

The Shape Resonance

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Abstract. For a class of Schrödinger operators $H := -(\hbar^2/2m)\Delta + V$ on $L^2(\mathbb{R}^n)$, with potentials having minima embedded in the continuum of the spectrum and non-trapping tails, we show the existence of shape resonances exponentially close to the real axis as $\hbar \rightarrow 0$. The resonant energies are given by a convergent perturbation expansion in powers of a parameter exhibiting the expected exponentially small behaviour for tunneling.

I. Introduction

The concept of shape resonance has been introduced in the early days of quantum mechanics to resolve the puzzle of alpha-decay [Ga, GuGo]. As in the case of tunneling, the configuration space of the particle with energy ε in a potential V contains a region $J(\varepsilon) := \{x \in \mathbb{R}^n, V(x) > \varepsilon\}$ which is classically non-accessible and which for some values of ε , separates \mathbb{R}^n into an exterior and interior region. The interior region stands for the nucleus, where the particle would be confined if it were not for the quantum mechanical tunneling through the barrier $J(\varepsilon)$ into the exterior. In the case of shape resonance the exterior extends typically to infinity (see Fig. 1 a and b below).

In the case of tunneling and in particular in the case of shape resonance one is interested in situations where barrier penetration is small. This is expected to hold in the semiclassical regime: $k^2 := \hbar/(2m)^{1/2}$ small compared to $d(\mathbf{C}, (\partial J)_{\text{ext}})$ which denotes the Agmon distance between the exterior part $(\partial J(\varepsilon))_{\text{ext}}$ of $\partial J(\varepsilon)$ and the set \mathbf{C} of points in the interior where V takes its minimal value v_0 ; d is derived from the metric $(ds)^2 := \max(0, V(x) - v_0) dx^2$.

In this introduction we shall describe the ideas of our analysis of shape resonances without going into precise technical definitions of the model (Sect. II).

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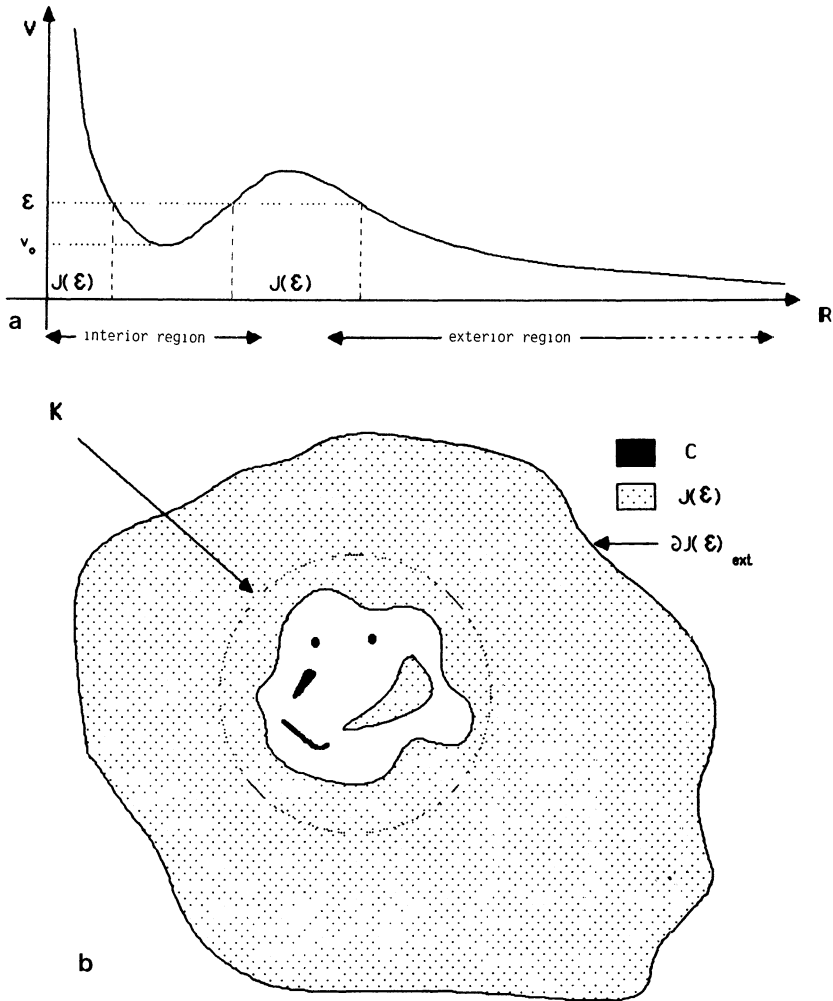


Fig. 1. **a** A possible graph of V in one dimension. **b** The classically inaccessible region $J(\epsilon)$ (shaded), the sphere K and the set C where V takes its minimal value v_0 inside K

Since the physical concept of resonances in quantum mechanics is difficult, we shall circumvent this problem by the following standard mathematical definition [AC]: let $H := -k^4 \Delta + V$ be the Schrödinger operator for the system under consideration. Then $\epsilon \in \mathbb{C}$ is called a resonant energy if the analytic function $F_\varphi(z) := (\varphi, (H - z)^{-1} \varphi)$ has a pole at $z = \epsilon$ on the second sheet for some $\varphi \in \mathbf{A}$, where \mathbf{A} denotes a properly chosen dense set of states, [it is tacitly assumed that $F_\varphi(z)$ has the analytic structure where the concept of “second sheet” makes sense].

In order to analyse the analytic structure of $F_\varphi(z)$ we use physical intuition as a guide and compare H with an operator H^D expected to be close to H in the semiclassical regime. H^D has by definition the same symbol as H but an additional Dirichlet boundary condition on some $n - 1$ dimensional convex surface $K \subset J(\epsilon)$ separating the interior from the exterior region (Fig. 1 b). To simplify the analysis

we consider the situation where K is a sphere. H^D is the direct sum of the two operators H_{int} and H_{ext} ; typically H_{int} has compact resolvent, hence discrete spectrum accumulating at most at infinity, and H_{ext} only essential spectrum. Since the spectrum of H^D is the union of the spectra of H_{int} and H_{ext} , it has point spectrum immersed in the continuum. So H^D describes a physical system very much the same as the one before. The only difference is the infinitely high and narrow wall (Dirichlet boundary condition) on top of the barrier $J(\varepsilon)$ which makes tunneling across $J(\varepsilon)$ impossible.

The spectrum of H_{int} for $k \searrow 0$ has been recently analysed in great detail (see in particular [CDS1, S2, HSj1]). In general the lowest eigenvalues of H_{int} – spectrum valued functions in the terminology of [CDS1] – get absorbed into v_0 for $k \searrow 0$. Furthermore, under certain assumptions on V near the set C of points where the minimum v_0 is reached, one can derive asymptotic expansions in rational powers of k for these eigenvalues. They depend very much on the geometrical properties of V near this set. In the simplest case where v_0 is a non-degenerate minimum, the harmonic approximation is valid, whereas degeneracies can lead to various polynomial behaviours in rational powers of k or even to groups of eigenvalues arbitrarily close to each other. We will not analyse in detail all these possibilities, but the abstract conditions on eigenvalues or group of eigenvalues will appear in the form of a suitable hypothesis (see Sect. IV).

So the energies considered here will be very close to v_0 in the classical limit, and for a suitable choice of the surface K containing C one expects that through the perturbation of H^D obtained by removing the Dirichlet boundary condition they will turn into resonances. In fact we shall prove in Sect. IV that the lowest eigenvalues of H_{int} have resonant energies exponentially close to them. Furthermore in the case of polynomial separation between them we shall derive in Sect. V a convergent tunneling expansion very much the same way as in the case of simple tunneling [CDS2].

The problem with removing the Dirichlet boundary condition on K is twofold: first it is very singular in as much as it changes the domain of the operator; secondly the point spectrum is immersed in the continuous spectrum; hence ordinary perturbation theory cannot be applied (this is a situation typical for resonances). Even worse than in other cases is the fact that the standard method of scaling does not apply in this case because scaling does not leave invariant the domain of H^D . The first problem can be avoided, using resolvents instead of operators. The second one can be overcome by the technique of exterior scaling introduced by Simon [S1]. This concept will be described in more details in the next chapter and Appendix II. Let us just notice that exterior scaling – although useful in this context – is a very brutal deformation of operators since it maps smooth functions into discontinuous functions; it does not even leave invariant the form domain of H . However other approaches to the problem – for instance deformations by a smooth scale function $\exp\theta(x)$ lead to more complicated kinetic energy terms (see [Hu] for a linearized version of this program and [Cy, Sig] for a similar approach in momentum space).

One of the technically most difficult parts of the shape resonance problem is the proof of the fact that resonant energies are only due to the perturbation by the Dirichlet boundary condition of $E_{\text{int}} \in \sigma(H_{\text{int}})$. For that one has to prove absence of

resonant energies for H_{ext} in a suitable neighbourhood of E_{int} . There are two possible approaches for that. The first one uses a numerical range argument and gives absence of resonant energies in a neighbourhood of the real axis. It is described for the case $n=1$ in [CDS3]. We will follow the second route and use a result about the absence of resonant energies in a suitable neighbourhood of a real point [BCD, K11]. It follows, in [BCD], Lavine's space localization method [L] and, in [K11], energy localization, Mourre's inequalities [M1], together with estimates on the rate of decay with respect to k of states which are localized in the classically forbidden region $J(\varepsilon)$ (see also Lemma II.3).

Our methods rely strongly on results about the classical limit of discrete energies' eigenvalues and localization properties of eigenfunctions for Schrödinger operators. They have been derived in two earlier publications for the case of one space dimension [CDS1, 2] and later extended to the n -dimensional case by Simon [S2, 3] and Helffer and Sjöstrand [HSj1, 2].

