

2

61
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THE SHAPE RESONANCE

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ABSTRACT : For a class of Schrödinger operators $H = \underbrace{-(D_x^2 + V(x))}_{\text{on } \mathbb{R}^n} + V$ 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.

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1

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, GuCo]. As in the case of tunneling the configuration space of the particle with energy \mathcal{E} in a potential V contains a region $J(\mathcal{E}) := \{x \in \mathbb{R}^n, V(x) > \mathcal{E}\}$ which is classically non accessible and which for some values of \mathcal{E} , 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 $J(\mathcal{E})$ into the exterior. In the case of shape resonance the exterior extends typically to infinity (fig. 1.a and b).

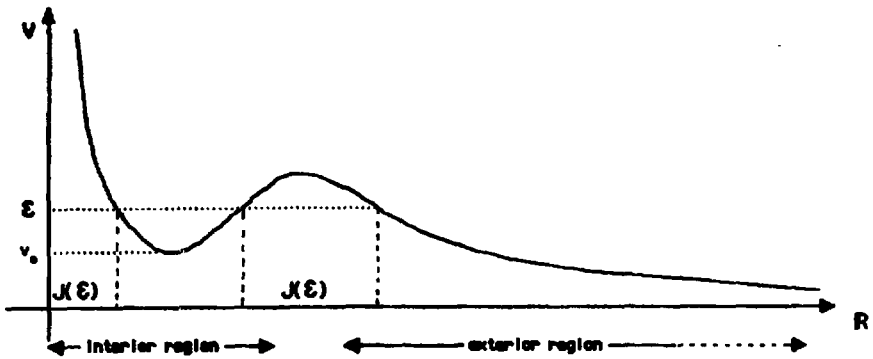


Fig. 1.a. A possible graph of V in one dimension

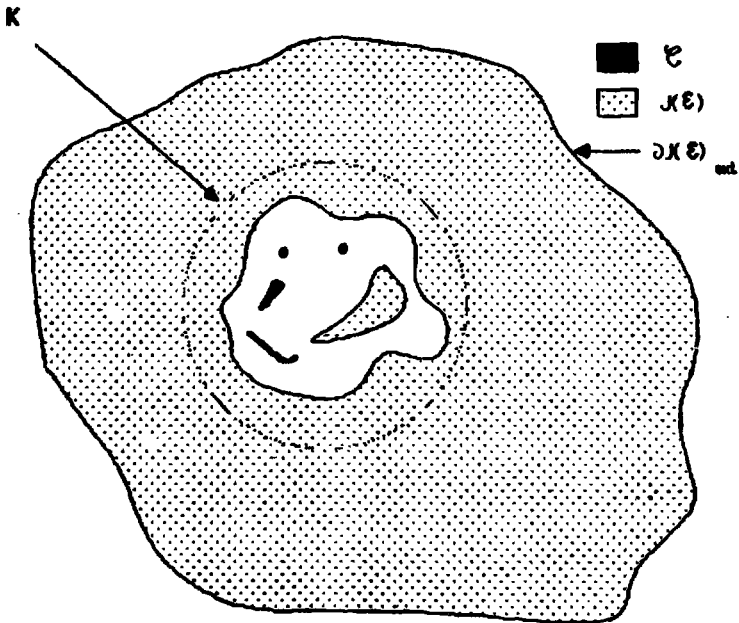


Fig. 1.b. The classically inaccessible region $J(\epsilon)$ (shaded), the sphere K and the set C where V takes its minimal value v_0 inside K .

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

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

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

In order to analyse the analytic structure of $F_{\phi}(z)$ we use physical intuition as a guide and compare H with an operator H^{\flat} expected to be close to H in the semiclassical regime. H^{\flat} has by definition the same symbol as H but an additional Dirichlet boundary condition on some $n-1$ dimensional convex surface $K \subset J(\mathcal{E})$ separating the interior from the exterior region (Fig.1.b). To simplify the analysis we consider the situation where K is a sphere. H^{\flat} 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 $J(\xi)$ which makes tunneling across $J(\xi)$ impossible.

The spectrum of H_{int} for $k \neq 0$ has been recently analysed in great details (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 $k \neq 0$. Furthermore, under certain assumptions on V near the set \mathcal{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 analyze in detail all these possibilities but the abstract conditions on eigenvalues or group of eigenvalues will appear in the form of suitable hypothesis (see chapter 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 \mathcal{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 Chapter 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 Chapter 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^p . The first problem can be avoided, using resolvents instead of operators. The second one can be overcome by the technic of exterior scaling introduced by Simon [S1] . This concept will be described in more details in the next section. 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 [G.Y] . However other approaches to the problem - for instance deformations by a smooth scale function $\exp\theta(x)$ lead to more complicated kinetic energy terms.

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 $E_{int} \in G(H_{int})$. 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 , K1] . It follows, in [BCD] , Lavine's space localization method [L] and , in [K1] , energy

7

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 $J(\xi)$ (see also Lemma IV.2).

Our methods rely strongly on results about the classical limit of discrete energy 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 Sjöstrand [HSj1,2].

Concerning the shape resonance problem let us mention some related works by M.S. Asbaugh and E.M. Harrel [AsH] who use differential equation technics, G. Jona-Lasinio, F. Martinelli and E. Scoppola [JMarSc] for an approach through stochastic methods, H. Siedentop [S1] for a quantitative analysis of resonance widths through local Birman Schwinger bounds, R. Lavine [L] where resonances are studied with the concept of local spectral density and H. Baumgartel [Ba] where a method closer to ours is initiated. See also a recent work by B. Helffer and J. Sjöstrand [HSj3,Sj].

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

II. THE MODEL

We consider a potential V which obeys the following hypothesis H1-5.

We begin by a smoothness property of V :

H1 : $V \in C^4(\mathbb{R}^n)$ with uniformly bounded derivatives..

To express the geometrical properties of V we need to use the notion of classically forbidden region at energy \mathcal{E} defined as follows :

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

Next V must have a local minimum v_0 which satisfies :

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

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

and

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

then $K \subset J(v_0)$ and $\mathcal{E} \subset \Omega_{int}$.

H3 : $\liminf_{|x| \rightarrow \infty} V(x) > v_0$

Hypothesis (H1) could be relaxed by requiring, for example, $V \in L^4_{loc}(\Omega_{int}) \oplus C^4(\Omega_{ext})$ only, modulo technicalities unrelated to shape resonance. 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 choosen as a sphere one could (e.g. if $J(v_0)$ is starlike) use angle dependant 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 :

$$K \subset J(\mathcal{E}) \text{ for } \mathcal{E} \text{ close enough to } v_0 \quad (2.4)$$

$$\overline{J(v_0)} \text{ is compact} \quad (2.5)$$

$$x \in \mathcal{C} \Rightarrow \nabla V(x) = 0 \quad (2.6)$$

So we choose, without loss of generality, $K := \{x \in \mathbb{R}^n, |x| = r_0\}$, $r_0 > 0$, to be a sphere having property (H2) and separating an interior region $\Omega_{int} := \{x \in \mathbb{R}^n, |x| < r_0\}$ from an exterior region $\Omega_{ext} := \{x \in \mathbb{R}^n, |x| > r_0\}$.

