Singular Rank One Perturbations

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In this paper $A = B + V$ represents a self-adjoint operator acting on a Hilbert space $\mathscr{H}$. We set a general theoric framework and obtain several results for singular perturbations of A of the type $A_\beta = A + \beta\tau^*\tau$ for τ a functional defined in a subspace of $\mathscr{H}$. In particular we apply these results to $H_\beta = -\Delta + V + \beta|\delta\rangle\langle\delta|$ where δ is the singular perturbation given by $\delta(\varphi) = \int_S \varphi\, d\sigma$ where S is a suitable hypersurface in $\mathbb{R}^n$.

Using the fact that the singular perturbation $\tau^*\tau$ is a sort of rank one perturbation of the operator A, it is possible to prove the invariance of the essential spectrum of A under these singular perturbations. The main idea is to apply an adequate Krein's formula in this singular framework.

As an additional result, we found the corresponding relationship between the Green's functions associated to the operators $H_0 = \Delta + V$ and H_β and we give a result about the existence of pure point spectrum (eigenvalues) of H_β. Also we study the case β goes to infinity.

I. INTRODUCTION

This article deals with singular perturbations of a self-adjoint operator $A : \mathscr{H} \to \mathscr{H}$, that is, $A_\beta = A + \beta\tau^*\tau$ where τ is a continuous functional defined on a linear subspace of the Hilbert space $\mathscr{H}$. For τ continuous in $\mathscr{H}$ the problem becomes a classical rank one perturbation which has been fully studied in the last decades. See for example[1],[2],[3] and the bibliography cited there.

A concrete example is $H_\beta = H_0 + \beta\,|\delta_S\rangle\langle\delta_S|$ where $H_0 = -\Delta + V(x)$ on the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n)$, and $V(x)$ is an adequate measurable real valued function defined on $\mathbb{R}^n$. Specifically, we shall consider H_β, a singular perturbation of H_0, of the type

$$H_\beta = H_0 + \beta\,|\delta_S\rangle\langle\delta_S| \tag{1}$$

with S the boundary of a bounded Lipschitz domain Ω in $\mathbb{R}^n$, β is a real parameter. and

$$\delta_S(\varphi) = \int_S \varphi\, d\sigma \tag{2}$$

where $d\sigma$ is the surface area element of the smooth surface S. This is a generalization of the delta distribution δ_a in one dimension, $\delta_a(\phi) = \phi(a)$, $\phi \in C_0^\infty$.

For singular perturbations that is, perturbations of the type δ-function in a point or the delta supported on a compact surface we mention[4]. Some authors, see[5], have characterized the domain of these operators in term of an adequate boundary conditions. Following this approach, we are able to relate it with a bounded operator in an adequate Sobolev space, where the difference of the corresponding resolvents behave as a true rank one operator, which allows us to formulate a Krein's identity in that context. We apply this identity for proving a version of Weyl's theorem for these kind of singular perturbations. Moreover it allows us to define singular perturbations in dimensions greater than one.

Also we mention[5] where the authors study the case of Schrödinger operators with δ and δ' potentials.

In[6] the authors study the resonance phenomena for $H_\beta = H_0 + \beta|\delta\rangle\langle\delta|$, where $H_0 = -\Delta$ on the half line $[0,\infty)$ and δ is a one point interaction. One expects a resonant behavior when β is large. The operator H_β converges in some sense to an operator H_∞ as $\beta \to \infty$, which has embedded eigenvalues, motivating the computations in Section 6.

Notations.
Throughout this paper, Δ denotes the spatial Laplace operator, $\Delta = \sum_{i=1}^n \dfrac{\partial^2}{\partial x_i^2}$. Green's function are denoted by: G_0 , G_β for $n \geq 2$ and for $n = 1$ we write g_0 , g_β and g_∞. The Sobolev space $\mathscr{H}^p(\mathbb{R}^n)$, $1 \leq p < \infty$ is defined as the subset of functions $f \in L^2(\mathbb{R}^n)$ such that f and its weak derivatives up to order p have a finite L^2 norm.

Our main example is the Schrödinger operator $H_0 = -\Delta + V(x)$ on $L^2(\mathbb{R}^n)$ under a singular perturbation given by interaction on a hypersurface S as the one defined in (1). For this reason, in all what follows we assume that the operator A is of the form $A = B + V$, where B and V are self–adjoint operators on $\mathscr{H}$, with V bounded relative to B and $B \geq 0$. We write $\mathscr{H}^2 = \mathscr{D}(B)$ with norm

$$\|\psi\|_2^2 = \|\psi\|^2 + \|B\psi\|^2. \tag{3}$$

with this $\|\cdot\|_2$ norm $\mathscr{H}^2$ becomes a Hilbert space with inner product $<u,v>_2 = <u,v> + <Bu,Bv>$. We denote its dual, the space of all linear bounded functional defined in $\mathscr{H}^2$, by $\mathscr{H}^{-2} = (\mathscr{H}^2)^*$. Also, $\mathscr{H}^1$ denotes the domain of $B^{1/2}$, with norm

$$\|\psi\|_1^2 = \|\psi\|^2 + \langle\psi, B\psi\rangle = \|\psi\|^2 + \|B^{1/2}\psi\|^2.$$

Notice that $\mathscr{H}^1$, $\mathscr{H}^2$ are linear subspaces of $\mathscr{H}$.

In the case of the Schrödinger operator $-\Delta + V(x)$ on $L^2(\mathbb{R}^n)$, the spaces $\mathscr{H}^1$, $\mathscr{H}^2$ are just the Sobolev's spaces $\mathscr{H}^1(\mathbb{R}^n)$ and $\mathscr{H}^2(\mathbb{R}^n)$ respectively.

Next we consider a a natural way to regard singular rank one perturbations of a self-adjoint operator A. If one writes formally these perturbations as $A_\beta = A + \beta\langle\varphi,\cdot\rangle\varphi$ where φ is a given functional, then we can think of A_β as a self-adjoint extension of the operator A restricted to the kernel of φ. In section 2 this approach is explained.

Section 3 is dedicated to the construction of the singular perturbed operator by using its corresponding quadratic form,

$$q_\beta(\varphi) = \int |\nabla\varphi(x)|^2 dx + \int V(x)|\varphi(x)|^2 dx + \beta\left|\int_S \varphi\, d\sigma\right|^2 .$$

This quadratic form leads to the definition of a self–adjoint operator H_β on $L^2(\mathbb{R}^n)$, including a description of its domain, a representation of its resolvent and the corresponding associated Green's function.