Concerning the shape resonance problem, let us mention some related works by Asbaugh and Harrell [AsHa] who use differential equation techniques, Jona-Lasinio et al. [JMarSc] for an approach through stochastic methods, Siedentop [Si] for a quantitative analysis of resonance widths through local Birman Schwinger bounds, Lavine [L] and Orth [O] where resonances are studied with the concept of spectral density, Baumgartel [Ba], where a method closer to ours is initiated, and Klein [K12] who studies predissociation with the techniques of this paper. See also a recent work by Helffer and Sjöstrand [HSj3, Sj].

This article is organized as follows: in Sect. II, we describe the model and the concept of exterior scaling to the extent it will be used. In Sect. III, the analysis of perturbation by the Dirichlet boundary condition is presented. Section IV concerns stability of eigenvalues of H_{int} . In the last chapter we explain the tunneling expansion based on the Brillouin-Wigner perturbation theory for nondegenerate eigenvalues of H_{int} . Since we are considering one parameter families of operators only, the nondegeneracy is generically true [vNW]. Further technicalities on Krein's formula and a rigorous investigation of exterior scaling are presented in two appendices.

II. The Model

We consider a potential V which obeys the following hypotheses H1–5. We begin with a smoothness property of V :

$$\text{H1: } V \in C^1(\mathbb{R}^n).$$

To express the geometrical properties of V we need to use the notion of classically forbidden region at energy ε defined as follows:

$$J(\varepsilon) := \{x \in \mathbb{R}^n, V(x) > \varepsilon\}. \quad (2.1)$$

Next, V must have a local minimum v_0 which satisfies:

$$\text{H2: there exists a sphere } K \text{ which splits } \mathbb{R}^n \text{ in two disjoint regions } \Omega_{\text{int}} \text{ and } \Omega_{\text{ext}} \text{ such that with the notations}$$

$$v_0 := \inf\{V(x), x \in \Omega_{\text{int}}\} \quad (2.2)$$

and

$$C := \{x \in \mathbb{R}^n, V \text{ has a local minimum at } x \text{ and } V(x) = v_0\}, \tag{2.3}$$

then $K \subset J(v_0)$ and $C \subset \Omega_{\text{int}}$.

$$\text{H3: } \limsup_{\infty} V(x) < v_0.$$

Hypothesis (H1) could be relaxed by requiring, for example, $V \in L^1_{\text{loc}}(\Omega_{\text{int}}) \oplus C^1(\Omega_{\text{ext}})$ only, modulo technicalities unrelated to shape resonances. Hypothesis (H2) is obviously rather restrictive in a way which is not physically relevant. We impose it for technical reasons in order to simplify the analytic continuation program (see below). To cover geometrical situations where K cannot be chosen as a sphere one could [e.g. if $J(v_0)$ is starlike] use angle dependent exterior scaling or non-homogeneous groups of transformations. This would lead to considerably more technicalities which we want to avoid here. Notice that (H1–3) imply:

$$K \subset J(\varepsilon) \quad \text{for } \varepsilon \text{ close enough to } v_0, \tag{2.4}$$

$$J(v_0) \text{ is compact,} \tag{2.5}$$

$$x \in C \Rightarrow \nabla V(x) = 0. \tag{2.6}$$

So we choose $K := \{x \in \mathbb{R}^n, |x| = r_0\}$, $r_0 > 0$, to be a sphere having property (H2) and separating an interior region $\Omega_{\text{int}} := \{x \in \mathbb{R}^n, |x| < r_0\}$ from an exterior region $\Omega_{\text{ext}} := \{x \in \mathbb{R}^n, |x| > r_0\}$ and ε such that $K \subset J(\varepsilon)$, where $J(\varepsilon)$ is the classically forbidden region [see (2.4)].

An important property in our analysis of shape resonances is that the part of V in Ω_{ext} does not create bound states or resonances close to ε . So we introduce the

Definition 1. The potential V is non-trapping in Ω_{ext} at energy ε (we shall abbreviate this by saying that ε is non-trapping, in short ε is NT), if the following condition¹ is satisfied:

$$\text{NT: } \exists S > 0, \forall x \in \Omega_{\text{ext}} \setminus J(\varepsilon), ((r - r_0)/r) [2(V(x) - \varepsilon) + r \nabla_r V(x)] < -S.$$

Consider now the n^{th} eigenvalue $E^D(k)$ of H_{int} ; such a family is called the n^{th} spectrum valued function and will be denoted simply by E^D . It is useful to define the property (NT) for E^D ; in fact it is clear that if (NT) holds for some ε it also holds nearby. By extension we will say:

E^D is non-trapping if $\exists k_0 > 0$ and $S > 0$ such that for any k , $0 < k < k_0$, $E^D(k)$ is NT with the fixed value S .

In some circumstances [for example if $v_0 = \limsup_{\infty} V(x)$], which we exclude here by (H3), it becomes necessary to allow S to depend on k in the above definition of non-trapping for the spectrum valued function E^D . In order to simplify the presentation of the main ideas of this approach to shape resonances we will not discuss such situations which are analysed in the one dimensional case in [CDS 3c]. Let us simply mention that this type of difficulty is related to the fact (well-known e.g. in the analysis of N -body Schrödinger operators) that in the range

¹ Obviously in the present context the last part of NT is equivalent to the more familiar virial condition: $2(V(x) - \varepsilon) + r \cdot \nabla_r V(x) < -S_1$ for some appropriately chosen $S_1 > 0$

of energy ($\liminf_{\infty} V(x)$, $\limsup_{\infty} V(x)$) there are threshold points where perturbation theory becomes rather delicate. We want to stress that under (H3), i.e. if $v_0 = \inf\{V(x), x \in \Omega_{\text{int}}\}$ is strictly larger than $\limsup_{\infty} V(x)$ and if $\varepsilon = v_0$ satisfies (NT), then the n^{th} spectrum valued function E^D of H_{int} is non-trapping since $\lim_{k \searrow 0} E^D(k) = v_0$. This is why we introduce another geometrical assumption on V :

H4: $v_0 = \inf\{V(x), x \in \Omega_{\text{int}}\}$ is non-trapping.

Let Δ and Δ^D denote the Laplacians defined on their natural domains $\mathcal{H}^2(\mathbb{R}^n)$ and $(\mathcal{H}_0^1 \cap \mathcal{H}^2)(\Omega_{\text{int}}) \oplus (\mathcal{H}_0^1 \cap \mathcal{H}^2)(\Omega_{\text{ext}})$. The kinetic operators are denoted by

$$H_0 := -k^4 \Delta \quad \text{and} \quad H_0^D := -k^4 \Delta^D =: -k^4 (\Delta_{\text{int}} \oplus \Delta_{\text{ext}}), \quad (k > 0).$$

We shall denote by H the selfadjoint operator which describes our system and is defined by $H := H_0 + V$, whereas $H^D := H_0^D + V =: H_{\text{int}} \oplus H_{\text{ext}}$ will be the operator describing the system where the particle is confined in Ω_{int} by the Dirichlet boundary condition on K . Notice that for notational simplicity we do not write explicitly the k dependence in all Schrödinger operators considered.

To perform the analytic deformation of the Schrödinger operator H by the exterior scaling $U(\theta)$, to be defined below, we need:

H5: $V(\theta) := U(\theta) V U(\theta)^{-1}$, $\theta \in \mathbb{R}$, has an analytic extension as a bounded operator into the strip $S_\alpha := \{\theta \in \mathbb{C}, |\text{Im} \theta| < \alpha\}$ for some $\alpha > 0$.

For computational reasons it is often simpler to use polar coordinates on \mathbb{R}^n . The coordinates transformation $x \rightarrow (r = |x|, \omega = x/|x|)$ induces the unitary mapping from $L^2(\mathbb{R}^n)$ onto $L^2(\mathbb{R}^+ \times S^{n-1})$ which maps $x \rightarrow f(x)$ into $(r, \omega) \rightarrow r^{(n-1)/2} f(r\omega)$. In the sequel we shall make free use of computing in either of the two representations. In particular we shall use the following notation for the Laplace operator on $L^2(\mathbb{R}^+ \times S^{n-1})$,

$$-\Delta = -\Delta_r + A/r^2, \quad A := B + (1/4)(n-1)(n-3),$$

where Δ_r denotes the radial Laplacian and $B \geq 0$ the Laplace-Beltrami operator on S^{n-1} , ∇_r will denote the radial derivative operator and prime indicate the result of the radial derivative on a function. The operators H and H^D will be analytically deformed by exterior scaling defined as follows [S1]:

Let $\theta \in \mathbb{R}$ and χ be the characteristic function of Ω_{ext} ; consider the following mapping in \mathbb{R}^n , expressed in polar coordinates:

$$(r, \omega) \rightarrow (r(\theta), \omega), \quad r(\theta) := r_0 + e^{\theta \chi(r)}(r - r_0).$$

It induces on $L^2(\mathbb{R}^n)$ the unitary transformation $U(\theta)$ called exterior dilation or exterior scaling, generated by

$$A := 0 \oplus (2i)^{-1} ((r - r_0) \nabla_r + \nabla_r (r - r_0)) \quad \text{on} \quad L^2(\mathbb{R}^n) = L^2(\Omega_{\text{int}}) \oplus L^2(\Omega_{\text{ext}}).$$

In terms of polar coordinates the action of $U(\theta)$ is given by:

$$\forall f \in L^2(\mathbb{R}^+ \times S^{n-1}), (U(\theta) f)(r, \omega) = e^{\theta \chi(r)/2} f(r(\theta), \omega).$$

