

Semiclassical Analysis for Hamiltonian in the Born-Oppenheimer Approximation

Senoussaoui Abderrahmane

Université d'Oran1, Faculté des Sciences Exactes & Appliquées, Département de Mathématiques
B.P. 1524 El-Mnaouer, Oran, Algeria

e-mail: senoussaoui_abdou@yahoo.fr, senoussaoui.abderahmane@univ-oran.dz

Abstract The purpose of this paper is to show that the operator $H(h) = -h^2 \Delta_x - \Delta_y + V(x, y)$, V is continuous (or $V \in L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$), and $V(x, y) \rightarrow \infty$ as $\|x\| + \|y\| \rightarrow \infty$, has purely discrete spectrum. We give an application to the harmonic oscillator.

Keywords Discrete spectrum; harmonic oscillator; locally compact operator.

2010 Mathematics Subject Classification 35J10, 35Q55

1 Introduction

The Born-Oppenheimer approximation is a method introduced in [1] to analyze the spectrum of molecules. It consists in studying the behavior of the associate Hamiltonian when the nuclear mass tends to infinity. This Hamiltonian can be written in the form:

$$H(h) = -h^2 \Delta_x - \Delta_y + V(x, y)$$

where $x \in \mathbb{R}^n$ represents the position of the nuclei, $y \in \mathbb{R}^p$ is the position of the electrons, h is proportional to the inverse of the square-root of the nuclear mass and $V(x, y)$ is the interaction potential.

In the last decade, many efforts have been made in order to study in the semiclassical limit the spectrum of $H(h)$ (see e.g. [2–7]). These authors have shown that in many situations it is still possible to perform, by Grushin's method, semiclassical constructions related to the existence of some hidden effective semiclassical operator.

In this paper, we study the semiclassical approximation to the eigenvalues and eigenfunctions of $H(h)$ for potentials $V(x, y)$ with $\inf_{\|x\| + \|y\| > R} V(x, y) > 0$, for some $R > 0$, in particular when $\lim_{\|x\| + \|y\| \rightarrow \infty} V(x, y) = \infty$. Our main result in this sense is to show that in this case the Hamiltonian $H(h)$ has a purely discrete spectrum. The technique used is based on the so called locally compact operator. The resolvent $R_{H(h)}(z) = (H(h) - z)^{-1}$, $\text{Im} z \neq 0$, of the operator $H(h)$ on $L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$ is typically not compact (however, it usually is on $L^2(\mathbb{X})$, when $\mathbb{X} \subset \mathbb{R}_x^n \times \mathbb{R}_y^p$ is compact). If $R_{H(h)}(z)$ is compact, then the spectrum $\sigma(R_{H(h)}(z))$ is discrete with zero the only possible point in the essential spectrum. Hence, one would expect that $H(h)$ has discrete spectrum with the only possible accumulation point at infinity (i.e., the essential spectrum $\sigma_{ess}(H(h)) = \emptyset$). In this way, the spectrum $\sigma(H(h))$ reflects the compactness of $R_{H(h)}(z)$. It turns out that these properties are basically preserved if, instead of $R_{H(h)}(z)$ being compact, it is compact only when restricted to any compact subset of $\mathbb{R}_x^n \times \mathbb{R}_y^p$. This is the notion of local compactness. From an analysis of this notion we will see that the discrete spectrum of $H(h)$ is determined by the behavior of $H(h)$ on bounded subsets of $\mathbb{R}_x^n \times \mathbb{R}_y^p$ and the essential spectrum of $H(h)$ is determined by the behavior of $V(x, y)$ in a neighborhood of infinity.

We introduce a specific family of sequences, called Zhislin sequences, which will allow us to characterize the class of locally compact, self-adjoint operators, representing Weyl sequences for a self-adjoint operator.

We finish our work by an application to calculate the spectrum of the harmonic oscillator of semiclassical Schrödinger operator and of the Hamiltonian in the Born-Oppenheimer approximation $H(h)$.