Also, in Section 4 we describe the Krein's formula and the corresponding Green's functions to obtain a characterization on H_β as self-adjoint operator on $L^2(\mathbb{R}^n)$.

In Section 5 we prove some spectral properties of H_β. Throughout Section 6 we will study the convergence of $H_\beta \to H_\infty$ as $\beta \to \infty$ and we focus on to study the spectral properties of the limit operator H_∞. Finally, for completeness in Section 6 we describe the limit operator H_∞.

II. ON SINGULAR PERTURBATIONS. ABSTRACT SETTING.

Let $\mathscr{H}$ be a Hilbert space with inner product $\langle\, ,\rangle$ and the corresponding norm $\|\,\|$. For a self-adjoint operator A defined in $\mathscr{H}$, with domain $\mathscr{D}(A)$, we consider the perturbation A_α given by

$$A_\beta = A + \beta\langle\varphi,\cdot\rangle\varphi .$$

with β a real parameter. When $\varphi \in \mathscr{H}$, the operator A_β is just a self-adjoint rank one perturbation of A, with the same domain $\mathscr{D}(A)$.

Instead, we consider

$$\varphi : \mathscr{D}(A) \longrightarrow \mathbb{C},$$

but φ not in $\mathscr{H}$, in which case we say that A_β *is a singular perturbation of* A .

Here, we also use $\langle\varphi,x\rangle$ to denote the action of φ on a vector $x \in \mathscr{D}(A)$.

We call $\mathscr{K} = \operatorname{Ker}\varphi = \{x \in \mathscr{H} : \langle\varphi,x\rangle = 0\}$. In some sense we expect that A_β restricted to $\mathscr{D}(A)\cap\mathscr{K}$ should coincide with A. We write $\hat{A} = A|_{\mathscr{D}(A)\cap\mathscr{K}}$. To assure the existence of self-adjoint extensions of $\hat{A}$, the following lemmas are needed, see[7] for more details.

Lemma II.1 *Let $\mathscr{D}$ be a dense subspace of a Hilbert space $\mathscr{H}$. Suppose that $\varphi : \mathscr{D} \longrightarrow \mathbb{C}$ is discontinuous. Then Ker(φ) is dense in $\mathscr{H}$.*

Proof. Since φ is discontinuous there exists a sequence $\{x_n\} \subset \mathscr{D}$ such that $\|x_n\| = 1$ and $|\varphi(x_n)| \to \infty$ as $n \to \infty$. Take $y \in \mathscr{D}$ and write

$$y = y - \frac{\varphi(y)}{\varphi(x_n)}x_n + \frac{\varphi(y)}{\varphi(x_n)}x_n .$$

Suppose $x \in \operatorname{Ker}(\varphi)^\perp$, hence since $y - \frac{\varphi(y)}{\varphi(x_n)}x_n \in \operatorname{Ker}(\varphi)$ we have the inequality

$$|\langle x,y\rangle| = |\langle x, \frac{\varphi(y)}{\varphi(x_n)}x_n\rangle| \le \|x\|\frac{|\varphi(y)|}{|\varphi(x_n)|} \to 0 \qquad \text{as } n\to\infty .$$

Therefore $\mathscr{D} \subset \operatorname{Ker}(\varphi)^{\perp\perp} = \overline{\operatorname{Ker}(\varphi)}$. Since $\mathscr{D}$ is dense $\mathscr{H} = \overline{\mathscr{D}} \subset \overline{\operatorname{Ker}(\varphi)}$ and therefore $\overline{\operatorname{Ker}(\varphi)} = \mathscr{H}$, so $\operatorname{Ker}(\varphi)$ is dense. □

As a direct consequence of the above lemma we can set the following result about self-adjoint extensions,

Lemma II.2 *Consider A a self-adjoint operator acting on $\mathscr{H}$. Assume φ is discontinuous in $\mathscr{D}(A)$ with respect to the norm of $\mathscr{H}$. Let $l : \mathscr{H} \to \mathbb{C}$ be the functional defined as $l(\psi) := \varphi((A+i)^{-1}\psi)$. If l is continuous on $\mathscr{H}$, then $\hat{A}$ is a densely defined symmetric operator with deficiency indices $(1,1)$.*

Proof. From Lemma II.1 it follows that the domain $D(\hat{A}) := \operatorname{Ker}(\varphi)$ is dense. Now for $\gamma \in \mathscr{H}$, we have

$$l(\gamma) = 0 \Leftrightarrow (A+i)^{-1}\gamma \in \operatorname{Ker}(\varphi) = D(\hat{A}) \Leftrightarrow \gamma \in \operatorname{Ran}(\hat{A}+i) .$$

Therefore

$$\operatorname{Ker}(l) = \operatorname{Ran}(\hat{A}+i) \tag{4}$$

and this set is closed by the continuity of l.

Now $\operatorname{Ker}(l) \neq \mathscr{H}$ because if $l(\psi) = 0$, for all $\psi \in \mathscr{H}$, from (4) and the basic criterion for selfadjointness we conclude that $\hat{A}$ is selfadjoint and therefore $\hat{A} = A$. That would mean that $\operatorname{Ker}(\varphi) = D(A)$ and therefore φ continuous in $D(A)$ which is a contradiction to the hypothesis. Since l is continuous and linear, by Riesz's lemma there exists $h \in \mathscr{H}$, $h \neq 0$, such that $\langle h,\cdot\rangle = l(\cdot)$.

Taking into account that $\operatorname{Ran}(\hat{A}+i)$ is closed and therefore equal to $\operatorname{Ker}((\hat{A})^* - i)^\perp$, we have

$$\{\gamma : \langle h,\gamma\rangle = 0\} = \operatorname{Ker}(l) = \operatorname{Ker}((\hat{A})^* - i)^\perp .$$

It follows that $\{c\,h : c \in \mathbb{C}\} = \{\gamma : \langle h,\gamma\rangle = 0\}^\perp = \operatorname{Ker}((\hat{A})^* - i))$. Therefore, $\dim(\operatorname{Ker}((\hat{A})^* - i)) = 1$. Since $\hat{A}$ has self-adjoint extensions, the deficiency indices are equal and $\dim(\operatorname{Ker}((\hat{A})^* + i)) = 1$.