Furthermore one finds easily

$$\begin{aligned} -\Delta^D(\theta) &:= -U(\theta)\Delta^D U(\theta)^{-1} = -e^{-2\theta x}\Delta_r^D + A/r(\theta)^2 =: -\Delta_{\text{int}} \oplus -\Delta_{\text{ext}}(\theta), \\ -\Delta(\theta) &:= -U(\theta)\Delta U(\theta)^{-1} = -e^{-2\theta x}\Delta_r + A/r(\theta)^2. \end{aligned}$$

Notice the important fact about the domains of the Laplacians (see Appendices I and II):

$$\begin{aligned} D(\Delta^D(\theta)) &:= U(\theta)D(\Delta^D(0)) = D(\Delta^D(0)) = (\mathcal{H}^2 \cap \mathcal{H}_0^1)(\Omega_{\text{int}}) \oplus (\mathcal{H}^2 \cap \mathcal{H}_0^1)(\Omega_{\text{ext}}), \\ D(\Delta(\theta)) &:= U(\theta)\mathcal{H}^2(\mathbb{R}^n) \neq D(\Delta(0)), \quad (\theta \neq 0) \\ &= \mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}}) \text{ plus boundary conditions on } K. \end{aligned}$$

More precisely

$$\begin{aligned} D(\Delta(\theta)) &= \{u \in \mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}}), u(r_0 + 0, \cdot) = e^{\theta/2} u(r_0 - 0, \cdot), \\ &\quad u'(r_0 + 0, \cdot) = e^{3\theta/2} u'(r_0 - 0, \cdot)\}. \end{aligned} \quad (2.7)$$

Hence in the first case the domain is θ -independent whereas in the second case not. It is therefore a remarkable fact that $\Delta(\theta)$ has an analytic extension in the sense that its resolvent can be analytically extended into the strip $S_{\pi/4}$. The analogous statement for the operator $\Delta^D(\theta)$ is easily seen with the associated quadratic form

$$\begin{aligned} t_0^D(\theta)[u] &:= (V_r u, e^{-2\theta x} V_r u) + (\sqrt{B}u, (1/r(\theta)^2)\sqrt{B}u) \\ &\quad + (1/4)(n-1)(n-3)(u, (1/r(\theta)^2)u) \end{aligned} \quad (2.8)$$

on the domain $\mathcal{H}_0^1(\Omega_{\text{int}}) \oplus \mathcal{H}_0^1(\Omega_{\text{ext}})$ (see Appendix I); as $V(\theta)$ is bounded analytic, (see H5) the image of H^D under $U(\theta)$, for real θ , extends into a selfadjoint holomorphic family for complex θ . We shall use the notation $H^D(\theta) =: H_{\text{int}} \oplus H_{\text{ext}}(\theta)$. In Appendix II we describe a perturbative method to show analyticity of $H(\theta)$ starting from the analyticity of $H^D(\theta)$.

To elucidate the terminology “non-trapping” we make the following

Remarks 2. 1. For computational reasons it is sometimes useful to have the following characterisation of non-trapping:

if $K \subset J(\varepsilon)$ and $\varepsilon > \limsup_{\infty} V(x)$ the potential V is non-trapping at energy ε if and only if there exist $S > 0$ and a compact set $\Omega \subset \mathbb{R}^n$ such that

$$\text{NT'1: } K \subset \Omega, \Omega \subset J(\varepsilon),$$

$$\text{NT'2: } \min\{V(x), x \in \partial\Omega \cap \Omega_{\text{ext}}\} \leq V|_{\Omega \cap \Omega_{\text{ext}}},$$

$$\text{NT'3: } ((r-r_0)/r)[2(V-\varepsilon) + rV_r V] < -S, (x \in \Omega_{\text{ext}} \setminus \Omega).$$

The proof is elementary and will not be given here (see [K11]).

2. The (NT) condition on ε guarantees that there are no resonances in an appropriate neighbourhood of ε due to the exterior of V [BCD, K11]; a precise statement is given in Lemma 3 below.

3. It can be shown that the following implication holds:

$$\varepsilon_1 < \varepsilon_2 \quad \text{and} \quad \varepsilon_1, \varepsilon_2 \text{ NT} \Rightarrow \forall \varepsilon \in [\varepsilon_1, \varepsilon_2], \quad \varepsilon \text{ is NT.}$$

4. On $\partial J(\varepsilon) \cap \Omega_{\text{ext}}$ one has $V(x) = \varepsilon$. Thus by (NT) we find: $\forall x \in \partial J(\varepsilon) \cap \Omega_{\text{ext}}, \nabla_r V(x) < 0$. In physical terms this means that the force on the exterior boundary of the classically forbidden region $J(\varepsilon)$ is repulsive.

5. The (NT) condition excludes a situation where the boundary of $J(\varepsilon)$ in Ω_{ext} is non-transversal to the vector field $\omega \nabla$. Due to $\varepsilon > \limsup_{\infty} V(x)$ for a non-trapping energy ε the classically forbidden region is bounded. A typical form is shown in Fig. 1 b.

6. If ε is NT then the boundary of $J(\varepsilon)$ in Ω_{ext} is diffeomorphic to K . The diffeomorphism is given by the integral lines of the vector field $\omega \nabla$.

7. Non-trapping conditions appear frequently in obstacle scattering problems for the wave equation, in particular in the discussion of resonance poles for the S -matrix and high energy asymptotic of the scattering phase (see e.g. Majda-Ralston [MajRa]). Recently Robert and Tamura introduced a non-trapping condition in their semiclassical analysis of potential scattering which is crucial for their investigations of the limiting absorption principle as $\hbar \searrow 0$. This is not surprising from the point of view developed here since one expects that resonances originating from classically trapped particles (e.g. shape resonances) become very sharp near the classical limit and will strongly influence the behaviour of Green's functions near such energies. A few years ago Lavine [L] already noticed the role of non-trapping conditions involving the virial:

$$2(V - E) + x \nabla V < 0 \tag{2.10}$$

in a commutator proof of the limiting absorption principle and in its analysis of the time delay operator. Condition (2.10) implies negative time delay; this means that a particle with energy E is accelerated by the potential V so that narrow resonances are not expected to occur near this energy. Condition (2.10) looks very much like (NT); it implies classical non-trapping in the sense of Robert and Tamura [RT]. Finally let us mention a nice classical interpretation of (NT) following Helffer and Sjöstrand's analysis of resonances [Sj, HSj3]. The left-hand side of (NT) is the Poisson bracket between the Hamiltonian H and the generator A of exterior scaling up to a certain term which vanishes in the classical limit (see [K11] for a discussion of this term). Hence (NT) imposes something like negativity of a Poisson bracket, thus the particle leaves any compact set in a finite time. Finally we should like to point out that negativity of the quantum analogue of Poisson brackets, namely commutators, is the basis of Mourre's investigations of propagation properties for solutions of the Schrödinger equation [M2].

Let us now state an essential consequence of the non-trapping condition (H4) which will play a crucial role in Sects. III and IV. The proof can be found in [BCD] or [K11].

Lemma 3. *Let (H1–5) be valid. Then there exist $\theta_0 \in S_{\omega}$, $\text{Im } \theta_0 > 0$, $k_0 > 0$ and a complex neighbourhood of $v_0 : v = \{z \in \mathbb{C}, |\text{Re } z - v_0| < \text{cte}, \text{Im } z > -\text{cte}\}$ such that*

$$\forall 0 < k < k_0, \forall z \in v, \|(H_{\text{ext}}(\theta_0) - z)^{-1}\| \leq \text{cte}. \tag{2.11}$$

All the constants are positive and independent of k and z .

III. Estimate on the Dirichlet Perturbation

In this section we shall give first convenient expressions for the difference of the resolvents of $H(\theta)$ and $H^D(\theta)$ which stands for the perturbation in our approach. After this, we shall obtain some basic quantitative estimates on this perturbation. It will depend crucially on the fact that the sphere K – separating the interior from the exterior region – is contained in the classically forbidden region $J(v_0)$. An important ingredient in the analysis of the perturbation by the Dirichlet boundary condition will be the trace operators on the sphere K .

Definition 1. If $f \in \mathcal{H}^1(\Omega_{\text{int}}) \oplus \mathcal{H}^1(\Omega_{\text{ext}})$, then T_{int} (respectively T_{ext}) denotes the trace of f_{int} (respectively f_{ext}) – restriction of f to Ω_{int} (respectively Ω_{ext}) – on K . If $T_{\text{int}}f = T_{\text{ext}}f$, we simply write Tf .

It is well known (see e.g. [LiMag]) that T_{int} (respectively T_{ext}) is a compact mapping from $\mathcal{H}^1(\Omega_{\text{int}})$ [respectively $\mathcal{H}^1(\Omega_{\text{ext}})$] to $L^2(K)$ and that T^* maps continuously $L^2(K)$ into $\mathcal{H}^{-1}(\mathbb{R}^n)$.