We now consider an energy \mathcal{E} such that $K \subset J(\mathcal{E})$ where $J(\mathcal{E})$ 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 \mathcal{E} . So we introduce the

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

$$NT : \exists S > 0, \forall x \in \Omega_{ext} \setminus J(\mathcal{E})$$

$$(2(r-r_0)/r)(V(x)-\mathcal{E}) - (x-r_0\omega)\nabla V(x) < -S.$$

Consider now the n th eigenvalue $E^{\mathcal{P}}(k)$ of H_{int} ; such a family is called the n th spectrum valued function in [CDS1] and will be denoted simply by $E^{\mathcal{P}}$. It is useful to define the property (NT) for E ; in fact it is clear that if (NT) holds for some \mathcal{E} it also holds near E . By extension we will say :

$E^{\mathfrak{P}}$ is non-trapping if $\exists k_0 > 0$ and $S > 0$ such that $\forall k < k_0, \epsilon = E^{\mathfrak{P}}(k)$ satisfies (NT).

In some circumstances (for example if $v_0 = \overline{\lim} V(x)$ 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 $E^{\mathfrak{P}}$. In order to simplify the presentation of the main ideas of this approach to shape resonances we will not discuss such situations which are analyzed in the one-dimensional case in [CUS3c]. Let us simply mention that this type of difficulty is not unrelated to the fact (well-known e.g. in the analysis of N -body Schrodinger operators) that in the range of energy ($\underline{\lim} V(x)$, $\overline{\lim} V(x)$) there are threshold points where perturbation theory becomes rather delicate. We want to stress that under (H3) i.e. if $v_0 = \inf \{V(x), x \in \Omega_{int}\}$ is strictly larger than $\overline{\lim} V(x)$ and if $\epsilon = v_0$ satisfies (NT), then the n^{th} spectrum valued function $E^{\mathfrak{P}}$ of H_{int} is non trapping since $\lim E^{\mathfrak{P}}(k) = v_0$. This is why we introduce another geometrical assumption on V :

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

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

$$H_0 := -k^2 \Delta \text{ and } H_0^{\mathfrak{P}} := -k^2 \Delta^{\mathfrak{P}} := -k^2 (\Delta_{int} \oplus \Delta_{ext}), (k > 0)$$

We shall denote by H the selfadjoint operator which describes our system and is defined by

$$H := H_0 + V$$

whereas

$$H := H_0^2 + V := H_{int} \oplus H_{ext}$$

will be the operator describing the system where the particle is confined in Ω_{int} by the Dirichlet boundary condition on K .

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

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

For computational reasons it is sometimes simpler to use polar coordinates on \mathbb{R}^n . The coordinate transformation $x \rightarrow (r=|x|, \omega = x/|x|)$ induces the unitary mapping from $L^2(\mathbb{R}^n)$ onto $L^2(\mathbb{R}^+ \times \mathbb{S}^{n-1})$ defined by $f \rightarrow \tilde{f} : (r, \omega) \rightarrow r^{\frac{n-1}{2}} f(r\omega)$. The normal vector field $\omega \nabla$ considered as an operator on $L^2(\mathbb{R}^n)$ turns into $d/dr - (n-1)/2r$ on $L^2(\mathbb{R}^+ \times \mathbb{S}^{n-1})$. 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 $L^2(\mathbb{R}^+ \times \mathbb{S}^{n-1})$

$$-\Delta = -(d/dr)^2 + \Lambda/r^2, \quad \Lambda := B + (1/4)(n-1)(n-3) \quad (2.7)$$

where $B \geq 0$ denotes the Laplace-Beltrami operator on \mathbb{S}^{n-1} .

The operators H and H^p 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

$$x \rightarrow r_\theta x/|x| + e^{\theta \chi(x)}(x - r_\theta x/|x|).$$

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

$$A := \mathbb{1} + (2i)^{-1} \{ (x - r_\theta \omega), \nabla \} \text{ on } L^2(\mathbb{R}^n) = L^2(\Omega_{int}) \oplus L^2(\Omega_{ext}).$$

In terms of polar coordinates the action of $U(\theta)$ has the following simple form : for $f \in L^1(\mathbb{R}^n \times \mathbb{S}^{n-1})$,

$$(U(\theta)f)(r, \omega) = e^{i\theta\chi(r)/2} f(r(\theta), \omega), \quad r(\theta) := r_0 + e^{i\theta\chi(r)}(r - r_0).$$

Furthermore one finds easily

$$\begin{aligned} -\Delta(\theta) &:= -U(\theta)\Delta U^{-1}(\theta) = -e^{-i\theta\chi} \left(\frac{d}{dr} \right)^2 + \wedge / r(\theta)^2 \\ -\Delta^2(\theta) &:= -U(\theta)\Delta^2 U^{-1}(\theta) = -e^{-i\theta\chi} \left(\left(\frac{d}{dr} \right)^2 \right)^2 + \wedge / r(\theta)^2 \\ &=: -\Delta_{int} \oplus -\Delta_{ext}(\theta). \end{aligned}$$

Notice the important fact about the domains of the Laplacians (see Appendix III):

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

More precisely

$$\begin{aligned} D(\Delta(\theta)) = \{ u \in \mathcal{H}^1(\Omega_{int}) \oplus \mathcal{H}^1(\Omega_{ext}), \quad u(r_0+0, \cdot) = e^{i\theta/2} u(r_0-0, \cdot), \\ (\omega \nabla u)(r_0+0, \cdot) = e^{i\theta/2} (\omega \nabla u)(r_0-0, \cdot) \} \end{aligned}$$

Hence in the first case the domain is θ -independent in the second case not. In fact the same holds for the corresponding form domains. 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 $S_{\pi/4}$ and that furthermore this extension is the resolvent of the operator $\Delta(\theta)$ with the associated quadratic form

$$t_0(\Theta)[u] := \left(\frac{d}{dr} u, e^{-2\Theta x} \frac{d}{dr} u \right) + \left(\frac{\sqrt{\Theta}}{r(\Theta)} u, \frac{\sqrt{\Theta}}{r(\Theta)} u \right) + \\ + (1/4)(n-1)(n-3) \left(\frac{1}{r(\Theta)} u, \frac{1}{r(\Theta)} u \right) \quad (2.8)$$

on the domain $\mathcal{H}_0^1(\Omega_{int}) \oplus \mathcal{H}_0^1(\Omega_{ext})$ with boundary condition on K :

$$u(r_0+0, \cdot) = e^{\Theta r_0} u(r_0-0, \cdot) \quad (2.9)$$

$t_0^2(\Theta)$ is similarly defined ; however the form domain $\mathcal{H}_0^1(\Omega_{int}) \oplus \mathcal{H}_0^1(\Omega_{ext})$ is independent of Θ , (for details on exterior scaling we refer to [GY] and a forthcoming article of Simon). In particular one finds [ref.cit] :

$$\mathcal{G}(H_0(\Theta)) = \mathcal{G}_{ess}(H_0^2(\Theta)) = \{ e^{-1\Theta} r, r > 0 \}.$$

This can also be proved using Krein's Formula [Kr] relating the resolvents of $H_0(\Theta)$ and $H_0^2(\Theta)$ (the problem can be analyzed on a fixed angular momentum sector). Finally as $V(\Theta)$ is bounded analytic, (see (H5)) one deduces easily that $H(\Theta)$ and $H^2(\Theta)$, the image of H and H^2 under $U(\Theta)$, for real Θ , extend into self adjoint holomorphic families for complex Θ . In Appendix II we describe an alternative method to define $H(\Theta)$ using Krein's formula.

To elucidate the terminology "non-trapping" we end up with the following.

