. The asymptotics are the following :

Theorem 2.4

$$\begin{split} If \ k > l & N(\lambda, H_1) \sim \gamma_1 \lambda^{\frac{l+k+1}{2l}} \\ if \ k = l & N(\lambda, H_1) \sim \gamma_2 \lambda^{\frac{2k+1}{2k}} \ln \lambda \\ if \ k < l & N(\lambda, H_1) \sim \gamma_3 \lambda^{\frac{2k+1}{2k}}. \end{split}$$

The constants γ_i depend only on k and l, but the first one γ_1 takes in account the trace of the operator $(-\Delta_z + z^{2k})^{-(k+1)/2l}$ in $L^2(\mathbf{R})$.

In the 2-dimensional case let us mention the results of B.Simon ([20]). He first recalls Weyl's famous result : let H be the Dirichlet Laplacian in a bounded region Ω in \mathbb{R}^2 , then the following asymptotics hold :

$$N(\lambda, H) \sim \frac{1}{2}\lambda |\Omega|$$

and then he considers special regions Ω for which the volume (denoted by $|\Omega|$) is infinite but the spectrum of the Laplacian is still discrete. These regions are of the type : $\Omega_{\mu} = \{(y, z); |y| | z |^{\mu} \leq 1\}.$

Actually the problem can be derived from the study of the asymptotics of Schrödinger operators with the homogeneous potential : $V(y, z) = |y|^{\alpha} |z|^{\beta}$.

In order to get these "non-Weyl" asymptotics, he uses the Feynman-Kac formula and the Karamata-Tauberian theorem, but the main tool is what he calls "sliced bread inequalities", which can be seen as a kind of Born-Oppenheimer approximation. More precisely let $H = -\Delta + V(y, z)$ be defined on \mathbf{R}^{n+p} , and denote by $\lambda_j(y)$ the eigenvalues of the operator $-\Delta_z + V(y, z)$ in $L^2(\mathbf{R}^p)$. (If the z's are electron coordinates and the y's are nuclear coordinates, the $\lambda_j(y)$ are the Born-Oppenheimer curves). He proves the following lemma :

$$\operatorname{Tr} e^{-tH} \leq \Sigma_j e^{-t(-\Delta_y + \lambda_j(y))}$$

(when the second term exists).

Thus he gets the two following coupled results :

Theorem 2.5 If $H = -\Delta + |y|^{\alpha} |z|^{\beta}$ and $\alpha < \beta$, then

$$N(\lambda, H) \sim c_{\nu} \lambda^{\frac{2\nu+1}{2}} \qquad (\nu = \frac{\beta+2}{2\alpha})$$

Corollary : if $H = -\Delta_{\Omega_{\mu}} \ (\mu > 1)$, then $N(\lambda, H) \sim c_{\mu} \lambda^{\frac{1}{2\mu+1}}$.

Theorem 2.6 If $H = -\Delta + |y|^{\alpha} |z|^{\alpha}$, then $N(\lambda, H) \sim \frac{1}{\pi} \lambda^{1+\frac{1}{\alpha}} \ln \lambda$ Corollary : if $H = -\Delta_{\Omega_{\mu}} \ (\mu = 1)$, then $N(\lambda, H) \sim \frac{1}{\pi} \lambda \ln \lambda$.

The constant c_{μ} depends only on μ , and the constant c_{μ} takes in account the trace of the operator $(-\Delta_z + |z|^{\beta})^{-\nu}$ in $L^2(\mathbf{R})$.

3 The min-max approach

The result presented in this section is based on the method of Courant and Hilbert, the min-max variational principle. It turns out that this method can be applied to operators in $L^2(\mathbf{R}^m)$ with principal symbols which can degenerate on some non bounded manifold of $T^*(\mathbf{R}^m)$. It is the case for the Schrödinger operator with a magnetic field $H = (D_x - A(x))^2$, which degenerates on $\{(x,\xi) \in T^*(\mathbf{R}^m); \xi = A(x)\}$. If the magnetic field B = dAfulfills the so-called magnetic bottle conditions (mainly : $\lim_{\infty} ||B(x)|| = \infty$) the spectrum is discrete ([1]) and the classical asymptotics were established by Colin de Verdière ([2]) using the min-max method. The semiclassical version of the result is given in ([24]).