Perturbation by the Dirichlet boundary condition factorises naturally into operators involving these traces as follows: consider the operators

$$\begin{aligned} A(\theta, a) &:= T_{\text{int}}(H(\theta) - a)^{-1}, \\ B(\theta, a) &:= B_{\text{int}}(a) \oplus B_{\text{ext}}(\theta, a), \\ B_{\text{int}}(a) &:= -T_{\text{int}}\nabla_r(H_{\text{int}} - a)^{-1}, \\ B_{\text{ext}}(\theta, a) &:= e^{-3\theta/2} T_{\text{ext}}\nabla_r(H_{\text{ext}}(\theta) - a)^{-1}, \end{aligned} \tag{3.1}$$

which are well defined on $L^2(\mathbb{R}^n) = L^2(\Omega_{\text{int}}) \oplus L^2(\Omega_{\text{ext}})$ with image in $L^2(K)$ for $\theta \in \mathbb{R}$ and $\text{Im} a > 0$. If $\theta = 0$ we write $A(\theta)$, $B(a)$ etc. Defining $R(\theta, a) := (H(\theta) - a)^{-1}$ and $R^D(\theta, a) := (H^D(\theta) - a)^{-1}$, we show in Appendix II that

$$\begin{aligned} A(\theta, a) &= k^4 TR(a) T^* B(\theta, a), \\ W(\theta, a) &:= R(\theta, a) - R^D(\theta, a) = k^4 A^*(\bar{\theta}, \bar{a}) B(\theta, a) = k^8 B^*(\bar{\theta}, \bar{a}) TR(a) T^* B(\theta, a). \end{aligned} \tag{3.2}$$

It is shown furthermore in Corollary A4 that (3.1, 2) extend to complex values of θ and a , provided $0 < \text{Im} \theta < \beta < \alpha$ and a does not belong to a certain sector of the complex plane $\Sigma_{\beta, k} = \{z \in \mathbb{C}, |\text{Arg}(z - \gamma_{\beta, k})| \leq \delta_{\beta, k} < \pi/2\}$ with real vertex $\gamma_{\beta, k}$ (the existence of this sector is proven in Appendix II). This will allow us to extend (3.2) analytically in a for fixed θ , $\text{Im} \theta > 0$ to some open sets having v_0 on their boundary. Here the non-trapping hypothesis (H4) is essential as well as Lemma II.3.

Lemma 2. *Let (H1–5) hold and let $a(k)$ be a complex valued function of k such that*

$$\text{Im} a(k) > 0 \quad \text{and} \quad \text{Re} a(k) - v_0 = o(1) \quad \text{as} \quad k \searrow 0. \tag{3.3}$$

Then there exist θ_0 , $\text{Im} \theta_0 > 0$ and $k_1 > 0$ such that for all k , $0 < k < k_1$:

- i) $a(k)$ is in the resolvent set of $H(\theta_0)$,
- ii) equalities (3.2) hold with $\theta = \theta_0$ and $a = a(k)$.

Proof. Let θ_0 , k_0 , v be the ones given by Lemma II.3 and let $k_1 < k_0$ such that for each fixed $k < k_1$, $a(k) \in v^+ := v \cap \{z \in \mathbb{C}, \text{Im} z > 0\}$. We choose some β such that

$\text{Im}\theta_0 < \beta < \alpha$; clearly $(\mathbb{C} \setminus \Sigma_{\beta,k}) \cap v^+$ is a non-empty open set. Since $R(\theta_0, a)$ is analytic in a belonging to the resolvent set of $H(\theta_0)$, then $R^D(\theta_0, a) + W(k_0, a)$ necessarily coincides with $R(\theta_0, a)$ in v^+ . Notice that $(\mathbb{C} \setminus \Sigma_{\beta,k})$ and v are connected open sets (see also Fig. 2 in Sect. IV). Since $a(k)$ belongs to v^+ , the proof is easily completed.

Now we are ready to state the main theorem of this section.

Theorem 3. *Assume (H1–5) and let $\theta_0 \in S_\alpha$ be as in Lemma 2. One has for any complex function $a(k)$ satisfying (3.3) and*

$$(\text{Im}a(k))^{-1} = O(k^{-p}) \quad \text{for some } p \in \mathbb{N}; \tag{3.4}$$

$$B(\theta_0, a) = O(k^{-3}), A(\theta_0, a) = O(k^{-1}), W(\theta_0, a) = O(1) \quad \text{as } k \searrow 0. \tag{3.5}$$

For the proof of Theorem 3 we need the following variant of the standard Sobolev inequalities:

Lemma 4. *Let χ be a $C_0^\infty(\mathbb{R}^n)$ function with value one on K . Then the following inequality holds:*

$$\|T_{\text{int}}f\|^2 \leq 2\|\chi f_{\text{int}}\| \|V_r \chi f_{\text{int}}\|,$$

and similarly in the exterior region.

Proof. We give the proof for the internal trace and omit the subscript int along the proof. The argument for T_{ext} is almost identical. By the fundamental theorem of calculus and the Schwarz inequality,

$$\begin{aligned} \|Tf\|^2 &= \|T\chi f\|^2 = \int_{S^{n-1}} d\omega |\chi f(r_0, \omega)|^2 = 2 \text{Re} \int_{S^{n-1} \times [0, r_0]} d\omega dr (V_r \chi f) \bar{\chi} \bar{f} \\ &\leq 2\|V_r \chi f\| \|\chi f\|. \end{aligned}$$

Notice that the proof for $n=1$ is slightly different.

We now proceed to the proof of Theorem 3 which is split into several steps:

Proof of Theorem 3. Using (3.2) it is sufficient to prove the two estimates:

$$B(\theta_0, a) = O(k^{-3}), \tag{3.6}$$

$$TR(a)T^* = O(k^{-2}), \tag{3.7}$$

once the validity of (3.2) has been checked in Lemma 2.

1) First we prove a quadratic estimate on the resolvent $(H_{\text{int}} - a)^{-1}$. Since $J(v_0)$ is open and $K \subset J(v_0)$ is compact there is a $\delta > 0$ and a radially symmetric $\chi \in C_0^\infty(\mathbb{R}^n)$, supported near K , $\chi = 1$ on K , such that $V(x) - (v_0) \geq 2\delta$, for $x \in \text{supp}\chi$; this implies in particular that $0 \notin \text{supp}\chi$. Since $v_0 - \text{Re}a(k)$ tends to zero as $k \searrow 0$, one has $V(x) - a \geq \delta$ for $x \in \text{supp}\chi$ and k small enough. We need the following straightforward identity:

$$\text{Re}\chi^2(H_{\text{int}} - a) = \chi(H_{\text{int}} - \text{Re}a)\chi - k^4(\chi')^2, \tag{3.8}$$

which is valid in the form sense on $\mathcal{H}_0^1(\Omega_{\text{int}})$. Hence for $\hat{u} \in D(H_{\text{int}})$, one gets

$$\delta\|\chi\hat{u}\|^2 + k^4\|V_r\chi\hat{u}\|^2 \leq \text{Re}(\chi\hat{u}, \chi u) + k^4\|\chi'\hat{u}\|^2 \quad (+ \text{cte}k^4\|\chi\hat{u}\|^2 \quad \text{if } n=2), \tag{3.9}$$

where $u := (H_{\text{int}} - a)\hat{u}$. Notice that (3.9) is also valid if χ is replaced by χ' or χ'' .

2) Let $u \in L^2(\Omega_{\text{int}})$, $\|u\| = 1$, we shall prove that

$$\chi(H_{\text{int}} - a)^{-1}u = O(1). \tag{3.10}$$

Due to (3.4), $\chi(H_{\text{int}} - a)^{-1}u = O(k^{-p})$. Inserting this estimate into (3.9) yields

$$\begin{aligned} \chi(H_{\text{int}} - a)^{-1}u &= O(k^{-p+2}) \quad \text{if } p > 2, \\ &= O(1) \quad \text{if } p \leq 2. \end{aligned}$$

Iterating this procedure leads to (3.10). Then inserting (3.10) in (3.9) we obtain

$$\nabla_r \chi(H_{\text{int}} - a)^{-1}u = O(k^{-2}), \tag{3.11 a}$$

and therefore

$$\chi \nabla_r (H_{\text{int}} - a)^{-1}u = O(k^{-2}), \tag{3.11 b}$$

because $\chi \nabla_r \hat{u} = \nabla_r \chi \hat{u} + \chi' \hat{u}$ and $\chi' \hat{u} = O(1)$ by (3.10). Notice that the estimates (3.11) are also valid when ∇_r is replaced by ∇ . We shall also use the estimate

$$\nabla_r \chi \nabla_r (H_{\text{int}} - a)^{-1}u = O(k^{-4}). \tag{3.12}$$

It is elementary to check that

$$\|\nabla_r \chi \nabla_r \hat{u}\|^2 \leq \|\chi \Delta \hat{u}\|^2 + \|\chi \nabla_r \hat{u}\| \|\chi'' \nabla_r \hat{u}\| + \text{cte} \|\nabla \chi' \hat{u}\|^2 + \text{cte} \|\chi \hat{u}\|^2;$$

using the boundedness of V on $\text{supp } \chi$, (3.10) and (3.11) we obtain on one hand that the three last terms on the right-hand side are globally $O(k^{-4})$ and on the other hand that $\chi \Delta \hat{u} = k^{-4} \chi(V - a)\hat{u} + k^{-4} \chi u = O(k^{-4})$. Hence (3.12) is proven.

3) Obviously by Lemma II.3,

$$\chi(H_{\text{ext}}(\theta_0) - a)^{-1} = O(1), \tag{3.13}$$

and using $-k^4 \cos 2 \text{Im } \theta_0 \Delta_r \leq \text{Re} - \Delta_{\text{ext}}(\theta_0) (+ \text{cte} k^4 \text{ if } n = 2)$ valid in the form sense on $\mathcal{H}_0^1(\Omega_{\text{ext}})$ we obtain

$$k^4 \cos 2 \text{Im } \theta_0 \|\nabla_r \hat{u}\|^2 \leq (\|u\| + \|(V(\theta_0) - a)\hat{u}\|) \|\hat{u}\| \quad (+ \text{cte} k^4 \|\hat{u}\|^2 \quad \text{if } n = 2) \tag{3.14}$$

with $\hat{u} \in D(H_{\text{ext}})$ and $u := (H_{\text{ext}}(\theta_0) - a)\hat{u}$.