2 Preliminaries

Let's recall some basic definitions on the spectrum of unbounded operator on Hilbert space.

Definition 1 Let A be a linear operator on a Hilbert space X with domain $D(A) \subset X$.

- (i) The spectrum of A , $\sigma(A)$, is the set of all points $\lambda \in \mathbb{C}$ for which $A - \lambda I$, I is the identity) is not invertible.
- (ii) The resolvent set of A , $\rho(A)$, is the set of all points $\lambda \in \mathbb{C}$ for which $A - \lambda I$ is invertible.
- (iii) If $\lambda \in \rho(A)$, then the inverse of $A - \lambda I$ is called the resolvent of A at λ and is written as $R_\lambda(A) = (A - \lambda I)^{-1}$.

Let us note that by definition, $\rho(A) = \mathbb{C} \setminus \sigma(A)$. We can classify $\sigma(A)$ as below:

Definition 2 Let A be a linear operator on a Hilbert space X with domain $D(A) \subset X$.

- (i) If $\lambda \in \sigma(A)$ is such that $\ker(A - \lambda I) \neq \{0\}$, then λ is an eigenvalue of A and any $u \in \ker(A - \lambda I)$, $u \neq 0$, is an eigenvector of A for λ and satisfies $Au = \lambda u$. Moreover, $\dim \ker(A - \lambda I)$ is called the (geometric) multiplicity of λ and $\ker(A - \lambda I)$ is the (geometric) eigenspace of A at λ .
- (ii) The discrete spectrum of A , $\sigma_{disc}(A)$, is the set of all eigenvalues of A with finite (algebraic) multiplicity and which are isolated points of $\sigma(A)$.
- (iii) The essential spectrum of A is defined as the complement of $\sigma_{disc}(A)$ in $\sigma(A)$: $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_{disc}(A)$.

Let $h \in]0, h_0]$, $h_0 > 0$, a small semiclassical parameter.

Theorem 1 *The spectrum of the self-adjoint operator $-h^2 \Delta_x - \Delta_y$ on $H^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$ is*

$$\sigma(-h^2 \Delta_x - \Delta_y) = \sigma_{ess}(-h^2 \Delta_x - \Delta_y) = [0, +\infty[, \text{ for all } h \in]0, h_0].$$

Proof The proof is similar as in [8, 9]. \square

Let $V \in L^2_{loc}(\mathbb{R}^n_x \times \mathbb{R}^p_y)$ and be real. We define $H(h) = -h^2\Delta_x - \Delta_y + V(x, y)$ on $D(-h^2\Delta_x - \Delta_y) \cap D(V)$, where $D(-h^2\Delta_x - \Delta_y) = H^2(\mathbb{R}^n_x \times \mathbb{R}^p_y)$ and :

$$D(V) = \left\{ \varphi \in L^2(\mathbb{R}^n_x \times \mathbb{R}^p_y); \int |V\varphi|^2 dx dy < +\infty \right\}.$$

Note that $C_0^\infty(\mathbb{R}^n_x \times \mathbb{R}^p_y) \subset D(H(h))$, so $H(h)$ is densely defined. The Hamiltonian in the Born-Oppenheimer approximation is symmetric on this domain:

$$\langle H(h)\varphi, \psi \rangle_{L^2(\mathbb{R}^n_x \times \mathbb{R}^p_y)} = \langle \varphi, H(h)\psi \rangle_{L^2(\mathbb{R}^n_x \times \mathbb{R}^p_y)}, \quad \forall \varphi, \psi \in C_0^\infty(\mathbb{R}^n_x \times \mathbb{R}^p_y), \quad \forall h \in]0, h_0].$$

Hence, we have that $D(H(h)) \subset D(H^*(h))$. Moreover, if $V \geq 0$, then $H(h) \geq 0$ as

$$\langle H(h)\varphi, \varphi \rangle_{L^2(\mathbb{R}^n_x \times \mathbb{R}^p_y)} = \|h\nabla_x \varphi\|^2 + \|\nabla_y \varphi\|^2 + \langle V\varphi, \varphi \rangle_{L^2(\mathbb{R}^n_x \times \mathbb{R}^p_y)} \geq 0$$

for any $\varphi \in D(H)$, $\forall h \in]0, h_0]$.