□

Lemma II.3 *Assume that B, V are self-adjoint operators acting on $\mathscr{H}$ with $\mathscr{D}(B) \subset \mathscr{D}(V)$. Consider $A = B + V$ and suppose that there exist positive constants a and b, with $b < 1$, such that*

$$\|V\psi\| \le a\|\psi\| + b\|B\psi\| , \tag{5}$$

for all $\psi \in \mathscr{D}(B)$. Then

(i) the operator V is A–bounded.

(ii) for all $z \in \mathbb{C}$, $\Im z \neq 0$: $V(A-z)^{-1}$ is bounded.

Proof. By the Kato-Rellich's Theorem condition (5) implies that $B+V$ is self-adjoint. Given $\psi \in \mathscr{D}(B)$ we have that $\|V\psi\| \le a\|\psi\| + b\|B\psi\| \le a\|\psi\| + b(\|A\psi\| + \|V\psi\|)$. Since $b<1$, we obtain at once that

$$\|V\psi\| \le \frac{a}{1-b}\|\psi\| + \frac{b}{1-b}\|A\psi\| \tag{6}$$

ending the proof of part (i).

Part (ii). Using (6), for any $\psi \in \mathscr{H}$ one has that

$$\begin{aligned}\|V(A-z)^{-1}\psi\| &\le \frac{a}{1-b}\,\|(A-z)^{-1}\psi\| + \frac{b}{1-b}\,\|A(A-z)^{-1}\psi\| \\ &= \frac{a}{1-b}\,\|(A-z)^{-1}\psi\| + \frac{b}{1-b}\,\|(I+z(A-z)^{-1})\psi\| \\ &\le c\|\psi\|.\end{aligned} \tag{7}$$

which proves (ii).

□

Consider a linear functional $\tau : \mathscr{H}^1 \to \mathbb{C}$. Thus if τ is continuous, that is $|\langle \tau, \psi\rangle| \le c\|\psi\|_1$, then it can be identified with an element of $\mathscr{H}^{-1}$, the dual of $\mathscr{H}^1$. On the other hand, if restriction of τ to $\mathscr{H}^2$ is continuous ($|\langle \tau, \psi\rangle| \le c\|\psi\|_2$), then τ belongs to $\mathscr{H}^{-2}$. We need to prove the following result which we will use afterward.

Lemma II.4 *Assume that $A = B+V$ with B, V satisfying conditions of Lemma II.3. Suppose that $\tau \in \mathscr{H}^{-2}$ ($\tau \in \mathscr{H}^{-1}$). Then there exists a positive constant c such that for all $\psi \in \mathscr{H}$ and z complex with $\Im z \neq 0$,*

$$|\tau(A-z)^{-1}\psi| \le c\|\psi\|. \tag{8}$$

Proof. We observe that for all $\psi \in \mathscr{H}$ we have that

$$\begin{aligned}B(A-z)^{-1} &= (A-V)(A-z)^{-1} \\ &= (A-z+z-V)(A-z)^{-1} \\ &= I + z(A-z)^{-1} - V(A-z)^{-1}.\end{aligned} \tag{9}$$

By continuity of τ in $\mathscr{H}^2$, there exists a positive constant c_1 such that $|\tau(A-z)^{-1}\psi|^2 \le c_1\|(A-z)^{-1}\psi\|_2^2$, that is,

$$|\tau(A-z)^{-1}\psi|^2 \le c_1\|(A-z)^{-1}\psi\|^2 + c_1\|B(A-z)^{-1}\psi\|^2$$

Using that $(A-z)^{-1}$ is bounded in $\mathscr{H}$, the identity (9) together with (7) imply (8).

□

As a first application we can take $H_\beta u = -\Delta u + Vu + \beta\tau^*\tau u$ with singular perturbation $\tau = \delta \in \mathscr{H}^{-1}(\mathbb{R}^n)$. A second one will be the partial derivative of the delta, that is, $H_\beta u = -\Delta u + Vu + \beta\tau_i^*\tau_i u$ where $\tau_i(\varphi) = -\int_S \frac{\partial\varphi}{\partial x_i}\,d\sigma$ as an element of $\mathscr{H}^{-2}(\mathbb{R}^n)$. Of course we need to prove that τ, τ_i are continuous on the corresponding spaces. All the details about $\tau \in \mathscr{H}^{-1}$, $\tau_i \in \mathscr{H}^{-2}$ will be developed along the next section.

III. SINGULAR PERTURBATIONS OF $H_0 = -\Delta + V$

In Section II the existence of self-adjoint extensions of $\hat{A}$ was proved in a general abstract setting. In this section we study the concrete example $H_\beta = -\Delta + V + \beta\tau^*\tau$ with V a measurable real valued function defined on $\mathbb{R}^n$. We use a different approach to establish the existence H_β as a self-adjoint operator. To this end we work with the quadratic form which it allows us to identify the domain of the operator H_β.

A. Examples of singular perturbations

Given a smooth compact surface S in $\mathbb{R}^n$ we define the linear functional τ as:

$$\tau(\varphi) = \int_S \varphi\,d\sigma. \tag{10}$$

Since S is compact, by the well known Trace's Theorem (for $n>1$), see[8], for $\varphi \in \mathscr{H}^1(\mathbb{R}^n)$, we obtain that

$$|\tau(\varphi)| \le |S|^{1/2}\|\varphi\|_{L^2(S)} \le C|S|^{1/2}\|\varphi\|_{\mathscr{H}^1} \tag{11}$$

which proves that $\tau : \mathscr{H}^1(\mathbb{R}^n) \to \mathbb{C}$ is continuous, that is, $\tau \in \left(\mathscr{H}^1\right)^*(\mathbb{R}^n) = \mathscr{H}^{-1}(\mathbb{R}^n)$. The corresponding adjoint operator $\tau^* : \mathbb{C} \to \mathscr{H}^{-1}(\mathbb{R}^n)$ is the bounded operator defined as $\tau^*(z) = z\tau$.