Proceeding as in the end of step 2 we get for all u in $L^2(\Omega_{\text{ext}})$ with $\|u\| = 1$:

$$\chi \nabla_r (H_{\text{ext}}(\theta_0) - a)^{-1}u = O(k^{-2}), \tag{3.15}$$

$$\nabla_r \chi \nabla_r (H_{\text{ext}}(\theta_0) - a)^{-1}u = O(k^{-4}). \tag{3.16}$$

4) We can now estimate $\|B(\theta_0, a)u\|^2 = \|B_{\text{int}}(a)u_{\text{int}}\|^2 + \|B_{\text{ext}}(\theta_0, a)u_{\text{ext}}\|^2$. Using Lemma 4 we deduce with (3.11, 12),

$$\|B_{\text{int}}(a)u_{\text{int}}\|^2 \leq 2\|\chi \nabla_r (H_{\text{int}} - a)^{-1}u_{\text{int}}\| \|\nabla_r \chi \nabla_r (H_{\text{int}} - a)^{-1}u_{\text{int}}\| = O(k^{-6}) \|u_{\text{int}}\|^2,$$

and a similar estimate for $B_{\text{ext}}(\theta_0, a)u_{\text{ext}}$ with (3.15, 16). Thus (3.6) is proven.

5) We now proceed to derive (3.7). Let $\eta \in L^2(S^{n-1})$, $\|\eta\| = 1$; then $u := T^* \eta \in \mathcal{H}^{-1}(\mathbb{R}^n)$ and $\hat{u} := R(a)T^* \eta \in \mathcal{H}^1(\mathbb{R}^n)$, because $R(a)$ can be viewed as a bounded map from $\mathcal{H}^{-1}(\mathbb{R}^n)$ into $\mathcal{H}^1(\mathbb{R}^n)$ (see e.g. [RS, p. 279; F, p. 13, 17]). By mimicking step 1 and 2 we derive $\chi R(a) = O(1)$ and $\nabla_r \chi R(a) = O(k^{-2})$; then using

Lemma 4 we have $\|TR(a)\| = O(k^{-1})$ and therefore

$$\|\chi\hat{u}\| = O(k^{-1}), \tag{3.17}$$

because $\|\chi\hat{u}\| \leq \|\chi\|_\infty \|R(a)T^*\| \|\eta\| = \|TR(a)\|$. By Lemma 4 again we have

$$\|TR(a)T^*\eta\|^2 \leq 2\|\chi\hat{u}\| \|\nabla_r\chi\hat{u}\| \leq k^{-2}(k^4\|\nabla_r\chi\hat{u}\|^2 + \|\chi\hat{u}\|^2). \tag{3.18}$$

Proceeding as in step 1, formula (3.8) and (3.9), we obtain [using suitable L^2 -approximation of u in $\mathcal{H}^{-1}(\mathbb{R}^n)$]:

$$\begin{aligned} \|TR(a)T^*\eta\|^2 &\leq k^{-2} \max(1, \delta^{-1}) [\operatorname{Re}(TR(a)T^*\eta, \eta) + k^4\|\chi'\hat{u}\|^2] \\ &\quad (+ k^2 \text{cte} \|\chi\hat{u}\|^2 \quad \text{if } n=2). \end{aligned}$$

Since by (3.17) $\|\chi\hat{u}\|$ and $\|\chi'\hat{u}\|$ are $O(k^{-1})$, this implies

$$\|TR(a)T^*\eta\|^2 \leq \text{cte} k^{-2} \|TR(a)T^*\eta\| + O(1),$$

thus (3.7) is proven.

IV. Stability of Eigenvalues of H^D

In this section we shall prove that every spectrum valued function E^D of H_{int} has a resonant energy E of H nearby for k sufficiently small provided assumption (H6) introduced below is satisfied. This stability of eigenvalues will be the basis for applying the Brillouin-Wigner perturbation theory in the following chapter. We prove it for groups of spectrum valued functions $J := \{E_1^D, \dots, E_N^D\}$ having the following property:

H6: there exist $b > 0$ and $k_0 > 0$ such that $\forall k \leq k_0$,

$$\text{cte} k^b \leq \Delta(k) \quad \text{and} \quad |J(k)|^2 / \Delta(k) = o(1),$$

where we use the notations

$$\Delta := \operatorname{dist}(J, \sigma(H_{\text{int}}) \setminus J) \quad \text{and} \quad |J| := \operatorname{Max}_{i,j} |E_i^D - E_j^D| =: \operatorname{diam} J.$$

These conditions are met in most interesting cases, as for instance if the harmonic approximation is valid and \mathbf{C} is finite (see [CDS1, S2, HSj1]).

Remark 1. Since J consists of spectrum valued functions which all converge to v_0 as $k \rightarrow 0$ one always has that $\lim_{k \rightarrow 0} |J(k)| = \lim_{k \rightarrow 0} \Delta(k) = 0$.

As a first step we prove the smallness of the resolvent of $R^D(\theta_0, a)$ [for $a(k)$ correctly chosen] on an appropriate loop in the complex plane. This will then be used to define the projector P of $H(\theta_0)$. Finally an argument involving analytic interpolation will prove that P has the same dimension as the corresponding projector P^D of H^D .

Remark 2. In the following lemma we shall consider a loop in the resolvent set of $H^D(\theta_0)$ around a given finite group J of spectrum valued functions obeying (H6) (see Fig. 2 below). To do it we shall use Lemma II.3. As the size of v is

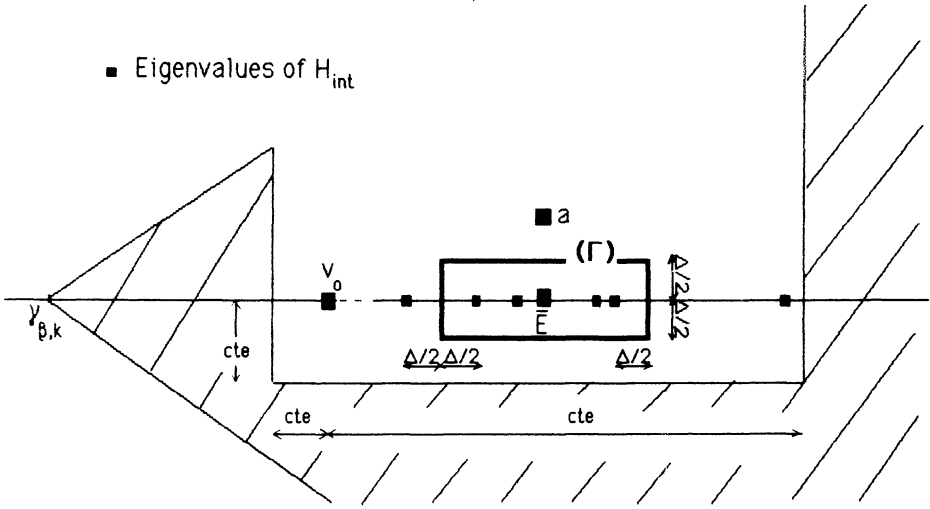


Fig. 2. The loop Γ around J in the neighbourhood v , and the sector $\Sigma_{\beta,k}$

k -independent and all the elements of J go to v_0 when $k \searrow 0$, this makes sure that $J \subset v$ for sufficiently small k . In Fig. 2 the non-shaded area is singularity free for $(H_{\text{ext}}(\theta_0) - z)^{-1}$.

Lemma 3. Assume (H1–5) and (H6) for a set $J = \{E_1^D, \dots, E_N^D\}$ of spectrum valued functions. Let $\theta_0 \in S_a$ be as in Lemma II.3, then there exist a complex valued function $a(k)$ satisfying (3.3) and a loop Γ around J such that: $(R^D(\theta_0, a) - (z - a)^{-1})^{-1} = o(1)$ uniformly in $z \in \Gamma$ as $k \searrow 0$.

Proof. Let \bar{E} be the barycenter of J , $a := \bar{E} + i\Delta$ and Γ the contour defined by the following figure (see Lemma II.3 and Remark 2) which implies in particular

$$\text{dist}(\Gamma, \sigma(H_{\text{int}})) \geq \Delta/2. \tag{4.1}$$

Since a obeys (3.3) (by construction) the resolvent $R^D(\theta_0, a)$ exists for k sufficiently small by Lemma II.3. Due to the identity

$$(R^D(\theta_0, a) - (z - a)^{-1})^{-1} = -(z - a) - (z - a)^2 R^D(\theta_0, z), \tag{4.2}$$

it is enough to have an estimate on $z - a$ and $R^D(\theta_0, a)$. By definition of $a(k)$ and Γ one gets

$$|z - a|^2 \leq |\text{Im} a + \Delta/2|^2 + ||J| + \Delta/2|^2 = 5\Delta^2/2 + |J|\Delta + |J|^2 = o(1).$$

Now we estimate $\|R^D(\theta_0, a)\| \leq \max(\|(H_{\text{int}} - z)^{-1}\|, \|(H_{\text{ext}}(\theta_0) - z)^{-1}\|)$. On one hand $\|(H_{\text{int}} - z)^{-1}\| = 1/\text{dist}(z, \sigma(H_{\text{int}})) \leq 2/\Delta$, on the other hand by Lemma II.3 $\|(H_{\text{ext}}(\theta_0) - z)^{-1}\| \leq \text{cte}$. Hence for k small enough,

$$\|(z - a)^2 R^D(\theta_0, a)\| \leq 5\Delta + 2|J| + 2|J|^2/\Delta = o(1),$$

which proves the lemma.