Remarks 2.

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

if $K \subset J(\mathcal{E})$ and $\mathcal{E} > \overline{\lim} V(x)$ the potential V is non-trapping at energy \mathcal{E} if and only if there exists $S > 0$ and a compact set $\Omega \subset \mathbb{R}^n$ such that

$$NT'1 : K \subset \bar{\Omega}, \Omega \subset J(\mathcal{E})$$

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

$$NT'3 : (2(r-r_0)/r)(V-\mathcal{E}) + (x-r_0\omega) \nabla V < -S, (x \in \Omega_{ext} \setminus \Omega).$$

The proof of this statement is elementary and will not be given here (see [K1]).

2. The (NT) condition on \mathcal{E} guarantees that there are no resonances in an appropriate neighbourhood of \mathcal{E} due to the exterior of V [BCD , K1] .

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

$$\mathcal{E}_1 < \mathcal{E}_2 \text{ and } \mathcal{E}_1, \mathcal{E}_2 \text{ NT} \implies \forall \mathcal{E} \in [\mathcal{E}_1, \mathcal{E}_2] \text{ , } \mathcal{E} \text{ is NT.}$$

4. On $\partial J(\mathcal{E}) \cap \Omega_{\text{ext}}$ one has $V(x) = \mathcal{E}$. Thus by (NT) we find

$$\forall x \in \partial J(\mathcal{E}) \cap \Omega_{\text{ext}} \text{ , } (\omega \nabla)V(x) < 0.$$

In physical terms this means that the force on the exterior boundary of the classically forbidden region $J(\mathcal{E})$ is repulsive.

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

6. If \mathcal{E} is NT then the boundary of $J(\mathcal{E})$ 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 eg. Majda-Ralston[MajRa]). Recently D. Robert and H. Tamura [RT] introduced a non-trapping condition in their semi-classical analysis of potential

scattering which is crucial for their investigation of the limiting absorption principle as $\hbar \rightarrow 0$. 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 behaviours of Green's function near such energies. A few years ago R. Lavine [L] already noticed the role of a non-trapping condition involving the virial :

$$2(V-E) + xVV < 0 \quad (2.10)$$

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 term which vanishes in the classical limit (see [K1] 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 the Poisson brackets, namely commutators, is the basis of Mourre's investigation of propagation properties for solutions of the Schrödinger equation [M2].

III. ESTIMATE ON THE DIRICHLET PERTURBATION

In this section we shall derive first convenient expressions for the difference of the resolvents of $H(\theta)$ and $H^{\mathfrak{D}}(\theta)$ 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 $T_{\text{int}} f$ denotes the trace of $f|_{\text{int}}$ (restriction of f to Ω_{int}) 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} (resp T_{ext}) is a bounded mapping from $\mathcal{H}^1(\Omega_{\text{int}})$ (resp $\mathcal{H}^1(\Omega_{\text{ext}})$) to $L^2(K)$. It follows that T_{int}^* maps continuously $L^2(K)$ into $\mathcal{H}^{-1}(\Omega_{\text{int}})$.

Perturbation by the Dirichlet boundary condition factorises naturally into two operators involving these traces as follows: Let a, θ be complex valued functions of k such that for some $k_0 > 0$:

$$\begin{aligned} \theta(k) \in S_d, \quad \text{Im}\theta(k) > 0 \quad (k_0 > k) \\ \text{Im}a(k) > 0, \quad \text{Im}\theta = o(\text{Im}a). \end{aligned} \quad (3.1)$$

A rough estimate on the numerical range of $H(\theta)$, $H^{\mathfrak{D}}(\theta)$ (see (3.6)) shows that a is in the resolvent set of $H(\theta)$ and $H^{\mathfrak{D}}(\theta)$ for k small enough. Hence the operators

$$\begin{aligned} A(\theta, a) &:= T_{\text{int}}(H(\theta) - a)^{-1} \\ B(\theta, a) &:= B_{\text{int}}(a) \oplus B_{\text{ext}}(\theta, a) \\ B_{\text{int}}(a) &:= -T_{\text{int}}(\omega \nabla)(H_{\text{int}} - a)^{-1} \\ B_{\text{ext}}(\theta, a) &:= e^{-1/\hbar} T_{\text{ext}}(\omega \nabla)(H_{\text{ext}}(\theta) - a)^{-1} \end{aligned} \quad (3.2)$$

are well defined on $L^2(\mathbb{R}^n) = L^2(\Omega_{\text{ext}}) \oplus L^2(\Omega_{\text{int}})$ with image in $L^2(\mathbb{R})$. If $\theta = 0$ we write $A(a)$ and $B(a)$. Defining $R(\theta, a) := (H(\theta) - a)^{-1}$ and $R^2(\theta, a) := (H^2(\theta) - a)^{-1}$ one has :

Lemma 2 . Let (H1-5) and (3.1) hold ; then , for k small enough,

$$W(\theta, a) := R(\theta, a) - R^2(\theta, a)$$

satisfies

$$W(\theta, a) = k^4 A^2(\theta, a) B(\theta, a). \quad (3.3)$$

Proof. This is a particular case of Krein's formula which relates different extensions of a symmetric operator $[Kr]$. The proof is essentially an application of Green's formula. Let u, v be elements of $L^2(\mathbb{R}^n)$ and $\hat{u} := R(\theta, a)u$, $\hat{v} := R^2(\theta, a)v$.

Then

$$(u, (R(\theta, a) - R^2(\theta, a))v) = -k^4 [(\hat{u}, \Delta^2(\theta)\hat{v}) - (\Delta(\theta)\hat{u}, \hat{v})] ,$$

since the term $V \cdot a$ cancels. If we insert the explicit form of the Laplacian in polar coordinates it is easily seen that the terms with the Laplace-Beltrami operators cancel too. So we are left with the difference of $(d/dr)^2$ and $((d/dr)^2)^2$. Partial integration leads to

$$(u, (R(\theta, a) - R^2(\theta, a))v) = -k^4 \int_{\mathbb{S}^{n-1}} d\omega \overline{\hat{u}(r_0 - 0, \omega)} (e^{-2ak} \hat{v}'(r_0 + 0, \omega) - \hat{v}'(r_0 - 0, \omega)) \quad (3.4)$$

where prime denotes partial derivative with respect to r . Notice that in the derivation of the above equation we used the boundary condition (2.9). Finally we recall that d/dr is equal to $\omega \nabla$ up to a multiplication operator ; hence Td/dr and $T\omega \nabla$ coincides on the domain of $H^2(\theta)$. This can be used on the r.h.s. of (3.4) and leads to the statement of the lemma.

Remark 3 .

It is worth noticing that $W(\theta, a)$ can be written in the more symmetric form (using a simple iteration of (3.3) :

$$W(\theta, a) = k^2 B^{\dagger}(\bar{\theta}, \bar{a}) T_{int} R(\theta, a) T_{int}^{\dagger} B(\theta, a)$$

It turns out that in fact $T_{int} R(\theta, a) T_{int}^{\dagger}$ does not depend on θ and equals $TR(a)T^{\dagger}$ (see Appendices I and II). So

$$W(\theta, a) = k^2 B^{\dagger}(\bar{\theta}, \bar{a}) T(H-a)^{-1} B(\theta, a).$$

In order to estimate the Dirichlet perturbation we proceed as follows. First we prove a crude estimate on the resolvents $R(\theta, a)$ and $R^{\dagger}(\theta, a)$ using a numerical range argument. After that we improve the result by a quadratic estimate. The arguments for the crude estimate of $R(\theta, a)$ and $R^{\dagger}(\theta, a)$ are very much the same. So we shall only present the one for $R(\theta, a)$ (in fact a much stronger estimate on $R^{\dagger}(\theta, a)$ than the one we will get here could be derived using the results of [BCD, XI]).