Thus, $\tau^*\tau : \mathscr{H}^1(\mathbb{R}^n) \to \mathscr{H}^{-1}(\mathbb{R}^n)$ and it is defined as

$$(\tau^*\tau)\varphi = \tau(\varphi)\tau = (\int_S \varphi\,d\sigma)\,\tau.$$

Next, by using (11), we prove that $\tau^*\tau$ is continuous on $\mathscr{H}^1(\mathbb{R}^n)$ since

$$\|\tau^*\tau(\varphi)\|_{\mathscr{H}^{-1}} = |\tau(\varphi)|\,\|\tau\|_{\mathscr{H}^{-1}} \le C^2|S|\,\|\varphi\|_{\mathscr{H}^1}. \tag{12}$$

In this way, $|\delta_S\rangle\langle\delta_S| = \tau^*\tau$ can be viewed as a bounded linear operator $\mathscr{H}^1(\mathbb{R}^n) \to \mathscr{H}^{-1}(\mathbb{R}^n)$, that is, it represents a singular rank one operator acting on $\mathscr{H}^1(\mathbb{R}^n)$, with range the subspace of dimension one generated by τ.

Similarly, for a fixed $i = 1,\dots,n$ we consider the sort of partial derivative of δ defined as:

$$\tau_i(\varphi) = -\int_S \frac{\partial\varphi}{\partial x_i}\,d\sigma. \tag{13}$$

Replacing φ by φ_x in (11) we see that $\tau_i : \mathscr{H}^2(\mathbb{R}^n) \longrightarrow \mathbb{C}$ is continuous, so $\tau_i \in \mathscr{H}^{-2}(\mathbb{R}^n)$. On the other hand, a direct computation shows that its adjoint $\tau_i^* : \mathbb{C} \longrightarrow \mathscr{H}^{-2}(\mathbb{R}^n)$ is given by $\tau_i^*(z) = z\tau_i$. Moreover, $\tau_i^*\tau_i : \mathscr{H}^2(\mathbb{R}^n) \longrightarrow \mathscr{H}^{-2}(\mathbb{R}^n)$ is also continuous and its range is the one dimensional space generated by τ_i.

By choosing an adequate real valued potential $V(x)$ in $L^\infty(\mathbb{R}^n)$ or any V suitable (5) the Hamiltonian $H_0 = -\Delta + V$ is an unbounded self-adjoint operator on the Hilbert space $L^2(\mathbb{R}^n)$, with domain the Sobolev space $\mathscr{H}^2(\mathbb{R}^n)$. On the other hand, it is actually a bounded operator when it is viewed from $\mathscr{H}^1(\mathbb{R}^n)$ to $\mathscr{H}^{-1}(\mathbb{R}^n)$. Clearly, $H_\beta = H_0 + \beta\,\tau^*\tau$ is also a bounded operator from $\mathscr{H}^1(\mathbb{R}^n)$ to $\mathscr{H}^{-1}(\mathbb{R}^n)$.

In the following we will use some results about semi-bounded quadratic form, see[9], page 276 for details. Remind that a quadratic form $q(u,u) : Q(q)\times Q(q) \longrightarrow \mathbb{C}$ is called *semibounded* if and only if tere exists a positive constant M such that $q(u,u) \geq -M\|u\|^2$ for all $u\in Q(q)$ and is *closed* if the dense domain $Q(q)$ is complete under the norm $\|u\|_q = \big(q(u,u)+(M+1)\|u\|^2\big)^{1/2}$.

On the other hand, by the spectral theorem for a self-adjoint operator A, A is unitary equivalent to a multiplication by x on $\oplus_n L^2(\mathbb{R}, d\mu_n)$. In this way we associate to A a quadratic form $q_A : \mathscr{D}(\sqrt{|A|}) \longrightarrow \mathbb{C}$

$$q_A(\varphi) = \oplus_n \int |x||\varphi(x)|^2\,d\mu_n(x)\,.$$

Clearly, $q_A(\varphi,\psi) = \langle\sqrt{|A|}\varphi, \sqrt{|A|}\psi\rangle$ and $Q(q_A) = \mathscr{D}(\sqrt{|A|})$.

The relationship between them is settled in the following results (see[9]),

Theorem III.1 *If q is a closed semibounded quadratic form then there exists a unique self-adjoint operator A such that $q = q_A$.*

As an application of the above theorem we define the quadratic form in $\mathscr{H}^1(\mathbb{R}^n)$ by

$$\begin{aligned} q_\beta(\varphi) = \int |\nabla\varphi(x)|^2dx + \int V(x)|\varphi(x)|^2(x)dx \\ +\beta\left|\int_S \varphi(x)d\sigma\right|^2 \end{aligned} \tag{14}$$

for $\beta\geq 0$. That is, the domain $\mathscr{D}(q_\beta) = \mathscr{H}^1(\mathbb{R}^n)$ for all $\beta \geq 0$.

Assume that V is real valued measurable function and there exists $M>0$ such that $V(x)\geq -M$ for all $x\in\mathbb{R}^n$. Then the next inequality holds:

$$\begin{aligned} \|\varphi\|^2_{q_\beta} &= q_\beta(u,u) + (M+1)\|u\|^2 \\ &= \int |\nabla\varphi(x)|^2 + \int V(x)|\varphi(x)|^2dx + (M+1)\int|\varphi(x)|^2dx \\ &\quad +\beta\left|\int_S \varphi(x)d\sigma\right|^2 \\ &\geq \int |\nabla\varphi(x)|^2dx + \int|\varphi(x)|^2dx \geq \|\varphi\|_1^2 \end{aligned}$$

So, it is enough to prove that the form q_β given by (14) is closed.

Proposition III.1 *The quadratic form q_β defined in (14) is closed.*

Proof. The assertion follows at once if we prove that $\mathscr{H}^1(\mathbb{R}^n)$ is a closed subset with the induced norm $\|\cdot\|_{q_\beta}$. Suppose that the sequence $\{\varphi_n\}_n \subset \mathscr{H}^1(\mathbb{R}^n)$ converges in the $\|\cdot\|_{q_\beta}$ norm to $\psi\in L^2(\mathbb{R}^n)$. Then $\{\varphi_n\}_n$ es Cauchy with the norm $\|\cdot\|_{q_\beta}$. By (15) we have that $\{\varphi_n\}_n$ es Cauchy with the norm $\|\cdot\|_1$. But $\mathscr{H}^1(\mathbb{R}^n)$ is complete, so $\psi\in\mathscr{H}^1(\mathbb{R}^n)$, ending the proof.