Theorem 4. *Assume (H1–5) and (H6) for a set $J = \{E_1^D, \dots, E_N^D\}$ of spectrum valued functions. Let θ_0 be as in Lemma II.3. Then there exists a loop Γ around J such that $P := -(2i\pi)^{-1} \int_{\Gamma} dz R(\theta_0, z)$ is well defined for k sufficiently small and has the same dimension as $P^D := -(2i\pi)^{-1} \int_{\Gamma} dz R^D(\theta_0, z)$.*

Proof. 1) Choose $a(k)$ and Γ as in the proof of Lemma 3 and let $\tilde{\Gamma} := \{\tilde{z} := (z-a)^{-1}, z \in \Gamma\}$; then by the functional calculus one also has: $P^D = -(2i\pi)^{-1} \int_{\tilde{\Gamma}} d\tilde{z} (R^D(\theta_0, a) - \tilde{z})^{-1}$. By the same argument it is enough to show that

$$P = -(2i\pi)^{-1} \int_{\tilde{\Gamma}} d\tilde{z} (R(\theta_0, a) - \tilde{z})^{-1} \quad (4.3)$$

is well defined and has the same dimension as P^D for k sufficiently small. For this we define the resolvent of $R(\theta_0, a)$ on the contour $\tilde{\Gamma}$ by the Neumann series:

$$(R(\theta_0, a) - \tilde{z})^{-1} := (R^D(\theta_0, a) - \tilde{z})^{-1} \sum_{n \geq 0} (W(\theta_0, a) (R^D(\theta_0, a) - \tilde{z})^{-1})^n. \quad (4.4)$$

Since by Lemma 3 $(R^D(\theta_0, a) - \tilde{z})^{-1}$ is $o(1)$ uniformly in $\tilde{z} \in \tilde{\Gamma}$ it is enough to have a k -independent bound on $W(\theta_0, a)$. This was the purpose of Theorem III.3. By construction of $a(k)$ all the assumptions of this theorem are met; hence the above definition of P makes sense.

2) To prove stability of dimension we construct an analytic interpolation between $R^D(\theta_0, a)$ and $R(\theta_0, a)$; consider $R(\theta_0, a, \beta) := R^D(\theta_0, a) + \beta W(\theta_0, a)$. The projection $P(\beta)$ defined in analogy to (4.3) is analytic in β and interpolates between P and P^D . Hence $\dim P = \dim P^D$.

Remark 5. A by-product of Theorem 4 is that Γ is inside the resolvent set of $H(\theta_0)$ and that the spectrum of $H(\theta_0)$ inside Γ is discrete with total algebraic multiplicity equal to the total multiplicity of the eigenvalues of H_{int} belonging to J .

In the next section we shall use the following

Corollary 6. *With the assumptions and notations of Theorem 4 and Γ chosen as in Lemma 3, let $Q^D := 1 - P^D$ and G be the closed set delimited by Γ . Then there exists k_0 such that for any $0 < k < k_0$ and z in G , $Q^D(R(\theta_0, a) - (z-a)^{-1})Q^D$ is bounded invertible on $\text{Ran } Q^D$; furthermore its inverse is $o(1)$ as $k \searrow 0$ uniformly in $z \in G$.*

Proof. Since by construction of Γ $\text{dist}(G, \sigma(Q^D H^D(\theta_0) Q^D)) \geq \Delta/2$, the corollary is clearly true if R is replaced by R^D (one need only to mimick the proof of Lemma 3). This allows us as in the proof of Theorem 4 to define the inverse of $Q^D(R(\theta_0, a) - \tilde{z})Q^D$ for $z \in G$ as a bounded operator on $\text{Ran } Q^D$ with the analogue of (4.4). The rest of the statement follows easily.

V. Tunneling Expansion

In this section we shall prove that the stability statement can be improved considerably. We demonstrate that the n^{th} eigenvalue E^D of H_{int} – if separated from the rest of the spectrum by a power in k – gives rise to a resonant energy exponentially close to E^D given by a convergent power series in a tunneling

parameter. The analysis is done here for nondegenerate eigenvalues only, generalizing a method we used in the multiple well case, [CDS2]. Instead of the Weinstein-Aronszajn determinant we use the Brillouin-Wigner formula for the computation of resonant energies.

Lemma 1. *Let E^D be the n^{th} eigenvalue of H_{int} . Assume E^D non-degenerate and furthermore (H1–5) and (H6) with $J = \{E^D\}$. Let P^D, P be the projectors defined according to Theorem IV.4. Then for a and θ_0 chosen as in Lemma IV.3 and k small enough the eigenvalue E associated to P satisfies:*

$$F - F^D = \text{trace } P^D W(\theta_0, a) P^D - \text{trace } P^D W(\theta_0, a) Q^D (Q^D R(\theta_0, a) Q^D - F)^{-1} Q^D W(\theta_0, a) P^D, \quad (5.1)$$

where we used the notation $F := (E - a)^{-1}$, $Q^D := 1 - P^D$.

Proof. The proof is split in two parts, a formal computation and verification of legality of the formal steps.

1. The formal argument is based on the equation $R(\theta_0, a)P = FP$ which is studied in the subspaces $\text{Ran } P^D$ and $\text{Ran } Q^D$ (to simplify notation θ_0 and a are suppressed):

$$P^D R P^D P + P^D R Q^D P = F P^D P, \quad Q^D R P^D P + Q^D R Q^D P = F Q^D P.$$

Eliminating $Q^D P$ from the second equation and inserting it into the first, then taking the trace yields (5.1).

2. The legal part of the argument concerns the existence of P, P^D and $(Q^D R Q^D - F)^{-1}$. The first two operators exist and are defined by a Cauchy integral according to Theorem IV.4. Since by Theorem IV.4 E has to be inside the loop Γ the third one exists by Corollary IV.6; hence the lemma is proved.

Now we are ready to state the main result of this chapter.

Theorem 2. *Let the assumptions of Lemma 1 be satisfied and E be the corresponding resonant energy. Then, for k small enough, E is given by a convergent power series in a tunneling parameter t :*

$$E = E^D + \sum_{n \geq 1} (\sigma_n t^n) / n!. \quad (5.2)$$

Furthermore the following estimates hold:

$$t = o(\exp(-2(1 - \varepsilon)k^{-2} d(K, \mathbf{C}))) \quad \text{and} \quad \forall n \geq 1 \quad \sigma_n = o(1) \quad (5.3)$$

for all $\varepsilon > 0$, where d denotes the pseudo-distance associated to the metric $(ds)^2 = \max(0, V(x) - v_0) dx^2$.

Proof. Let

$$\begin{aligned} t(\theta) &:= k^4 \text{trace } |B(\theta, a) P^D A^*(\bar{\theta}, \bar{a})|, \\ \sigma(\theta, \tilde{z}) &:= k^4 (t(\theta))^{-1} \text{trace } P^D A^*(\bar{\theta}, \bar{a}) \{1 - M(\theta, \tilde{z})\} B(\theta, a) P^D, \\ M(\theta, \tilde{z}) &:= k^4 B(\theta, a) Q^D (Q^D R(\theta, a) Q^D - \tilde{z})^{-1} Q^D A^*(\bar{\theta}, \bar{a}), (\tilde{z} \in \tilde{\Gamma}), \end{aligned}$$

where

$$a := E^D + i\Delta, \theta = \theta_0, \Gamma := \{z \in \mathbf{C}, |z - E^D| = \Delta/2\}$$

with $\Delta := \text{dist}(E^D, \sigma(H_{\text{int}}) \setminus E^D)$ according to Lemma IV.3. Since by Corollary IV.6, the operator $(Q^D R(\theta, a) Q^D - \tilde{z})^{-1}$ is well defined and analytic in \tilde{z} for $\tilde{z} = (z - a)^{-1}$, z inside Γ , hence $\sigma(\theta, \tilde{z})$ also is.

Now we prove that Lagrange's inversion formula [Di, p. 250] can be applied to the implicit Eq. (5.1) for F (very much in the same way as in [CDS2]) that we rewrite:

$$F - F^D = t(\theta) \sigma(\theta, F). \tag{5.4}$$

For this, it is enough that $t(\theta)$ obeys an estimate (5.3) and that $\sigma(\theta, \tilde{z})$ be $O(1)$ on $\tilde{\Gamma}$. We postpone the analysis of $t(\theta)$ and notice that by standard inequalities,

$$|\sigma(\theta, \tilde{z})| \leq \|1 - M(\theta, \tilde{z})\|,$$

where by Corollary IV.6 and Theorem III.3 $M(\theta, \tilde{z})$ is $o(1)$ on $\tilde{\Gamma}$. Then the solution of (5.4) is given by the convergent series:

$$F = F^D + \sum_{n \geq 1} (\tilde{\sigma}_n(\theta) t^n(\theta)) / n!, \tag{5.5}$$

where

$$\tilde{\sigma}_n(\theta) := (d/dz)^{n-1} \sigma^n(\theta, \tilde{z}) \upharpoonright_{\tilde{z} = (E^D - a)^{-1}}. \tag{5.6}$$

Now it turns out that $t(\theta)$, $\sigma(\theta, \tilde{z})$, and $\tilde{\sigma}_n(\theta)$ are in fact independent of θ . This follows from the following remarks. First, $B(\theta, a) P^D$ and $A(\theta, a) P^D$ are θ -independent; in fact setting $P^D \varphi^D = \varphi^D$, $\|\varphi^D\| = 1$, one has $B(\theta, a) \varphi^D = B_{\text{int}}(a) \varphi^D$, which is manifestly θ -independent because $\varphi^D \in \mathcal{H}_0^1(\Omega_{\text{int}})$. Then according to the first equality of (3.2) and Lemma III.2 one sees that:

$$A(\theta, a) \varphi^D = k^4 TR(a) T^* B(a) \varphi^D. \tag{5.7}$$

Notice that $\sigma(\theta, \tilde{z})$ is also θ -independent since it is analytic in θ and independent of it for real variation of θ . Thus we omit in the sequel to write θ when it is not necessary. Then we can estimate the parameter

$$t := k^4 \text{trace} |B(a) P^D A^*(a)| \leq k^4 \|B(a) \varphi^D\| \|A(a) \varphi^D\|.$$

As shown in the proof of Theorem III.3,

$$\|B(a) \varphi^D\|^2 \leq 2|E^D - a|^{-2} \|\chi \nabla_r \varphi^D\| \|\nabla_r \chi \nabla_r \varphi^D\|.$$

By Agmon's decay estimates both terms are $o(\exp -(1 - \varepsilon) k^{-1} d(K, \mathbf{C}))$, if we take χ supported in a sufficiently small neighbourhood of K [Ag, CDS1, S2, HSj1]. To estimate $\|A(a) \varphi^D\|$ we use (5.7) and $\|TR(a) T^*\| = O(k^{-2})$ as shown in Theorem III.3. Then the above bound on $\|B(a) \varphi^D\|$ implies (5.3).