The sectorial forms $t_0(\theta)$ and $t_0^{\dagger}(\theta)$ have both numerical range in the lower complex half plane for $\text{Im} \theta$ non negative and sufficiently small. This is easily seen by inspection of equation (2.9) and

$$-(1/2)\text{Arg}(z(\theta))^{-2} = \text{Arg}z(\theta) - \text{Arctan} \frac{(v-r_0)\sin \theta}{v_0 + (v-r_0)\cos \theta} \in (0, \pi/2) \quad (3.5)$$

where $\theta = i\phi$, is non negative and small enough. The numerical range of $t(\theta)$ differs only slightly from the one of $t_0(\theta)$ since $V(\theta)$ is bounded and differentiable in θ . Hence there is a constant $C > 0$ such that for $\text{Im} \theta > 0$:

$$NR H(\theta) \subset \{ z \in \mathbb{C}, \text{Im} z < C \text{Im} \theta \} \quad (3.6a)$$

where NR denotes numerical range.

Remark 4 . The estimate on the numerical range can be improved by adding to (H1-2), (H5) the following assumptions :

$$(xV) \forall(x) \notin 0 \quad (x \in \Omega_{\text{int}}) \implies NR(H(\Theta)) \subset \{z \in \mathbb{C}, \text{Im}z < C(\text{Im}\Theta)^2\} \quad (3.6b)$$

$$\text{Im}V(\Theta) \leq 0 \quad (x \in \Omega_{\text{int}}, \Theta \in S_d) \implies NR(H(\Theta)) \subset \{z \in \mathbb{C}, \text{Im}z \leq 0\} . \quad (3.6c)$$

(3.6b) is shown by making a Taylor expansion of $V(\Theta)$. (3.6) is the basis for a rough estimate on the resolvent :

$$\|R(\Theta, a)\| \leq (\text{Im}a - n(\Theta))^{-1}, \quad (\text{Im}a > n(\Theta)) , \quad (3.7)$$

where $n(\Theta)$ denotes $C\text{Im}\Theta$, $C(\text{Im}\Theta)^2$ or zero depending on whether we are in the general case (3.6a) or (3.6b,c). An example for the last class of potentials is $V(x) = (a + bx^m)^2$, $a > 0$, $b > 0$, $m \in \mathbb{N}$. Notice that (3.6b) and (3.6c) will not be used in the following. (3.6b) is of course again a kind of non-trapping condition but much stronger than (NT). (3.6c) is a Herglotz property of the potential; if it holds many technically difficult problems get much simpler.

Now we are prepared to state the main result of this section

Theorem 5 . Assume (H1-2) and (H5) and let a, Θ satisfy (3.1) and $(\text{Im}\Theta)^{-1} = O(k^{-p})$ for some $p \in \mathbb{N}$. Assume furthermore that $\text{dist}(\text{Re}a, v_0) = o(1)$. Then :

$$A(\Theta, a) = O(k^{-1}); \text{ and } B(\Theta, a) = O(k^{-3}).$$

By lemma 2 this result implies that $W(\Theta, a)$ is $O(1)$ in k . The basic idea of proof is that the two resolvents differ essentially only in the classically forbidden region. For the proof of theorem 5 we will need the following variant of the standard Sobolev inequalities.

Lemma 6 : Let χ be a $C_0^\infty(\mathbb{R}^n)$ function with value one on K . Then the following inequalities hold

$$\|T_{int} f\|^2 \leq \begin{cases} 2 \|\chi f_{int}\| \|\nabla \chi f_{int}\|, & (n \in \mathbb{N} \setminus \{2\}) \\ 2 \|\chi f_{int}\| (\|\nabla \chi f_{int}\| + (2\epsilon_0)^{-1} \|\chi f_{int}\|), & (n=2). \end{cases}$$

We give a proof for the internal trace and omit the subscript int along this proof. The argument for T_{ext} is almost identical. By the fundamental theorem of calculus and Schwartz's inequality

$$\begin{aligned} \|Tf\|^2 - \|T\chi f\|^2 &= \int_{S^{n-1}} d\omega |\chi f(r_0, \omega)|^2 - 2\text{Re} \int_{S^{n-1}} d\omega \int_0^{r_0} dr \frac{d}{dr} \overline{\chi f} \chi f \\ &\leq 2 \left\| \frac{d}{dr} \chi f \right\| \|\chi f\| \end{aligned}$$

The radial derivative can be controlled by the Euclidean gradient

$$\begin{aligned} \left\| \frac{d}{dr} \chi f \right\|^2 &= \|\nabla \chi f\|^2 - \left(\chi f, \frac{\Delta}{r^2} \chi f \right) \\ &\leq \begin{cases} \|\nabla \chi f\|^2 & , (n \in \mathbb{N} \setminus \{2\}) \\ \|\nabla \chi f\|^2 + (2\epsilon_0)^{-1} \|\chi f\|^2 & , (n=2) \end{cases} \end{aligned}$$

where we used the fact $B = -\wedge - (1/4)(n-1)(n-3) \geq 0$. Hence the lemma is proved.

We now proceed to the proof of theorem 5 which will be split into several steps.

Proof of theorem 5.

1) First we prove a quadratic estimate on the resolvent $R(\theta, a)$.

Since $J(v_0)$ is open and $K \subset J(v_0)$ is compact there is a $\delta > 0$ and $\chi \in C_0^\infty(\mathbb{R}^n)$, radially symmetric, supported near K , $\chi = 1$ on K , such that $(V(x) - v_0) \gg \delta^{-1}$ for $x \in \text{Supp } \chi$. Since both $v_0 - \text{Re} a$ and $\text{Im } \theta$ tend to zero as $k \rightarrow 0$ (we can assume $\text{Re } \theta = 0$ without restricting generality) one has

$$2\operatorname{Re}((V(\Theta, x) - a) \chi \hat{u}) \geq \delta^{-4}, \quad (x \in \operatorname{supp} \chi, k < k_0). \quad (3.8)$$

Hence one gets, for $\hat{u} \in D(H(\Theta))$, the inequality :

$$\operatorname{Re}(\chi \hat{u}, (V(\Theta) - a) \chi \hat{u}) \geq \inf \{ \operatorname{Re}(V(\Theta, x) - a), x \in \operatorname{supp} \chi \} \|\chi \hat{u}\|^2,$$

which implies

$$\|\chi \hat{u}\|^2 \leq 2\delta \operatorname{Re}(\chi \hat{u}, (H(\Theta) - a) \chi \hat{u}), \quad (k < k_0). \quad (3.9)$$

This is because the real part of $H_0(\Theta)$ is positive. If we denote $u = (H(\Theta) - a) \hat{u}$ we get from (3.9) the quadratic estimate

$$(\|\chi \hat{u}\|^2 - \delta \|\chi u\|^2) \leq \delta^2 \|\chi u\|^2 + \operatorname{const} k^4 \|\chi \hat{u}\|^2 \quad (3.10)$$

To get this last inequality from (3.9) one has to commute $H_0(\Theta)$ with χ . This is the origin of the last term. In deriving it we have made use of the estimate

$$\operatorname{Re}(\chi \hat{u}, [-\Delta(\Theta), \chi] \hat{u}) \leq \operatorname{const} \|(\nabla \chi) \hat{u}\|^2$$

which can be proved by partial integration noting that $\nabla(\Theta) - \nabla(\bar{\Theta}) \in C$, where C denotes complex conjugation. It is important here that multiplication by χ maps the domain of $H(\Theta)$ into itself. Furthermore we can repeat the argument with χ' replacing χ without changing δ and the constant in (3.10) because $\operatorname{supp} \chi' \subset \operatorname{supp} \chi$.