Remark. Note that the quadratic form $\tilde{q}_\beta$, which corresponds to $\frac{\partial\delta}{\partial x_i}$,

$$\tilde{q}(\varphi) = \int |\nabla\varphi(x)|^2 + \int V|\varphi(x)|^2dx + \beta\left|\int_S \frac{\partial\varphi}{\partial x_i}(x)dx\right|^2$$

with form domain $\mathscr{H}^2(\mathbb{R}^n)$ is bounded below but it is not closed.

It remains to describe the domain of H_β acting on $L^2(\mathbb{R}^n)$ that we settle in the next result.

Theorem III.2 *Assume that V is a real valued measurable function, Δ-bounded and $V(x)\geq -M$ for $x\in\mathbb{R}^n$. Let $H_0 = -\Delta + V$ be the operator acting on $\mathscr{H}^1(\mathbb{R}^n)$ and τ given by (2). Then the singular perturbed operator,*

$$H_\beta = H_0 + \beta\,\tau^*\tau\,,\quad \beta\in\mathbb{R}$$

is a self-adjoint unbounded operator with domain D_β contained in $\mathscr{H}^2(\mathbb{R}^n - S)\cap\mathscr{H}^1(\mathbb{R}^n)$.

Moreover, this unbounded self-adjoint operator, again called H_β, it satisfies that

$$(-\Delta + V + \beta\tau^*\tau)\varphi(x) = (-\Delta+V)\varphi(x)\,.$$

for all $x\notin S$, $\varphi\in\mathscr{H}^2(\mathbb{R}^n - S)$.

Proof. By Theorem III.1 there exists a self–adjoint operator H_β whose form is precisely q_β and its form domain is $\mathscr{H}^1(\mathbb{R}^n)$. Next, we give a precise characterization of this operator and its domain.

Let us consider φ in the domain D_β of the operator H_β. Then,

$$\langle H_\beta\varphi, v\rangle = Q_\beta(\varphi, v), \tag{15}$$

for any $v\in\mathscr{H}^1(\mathbb{R}^n)$. Moreover, choosing a test function $v\in C_0^\infty(\mathbb{R}^n)$, with support disjoint of the surface S, one has that $\langle H_\beta\varphi, v\rangle = \int\overline{\nabla\varphi}\cdot\nabla v + V\overline{\varphi}v$ in the weak sense.

Using elliptic regularity we get that $H_\beta\varphi = -\Delta\varphi + V\varphi$, in the strong sense. In other words, if $\varphi\in\mathscr{H}^2(\mathbb{R}^n - S)$ then $H_\beta\varphi = -\Delta\varphi + V\varphi$ on $\mathbb{R}^n - S$.

On the other hand, by choosing $v\in C_0^\infty$, such that $v\equiv 1$ in a neighborhood of S, we have

$$\langle H_\beta\,\varphi, v\rangle \;=\; \int\Big(\overline{\nabla\varphi}\cdot\nabla v + V\overline{\varphi}v\Big)\,dx + \beta|S|\int_S\overline{\varphi}. \tag{16}$$

But, $\int\overline{\nabla\varphi}\cdot\nabla v = \int_S\overline{\nabla\varphi}\cdot\nabla v + \int_{\mathbb{R}^n-\Omega}\overline{\nabla\varphi}\cdot\nabla v$. Then, it follows that φ satisfies the boundary condition,

$$\int_S(\nabla\varphi_+ - \nabla\varphi_-)\cdot\mathbf{N} +\ \beta|S|\int_S\varphi = 0, \tag{17}$$

where $\mathbf{N}$ is the outwards normal to Ω on the boundary S $\varphi_\pm(x) := \lim_{t\to\pm 0}\varphi(x+t\mathbf{N})$ for all $x\in S$. $\square$

IV. RESOLVENT IDENTITIES

In the previous sections it has been proved, under adequate conditions on the operator A and the functional τ, that the operator $A_\beta = A + \beta\tau^*\tau$ is well defined from $\mathscr{H}^1 \longrightarrow \mathscr{H}^{-1}$ with $A = B + V$. Moreover, it is continuous there. Our next step is to study the existence of the inverse operator $(A_\beta - zI)^{-1}$, $z \in \mathbb{C}, \Im z \neq 0$.

Similarly, if $\tau : \mathscr{H}^2 \longrightarrow \mathbb{C}$ is continuous then $\tau^*\tau : \mathscr{H}^2 \longrightarrow \mathscr{H}^{-2}$ is also continuous. Under these conditions in both cases it follows that $A_\beta = A + \beta\tau^*\tau$ is well defined and continuous. Let start by setting a trivial result,

Lemma IV.1 *If $z \in \mathbb{C}$, $\Im z \neq 0$ then for any β, $(A_\beta - z)$ is one to one.*

Proof. Consider $u \in \mathscr{H}^1$ such that $(A_\beta - z)u = 0$. Then,

$$0 = \langle (A_\beta - z)u, u\rangle = \langle u, Bu\rangle + \langle Vu, u\rangle + \beta|\tau(u)|^2 - \bar{z}\|u\|^2 .$$

Taking the imaginary part in the above identity and using that B, V are self-adjoint operators we deduce that $u = 0$. The case $\mathscr{H}^2$ is similar. □

Lemma IV.2 *(Krein's Formula) Let us denote by $R_\beta(z) := (A_\beta - z)^{-1}$. Assume that the unperturbed operator A satisfies that $(A - z)\mathscr{H}^1 = \mathscr{H}^{-1}$, $z \in \mathbb{C}$, $\Im z \neq 0$. Then*

$$R_\beta(z) = R_0(z) - \frac{\beta}{1 + \beta\tau R_0(z)\tau^*} R_0(z)\tau^*\tau R_0(z) \qquad (18)$$

where $R_0(z) = (A - z)^{-1}$.