Finally we prove the estimates on the coefficients $\tilde{\sigma}_n$ and σ_n . We use the Cauchy formula to estimate the $\tilde{\sigma}_n$:

$$\tilde{\sigma}_n = (n - 1)! (2i\pi)^{-1} \int_{\tilde{\Gamma}} \sigma^n(\tilde{z}) (F^D - \tilde{z})^{-n} d\tilde{z}.$$

We already know that as $k \searrow 0$, $\sigma(\tilde{z})$ is uniformly bounded on $\tilde{\Gamma}$ with respect to k . We consider now the identity

$$(F^D - z)^{-1} = -(z - a) - (z - a)^2 (E^D - z)^{-1}.$$

With the choice of a, Γ made above we have $(F^D - z)^{-1} = O(\Delta)$ and $\tilde{\sigma}_n = O(\Delta^{n-1})$. Now, to obtain a bound on σ_n we write the following identities:

$$F - F^D = \sum_{n \geq 1} (t^n \tilde{\sigma}_n)/n! = (E^D - E)/((E - a)(E^D - a)),$$

thus

$$E^D - E = \sum_{n \geq 1} (E - a)(E^D - a)(t^n \tilde{\sigma}_n/n!).$$

Hence

$$\sigma_n = (a - E)(E^D - a)\tilde{\sigma}_n = O(\Delta^{n+1}) = o(1).$$

Appendix I. The Family $\{\Delta^D(\theta)\}$

The purpose of this appendix is to show the following:

Theorem A1. *The family of operators $\{\Delta^D(\theta), |\text{Im } \theta| < \pi/4\}$ as defined in Sect. II, is a selfadjoint holomorphic family of type A. In particular*

- i) $D(\Delta^D(\theta)) = (\mathcal{H}_0^1 \cap \mathcal{H}^2)(\Omega_{\text{int}}) \oplus (\mathcal{H}_0^1 \cap \mathcal{H}^2)(\Omega_{\text{ext}})$,
- ii) $-\Delta^D(\theta)$ is m -sectorial with vertex 0 and semi-angle $2|\text{Im } \theta|$.

Proof. It is standard that $D(\Delta^D)$ is given by i) when $\theta = 0$. Since $\Delta_{\text{int}}(\theta) = \Delta_{\text{int}}$ for any θ , we concentrate only on $\Delta_{\text{ext}}(\theta)$ and analyse

$$T(\theta) := -e^{2\theta} \Delta_{\text{ext}}(\theta) = -\Delta_r + g(r, \theta)A \quad \text{with} \quad D(T(\theta)) := D := D(\Delta_{\text{ext}}(\theta)),$$

where $g(r, \theta) := e^{2\theta}/r(\theta)^2 =: g_1 + ig_2$; g_1 and g_2 being respectively the real and imaginary part of g , are in $(L^\infty \cap C^\infty)([r_0, \infty))$ as well as their derivatives. Since $U(\theta)$ is unitary, since $U(\theta)D = D$ for $\theta \in \mathbb{R}$, and since there is the obvious symmetry due to $H(\bar{\theta}) = H(\theta)^*$ it is sufficient to consider only $\theta \in i\mathbb{R}^+$.

First notice that $\text{Re } T(\theta) = -\Delta_r + g_1 A$ is uniformly elliptic (up to a constant if $n = 2$) thus selfadjoint on D (see [K, p. 353]). Secondly, using the following identity in the form sense on D ,

$$\Delta_r^2 + g_1^2 A^2 = (\text{Re } T(\theta))^2 + 2A^{1/2} g_1^{1/2} \Delta_r g_1^{1/2} A^{1/2} + 2((g_1^{1/2})^2) A,$$

one deduces easily, for $n \neq 2$ (if $n = 2$ replace A by $A + 1/4$),

$$g_1^2 A^2 \leq (\text{Re } T(\theta))^2 + C g_1 A, \quad C := 2\|(g_1')^2/g_1\|_\infty^2,$$

which implies, after a quadratic type estimate,

$$\|g_1 A u\| \leq \|\text{Re } T(\theta) u\| + C \|u\| \quad \text{on } D.$$

Now we have $\|\text{Im } T(\theta) u\| \leq \|g_1/g_2\|_\infty (\|\text{Re } T(\theta) u\| + C \|u\|)$ on D , which shows that $T(\theta)$ is m -sectorial because $\|g_2/g_1\|_\infty$ is smaller than one as long as $\text{Im } \theta < \pi/4$. The semi-angle of sectoriality is given by (note that $g_2 \geq 0$)

$$0 \leq \text{tg Arg}(T(\theta)u, u) \leq \|g_2/g_1\|_\infty = \text{tg } 2 \text{Im } \theta.$$

Since D is contained in the form domain of $T(\theta)$, $\Delta_{\text{ext}}(\theta) = e^{-2\theta} T(\theta)$ by a standard property of Friedrich's extensions of sectorial operators (see [K, p. 325–326]).

Appendix II. Exterior Scaling and Krein’s Formula

We provide here a proof of the analyticity in θ of $R(\theta, a) := (H(\theta) - a)^{-1}$, where $H(\theta) = -k^4 \Delta(\theta) + V(\theta)$ is defined as in Sect. II for $\theta \in \mathbb{R}$ through the exterior scaling $U(\theta)$ associated to the sphere $K = \{x \in \mathbb{R}^n, |x| = r_0\}$. We assume here

A: $V(\theta) := U(\theta) V U(\theta)^{-1}$, $\theta \in \mathbb{R}$ has an analytic extension into the strip $S_\alpha := \{\theta \in \mathbb{C}, |\text{Im} \theta| < \alpha\}$ for some $0 < \alpha \leq \pi/4$ as a family of operators relatively bounded to Δ^D with zero relative bound.

From Theorem A1 and hypothesis (A) we deduce easily that $H^D(\theta) := -k^4 \Delta^D(\theta) + V(\theta)$ is a type A analytic family in S_α of m -sectorial operators. So it is natural to use a perturbative argument based on the following form of Krein’s formula [Kr]. Since we shall use in the sequel the results of this lemma with complex θ , it is formulated in order to respect formally the analyticity in θ , though θ is for the moment real.

Lemma A2. *Let V satisfy (A) and $\theta \in \mathbb{R}$, $\text{Im} a \neq 0$, then $W(\theta, a) := R(\theta, a) - R^D(\theta, a)$ obeys*

$$W(\theta, a) = k^4 A^*(\bar{\theta}, \bar{a}) B(\theta, a) = k^8 B^*(\bar{\theta}, \bar{a}) TR(a) T^* B(\theta, a), \tag{A.2.1}$$

where $A(\theta, a)$ and $B(\theta, a)$ are given by (3.1).

Proof. It is essentially an application of Green’s formula. Let u and v be elements of $L^2(\mathbb{R}^n)$ and $\hat{u} := R(\bar{\theta}, \bar{a})u$, $\hat{v} := R^D(\theta, a)v$. Then

$$(u, (R(\theta, a) - R^D(\theta, a))v) = -k^4 [(\hat{u}, \Delta^D(\theta)\hat{v}) - (\Delta(\bar{\theta})\hat{u}, \hat{v})],$$

since the $V - a$ term cancels. If we insert the explicit form of the Laplacian in polar coordinates it is easily seen that the terms with Laplace Beltrami operators cancel too. So we are left with the difference of Δ , and Δ^D . Partial integration leads to

$$(u, (R(\theta, a) - R^D(\theta, a))v) = k^4 \int_{S^{n-1}} d\omega \bar{\hat{u}}(r_0 - 0, \omega) \times (e^{-3\theta/2} \hat{v}'(r_0 + 0, \omega) - \hat{v}'(r_0 - 0, \omega)), \tag{A.2.2}$$

which is just the first equality of (A.2.1). Notice that in the derivation of the above equation we used the boundary condition,

$$\hat{u}(r_0 + 0, \cdot) = e^{\theta/2} \hat{u}(r_0 - 0, \cdot),$$

which follows from the fact that $\hat{u} = U(\theta) R(a) U(\theta)^{-1} u \in U(\theta) \mathcal{H}^2(\mathbb{R}^n)$.

Now by a simple iteration of (A.2.1), using $T_{\text{int}} R^D(\theta, a) = 0$, we get $A(\theta, a) = k^4 T_{\text{int}} A^*(\bar{\theta}, \bar{a}) B(\theta, a)$. Since $T_{\text{int}} U(\theta) = T_{\text{int}}$ as mappings from $\mathcal{H}^1(\Omega_{\text{int}})$ to $L^2(K)$ and $R(a)$ can be viewed as a bounded map from $\mathcal{H}^{-1}(\mathbb{R}^n)$ onto $\mathcal{H}^1(\mathbb{R}^n)$, we obtain

$$A(\theta, a) = k^4 TR(a) T^* B(\theta, a), \tag{A.2.3}$$

because $T_{\text{int}} A^*(\bar{\theta}, \bar{a}) = T_{\text{int}} (TR(a) U(\theta)^{-1})^* = T_{\text{int}} U(\theta) R(a) T^* = TR(a) T^*$ which proves the second equality of (A.2.1).