In ([14]), the min-max method is performed to get semiclassical asymptotics for a large class of degenerate potentials, namely potentials of the following form : $x = (y, z) \in \mathbf{R}^n \times \mathbf{R}^p$, n + p = m, $m \ge 2$

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

$$g \in C(\mathbf{R}^p; \mathbf{R}_+), \ g(tz) = t^a g(z) \ (a > 0) \ \forall t > 0 \ , \ g(z) > 0 \ \forall z \neq 0.$$
(3.1)

The spectrum of the operator $-\Delta_z + g(z)$ in $L^2(\mathbf{R}^p)$ is discrete and positive. Let us denote by μ_i its eigenvalues. It is easy to make the following remark : **Remark 3.1** If $f(y) \to +\infty$ as $|y| \to +\infty$ then $H_h = -h^2\Delta + V$ has a compact resolvent.

Of course if f was supposed to be homogeneous, the asymptotics would be given by Theorem 2.3. Here the assumption on f is only a locally uniform regularity :

 $\exists b, c > 0 \text{ s.t. } c^{-1} \leq f(y) \text{ and } |f(y) - f(y')| \leq cf(y)|y - y'|^b$, for any y, y' verifying $|y - y'| \leq 1$.

Theorem 3.2 Let us assume the previous conditions on f and g. Then there exists $\sigma, \tau \in]0, 1[$ such that, for any $\lambda > 0$, one can find $h_0 \in]0, 1[$, $C_1, C_2 > 0$ in order to have

$$(1-h^{\sigma}C_{1})n_{h,f}(\lambda-h^{\tau}C_{2}) \leq N(\lambda;H_{h}) \leq (1+h^{\sigma}C_{1})n_{h,f}(\lambda+h^{\tau}C_{2}) \quad \forall h \in]0, h_{0}[$$

$$if \ n_{h,f}(\lambda) = h^{-n}(2\pi)^{-n}v_{n} \int_{\mathbf{R}^{n}} \Sigma_{j\in\mathbf{N}} [\lambda-h^{2a/(2+a)}f^{2/(2+a)}(y)\mu_{j}]_{+}^{n/2}dy \ .$$

Provided some additional conditions on f, the previous result can be refined as follows :

Theorem 3.3 If moreover one can find a constant C_3 such that, for any $\mu > 1$:

$$\int_{\{y,f(y)<2\mu\}} f^{-p/a}(y) dy \le C_3 \int_{\{y,f(y)<\mu\}} f^{-p/a}(y) dy ,$$

then one can take $C_2 = 0$ in Theorem 7:

$$(1 - h^{\sigma}C_1)n_{h,f}(\lambda) \le N(\lambda; H_h) \le (1 + h^{\sigma}C_1)n_{h,f}(\lambda) \quad \forall h \in]0, h_0[$$

Remark 3.4 If moreover $f^{-p/a} \in L^1(\mathbf{R}^n)$ and $g \in C^1(\mathbf{R}^p \setminus \{0\})$, then the formula (1) holds.

The proof of Theorem 3.2 uses a suitable covering of \mathbb{R}^n , so that the min-max variational principle allows to deal with Dirichlet and Neumann problems in cylinders for the restrained operator (with a fixed y). The proof of Theorem 3.3 is based on an asymptotic formula of the moment of eigenvalues of $-h^2\Delta_z + g(z)$, which is again obtained using the min-max principle.

As a conclusion, let us notice that if there is some information on the growth of f, then the asymptotics can be computed in terms of power of h:

Remark 3.5 If there exists k > 0 and C > 0 such that $\frac{1}{C}|y|^k \leq f(y) \leq C|y|^k$ for |y| > 1, then

$$\begin{split} & if \ k > a \qquad N(\lambda, H_h) \approx h^{-m} \\ & if \ k = a \quad N(\lambda, H_h) \approx h^{-m} \ln \frac{1}{h} \\ & if \ k < a \qquad N(\lambda, H_h) \approx h^{-n - \frac{pa}{k}} \end{split}$$

4 **Born-Oppenheimer-type** estimates

In last section we have investigated the asymptotic behavior of the number of eigenvalues less than λ of $\widehat{H}_h = -h^2 \Delta + f(y)g(z)$.