Proof. By Lemma IV.1 and the hypothesis $(A - z)\mathscr{H}^1 = \mathscr{H}^{-1}$ we have that $(A - z) : \mathscr{H}^1 \longrightarrow \mathscr{H}^{-1}$ is invertible with inverse $R_0(z) : \mathscr{H}^{-1} \longrightarrow \mathscr{H}^1$. Clearly,

$$R_\beta(z) - R_0(z) = -\beta R_0(z)\tau^*\tau R_\beta(z) \qquad (19)$$

which makes sense in $\mathrm{Ran}(A_\beta - z)$ which it is a subspace of $\mathscr{H}^{-1}$. On the other hand, the range of $R_\beta(z)$ is a subspace of $\mathscr{H}^1$ for any β, this allows us to apply τ by the left in (19), having that $\tau R_\beta = \tau R_0 - \beta\tau R_0\tau^*\tau R_\beta$. But, $\tau R_0(z)\tau^*$ is a complex number and $1 + \beta\tau R_0(z)\tau^*$ is not zero otherwise $\tau R_0(z) = 0$ and then τ is the zero functional. So,

$$\tau R_\beta = \frac{1}{1 + \beta\tau R_0(z)\tau^*}\tau R_0(z) .$$

By replacing the above equality in (19) we obtain identity (18). □

As a consequence of the previous lemma we can extend Krein's formula to $\mathscr{H}^{-1}$ by the obvious manner, since $R_0(z)$ has the property $(A - z)\mathscr{H}^1 = \mathscr{H}^{-1}$.

Corollary IV.1 *Let us define $R_\beta(z)$ by identity (18) in $\mathscr{H}^{-1}$. Then $(A_\beta - z)R_\beta = I_{\mathscr{H}^{-1}}$.*

Finally we summarize these results in the following theorem

Theorem IV.1 *Consider $A_\beta = A + \beta\tau^*\tau$ with A self-adjoint and $(A - z)\mathscr{H}^1 = \mathscr{H}^{-1}$. Then, for any $z \in \mathbb{C}$, $\Im z \neq 0$ one has that the operator $(A_\beta - z) : \mathscr{H}^1 \longrightarrow \mathscr{H}^{-1}$ is a bijection and its resolvent satisfies (18).*

Notice that the above results are valid in $\mathscr{H}^1$ subspace of $\mathscr{H}$. For the case $\mathscr{H}^2$ see remark below.

Remark. If $\tau \in (\mathscr{H}^2 - \mathscr{H}^0)$ with $\Im z \neq 0$ then $(A - z)\mathscr{H}^2 = \mathscr{H}^0$ and $(A_\beta - z)\mathscr{H}^2 = \mathscr{H}^0 + \mathrm{Gen} < \tau >$ where $\mathrm{Gen} < \tau >$ is the linear subspace generated by τ. Thus the resolvents $R_0(z)$, R_β are well defined in different subspaces of $\mathscr{H}^{-2}$. Notice that $R_0(z) = R_\beta$ in $\mathscr{H}^0$.

We notice that the above results are true for suitable conditions on the perturbation $\tau^*\tau$, for instance, continuity is one of them. But, as we will show next, for the concrete example $H_0 = -\Delta + V$ with singular perturbations of the type (10) or (13) it is possible to be precise.

Let us consider $H_0 = -\Delta + V$ and denote by $G_0(x, y; z)$ the corresponding Green's function associated to the equation $-\Delta + V$. In other words, for $f \in L^2(\mathbb{R}^n)$ it is well known that

$$u(x) = \int_{\mathbb{R}^n} G_0(x, y; z) f(y)\, dy$$

is the solution of $(H_0 - z)u = f$ with $u \in \mathscr{H}^2(\mathbb{R}^n)$ that is, $u = R_0(z)f$.

We will see that the numeric factor $\tau R_0(z)\tau^*$ which appears in (18) can be computed explicitly if some information is known about the free resolvent $R_0(z)$. We know that $R_0(z)\tau(x) = \int_{\mathbb{R}^n} G_0(x, y; z) f(y)\, dy$. So,

$$\tau R_0(z)\tau^*(\xi) = \xi \int_{\mathbb{R}^n}\int_S G_0(x, y; z) f(y)\, dS_x\, dy .$$

Given $f \in \mathscr{H}^1$ with compact support

$$\begin{aligned}(R_\beta(z)f)(x) &= R_0(z)f(x) - \frac{\beta}{1 + \beta\tau R_0(z)\tau^*}(R_0(z)\tau^*\tau R_0(z)f)(x)\\ &= R_0(z)f(x) - \\ &\quad \frac{\beta}{1 + \beta\tau R_0(z)\tau^*}\int G_0(x, y : z)(\tau^*\tau R_0 f)(y)\, dy\end{aligned}$$

Then $f \in \mathscr{H}^{-1}$, $R_0 f \in \mathscr{H}^1$ and

$$\tau R_0 f = \int_S R_0 f \in \mathbb{C}, \quad \tau^*\tau R_0(z)f = \int_S R_0 f\,\tau \in \mathscr{H}^{-1}.$$

That is, we have proven the following result,

Proposition IV.1 *Let $H_0 : \mathscr{H}^1(\mathbb{R}^n) \to \mathscr{H}^{-1}(\mathbb{R}^n)$ be a bounded operator. Assume that G_0 is the Green's function (or the kernel) of $R_0(z)$. Assume that $H_\beta = H_0 + \beta\tau\tau^*$ is a singular rank one perturbation of H_0. Then*

$$R_\beta(z) = R_0(z) - \kappa_\beta(z)R_0\tau^*\tau R_0(z)$$

where $\kappa_\beta(z) = \dfrac{\beta}{1 + \beta\int_S\int_S G_0(x, y; z)\, dS_x\, dS_y}$.

As mentioned in the Introduction, one of the motivation of this work is the study of dynamical resonances for singular Hamiltonians. The usual stationary theory characterizes resonances as poles of a suitable continuation of the Hamiltonian's resolvent. Proposition IV.1 says that the poles of R_β are exactly the poles of $\kappa_\beta(z)$, which are the roots of $1+\beta\int_S\int_S G_0(x,y;z)\,dS_x\,dS_y$.

The next corollary is a direct consequence of the above proposition,

Corollary IV.2 *Let G_β be the corresponding Green's function associated to H_β. Then*

$$G_\beta(z) = G_0(z) - \kappa_\beta(z) G_0(z)$$

We already know that $R_\beta : \mathscr{H}^{-1}(\mathbb{R}^n) \to \mathscr{H}^1(\mathbb{R}^n)$ is well defined. Next we characterize the L^2 range of R_β.