Theorem 2 Let $V \in L^2_{loc}(\mathbb{R}^n_x \times \mathbb{R}^p_y)$ and $V \geq 0$. Then the operator $H(h)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n_x \times \mathbb{R}^p_y)$, for all $h \in]0, h_0]$.

Proof See [8, Theorem 7.6, page 73], [9]. \square

3 Locally Compact Operators and Their Application to the Born-Oppenheimer Operator

Definition 3 Let A be a closed operator on $L^2(\mathbb{R}^n)$ with $\rho(A) \neq \emptyset$, let χ_B be the characteristic function for a set $B \subset \mathbb{R}^n$. Then A is locally compact if for each bounded set B , $\chi_B(A - \lambda)^{-1}$ is compact for some (and hence all) $\lambda \in \rho(A)$.

Example 1 Δ is locally compact on $L^2(\mathbb{R}^3)$. Note that $\chi_B(1 - \Delta)^{-1}$ has kernel

$$\chi_B(x) [4\pi \|x - y\|]^{-1} e^{-\|x-y\|},$$

which belong to $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. By Hilbert-Schmidt theorem [8-10], $\chi_B(1 - \Delta)^{-1}$ is compact. We mention that the same compactness result holds in n dimension (see [9]).

Example 2 $(-\Delta)^{\frac{1}{2}}$, the positive square root of $(-\Delta) \geq 0$ is locally compact. Indeed, note that it suffices to show that $A^* = \chi_B \left(i + (-\Delta)^{\frac{1}{2}} \right)^{-1}$ is compact. As $A = \left(-i + (-\Delta)^{\frac{1}{2}} \right)^{-1} \chi_B$, we have

$$A^*A = \chi_B(1 - \Delta)^{-1} \chi_B,$$

and by (1) above, A^*A is compact. Now we claim that this implies that A is compact, for if $u_n \xrightarrow{w} 0$ (weakly convergence),

$$\|Au_n\|^2 = \langle u_n, A^*Au_n \rangle \leq \|u_n\| \|A^*Au_n\|,$$

and as the sequence $(u_n)_n$ is uniformly bounded and $A^*Au_n \xrightarrow{s} 0$ (strongly convergence), we have $Au_n \xrightarrow{s} 0$. Hence, A is compact.

We now show that certain classes of Hamiltonian operators $H(h) = -h^2\Delta_x - \Delta_y + V(x, y)$ are locally compact.

Theorem 3 *Let V be continuous (or $V \in L^2_{loc}(\mathbb{R}_x^n \times \mathbb{R}_y^p)$), $V \geq 0$, and $V \rightarrow +\infty$ as $\|x\| + \|y\| \rightarrow \infty$. Then $H(h) = -h^2\Delta_x - \Delta_y + V(x, y)$ is locally compact, for every $h \in]0, h_0]$.*

Proof Note that $H(h)$ is self-adjoint by the Kato inequality [11], and $H(h) \geq 0$, $\forall h \in]0, h_0]$. We first make the following claim:

$(-h^2\Delta_x - \Delta_y)^{1/2}$ is $H^{1/2}(h)$ -bounded and $(-h^2\Delta_x - \Delta_y + 1)^{1/2}$ is $(H(h) + 1)^{1/2}$ -bounded.