Theorem 3.2 gives us a hint of what should eigenvalues of \hat{H}_h look like. This can be done using Born-Oppenheimer-type methods.

We assume as in last section that : $g \in C^{\infty}(\mathbf{R}^m \setminus \{0\})$ is homogeneous of degree a > 0, and assume the following for f:

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

$$0 < f(0) = \inf_{y \in \mathbb{R}^n} f(y)$$

$$f(0) < \liminf_{|y| \to \infty} f(y) = f(\infty)$$

$$\partial^2 f(0) > 0$$

$$(4.1)$$

 $\partial^2 f(0)$ denotes the hessian matrix in 0.

Using homogeneity 4.1

By dividing \widehat{H}_h by f(0), we can change the parameter h and assume that

$$f(0) = 1 . (4.2)$$

Let us define : $\hbar = h^{2/(2+a)}$ and change z in $z\hbar$; we can use the homogeneity of q (3.1) to get :

$$sp(\widehat{H}_h) = \hbar^a sp(\widehat{H}^\hbar),$$
 (4.3)

with $\hat{H}^{\hbar} = \hbar^2 D_y^2 + D_z^2 + f(y)g(z)$. Let us denote as usually the increasing sequence of eigenvalues of D_z^2 + g(z), (on $L^2(\mathbb{R}^m)$), by $(\mu_j)_{j>0}$.

The associated eigenfunctions will be denoted by $(\varphi_j)_j$:

By homogeneity (3.1) the eigenvalues of $Q_y(z, D_z) = D_z^2 + f(y)g(z)$, on $L^2(\mathbb{R}^m)$), for a fixed y, are given by the sequence $(\lambda_j(y))_{j>0}$, where : $\lambda_j(y) = \mu_j f^{2/(2+a)}(y)$. So as in [15] we get :

$$\widehat{H}^{\hbar} \geq \left[\, \hbar^2 D_y^2 \, + \, \mu_1 f^{2/(2+a)}(y) \, \right] \, . \tag{4.4}$$

This estimate is sharp as we will see below.

Then using the same kind of estimate as (4.4), one can see that

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

$$(4.5)$$

We are in the Born-Oppenheimer approximation situation described by A. Martinez in [13] : the "effective" potential is given by $\lambda_1(y) = \mu_1 f^{2/(2+a)}(y)$, the first eigenvalue of Q_y , and the assumptions on f ensure that this potential admits one unique and nondegenerate well $U = \{0\}$, with minimal value equal to μ_1 . Hence we can apply theorem 4.1 of [13] and get :

Theorem 4.1 Under the above assumptions, for any arbitrary C > 0, there exists $h_0 > 0$ such that, if $0 < \hbar < h_0$, the operator (\widehat{H}^{\hbar}) admits a finite number of eigenvalues $E_k(\hbar)$ in $[\mu_1, \mu_1 + C\hbar]$, equal to the number of the eigenvalues e_k of $D_y^2 + \frac{\mu_1}{2+a} < \partial^2 f(0) y, y > in [0, +C]$ such that :

$$E_k(\hbar) = \lambda_k(\widehat{H}^{\hbar}) = \lambda_k \left(\hbar^2 D_y^2 + \mu_1 f^{2/(2+a)}(y) \right) + \mathbf{O}(\hbar^2) .$$
(4.6)

More precisely $E_k(\hbar) = \lambda_k(\widehat{H}^{\hbar})$ has an asymptotic expansion

$$E_k(\hbar) \sim \mu_1 + \hbar (e_k + \sum_{j\geq 1} \alpha_{kj} \hbar^{j/2}).$$
 (4.7)