2. $\forall u \in L^2(\mathbb{R}^n)$, $\|u\| = 1$, and choose a, Θ, p according to the assumptions of the theorem. We shall demonstrate that

$$\chi R(\Theta, a)u = o(1) \quad (3.11)$$

Due to (3.1) and (3.7) one gets

$$\chi R(\Theta, a)u = o(k^{-p}) \quad (3.12)$$

Inserting this result into the quadratic estimate (3.10) we

conclude that the power p in the above estimate can be reduced :

$$\chi R(\theta, a)u = \begin{cases} O(k^{-p+2}) , & (p > 2) \\ O(1) & , (p \leq 2) \end{cases} \quad (3.13)$$

Iterating this procedure leads to (3.11).

3. By an analogous argument one can get an estimate on the gradient of the resolvent. We shall prove

$$\nabla \chi (R(\theta, a)u)_{,mk} = O(k^{-2}) \quad (3.14)$$

starting from

$$\|\nabla \chi \hat{u}\|^2 \leq k^{-4} \delta \operatorname{Re}(\chi \hat{u}, (H(\theta) - a)\chi \hat{u}) \quad , (k < k_0)$$

which holds in analogy to (3.9). The r.h.s. is again of the same type and is estimated as before. This leads to (3.14).

4. To estimate $A(\theta, a)$ we use its explicit form in terms of the trace $T_{,mk}$ and the resolvent $R(\theta, a)$:

$$\|A(\theta, a)u\|^2 = \|T_{,mk} R(\theta, a)u\|^2 \leq 2 \|\chi \hat{u}_{,mk}\| \|\nabla \chi \hat{u}_{,mk}\| = O(k^{-1}).$$

The first inequality follows from lemma 6, the second from (3.11) and (3.14) of paragraph 2 and 3 above. This proves the first statement of the theorem.

5. To get an estimate on $B(\theta, a)$ one proceeds along the same lines as before. Therefore we indicate just those points which differ from the argument for $A(\theta, a)$.

By definition one has

$$\begin{aligned} \|B(\theta, a)u\|^2 &= \|B_{,mk}(a)u\|^2 + \|B_{\theta, mk}(\theta, a)u\|^2 \\ \|B_{,mk}(a)u\|^2 &= \|T_{,mk} u \mathcal{N} \hat{u}\|^2 \quad \text{with } u = (H^{\mathfrak{D}}(\theta) - a)\hat{u} \end{aligned}$$

and an analogous form for $B_{ext}(\Theta, a)$. By lemma 6 we get :

$$\|B_{int}(a)u\|^2 \leq 2 \|\chi \omega \nabla \hat{u}_{int}\| \|\nabla \chi \omega \nabla \hat{u}_{int}\|.$$

The only term which has not yet been estimated is $\Delta \chi \hat{u}_{int}$.
But this one is in fact particularly simple because

$$\chi \Delta \hat{u}_{int} = k^{-2} \chi (u_{int} - (v-a) \hat{u}_{int}).$$

The r.h.s. is up to the term k^{-2} of order one. For the first term this follows from normalization of u , for the second one from (3.11), and boundedness of v .

The estimate for $B_{ext}(\Theta, a)$ is reduced to an estimate on $\Delta \chi \hat{u}_{ext}$ which is now Θ -dependent. Since

$$\|(\Delta - \Delta(\Theta)) \chi \hat{u}_{ext}\| \leq c|\Theta| \left\{ \|\Delta(\chi \hat{u}_{ext})\| + \|\chi \hat{u}_{ext}\| \right\}$$

one has

$$\|\Delta \chi \hat{u}_{ext}\| \leq 2 \|\Delta(\Theta) \chi \hat{u}_{ext}\| + c|\Theta| \|\chi \hat{u}_{ext}\|$$

Repeating the argument above gives $\Delta \chi \hat{u}_{ext} = O(k^{-2})$ as before.

This concludes the proof of theorem 5.

IV. STABILITY OF EIGENVALUES OF H

In this section we shall prove that every spectrum valued function E^p 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 section. We prove it here for groups of spectrum valued functions $I = \{E_1^p, \dots, E_n^p\}$ having the following property :

H6 : there exists $b > 0$, $k_0 > 0$ such that

$$\forall k < k_0, \|I\|(k) \leq \text{const} k^b \leq \text{const} \Delta(k),$$

where we use the notation

$$\Delta := \text{dist}(I, G(H_{int}) \setminus I)$$

$$\|I\| := \text{Max}_{i,j} |E_i - E_j| =: \text{diam } I$$

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

Remark 1 . Since I consists of spectrum valued functions which all converge to v_0 as $k \rightarrow 0$ one always has that

$$\lim_{k \rightarrow 0} \|I\|(k) = \lim_{k \rightarrow 0} \Delta(k) = 0$$

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

Now we state the main technical lemmas of this section. First we give a result of [ECD, K1] under a form convenient for our purpose.

Lemma 2 . Let (H1-5) be valid and let Θ be a G_u -valued function of k such that $\text{Im}\Theta > 0$ and $(\text{Im}\Theta)^{-1} = O(k^{-p})$ for some $p \in \mathbb{N}$. Then there exists $k > 0$ and a complex neighbourhood \mathcal{V}_Θ of v_0 such that

$$\forall 0 < k < k_\Theta, \quad z \in \mathcal{V}_\Theta, \quad \|(H_{\text{ext}}(\Theta) - z)^{-1}\| \leq \text{const}(\text{Im}\Theta)^{-1}. \quad (4.1)$$

In particular \mathcal{V}_Θ can be chosen as follows :

$$\mathcal{V}_\Theta = \{z = v_0 + w_1 + iw_2, \quad |w_1| < \text{const}, \quad -\text{const}\text{Im}\Theta < w_2\}.$$

All the constants which appear here are positive and independent of k and z .

Remark 3 . In the following lemma we shall consider a loop in the resolvent set of $\mathcal{R}^\beta(\Theta)$ around a given finite group I of spectrum valued functions obeying (H6), (see fig. 2). To do it we shall use lemma 2. As the size of \mathcal{V}_Θ along the real axis is k -independent and all the elements of I go to v_0 when $k \rightarrow 0$, this makes sure that $I \subset \mathcal{V}_\Theta$ for sufficiently small k . In fig.2 the non-shaded area is singularity free for $(H_{\text{ext}}(\Theta) - z)^{-1}$.

Lemma 4 . Assume (H1-5) and let $I = \{E_1^\beta, \dots, E_n^\beta\}$ be a set of spectrum valued functions satisfying (H6). Then there exists a and Θ , two complex valued functions of k , satisfying (3.1) and $\text{Im}\Theta > 0$, and a loop Γ around I such that

$$(\mathcal{R}^\beta(\Theta, a) - (z-a)^{-1})^{-1} = o(1), \quad (z \in \Gamma).$$

Proof . Let \bar{E} be the barycenter of I . By (H6), $\|I\| \leq \text{const}\Delta$, where Δ denotes the distance of I to the rest of the spectrum of H_{int} .