We are now ready to prove

Theorem A3. *Let V satisfy (A). Then the family of operators $\{H(\theta), \theta \in S_\alpha\}$ is analytic. Furthermore $H(\theta)$ is characterised by $u \in D(H(\theta)) \Leftrightarrow$*

- i) $u \in \mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}}),$
- ii) $u(r_0 + 0, \cdot) = e^{\theta/2} u(r_0 - 0, \cdot),$
- iii) $u'(r_0 + 0, \cdot) = e^{3\theta/2} u'(r_0 - 0, \cdot),$

where prime denotes the derivative with respect to r , and

$$H(\theta)u = -k^4 \Delta(\theta)u + V(\theta)u.$$

Proof. Obviously it is sufficient to verify the statement of the theorem for $k > 0$ and $\theta \in S_\beta$, where k and $0 < \beta < \alpha$ are arbitrary but fixed. Due to (A) and Theorem A1 $H^D(\theta)$ is analytic and “uniformly” m -sectorial on S_β , i.e. the numerical range is contained in a θ -independent sector $\Sigma_{\beta,k}$. The sector has the following form:

$$\Sigma_{\beta,k} = \{z \in \mathbb{C}, |\text{Arg}(z - \gamma_{\beta,k})| \leq \delta_{\beta,k} < \pi/2\}, \quad \gamma_{\beta,k} \in \mathbb{R}. \tag{A.2.4}$$

Thus for a outside this sector $R^D(\theta, a)$ is analytic on S_β as a bounded operator on $L^2(\mathbb{R}^n)$ as well as a mapping from $L^2(\mathbb{R}^n)$ to $\mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}})$. Hence due to (A.2.1), $B(\theta, a)$ and so $R(\theta, a)$ have an analytic extension to S_β . Let us denote again this extension by $R(\theta, a) = R^D(\theta, a) + W(\theta, a)$. It coincides with $R(\theta, a)$ for real θ ; to complete the proof of analyticity of $\{H(\theta), \theta \in S_\beta\}$ it remains to show that $R(\theta, a)$ still is a resolvent for complex θ . It is well known [K, p. 428] that this holds if two conditions are satisfied. The first one is the resolvent equation which is satisfied here by analyticity since it holds for real θ . The second one is the condition $\ker R(\theta, a)u = \{0\}$. To prove it and for our next purposes we need the following key result:

$$\forall \theta \in S_\alpha, \forall u \in L^2(\mathbb{R}^n), (-k^4 \Delta(\theta) + V(\theta) - a) W(\theta, a)u = 0 \text{ as a distribution on } \mathbb{R}^n \setminus K \text{ or equivalently} \tag{A.2.5}$$

$$\forall \theta \in S_\alpha, \forall u \in L^2(\mathbb{R}^n), \forall \hat{v} \in C_0^\infty(\mathbb{R}^n \setminus K), ((H^D(\bar{\theta}) - \bar{a})\hat{v}, W(\theta, a)u) = 0;$$

it can be verified as follows: let $v := (H^D(\bar{\theta}) - \bar{a})\hat{v}$ [notice that $C_0^\infty(\mathbb{R}^n \setminus K)$ is contained in $D(H^D(\theta))$ for any $\theta \in S_\alpha$], then

$$((H^D(\bar{\theta}) - \bar{a})\hat{v}, W(\theta, a)u) = k^8 (B(\bar{\theta}, \bar{a})v, TR(a)T^*B(\theta, a)u) = 0,$$

because

$$B(\bar{\theta}, \bar{a})v = -T_{\text{int}} \nabla_r \hat{v}_{\text{int}} \oplus e^{-3\bar{\theta}/2} T_{\text{ext}} \nabla_r \hat{v}_{\text{ext}} = 0.$$

Now if u satisfies $R(\theta, a)u = 0$, then $\forall \hat{v} \in C_0^\infty(\mathbb{R}^n \setminus K)$ one has $(v, R^D(\theta, a)u) + (v, W(\theta, a)u) = 0$; thus by (A.2.5) $(\hat{v}, u) = 0$, hence $u = 0$. Up to now we have shown that $\{R(\theta, a), \theta \in S_\beta\}$ is an analytic family of resolvents providing an analytic continuation of $R(\theta, a)$, $\theta \in \mathbb{R}$.

We turn now to the characterisation of $H(\theta)$ which is defined by $H(\theta) - a = R(\theta, a)^{-1}$. If \hat{u} belongs to $D(H(\theta)) = \text{Ran } R(\theta, a)$ and $u = (H(\theta) - a)\hat{u}$, then for any $\hat{v} \in C_0^\infty(\mathbb{R}^n \setminus K)$, one has using (A.2.5),

$$\begin{aligned} ((-k^4 \Delta(\bar{\theta}) + V(\bar{\theta}) - \bar{a})\hat{v}, \hat{u}) &= ((H^D(\bar{\theta}) - \bar{a})\hat{v}, R(\theta, a)u) \\ &= ((H^D(\bar{\theta}) - \bar{a})\hat{v}, R^D(\theta, a)u) = (\hat{v}, u), \end{aligned}$$

which proves that $\hat{u} \in \mathcal{H}_{\text{loc}}^2(\Omega_{\text{int}}) \oplus \mathcal{H}_{\text{loc}}^2(\Omega_{\text{ext}})$, and $H(\theta)\hat{u} = (-k^4\Delta(\theta) + V(\theta))\hat{u}$. In fact $\hat{u} \in \mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}})$, since $R^D(\theta, a)$ and $W(\theta, a)$ (see Lemma A7) map continuously $L^2(\mathbb{R}^n)$ into $\mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}})$. Then if we consider the two operators: $(-T_{\text{int}} \oplus e^{-\theta/2} T_{\text{ext}})R(\theta, a)$ and $(-T_{\text{int}}V_r \oplus e^{-3\theta/2} T_{\text{ext}}V_r)R(\theta, a)$, they are well defined and bounded analytic on S_α . As they vanish for real θ (see 2.7) they also vanish on S_α . Hence we have proven that \hat{u} obeys i)–iii).

To verify that a vector \hat{u} which fulfills i)–iii) is actually in $D(H(\theta))$, one has to exhibit a vector u in $L^2(\mathbb{R}^n)$ such that $\hat{u} = R(\theta, a)u$. One can check by direct computation that $u := (-k^4\Delta(\theta) + V(\theta) - a)\hat{u}$ is the good candidate.

As a by-product of Theorem A3 one has the following

Corollary A4. *For any $0 \leq \beta < \alpha$ and $k > 0$, there exists a sector $\Sigma_{\beta, k}$ in the complex plane of the form (A2.4) such that if a is taken outside this sector (A2.1) is valid for any $\theta \in S_\beta$.*

Remark A5. In fact since in this paper we assume that $V(\theta)$ is bounded, the numerical range of $H^D(\theta)$ is contained in $\{z \in \mathbb{C}, \text{Im } z \leq \text{cte Im } \theta\}$ if $\text{Im } \theta \geq 0$; hence one may use this domain instead of $\Sigma_{\beta, k}$. We shall not use this possibility.

Remark A6. Notice that for real θ one has from the definition of $H(\theta)$ the relation

$$\forall \alpha \in \mathbb{R}, R(\theta + \alpha, a) = U(\alpha) R(\theta, a) U(\alpha)^{-1}. \tag{A2.6}$$

This property extends to complex values of θ since both sides of this equality have an analytic extension in θ in the strip S_β provided a is taken outside $\Sigma_{\beta, k}$. The role of (A2.6) is essential in deriving the most important consequence of the analyticity of $H(\theta)$ namely independence of the isolated eigenvalues of $H(\theta)$ with respect to θ and existence of an analytic continuation of expectation values $(\varphi, (H - z)^{-1} \varphi)$ when φ is an analytic vector with respect to the group $U(\theta)$, $\theta \in \mathbb{R}$ (see [AC]); these properties in turn are basic for the interpretation of complex isolated eigenvalues of $H(\theta)$ as resonances.

Lemma A7. *For any a, θ, k such that a lies outside the sector $\Sigma_{\beta, k}$ described in (A2.4), $W(\theta, a)$ maps continuously $L^2(\mathbb{R}^n)$ into $\mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}})$.*

Proof. Since V is relatively bounded to Δ^D , it is sufficient to consider the case $V = 0$. Obviously $B_{\text{int}}(a)$ is bounded from $L^2(\Omega_{\text{int}})$ to $\mathcal{H}^{1/2}(K)$ (see [LiMag, p. 47]). Since $B_{\text{int}}^*(a)u = f$ is equivalent to the elliptic boundary value problem in Ω_{int} : $(-\hbar^2\Delta - a)f = u$ and $T_{\text{int}}f = u$, elliptic regularity implies that $B_{\text{int}}^*(a)$ maps continuously $\mathcal{H}^s(K)$ into $\mathcal{H}^{s+1/2}(\Omega_{\text{int}})$ for any $s \geq 0$ (see [LiMag, p. 176]). The similar statements are true for $B_{\text{ext}}(\theta, a)$ and its adjoint since $H_{\text{ext}}(\theta)$ is uniformly elliptic (see Theorem A1). Again by elliptic regularity one can deduce that $A^*(a)$ is bounded from $\mathcal{H}^s(K)$ into $\mathcal{H}^{s+3/2}(\mathbb{R}^n)$ ($s \geq 0$), hence $TR(a)T^* = TA^*(a)$ maps continuously $\mathcal{H}^s(K)$ into $\mathcal{H}^{s+1}(K)$ ($s \geq 0$). So we have the chain of bounded mappings:

$$L^2(\mathbb{R}^n) - B(\theta, a) \rightarrow \mathcal{H}^{1/2}(K) - TR(a)T^* \rightarrow \mathcal{H}^{3/2}(K) - B^*(\theta, a) \rightarrow \mathcal{H}^2(\Omega_{\text{int}}) \oplus \mathcal{H}^2(\Omega_{\text{ext}}),$$

which in view of (A2.1) and Corollary A4 proves the lemma.

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