If $E_k(\hbar)$ is asymptotically non degenerate, then there exists a quasimode

$$\phi_k^{\hbar}(y,z) \sim \hbar^{-m_k} e^{-\psi(y)/\hbar} \sum_{j\geq 0} \hbar^{j/2} a_{kj}(y,z) ,$$
 (4.8)

satisfying

$$C_{0}^{-1} \leq \|\hbar^{-m_{k}}e^{-\psi(y)/\hbar}a_{k0}(y,z)\| \leq C_{0} \\ \|\hbar^{-m_{k}}e^{-\psi(y)/\hbar}a_{kj}(y,z)\| \leq C_{j} \\ \|\left(\hat{H}^{\hbar}-\mu_{1}-\hbar e_{k}-\sum_{1\leq j\leq J}\alpha_{kj}\hbar^{j/2}\right) \\ \hbar^{-m_{k}}e^{-\psi(x)/\hbar}\sum_{0\leq j\leq J}\hbar^{j/2}a_{kj}(x,y)\| \leq C_{J}\hbar^{(J+1)/2}$$

$$(4.9)$$

The formula (4.7) implies

$$\lambda_k(\widehat{H}^{\hbar}) = \mu_1 + \hbar \lambda_k \left(D_y^2 + \frac{\mu_1}{2+a} < \partial^2 f(0) \ y \ , \ y \ > \right) + \mathbf{O}(\hbar^{3/2}) \ , \ (4.10)$$

and when k = 1, one can improve $O(\hbar^{3/2})$ into $O(\hbar^2)$. The function ψ is defined by : $\psi(y) = d(y, 0)$, where d denotes the Agmon distance related to the degenerate metric $\mu_1 f^{2/(2+a)}(y) dy^2$.

4.2 Improving Born-Oppenheimer methods

We are interested now with the lower energies of \widehat{H}^{\hbar} . Let us make the change of variables

$$(y, z) \to (y, f^{1/(2+a)}(y)z)$$
. (4.11)

The Jacobian of this diffeomorphism is $f^{m/(2+a)}(y)$, so we perform the change of test functions : $u \to f^{-m/(4+2a)}(y)u$, to get a unitary transformation.

Thus we get that

$$sp\left(\hat{H}^{\hbar}\right) = sp\left(\hat{H}^{\hbar}\right)$$

$$(4.12)$$

where \widetilde{H}^{\hbar} is the self-adjoint operator on $L^2(\mathbb{R}^n \times \mathbb{R}^m)$ given by

$$\widetilde{H}^{\hbar} = \hbar^{2} D_{y}^{2} + f^{2/(2+a)}(y) (D_{z}^{2} + g(z))
+ \hbar^{2} \frac{2}{(2+a)f(y)} (\nabla f(y) D_{y})(z D_{z})
+ i\hbar^{2} \frac{1}{(2+a)f^{2}(y)} (|\nabla f(y)|^{2} - f(y)\Delta f(y)) [(z D_{z}) - i\frac{m}{2}]
+ \hbar^{2} \frac{1}{(2+a)^{2}f^{2}(y)} |\nabla f(y)|^{2} [(z D_{z})^{2} + \frac{m^{2}}{4}]$$
(4.13)

The only significant role up to order 2 in \hbar will be played actually by the first operator, namely : $\widetilde{H}_1^{\hbar} = \hbar^2 D_y^2 + f^{2/(2+a)}(y) \left(D_z^2 + g(z)\right)$.

This leads to :

Theorem 4.2 .

Under the assumptions (3.1) and (4.1), for any fixed integer N > 0, there exists a positive constant $h_0(N)$ verifying : for any $\hbar \in]0, h_0(N)[$, for any $k \leq N$ and any $j \leq N$ such that

$$\mu_j < \mu_1 f^{2/(2+a)}(\infty) ,$$

there exists an eigenvalue $\lambda_{jk} \in sp_d(\widehat{H}^{\hbar})$ such that

$$|\lambda_{jk} - \lambda_k \left(\hbar^2 D_z^2 + \mu_j f^{2/(2+a)}(z) \right) | \leq \hbar^2 C.$$
 (4.14)

Consequently, when k = 1, we have

$$|\lambda_{j1} - \left[\mu_j + \hbar(\mu_j)^{1/2} \frac{tr((\partial^2 f(0))^{1/2})}{(2+a)^{1/2}}\right]| \leq \hbar^2 C.$$
 (4.15)