Let $a := \bar{E} + i(|I| + \Delta)$ and Γ the contour defined by the following figure (see lemma 2 and remark 3):

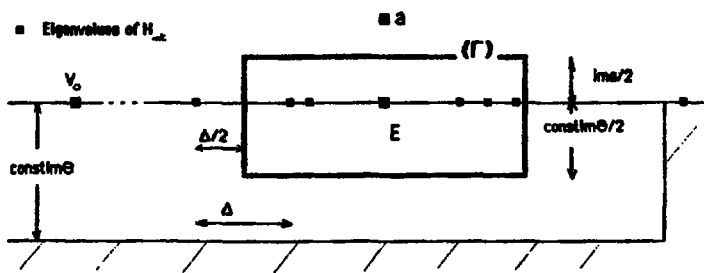


Fig. 2. The loop Γ around a in the neighbourhood U_θ .

Let $\varepsilon \in (0, 1)$ and define $\text{Im } \theta = (\Delta + |\varepsilon|)$, $\text{Re } \theta = 0$. Let us show that :

$$\| (R^\theta(\theta, a) - (z-a)^{-1})^{-1} \| \leq \text{const}(\Delta + |\varepsilon|)^{1-\varepsilon}$$

which is sufficient (see remark 1).

Since $\text{Im } \theta = o(\text{Im } a)$ (by construction) the resolvent $R^\theta(\theta, a)$ exists for k sufficiently small. Due to the identity

$$(R^\theta(\theta, a) - (z-a)^{-1})^{-1} = -(z-a) - (z-a)^2 R^\theta(\theta, z) \quad (4.2)$$

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

$$|z-a| \leq \text{const}(\Delta + |\varepsilon|)$$

Now we estimate

$$\| R^\theta(\theta, z) \| \leq \max(\| (H_{\text{int}} - z)^{-1} \|, \| (H_{\text{ext}}(\theta) - z)^{-1} \|).$$

On one hand

$$\| (H_{\text{int}} - z)^{-1} \| = 1/\text{dist}(z, \sigma(H_{\text{int}})) \leq \max(2\Delta^{-1}, \text{const}(\Delta + |\varepsilon|)^{1-\varepsilon}).$$

On the other hand by Lemma 2

$$\| (H_{\text{ext}}(\Theta) - z)^{-1} \| \leq \text{const} (\text{Im} \Theta)^{-1} = \text{const} (\Delta + |I|)^{-1-k}$$

Hence

$$\| (z-a)^k R^D(\Theta, z) \| \leq \text{const} \max(\Delta^k (\Delta + |I|)^2, (\Delta + |I|)^{1-k})$$

Since $\Delta + |I| \leq \text{const} \Delta$ one gets the result of the lemma.

Theorem 5. Let $I = \{E_1^3, \dots, E_n^3\}$ be a group of spectrum valued functions of H_{int} obeying (H5). Assume conditions (H1-5); then there exists a complex valued function Θ of k , $\text{Im} \Theta > 0$, and a loop Γ around I such that

$$P := -(2i\pi)^{-1} \int_{\Gamma} dz R(\Theta, z)$$

is well defined for k sufficiently small and has the same dimension as

$$P^D := -(2i\pi) \int_{\Gamma} dz R^D(\Theta, z).$$

Proof .1. Choose a, Θ and Γ as in the proof of lemma 4 and let

$\tilde{\Gamma} = \{ \tilde{z} = (z-a)^{-1}, z \in \Gamma \}$; then by the functional calculus one also has :

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

By the same argument it is enough to show that

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

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

$$(R(\Theta, a) - \tilde{z})^{-1} = (R^D(\Theta, a) - \tilde{z})^{-1} \sum_{n \geq 0} (W(\Theta, a) (R^D(\Theta, a) - \tilde{z})^{-1})^n$$

Since $(R^{\triangleright}(\theta, a) - \tilde{z})^{-k}$ is $o(1)$ on $\tilde{\Gamma}$ it is enough to have a k -independent bound on $W(\theta, a)$. This was the purpose of theorem III.5. By construction of a and θ 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 $R^{\triangleright}(\theta, a)$ and $R(\theta, a)$; consider

$$R(\theta, a, \beta) := R^{\triangleright}(\theta, a) + \beta W(\theta, a).$$

The projections $P(\beta)$ defined in analogy to (4.3) are analytic in β and interpolate between P and P^{\triangleright} . Hence $\dim P = \dim P^{\triangleright}$.

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^n 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^n 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^n be the n -th eigenvalue of H_{int} . Assume E^n non degenerate and furthermore (H1-5) and (H6) with $1-\{E^n\}$. Let P^n, P be the projectors defined according to theorem IV.5. Then for suitable a and θ the eigenvalue E associated to P satisfies :

$$E - E^n = \text{Trace } P^n W(\theta, a) P^n - \text{Trace } P^n W(\theta, a) Q^n \times \quad (5.1)$$

$$\times (Q^n R(\theta, a) Q^n - F)^{-1} Q^n W(\theta, a) P^n$$

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

Proof. The proof is split into two parts, a formal computation and verification of legality of the formal steps. Here θ and a are taken as in theorem IV.5.

1. The formal argument is based on the equation $R(\theta, a)P = FP$ which is studied in the subspaces range of P^n and range of Q^n (to simplify notation θ and a are suppressed).

$$P^n R P^n P + P^n R Q^n P = F P^n P$$

$$Q^n R P^n P + Q^n R Q^n P = F Q^n P$$

Eliminating $Q^n P$ 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^{\flat} and $(Q^{\flat} R Q^{\flat} - F)^{-1}$. The first two operators exist and are defined by a Cauchy integral according to theorem IV.5.

Now consider

$$\begin{aligned} Q^{\flat} R Q^{\flat} - F &= Q^{\flat} R^{\flat} Q^{\flat} + Q^{\flat} W Q^{\flat} - F \\ &= Q^{\flat} R_{int} Q^{\flat} + R_{ext} + Q^{\flat} W Q^{\flat} - F . \end{aligned}$$

Since by theorem IV.5, F has to be inside the loop $\tilde{\Gamma} = \{(z-a)^{\pm 1}, z \in \Gamma\}$ and the spectra of $Q^{\flat} R_{int} Q^{\flat}$ and R_{ext} are outside at a distance of order Δ (by our choice of Θ) and since furthermore W is $O(1)$, we get the a priori estimate on the range of Q^{\flat}

$$\|(Q^{\flat} R Q^{\flat} - F)u\| \geq c(k)\|u\|, \quad c(k)^{-1} = o(1). \quad (5.2)$$

Hence by standard arguments the inverse of $Q^{\flat} R Q^{\flat} - F$ exists and the lemma is proved.

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

Theorem 2 : Let the assumption 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 :

$$E = E^{\flat} + \sum_{n \geq 1} \frac{G_n}{n!} t^n .$$

Furthermore the following estimates hold :

$$t^{-1} = o(\exp(-2(1-\varepsilon)k^2 d(K, \mathcal{C}))) \quad (5.3)$$

for all $\varepsilon > 0$ where d denotes the pseudo-distance associated to the metric $(ds)_1^2 = \max(0, V(x) - v_0) dx^2$

and

$$G_n = o(1),$$

Proof . Let

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

where a , Θ and Γ are chosen according to lemma IV.4. So as shown in the proof of Lemma 1, the operator $(Q^B R(\Theta, a) Q^B - \tilde{z})^{-1}$ is well defined and analytic in \tilde{z} for $\tilde{z} = (z-a)^{-1}$, z inside Γ ; hence $\mathcal{G}(\Theta, \tilde{z})$ also is.