Indeed, since $-h^2\Delta_x - \Delta_y \geq 0$ and $H(h) \geq 0$, all the operators $(-h^2\Delta_x - \Delta_y)^{1/2}$, $H^{1/2}(h)$ and $(H(h) + 1)^{1/2}$ are well defined. We have a simple estimate for any $u \in C_0^\infty(\mathbb{R}_x^n \times \mathbb{R}_y^p)$,

$$\begin{aligned} \left\| (-h^2\Delta_x - \Delta_y)^{\frac{1}{2}} u \right\|^2 &= \langle u, (-h^2\Delta_x - \Delta_y) u \rangle \leq \langle u, H(h) u \rangle \leq \langle u, (H(h) + 1) u \rangle \\ &\leq \| (H(h) + 1) u \|^2. \end{aligned} \quad (1)$$

This estimate extends to all $u \in D(H^{1/2}(h))$. Consequently, equation (1) shows that $(-h^2\Delta_x - \Delta_y)^{\frac{1}{2}}$ is $H^{1/2}(h)$ -bounded. Also, as we have

$$\langle u, H(h) u \rangle \leq \left\| H^{1/2}(h) u \right\|^2,$$

which follows from the Schwarz inequality, it follows from this and the third term of (1) that $(-h^2\Delta_x - \Delta_y)^{\frac{1}{2}}$ is $H^{1/2}(h)$ -bounded.

We have

$$\begin{aligned} \chi_B (1 + H(h))^{-1/2} &= \\ \chi_B (1 + H(h))^{-1} \left(1 + (-h^2\Delta_x - \Delta_y)^{1/2} \right)^{-1} \left(1 + (-h^2\Delta_x - \Delta_y)^{1/2} \right) (1 + H(h))^{-1/2} & \end{aligned} \quad (2)$$

and by Example 2, the first factor on the right in (2) is compact, the second is bounded, and so $\chi_B (1 + H)^{-1/2}$ is compact. To prove the theorem, simply write

$$\chi_B (1 + H(h))^{-1} = \chi_B (1 + H(h))^{-\frac{1}{2}} (1 + H(h))^{-\frac{1}{2}},$$

and observe that the right side is a product of a compact and a bounded operator and is hence compact. \square

3.1 Spectral Properties of Locally Compact Operators

A specific family of sequences, called Zhislin sequences [12], which will allow us to characterize the essential spectrum σ_{ess} of locally compact, self-adjoint operators.

Definition 4 Let $B_k = \{x \in \mathbb{R}^n : \|x\| \leq k, k \in \mathbb{N}\}$. A sequence $(u_n)_n$ is a Zhislin for a closed operator A and $\lambda \in \mathbb{C}$ if $u_n \in D(A)$,

$$\|u_n\| = 1, \text{supp}u_n \subset \{x; x \in \mathbb{R}^n \setminus B_n\} \text{ and } \|(A - \lambda)u_n\| \rightarrow 0 \text{ as } n \rightarrow \infty.$$

By Weyl's criterion [9], it is clear that if A is self-adjoint and there exists a Zhislin sequence for A and λ , then $\lambda \in \sigma_{ess}(A)$.

Definition 5 Let A be a closed operator. The set of all $\lambda \in \mathbb{C}$ such that there exists a Zhislin sequence for A and λ is called the Zhislin spectrum of A , which we denote by $Z(A)$.

Notation 1 The commutator of two linear operators A and B is defined formally by $[A, B] = AB - BA$.

Let $B(x, R)$ denote the ball of radius R centered at the point x . Our main theorem states that the essential spectrum is equal to the Zhislin spectrum of a self-adjoint, locally compact operator that is also local in the sense of (3) ahead.

Theorem 4 Let A be a self-adjoint and locally compact operator on $L^2(\mathbb{R}^n)$. Suppose that A also satisfies

$$\left\| [A, \phi_n(x)] (A - i)^{-1} \right\| \rightarrow 0, \text{ as } n \rightarrow \infty \quad (3)$$

where $\phi_n(x) = \phi(x/n)$ for some $\phi \in C_0^\infty(\mathbb{R}^n)$, $\text{supp}\phi \subset B(0, 2)$, $\phi \geq 0$ and $\phi|_{B(0,1)} = 1$. Then $\sigma_{ess}(A) = Z(A)$.