Theorem IV.2 *Let $R_\beta : \mathscr{H}^{-1}(\mathbb{R}^n) \to \mathscr{H}^1(\mathbb{R}^n)$ be the resolvent of H_β. Then*

$$R_\beta L^2 = \{\varphi \in \mathscr{H}^1 : \varphi \in \mathscr{H}^2(\mathbb{R}^n - S) : \int_S \left(\frac{\partial\varphi}{\partial\nu^+} - \frac{\partial\varphi}{\partial\nu^-} \right) dS = \beta \int_S \varphi\, dS \}\,.$$

Theorem IV.3 *There exists a self-adjoint operator H_β on $L^2(\mathbb{R}^n)$ with domain $\mathscr{D}_\beta$ contained in $\mathscr{H}^1(\mathbb{R}^n)$ such that $R_\beta(z) = (H_\beta - zI)^{-1}$ in $L^2(\mathbb{R}^n)$.*

V. SPECTRAL PROPERTIES OF H_β

In this section we study some spectral properties of the operator $H_\beta = H_0 + \beta|\delta_S\rangle\langle\delta_S|$.

Our goal is to characterize the essential spectrum of H_β and to study the existence of eigenvalues of finite multiplicity for H_β. Regarding the essential spectrum we can not apply directly the Weyl's theorem to H_β, since the perturbation is not a true compact self-adjoint operator. For the non-singular case, that is , when the perturbation $\beta|\delta_S\rangle\langle\delta_S|$ is a genuine rank one perturbation, the analysis of the spectrum for a perturbation of a absolutely continuous operator is treated in detail in[2].

In the next result we set some conditions to fix this problem.

Proposition V.1 *Assume that $H_0 \geq c_1$ and there exists a positive constant c such that $H_0 + c \geq c + c_1 > 0$. Then $\sigma_{ess}(H_\beta) = \sigma_{ess}(H_0)$.*

Proof. By the assumptions H_0 and H_β are self-adjoint operators.

Let us call $R_{c,\beta} = (H_\beta + c)^{-1}$ for $\beta \geq 0$. The choice of c gives that $R_{c,\beta}$ is a self-adjoint operator. By Krein identity, Lemma 18

$$R_\beta = R_0 - \frac{\beta}{1+\beta\langle\delta_S, R_0\delta_S\rangle} R_0|\delta_S\rangle\langle\delta_S|R_0\,.$$

We observe that

$$\begin{aligned}(R_0|\delta_S\rangle\langle\delta_S|R_0)\,\varphi &= \langle\delta_S, R_0\varphi\rangle\, R_0\,\delta_S = \langle R_0^*\,\delta_S, \varphi\rangle\, R_0\,\delta_S \\ &= |R_0\,\delta_S\rangle\langle R_0\,\delta_S|\varphi\,.\end{aligned}$$

So, the operator $\langle R_0|\,\delta_S\rangle\langle\delta_S|R_0$ is a rank one operator on $L^2(\mathbb{R}^n)$ since

$$(R_0\,\delta_S)(x) = \int_{\mathbb{R}^n} g_0(x,y)\delta_S(y)dy = \int_S g_0(x,y)d\sigma(y) \in L^2(\mathbb{R}^n)$$

We conclude that $R_\beta - R_0$ is a rank one operator. So by Weyl's theorem $\sigma_{\text{ess}}(R_\beta) = \sigma_{\text{ess}}(R_0)$ and it follows that $\sigma_{\text{ess}}(H_\beta) = \sigma_{\text{ess}}(H_0)$

□

For example, for $H_0 = -\Delta$ in $L^2(\mathbb{R}^n)$ we can say that the singular perturbation H_β has no isolated eigenvalues of infinite multiplicity.

As a consequence of the above results one has that

Proposition V.2 *Suppose that V is a real valued potential on $L^2(\mathbb{R}^n)$, bounded below and let $H_0 = -\Delta + V$ be a self-adjoint operator on $L^2(\mathbb{R}^n)$. Then $H_\beta = H_0 + \beta\,|\delta_S\rangle\langle\delta_S|$ has the same essential spectrum of H_0.*

Next we will study the existence of isolated eigenvalues of finite multiplicity for thr perturbed operator H_β. We set $\mathscr{D}_\beta$ for the domain of H_β.

Let us assume that the operator $H_0 = -\Delta + V(x)$ has no eigenvalues in an interval J. In the other hand, if $E_0 \in J$ is an eigenvalue of $H_\beta = H_0 + \beta|\delta >< \delta|$, then there exists a nontrivial $\psi \in \mathscr{D}_\beta$ such that, $H_\beta\psi = E_0\psi$. But E_0 is also a generalized eigenvalue, since $\psi \in \mathscr{H}^1$ and

$$-\Delta\psi + V(x)\psi + \beta(\int_S \psi)\,\delta = E_0\,\psi\,.$$

This identity is valid in the space $\mathscr{H}^{-1}(\mathbb{R}^n)$. We note that $\int_S \psi \neq 0$, otherwise E_0 would be an eigenvalue of H_0. Therefore we have that δ belongs to the range of the operator $H_0 - E_0$ and

$$\int_S \psi - \beta \int_S \psi \int_S (H_0 - E_0)^{-1}\delta = 0$$

That is, β and E_0 must satisfy the condition

$$1 - \beta \int_S (H_0 - E_0)^{-1}\delta = 0\,. \tag{20}$$

Theorem V.1 *Assume that the operator $H_0 = -\Delta + V(x)$ has no eigenvalues in an interval J. Suppose that $E_0 \in J$ is an eigenvalue of $H_\beta = H_0 + \beta\,|\delta_S\rangle\langle\delta_S|$ for some $\beta > 0$. Then identity* (20) *holds and*

$$\psi = (H_0 - E_0)^{-1}\delta \tag{21}$$

is its corresponding eigenvector.

Conversely, if (20) *is satisfied then E_0 is an eigenvalue of H_β and ψ given in* (21) *is its corresponding eigenvector.*

Proof. Since E_0 is an eigenvalue then there exists $\psi \in \mathscr{D}(H_\beta)$ such that

$$(H_0 - E_0)\psi = -\beta\langle\delta, \psi\rangle\,\delta\,. \tag{22}$$

Now, $(H_0 - E_0) : \mathscr{H}^1(\mathbb{R}^n) \to \mathscr{H}^{-1}(\mathbb{R}^n)$ is one to one in $\mathscr{D}(H_\beta) \subset \mathscr{H}^1(\mathbb{R}^n)$ so $(H_0 - E_0)^{-1}\delta$ makes sense. Then we conclude that

$$\psi = -\beta \langle \delta, \psi \rangle (H_0 - E_0)^{-1} \delta . \tag{23}$$

Hence, $\langle \delta, \psi \rangle = -\beta \langle \delta, \psi \rangle \langle \delta, (H_0 - E_0)^{-1}\delta \rangle$. Clearly, $\langle \delta, \psi \rangle \neq 0$, otherwise by (22) E_0 would be an eigenvalue of H_0. We conclude that (20) holds and (23) gives explicitly the corresponding eigenvector ψ.