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

$$F - P^B = t(\Theta) \mathcal{G}(\Theta, F). \tag{5.4}$$

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

$$|\mathcal{G}(\Theta, \tilde{z})| \leq \|1 - M(\Theta, \tilde{z})\|$$

where by (5.2) $M(\Theta, z)$ is $o(1)$ on $\tilde{\Gamma}$. Then the solution of (5.4) is given by the convergent series.

$$F - P^B = \sum_{n \geq 1} \frac{\tilde{G}_n(\Theta)}{n!} t^n(\Theta) \tag{5.5}$$

where

$$\tilde{G}_n(\Theta) := (d/dz)^{n-1} \mathcal{G}(\Theta, z) \Big|_{z=(E^B - a)^{-1}} \tag{5.6}$$

Now it turns out that $t(\Theta)$, $\mathcal{G}(\Theta, \tilde{z})$ and $\tilde{G}_n(\Theta)$ are in fact independent of Θ and can be taken at $\Theta = 0$. This follows from the following remarks. First; $B(\Theta, a) P^B$ and $A(\Theta, a) P^B$ are Θ -independent; in fact setting $P^B \tilde{P}^B = P^B$, $\|P^B\| = 1$ one has $B(\Theta, a) \tilde{P}^B = B_{\text{int}}(a) P^B$ which is manifestly Θ -independent because

$\xi^p \in \mathcal{K}_0^k(\Omega_{\text{int}})$. Then according to Remark III.3,

$$\begin{aligned} A(\Theta, a) \xi^p &= k^4 T_{\text{int}} R(\Theta, a) T_{\text{int}}^* B(\Theta, a) \xi^p \\ &\approx k^4 \text{TR}(a) T^* B(a) \xi^p \end{aligned} \quad (5.7)$$

is also Θ -independent. Since $\mathcal{G}(\Theta, \tilde{z})$ is obviously analytic in Θ and independent of it for real Θ the quantities appearing in (5.5) and (5.6) can be estimated at $\Theta = 0$ (thus we shall omit in the sequel to write Θ). It remains to estimate the parameter

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

As shown in the proof of theorem III.5

$$\|B(a) \xi^p\| \leq 2 |E^p - a|^{-1} \|\chi \omega \xi^p\| \|\nabla \chi(\omega \nabla) \xi^p\|.$$

By Agmon's decay estimates both terms are $o(\exp(-(1-\epsilon)k^4 d(K, \mathcal{E})))$, if we take χ supported in a sufficiently small neighbourhood of K [Ag, CUS1, S2, HSj1]. To estimate $\|A(a) \xi^p\|$ we use (5.7) and $\| \text{TR}(a) T^* \| = O(k^{-2})$ as shown in Appendix I. Then the above bound on $\|B(a) \xi^p\|$ implies (5.3). Finally we prove the estimates on the coefficients $\tilde{\mathcal{G}}_n$ and \mathcal{G}_n .

We use the Cauchy formula to estimate the $\tilde{\mathcal{G}}_n$:

$$\tilde{\mathcal{G}}_n = (n-1)! (2i\pi)^{-1} \int_{\tilde{\Gamma}} \mathcal{G}(\tilde{z}) (E^p - \tilde{z})^{-n} d\tilde{z}.$$

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

$$(E^p - \tilde{z})^{-n} = -(z-a) - (z-a)^2 (E^p - z)^{-1}.$$

In the case of a single eigenvalue, $|\mu| = 0$. It is easy to see that we may make a slightly modified choice of a , Θ , $\tilde{\Gamma}$ of lemma IV.4 as follows

$$a = E^2 + i\Delta, \operatorname{Im} \Theta = \operatorname{const} \Delta,$$

$$\Gamma = \{z \in \mathbb{C}, |z - E^2| = \operatorname{const} \Delta\}$$

with $\Delta := \operatorname{dist}(E^2, \mathcal{G}(H_{\text{int}} \setminus E^2))$.

Thus $(F^2 - \bar{z})^k = O(\Delta)$ and $\tilde{\mathcal{G}}_n = O(\Delta^{n-1})$.

Now, to obtain a bound on \mathcal{G}_n we write the following identities:

$$F - F^2 = \sum_{n \geq 1} t^n \frac{\tilde{\mathcal{G}}_n}{n!} = (E^2 - E)/(E - a)(E^2 - a)$$

thus

$$E^2 - E = \sum_{n \geq 1} \frac{t^n}{n!} (E - a)(E^2 - a)$$

Hence

$$\mathcal{G}_n = O((E - a)(E^2 - a)) \tilde{\mathcal{G}}_n = O(\Delta^{n-1}) = o(1).$$

APPENDIX I

We derive here a technical estimate on $\text{TR}(a)T^\theta$ needed in the proof of the main theorem V.2. We also emphasize that this result could be used to obtain an alternative proof of the estimate on the size of the perturbation $W(\Theta, a)$. In fact one has (see Remark III.3. and Appendix II)

$$W(\Theta, a) = k^2 B^a(\bar{\Theta}, \bar{a}) \text{TR}(a) T^B(\Theta, a)$$

so that for complex Θ only an investigation of the "unperturbed" Dirichlet operator is needed.

Lemma A.1. Let a be a complex valued function of k satisfying $(\text{Im} a)^{-1} = O(k^{-p})$ for some $p \in \mathbb{N}$ and $|\text{Re} a - \gamma| = o(1)$ as $k \rightarrow 0$. Then for some $k_0 > 0$ one has for some constant C :

$$\|\text{TR}(a)T^\theta\| \leq C(k^{-2}) \quad (k < k_0).$$

Proof. Let $\gamma \in L^1(S^{n-1})$, $\|\gamma\| = 1$; then $u = T^\theta \gamma \in \mathcal{H}^{-1}(\mathbb{R}^n)$ and $R(a)T^\theta \gamma \in \mathcal{H}^1(\mathbb{R}^n)$, 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 p279 ; F pl3, 17]). By Lemma III.6 one has with $\hat{u} = R(a)u$ and for k small enough

$$\|\text{TR}(a)T^\theta \gamma\|^2 \leq 2k^{-1} \|\chi \hat{u}\| (k^2 \|\nabla \chi u\|^2 + \|\chi \hat{u}\|^2)^{1/2}$$

Proceeding as in the proof of theorem III.5 with $\Theta = 0$ one obtains (using suitable L^2 -approximations of u in \mathcal{H}^{-1}):

$$\begin{aligned} \|\text{TR}(a)T^\theta \gamma\|^2 &\leq \text{const} k^{-1} [\text{Re}(\text{TR}(a)T^\theta \gamma, \gamma) + k^2 \|\chi \hat{u}\|^2] \\ &\leq \text{const} [k^{-1} \|\text{TR}(a)T^\theta \gamma\| + k^2 \|\chi \hat{u}\| \|\hat{u}\|] \end{aligned}$$

Now $\|\hat{u}\| = \|R(a)T^\theta \gamma\| \leq \|\text{TR}(a)\|$ and by theorem III.5, $\|\text{TR}(a)\| = O(k^{-1})$.