Proof

- (i) It is immediate that $Z(A) \subset \sigma_{ess}(A)$, by Weyl's criterion. To prove the converse, suppose $\lambda \in \sigma_{ess}(A)$. Then there exists a Weyl sequence $(u_n)_n$ for A and λ : $\|u_n\| = 1$, $u_n \xrightarrow{w} 0$ and $\|(A - \lambda)u_n\| \rightarrow 0$. Let ϕ_n be as in the statement of the theorem, and let $\bar{\phi}_n = 1 - \phi_n$. We first observe that $(i - A)u_n \xrightarrow{w} 0$, because

$$(i - A)u_n = (\lambda - A)u_n + (i - \lambda)u_n \quad (4)$$

and the first term goes strongly to zero whereas the second goes weakly to zero. Next, note that by local compactness, for any fixed n , $\phi_n u_m \xrightarrow{w} 0$ as $m \rightarrow \infty$. This can be seen by writing

$$\phi_n u_m = \phi_n (i - A)^{-1} (i - A) u_m, \quad (5)$$

and noting that by (4), $(i - A)u_m \xrightarrow{w} 0$ and $\phi_n (i - A)^{-1}$ is compact. Consequently, $\|\phi_n u_m\| \rightarrow 0$ and $\|\bar{\phi}_n u_m\| \rightarrow 1$ for any fixed n as $m \rightarrow \infty$.

- (ii) We want to construct a Zhislin sequence from $\bar{\phi}_n u_m$. To this end, it remains to consider

$$\|(\lambda - A)\bar{\phi}_n u_m\| \leq \|\bar{\phi}_n\| \|(\lambda - A)u_m\| + \|[A, \phi_n]u_m\|. \quad (6)$$

The commutator term is analyzed using (4):

$$\|[A, \phi_n]u_m\| \leq \left\| [A, \phi_n] (i - A)^{-1} \right\| (\|(\lambda - A)u_m\| + |i - \lambda|),$$

since $\|u_m\| = 1$. This converges to zero as $n \rightarrow \infty$ uniformly in m because the sequence $((\lambda - A)u_m)_m$ is uniformly bounded, say by M , so

$$\|[A, \phi_n]u_m\| \leq \|[A, \phi_n](i - A)^{-1}\| (M + |i - \lambda|) \rightarrow 0, \text{ as } n \rightarrow \infty.$$

(iii) To construct the sequence, it follows from (6) that for each k there exists $n(k)$ and $m(k)$ such that $n(k) \rightarrow \infty$ and $m(k) \rightarrow \infty$ as $k \rightarrow \infty$, and

$$\left\| \bar{\phi}_{n(k)} u_{m(k)} \right\| \geq 1 - k^{-1} \quad (7)$$

and

$$\left\| (\lambda - A) \bar{\phi}_{n(k)} u_{m(k)} \right\| \leq k^{-1}, \quad (8)$$

as $k \rightarrow \infty$. We define $v_k = \bar{\phi}_{n(k)} u_{m(k)} \left\| \bar{\phi}_{n(k)} u_{m(k)} \right\|^{-1}$. It then follows that $(v_k)_k$ is a Zhislin sequence for A and λ by (7)-(8) and the fact that $\text{supp} v_k \subset \mathbb{R}^n \setminus B_{2k}$. Hence, $\lambda \in Z(A)$ and $\sigma_{ess}(A) \subset Z(A)$. \square

We will now apply these ideas to compute $\sigma_{ess}(H(h))$ of the locally compact Hamiltonian in the Born-Oppenheimer approximation operators $H(h) = -h^2 \Delta_x - \Delta_y + V(x, y)$.