On the other hand, suppose that (20) holds and let $\psi = (H_0 - E_0)^{-1}\delta$. Then $1 + \beta \langle \delta, \psi \rangle = 0$. Thus,

$$\begin{aligned}(H_\beta - E_0)\psi &= (H_0 - E_0)\psi + \beta \langle \delta, \psi \rangle \delta \\ &= (1 + \beta \langle \delta, \psi \rangle)\delta = 0\end{aligned}$$

which proves the reciprocal. □

VI. THE LIMITING OPERATOR H_∞. CASE $n = 1$

For dimension $n = 1$ we have an straightforward result. That is, since g_0 is the Green's function associates to R_0 then by taking $\beta \to \infty$ in Krein's formula (18), we obtain that

$$R_\infty(z) = R_0(z) - \frac{1}{g_0(a,a;z)}\, g_0(a,y;z)\, g_0(x,a;z) .$$

We denote by $g_\infty(x,y;z) = g_0(x,y;z) - \frac{1}{g_0(a,a)}\, g_0(a,y)\, g_0(x,a)$. Using (18) it follows that $g_\infty(a,y;z) = g_\infty(x,a;z) = 0$.

Proposition VI.1 *The function $u(x) = \int_a^\infty g_\infty(x,y;z)\varphi(y)dy$ is a solution of the boundary value problem*

$$\begin{cases} (-\Delta u + V - z)u = \varphi, & \text{in } [0,\infty) \\ u(a) = 0 \\ u(0) = 0 \end{cases}$$

Furthermore, if the support of φ is contained on $[0,a]$ then u has the same properties as well. The same in true for $[a,\infty)$.

In short, g_∞ is the Green's function associated to the operator

$$H_\infty = (-\Delta_{[0,a]} + V) \oplus (-\Delta_{[a,\infty)}) + V$$

which resolvent is $R_\infty(z) = R_0(z) - \frac{1}{g_0(a,a)}\, g_0(a,y)\, g_0(x,a)$. Here $-\Delta_{[p,q]}$ denotes de negative Laplace operator with Dirichlet boundary conditions at p and q. Notice that the result is true only for dimension $n = 1$.

The next results follows at once.

Corollary VI.1 *The operator $R_\infty(z)$, $\Im z \neq 0$ leaves invariant the spaces $L^2[0,a]$ and $L^2[a,\infty]$. Moreover, for $\varphi \in L^2$, the state $\psi = R_\infty(z)\varphi$ satisfies the boundary value problem*

$$(-\Delta - z)\psi = \varphi, \quad \psi(0) = 0, \psi(a) = 0, \quad \textit{for } 0 < x < a$$

and for $a < x$,

$$(-\Delta - z)\psi = \varphi, \quad \psi(a) = 0, \psi \in \mathscr{H}^2 .$$

This corollary shows that $R_\infty(z) = (H_\infty - z)^{-1}$ where $H_\infty = -\Delta_{(0,a)} \bigoplus -\Delta_{(a,\infty)}$.

A. Case $V = 0$

For the operator $H_0 = -\Delta$ on the Hilbert space $L^2([0,\infty))$ with $\varphi(0) = 0$ we have an explicit representation of its Green's function $g_0(x,y;z)$, that is, g_0 is the fundamental solution of the equation $\Delta_x g_0 = \delta(x-y)$ with initial data $g_0(0,y;z) = 0$,

$$g_0(x,y;z) = -\frac{i}{2\sqrt{z}} \left(e^{i\sqrt{z}|x+y|} - e^{i\sqrt{z}|x-y|} \right), \quad \text{with } \Im z > 0.$$

Lemma VI.1 *Suppose that $0 < x < a < y$ (or $0 < y < a < x$). Then $g_\infty(x,y;z) = 0$.*

Proof. Assuming that $0 < x < a < y$. Then have that

$$g_0(x,y;z) = -\frac{i}{2\sqrt{z}} \left(e^{i\sqrt{z}(x+y)} - e^{i\sqrt{z}(y-x)} \right) .$$

Thus,

$$g_\infty(x,y;z) = g_0(x,y;z) - \frac{g_0(a,y;z)g_0(x,a;z)}{g_0(a,a;z)} , .$$

A direct computation proves that

$$\begin{aligned}\frac{g_0(a,y;z)g_0(x,a;z)}{g_0(a,a;z)} &= \frac{i\, e^{i\sqrt{z}a}}{2\sqrt{z}} \frac{[e^{i\sqrt{z}x} - e^{-i\sqrt{z}x}]\,[e^{i\sqrt{z}a} - e^{-i\sqrt{z}a}]}{(e^{2i\sqrt{z}a} - 1)e^{-i\sqrt{z}y}} \\ &= \frac{i\, e^{i\sqrt{z}a}\, e^{-i\sqrt{z}a}}{2\sqrt{z}}\, [e^{i\sqrt{z}x} - e^{-i\sqrt{z}x}]\, e^{i\sqrt{z}y} \\ &= -g_0(x,y;z).\end{aligned}$$

The case $0 < y < a < x$ is similar, ending the proof. □

The next results follows at once.

Corollary VI.2 *The operator $R_\infty(z)$, $\Im z \neq 0$ leaves invariant the spaces $L^2[0,a]$ and $L^2[a,\infty]$. Moreover, for $\varphi \in L^2$, the state $\psi = R_\infty(z)\varphi$ satisfies the boundary value problem*

$$(-\Delta - z)\psi = \varphi, \quad \psi(0) = 0, \psi(a) = 0, \quad \textit{for } 0 < x < a$$

and for $a < x$,

$$(-\Delta - z)\psi = \varphi, \quad \psi(a) = 0, \psi \in \mathscr{H}^2 .$$

This corollary shows that $R_\infty(z) = (H_\infty - z)^{-1}$ where $H_\infty = -\Delta_{(0,a)} \bigoplus -\Delta_{(a,\infty)}$.

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