So finally :

$$\|TR(a)T^{-n}\| \leq \text{const}[k^{-1}\|TR(a)\|^{n+1}].$$

The proof is now easily completed.

APPENDIX II

We provide here an alternative proof of the analyticity in Θ of $R(\Theta, z) = (H(\Theta) - z)^{-1}$. As mentioned earlier, this is not a priori easy since the domain and form domain associated to $H(\Theta)$, $\Theta \in S_q$ depend on Θ . However the family $\{H^\delta(\Theta), \Theta \in S_q\}$ is analytic of type A; so it is natural to try to use a perturbative argument. All we need to show is the following result:

Lemma A.2. Let $\Theta_0 \in \mathbb{R}$ and $z_0 \in \mathbb{C}$, $\text{Im} z_0 \neq 0$; then there exists a complex open neighbourhood $\mathcal{V}(\Theta_0)$ of Θ_0 such that $(H(\Theta) - z_0)^{-1}$ has an analytic continuation from $\mathcal{V}(\Theta_0) \cap \mathbb{R}$ to $\mathcal{V}(\Theta_0)$.

Proof. The lemma obviously holds for $H^\delta(\Theta)$ instead of $H(\Theta)$. Let $\mathcal{V}(\Theta_0)$ be the corresponding open set; then

$$R(\Theta, z_0) = R^\delta(\Theta, z_0) + W(\Theta, z_0)$$

holds for $\Theta \in \mathcal{V}(\Theta_0) \cap \mathbb{R}$ (here we use the notations introduced in Chapter III). One has for real Θ and by Lemma III.2:

$$W(\Theta, z_0) = K^+ A^+(\bar{\Theta}, \bar{z}_0) B(\Theta, z_0) = K^+ B^+(\bar{\Theta}, \bar{z}_0) T_{\text{int}} R(\Theta, z_0) T_{\text{int}}^+ B(\Theta, z_0).$$

$$\text{Now } T_{\text{int}} R(\Theta, z_0) T_{\text{int}}^+ = T_{\text{int}} U(\Theta) R(z_0) U^{-1}(\Theta) T_{\text{int}}^+ = T_{\text{int}} R(z_0) T_{\text{int}}^+$$

since obviously $T_{\text{int}} U(\Theta) = T_{\text{int}}$ for $\Theta \in \mathbb{R}$.

So consider now for $\Theta \in \mathcal{V}(\Theta_0)$:

$$W(\Theta, z_0) = K^+ B^+(\bar{\Theta}, \bar{z}_0) T R(z_0) T^+ B(\Theta, z_0).$$

Since $B(\Theta, z_0)$ is obviously analytic in $\mathcal{V}(\Theta_0)$, the family $\{W(\Theta, z_0), \Theta \in \mathcal{V}(\Theta_0)\}$ also is. Then let

$$\tilde{R}(\Theta, z_0) = R^\delta(\Theta, z_0) + W(\Theta, z_0).$$

This family of operators is analytic in $\mathcal{V}(\Theta_0)$ and coincides with $R(\Theta, z_0)$ for $\Theta \in \mathcal{V}(\Theta_0) \cap \mathbb{R}$. It remains to show that it is a family of resolvents; it is well-known, [K, P428] 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 $\ker \tilde{R}(\Theta, z) = \{0\}$; it can be verified as follows :

Let u satisfy $\tilde{R}(\Theta, z_0)u = 0$; then $\forall \hat{v} \in C_0^\infty(\mathbb{R} \setminus K)$ one has

$$(v, R^2(\Theta, z_0)u) + (v, W(\Theta, z_0)u) = 0.$$

with $v = :H^2(\bar{\Theta}) - \bar{z}_0) \hat{v}$ (notice that $C_0^\infty(\mathbb{R} \setminus K) \subset D(H^2(\Theta))$)

$\forall \Theta \in S_0$). Hence :

$$(\hat{v}, u) + k^2 (B(\bar{\Theta}, \bar{z}_0)v, TR(z_0)T^* B(\Theta, z_0)u) = 0.$$

But

$$B(\bar{\Theta}, \bar{z}_0)v = -T_{\text{int}}(\omega \nabla) \hat{v}_{\text{int}} \oplus e^{-ikx} T_{\text{ext}}(\omega \nabla) \hat{v}_{\text{ext}} = 0.$$

From this follows $(\hat{v}, u) = 0$ hence $u = 0$. Thus $\tilde{R}(\Theta, z_0)$ is an analytic family of resolvents providing the analytic continuation of $R(\Theta, z_0)$ to $\mathcal{V}(\Theta)$.

APPENDIX III

The purpose of this appendix is to show the following

Theorem A3. The family of operators $\{\Delta^2(\theta), |\operatorname{Im}\theta| < \pi/4\}$ as defined in chapter II, is a self adjoint holomorphic family of type A. In particular

- 1) $D(\Delta^2(\theta)) = (\mathcal{H}_0^1 \cap \mathcal{H}_1^1)(\Omega_{\text{int}}) \oplus (\mathcal{H}_0^1 \cap \mathcal{H}_1^1)(\Omega_{\text{ext}})$
- ii) $-\Delta^2(\theta)$ is m -sectorial with vertex 0 and semi-angle $|2\operatorname{Im}\theta|$.

Proof. It is standard that $D(\Delta^2) = (\mathcal{H}_0^1 \cap \mathcal{H}_1^1)(\Omega_{\text{int}}) \oplus (\mathcal{H}_0^1 \cap \mathcal{H}_1^1)(\Omega_{\text{ext}})$. Since $\Delta_{\text{int}}(\theta) = \Delta_{\text{int}}$ for any θ , we concentrate only on $\Delta_{\text{ext}}(\theta)$ and analyze

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

where

$$g(r, \theta) := e^{i\theta} / r(\theta)^2 =: g_r + i g_i$$

g_r and g_i , 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, $U(\theta)D = D$ 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 $\operatorname{Re}T(\theta) = -\Delta_r + g_r \Lambda$ is uniformly elliptic thus self adjoint on D (see [K p353]). Secondly, using the following identity in the form sense on D

$$\Delta_r^2 + g_r^2 \Lambda^2 = (\operatorname{Re}T(\theta))^2 + 2\Lambda^{1/2} g_r^2 \Delta_r \Lambda^{1/2} + 2((g_r^2)')^2$$

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

$$g_r^2 \Lambda^2 \leq (\operatorname{Re}T(\theta))^2 + C g_r \Lambda, \quad C := (1/2) \| (g_r^2)' / g_r \|_\infty^2$$

which implies, after a quadratic type estimate,

$$\|g_1 \wedge u\| \leq \|ReT(\theta)u\| + c \|u\| \quad \text{on } D.$$

Now we have

$$\|ImT(\theta)u\| \leq \|g_2/g_1\|_\infty (\|ReT(\theta)u\| + c \|u\|) \quad \text{on } D,$$

which shows that $T(\theta)$ is m -sectorial because $\|g_2/g_1\|_\infty$ is smaller than 1 as long as $Im\theta < \pi/4$.

The semi angle of sectoriality is given by (note that $g_2 \gg 0$)

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

Since $D \subset D(t_0^3(\theta))$, $\Delta_{t_0^3}(\theta) = e^{-3\theta} T(\theta)$ by a standard property of Friedrichs extension of sectorial operators (see [K p325-326]).

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