Theorem 5 *Assume that $V \geq 0$, V is continuous (or $V \in L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$), and $V(x, y) \rightarrow \infty$ as $\|x\| + \|y\| \rightarrow \infty$. Then $H = -h^2 \Delta_x - \Delta_y + V(x, y)$ has purely discrete spectrum.*

Proof By Theorem 3, the self-adjoint operator H is locally compact. Suppose that $h = 1$, and $H(1) = H$ for simplification. Let $\phi_q(X)$ be as in Theorem 4, with $q = n + m$ and $X = (x, y)$. We must verify (3). A simple calculation gives

$$[H, \phi_q] = \frac{2}{q} \phi'_q \nabla_X - \frac{1}{q^2} \phi''_q, \quad (9)$$

where ϕ'_q and ϕ''_q are uniformly bounded in q . For any $u \in D(H)$, it follows as in (1) that

$$\|\nabla_X u\|^2 \leq \langle u, -\nabla_X u \rangle \leq \langle u, (H + 1)u \rangle,$$

by the positivity of V . Taking $u = (H + 1)^{-1}v$ for any $v \in L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$, it follows that $\nabla_X (H + 1)^{-1}$ and, consequently, $\nabla_X (H - i)^{-1}$ are bounded. This result and (9) verify (3).

Hence, it follows by Theorem 4 that $Z(H) = \sigma_{ess}(H)$. We show that $Z(H) = \{\infty\}$. If $\lambda \in Z(H)$, then there exists a Zhislin sequence $(u_q)_q$ for H and λ . By the Schwarz inequality, we compute a lower bound,

$$\begin{aligned} \|(\lambda - H)u_q\| &\geq |\langle u_q, (\lambda - H)u_q \rangle| \geq \|\nabla_X u\|^2 + \langle u_q, V u_q \rangle - |\lambda| \\ &\geq \left[\inf_{(x,y) \in \mathbb{R}_x^n \times \mathbb{R}_y^p \setminus B(0,q)} V(x, y) \right] - \lambda. \end{aligned} \quad (10)$$

As $q \rightarrow \infty$, the left side of (10) converges to zero whereas the right side diverges to $+\infty$ unless $\lambda = +\infty$. Then $\sigma_{ess}(H) = \{\infty\}$, that is, it is empty. \square

4 Application to the Harmonic Oscillator

The semiclassical Schrödinger operator is $P(h) = -h^2\Delta + V$ on $L^2(\mathbb{R}^n)$. We treat h as an adjustable parameter of the theory. We will study the semiclassical approximation to the eigenvalues and eigenfunctions of $P(h) = -h^2\Delta + V$ for potentials V with in particular when $\lim_{\|x\| \rightarrow \infty} V(x) = \infty$. Because the small parameter h appears in front of the differential operator $-\Delta$, it may not be clear what is happening as h is taken to be small. It is more convenient, and perhaps more illuminating, to change the scaling. Letting $\lambda = 1/h$, we rewrite the Schrödinger operator as

$$P(\lambda) = -\Delta + \lambda^2 V = h^{-2} P(h),$$

looking at $P(\lambda)$, we see that the semiclassical approximation involves $\lambda \rightarrow \infty$.

Definition 6 Let A be a real $n \times n$ matrix, A is a positive definite matrix if $\langle Ax, x \rangle_{\mathbb{R}^n} > 0$, for all $x \in \mathbb{R}^n$.

Definition 7 Let A be a symmetric, positive definite matrix. The Schrödinger operator of type:

$$K(\lambda) = -\Delta + \lambda^2 \langle Ax, x \rangle_{\mathbb{R}^n} \quad (11)$$

is said to be the harmonic oscillator.

Here $\langle x, Ax \rangle_{\mathbb{R}^n} = \sum_{i,j=1}^n a_{ij} x_i x_j$ is the Euclidean quadratic form which is bounded from below by

$$\langle Ax, x \rangle_{\mathbb{R}^n} \geq \lambda_{\min} \|x\|^2,$$

where λ_{\min} is the smallest eigenvalue of A and is strictly positive.

We see that $K(\lambda)$ is positive with a lower bound strictly greater than zero. Since the harmonic oscillator is continuous and $V_{har}(x) = \langle x, Ax \rangle_{\mathbb{R}^n} \rightarrow \infty$, as $\|x\| \rightarrow \infty$, the harmonic oscillator Hamiltonian (11) is self-adjoint. Moreover, the spectrum of $K(\lambda)$, $\sigma(K(\lambda))$, is purely discrete by Theorem 5.