4.3 Middle energies

We can refine the preceding results when $a \ge 2$, $g \in C^{\infty}(\mathbb{R}^m)$ and $f(\infty) = \infty$. We get then sharp localization near the μ_j 's for much higher values of j's. More precisely we prove :

Theorem 4.3 . Assume the preceding properties, and consider j such that $\mu_j \leq \hbar^{-2}$;

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

$$|\lambda_{jk} - \lambda_k \left(\hbar^2 D_y^2 + \mu_j f^{2/(2+a)}(y) \right) | \leq C \mu_j \hbar^2 .$$
 (4.16)

Consequently, when k = 1, we have

$$|\lambda_{j1} - \left[\mu_j + \hbar(\mu_j)^{1/2} \frac{tr((\partial^2 f(0))^{1/2})}{(2+a)^{1/2}}\right] | \leq C\mu_j \hbar^2.$$
(4.17)

4.4 An application

We can apply the previous methods for studying Schrödinger operators on $L^2(\mathbb{R}^d_s)$ with $d \geq 2$,

$$P^h = -h^2 \Delta + V(s) \tag{4.18}$$

with a real and regular potential V(s) satisfying

$$V \in C^{\infty}(\mathbb{R}^{d}; [0, +\infty[))$$

$$\liminf_{|s|\to\infty} V(s) > 0$$
(4.19)

$$\Gamma = V^{-1}(\{0\}) \text{ is a regular hypersurface.}$$

Moreover we assume that Γ is connected and that there exist $m \in \mathbb{N}^*$ and $C_0 > 0$ such that for any s verifying $d(s, \Gamma) < C_0^{-1}$

$$C_0^{-1} d^{2m}(s, \Gamma) \leq V(s) \leq C_0 d^{2m}(s, \Gamma)$$
 (4.20)

(d(E, F) denotes the euclidian distance between E and F).

We choose an orientation on Γ and a unit normal vector N(s)on each $s \in \Gamma$, and then, we can define the function on Γ ,

$$f(s) = \frac{1}{(2m)!} \left(N(s) \frac{\partial}{\partial s} \right)^{2m} V(s) , \quad \forall s \in \Gamma .$$
 (4.21)

Then by (4.19) and (4.20), f(s) > 0, $\forall s \in \Gamma$.

Finally we assume that the function f achieves its minimum on Γ on a finite number of discrete points:

$$\Sigma_0 = f^{-1}(\{\eta_0\}) = \{s_1, \dots, s_{\ell_0}\}, \quad if \quad \eta_0 = \min_{s \in \Gamma} f(s), \quad (4.22)$$

and the hessian of f at each point $s_j \in \Sigma_0$ is non degenerate.

 $Hess(f)_{s_j}$ has d-1 non negative eigenvalues

$$\rho_1^2(s_j) \leq \ldots \leq \rho_{d-1}^2(s_j), \quad (\rho_j(s_j) > 0).$$

The eigenvalues $\rho_k^2(s_j)$ do not depend on the choice of coordinates. We denote

$$Tr^+(Hess(f(s_j))) = \sum_{\ell=1}^{d-1} \rho_\ell(s_j).$$
 (4.23)

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

Theorem 4.4 Under the above assumptions, for any $N \in \mathbb{N}^*$, there exist $h_0 \in]0,1]$ and $C_0 > 0$ such that, if $\mu_j << h^{-4m/(m+1)(2m+3)}$, 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.

$$\left| \begin{array}{l} \lambda_{j\ell\alpha}^{h} - h^{2m/(m+1)} \left[\eta_{0}^{1/(m+1)} \mu_{j} + h^{1/(m+1)} \mu_{j}^{1/2} \mathcal{A}_{\ell}(\alpha) \right] \right| \\ \leq h^{2} \mu_{j}^{2+3/2m} C_{0} ; \\ \text{with } \mathcal{A}_{\ell}(\alpha) = \frac{1}{\eta_{0}^{m/(2m+2)} (m+1)^{1/2}} \left[2\alpha \rho(s_{\ell}) + Tr^{+}(Hess(f(s_{\ell}))) \right] \\ (\alpha \rho(s_{\ell}) = \alpha_{1} \rho_{1}(s_{\ell}) + \dots + \alpha_{d-1} \rho_{d-1}(s_{\ell})) . \end{array}$$