We would like to find out how the eigenvalues of $K(\lambda)$ depend on the parameter λ .

Definition 8 Two operators A and B , with $D(A) = D(B) = D$, are called similar if there exists a bounded, invertible operator C such that $CD \subset D$ and $A = CBC^{-1}$.

Proposition 1 If A and B are similar, then $\sigma(A) = \sigma(B)$.

Proof It suffices to show that

$$\mu \in \rho(A) \iff \mu \in \rho(B)$$

where $\rho(A) := \mathbb{C} \setminus \sigma(A)$ is the resolvent set. This comes from

$$A - \lambda I = C(B - \lambda I)C^{-1}. \quad \square$$

Definition 9 For $\theta \in \mathbb{R}_+$, we define, the so-called dilation group, is a map on any $\psi \in C_0^\infty(\mathbb{R}^n)$ by

$$U_\theta \psi(x) = \theta^{n/2} \psi(\theta x).$$

Lemma 1 The dilation U_θ is a unitary on $L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$, and

$$(U_\theta)^* = (U_\theta)^{-1} = U_{\theta^{-1}}.$$

We have also, for $\theta, \theta' \in \mathbb{R}_+$,

$$U_\theta U_{\theta'} = U_{\theta+\theta'}.$$

Proof The proof is straightforward and is omitted. \square

We now claim that $U_{\lambda^{-\frac{1}{2}}}$ implements a similarity transformation on $K(\lambda)$ by

$$U_{\lambda^{-\frac{1}{2}}} K(\lambda) U_{\lambda^{-\frac{1}{2}}}^{-1} = \lambda K \quad (12)$$

where

$$K = -\Delta + \langle Ax, x \rangle_{\mathbb{R}^n} \quad (13)$$

Now we compute the spectrum of the harmonic oscillator K .

Proposition 2 The eigenvalues of K are given by

$$\sigma(K) = \left\{ \sum_{i=1}^n (2n_i + 1) w_i; n_i \in \mathbb{Z}_+ \cup \{0\} \right\},$$

where $\{w_i^2\}_{i=1}^n$ are the eigenvalues of the matrix A .

Proof The proof is by induction on the dimension $n \in \mathbb{N}^*$.

For $n = 1$, the Hermite polynomials \mathcal{H}_p are defined by

$$\left(\frac{d}{dx} \right)^2 \left(e^{-x^2} \right) = (-1)^p \mathcal{H}_p e^{-x^2}.$$

We recall that they satisfy the relations

$$\mathcal{H}_0 = 1 \text{ and } \mathcal{H}_{p+1} = \left(-\frac{d}{dx} + 2x \right) \mathcal{H}_p, p \geq 0.$$

Hermite functions Ψ_n are defined by

$$\Psi_p = C_p \mathcal{H}_p e^{-x^2/2}, \text{ where } C_p = (\sqrt{\pi} 2^p p!)^{-1/2}.$$

For $p \geq 1$, we have

$$\left(\frac{d}{dx} + x \right) \Psi_0 = 0 \quad (14)$$

and

$$\left(-\frac{d}{dx} + x \right) \Psi_p = \sqrt{2(p+1)} \Psi_{p+1}. \quad (15)$$

Now, if H is the harmonic oscillator in one dimension

$$H = -\left(\frac{d}{dx}\right)^2 + x^2,$$

it follows from (14) and (15) that

$$H\Psi_p = (2p + 1)\Psi_p. \quad \square$$

Corollary 1 As a consequence of Proposition 1 and (12), $\sigma(K(\lambda)) = \lambda\sigma(K)$, where $\sigma(K)$ is independent of λ . Hence the eigenvalues of $K(\lambda)$ depend linearly on λ . Moreover, the multiplicities of the related eigenvalues are the same. Now

$$\sigma(K(\lambda)) = \left\{ \sum_{i=1}^n (2n_i + 1)\lambda w_i; n_i \in \mathbb{Z}_+ \cup \{0\} \right\}$$

where $\{w_i\}_{i=1}^n$ are the eigenvalues of the matrix A . The eigenfunctions are related through

the unitary operator $U_{\lambda^{-\frac{1}{2}}}$. If Ψ_p are the eigenfunctions of K , then $\widetilde{\Psi}_p = U_{\lambda^{-\frac{1}{2}}}\Psi_p$ are the eigenfunctions of $K(\lambda)$.

5 Conclusion

The semiclassical harmonic oscillator $P(h) = -h^2\Delta + \langle Ax, x \rangle_{\mathbb{R}^n}$ has purely discrete spectrum

$$\sigma(P(h)) = \{he_j, j \in \mathbb{Z}_+ \cup \{0\}\}$$

where $e_j \in \sigma(K)$.

In general, we can give the spectrum the harmonic oscillator in the Born-Oppenheimer Approximation

$$H(h) = -h^2\Delta_x - \Delta_y + \langle Ax, x \rangle_{\mathbb{R}^n} + \langle By, y \rangle_{\mathbb{R}^p} \text{ on } L^2(\mathbb{R}_x^n \times \mathbb{R}_y^p)$$

where A and B are two symmetric, positive definite matrix. Hence,

$$\sigma(H(h)) = \sigma_{disc}(H(h)) = \left\{ \sum_{i=1}^n (2n_i + 1)hw_i + \sum_{i=1}^p (2n_i + 1)\mu_i, n_i \in \mathbb{Z}_+ \cup \{0\} \right\}$$

where $\{w_i\}_{i=1}^n$ and $\{\mu_i\}_{i=1}^p$ are respectively the eigenvalues of the matrix A and B .

Acknowledgements

This work is supported by Laboratory of Fundamental and Applied Mathematics of Oran.

References

- [1] Born, M. and Oppenheimer, R. Zur Quantentheorie der molekeln. *Annal. Phys.* 1927. 84(20): 457–484.
- [2] Gérard, C., Martinez, A. and Sjöstrand, J. A mathematical approach to the effective Hamiltonian in perturbed periodic problems. *Comm. Math. Physics.* 1991. 142(4): 217–244.
- [3] Klein, M., Martinez, A., Seiler, R. and Wang, X. P. On the Born-Oppenheimer expansion for polyatomic molecules. *Comm. Maths. Phys.* 1992. 143(3): 607–639.
- [4] Martinez, A. Développements asymptotiques et effet tunnel dans l’approximation de Born-Oppenheimer. *Ann. I.H.P.* 1989. 49(3): 239–257.
- [5] Martinez, A. and Messirdi, B. Resonances of diatomic molecules in the Born-Oppenheimer approximation. *Comm. P.D.E.* 1994. 19(7/8): 1139–1162.
- [6] Messirdi, B. and Senoussaoui, A. Méthode BKW formelle et spectre des molécules polyatomiques dans l’approximation de Born-Oppenheimer. *Canadian J. of Phys.* 2001. 79(4): 757–771.
- [7] Messirdi, B., Senoussaoui, A. and Djelouli, G. Resonances of polyatomic molecules in the Born-Oppenheimer approximation. *J. Maths. Phys.* 2005. 46(103506): 1–14.
- [8] Hislop, P. D. and Sigal, I. M. *Introduction to Spectral Theory with Applications to Schrödinger Operators*. Applied Mathematical Sciences Volume 113. New York: Springer-Verlag. 1996.
- [9] Reed, M. and Simon, B. *Methods of Modern Mathematical Physics*. Vols I, II and IV, New York: Academic Press. 1972.
- [10] Simon, B. *Trace Ideals and Their Applications*. Cambridge: Cambridge University Press. 1979.
- [11] Kato, T. *Perturbation Theory for Linear Operators*. 2nd Edition. Berlin: Springer-Verlag. 1980.
- [12] Zhislin, G. Discussion of the spectrum of the Schrödinger operator for systems of several particles. *Tr. Mosk. Mat. Obs.* 1960. 9: 81–128.