References

- [1] J.Avron, I Herbst, B.Simon, *Duke.Math.J.***45** (1978), 847-883.
- [2] Y.Colin de Verdière, L'asymptotique de Weyl pour les bouteilles magnétiques, Comm. Math. Phys. 105 (1986), 327-335.
- [3] J.S.de Wet and Mandl, On the asymptotic distribution of eigenvalues, Proc. Roy. Soc. London Ser. 200 (1950), 572-580.
- [4] B. Helffer : Introduction to the semiclassical analysis for the Schrödinger operator and applications. Springer lecture Notes in Math., n⁰ 1336 (1988).
- [5] B. Helffer, D. Robert, Propriétés asymptotiques du spectre d'opérateurs pseudo-différentiels sur \mathbb{R}^n . Comm. in P.D.E., 7(7),(1982),p.795-882.
- [6] B. Helffer, D. Robert, Comportement semi-classique du spectre des hamiltoniens quantiques hypoelliptiques. Annales ENS Pise IV, 9,(3),(1982),p.405-431.
- [7] B. Helffer, J. Sjoestrand, Multiple wells in the semi-classical limit. I. Comm. in P.D.E., 9, (4), (1984), p.337-408.
- [8] B. Helffer, J. Sjoestrand, Puits multiples en mecanique semi-classique.
 VI. Ann. Institut H. Poincaré, Phys. Theor., 46,(4),(1987),p.353-372.
- [9] L. Hörmander, The Weyl calculus of pseudo-differential operators. Comm. Pure Appl. Math., 32, (1979), p.359-443.
- [10] V. Ivrii, Microlocal analysis and precise spectral asymptotic. Springer, Berlin 1998.
- [11] B.M.Levitan, On the asymptotic behavior of Green's function and its expansion in eigenvalues of Schrödinger's equation, *Math.USSR-Sb.41* 83 (1957), 439-458.
- [12] A.G.Kostjucenko, Asymptotic distribution of the eigenvalues of elliptic operators, *Soviet Math.Dokl.*5 (1964), 1171-1175.

- [13] A. Martinez, Développement asymptotiques et effet tunnel dans l'approximation de Born-Oppenheimer. Ann. Inst. Henri Poincaré, Vol. 49,(3),(1989), 239-257.
- [14] A. Morame, F. Truc, Semiclassical Eigenvalue Asymptotics for a Schrödinger Operator with Degenerate Potential. Asymptotic Anal., 22(1), (2000), 39-49.
- [15] A. Morame, F. Truc, Accuracy on eigenvalues for a Schrödinger Operator with a Degenerate Potential in the semi-classical limit. Cubo, A Journal of Mathematics, 9 (2),(2007), 1-14.
- [16] M.Reed and B.Simon, Methods of Modern Mathematical Physics IV, Academic press, New York, 1978.
- [17] D.Robert, Comportement asymptotique des valeurs propres d'opérateurs du type de Schrödinger à potentiel dégénéré, J.Math.Pures Appl.61 (1982), 275-300.
- [18] G.V.Rosenbljum, Asymptotics of the eigenvalues of the Schrödinger operator, Math. USSR-Sb.22(3) (1974), 349-371.
- [19] M.A. Shubin, Pseudodifferential operators and spectral theory. Springer-Verlag, Berlin 1987.
- [20] B.Simon, non classical eigenvalue asymptotics, J.Funct.Anal.53 (1983), 84-98.
- [21] B. Simon : Semi-classical analysis of low lying eigenvalues I. Ann. Inst. H. Poincaré, 38, (1983), p. 295-307.
- [22] M.Z.Solomyak, Asymptotics of the spectrum of the Schrödinger operator with nonregular homogeneous potential, *Math. USSR-Sb.*55(1) (1986), 19-37.
- [23] E.C.Titchmarsh, On the asymptotic distribution of eigenvalues, Quart.J.Math.Oxford Ser.(2)5(1954), 228-240.
- [24] F. Truc, Semi-classical asymptotics for magnetic bottles, Asympt.Anal.15 (1997), 385-395.