A Simple Model for Predissociation*

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Abstract

We analyse a very simple class of one dimensional two by two matrix Schrödinger operators. Their diagonal part has embedded eigenvalues in the continuous spectrum which become resonances when the off-diagonal part is turned on. Our analysis is semiclassical and contains a regular perturbative calculus of these resonances, asymptotics of the Fermi rule contribution to the width of these as well as lower bounds on the corresponding life time.

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1 Introduction

We start directly exposing the model; the discussion about the content of this paper is split in several parts which are put at the end of their relevent sections.

1.1 The Model

Let

$$H := H^d + W, \quad H^d := \begin{pmatrix} H^1 & 0 \\ 0 & H^2 \end{pmatrix}, \quad W := \begin{pmatrix} 0 & V^{1,2} \\ V^{2,1} & 0 \end{pmatrix}$$

be a matrix Schrödinger operator acting on $L^2(I\!R) \oplus L^2(I\!R) =: \mathcal{H}$, where

$$\begin{aligned} H^k &:= D^2 + V^k, \quad k = 1, 2, \quad D := \frac{\hbar}{i}\frac{d}{dx}, \\ V^2(x) &:= x^2, \quad V^{1,2} := \hbar(tD + Dt) = -V^{2,1}. \end{aligned}$$

Dilation and translation analyticity of the potentials play here an important role; we assume

V^1 and it are bounded analytic multiplication operators in $\Sigma_{\beta_0,\eta_0} := \{z \in \mathbb{C}, |\mathrm{Arg}\, z| < \beta_0$ or $|\mathrm{Im}\, z| < \eta_0\}$, *$\beta_0, \eta_0$ being both strictly positive; V^1 and it are real on $I\!R$.* **(H1)**

The images of all operators under the scaling $x \to e^\theta x$ will be denoted when necessary by a subcript θ. With these assumptions we have the following

theorem 1. H_θ, H^i_θ, i=1,2 are selfadjoint analytic families of type A for all θ such that $|\mathrm{Im}\, \theta| < \hat\beta_0 := \min\{\beta_0, \frac{\pi}{4}\}$ with domains

$$\begin{aligned} \mathcal{D}(H_\theta) &= \mathcal{D}(H^1_\theta) \oplus \mathcal{D}(H^2_\theta), \\ \mathcal{D}(H^1_\theta) &= \mathcal{H}^2(I\!R), \quad \mathcal{D}(H^2_\theta) = \mathcal{H}^2 \cap \hat{\mathcal{H}}^2(I\!R). \end{aligned}$$

The definition of "type A family" may be found in [Ka, Ch.VII §2.1]. $\mathcal{H}^n(I\!R)$ denotes the usual Sobolev space and $\hat{\mathcal{H}}^n$ its Fourier image. The proof of this theorem is rather standard. For H^1_θ it is obvious, since V^1_θ is bounded analytic; for H^2_θ a detailed proof can be found in [BCD2]. H_θ can be treated perturbatively as in [DEŠ]; in the form sense on $\mathcal{D}(H^d_\theta)$ one has

$$|e^\theta W_\theta|^2 \le \hbar^2\{8\|t_\theta\|^2 D^2 + 2\hbar^2\|t'_\theta\|^2\} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

which shows that W_θ is H^d-bounded with relative bound zero.

In order to have a reasonable spectrum for H^1 we assume

$\exists \varepsilon > 0,\ \exists v_\infty < 0,\ \forall 0 < |\mathrm{Im}\, \theta| < \beta_0, \quad V^1_\theta = v_\infty + \mathcal{O}(x^{-1-\varepsilon})$, *as $|x|$ tends to infinity.* **(H2)**

This implies in particular that the essential spectrum of H^1_θ is simply:
$\sigma_{ess}(H^1_\theta) = v_\infty + e^{-2\theta} I\!R_+$.

1.2 Discussion and Further Hypothesis

H^2 has only discrete spectrum, $\sigma(H^2) = (2\mathbb{N}+1)\hbar$. When θ equals zero, these eigenvalues are embedded in the continuous spectrum of H^1. The effect of the perturbation W is usually to couple these bound states to the scattering states of H^1. If the quantum system is initially prepared in a state $0 \oplus \varphi^2$, φ^2 being a bound state of H^2, it will eventually turn into a scattering state. The mechanism behind this effect is very similar to the one which causes the existence of shape resonances, viz. tunneling through the potential barrier (see e.g. [CDKS, HeSj]).

If the two potentials V^1 and V^2 cross one can reduce the problem for the lowest energies to a shape resonance situation [K]; the relevent effective potential is $\min\{V^1, V^2\}$ which possesses a well, separated from the escaping regions by a potential barrier.

Here we want to address explicitly the case with no crossing of V^1 and V^2: we assume

$$\max V^1 < \min V^2 = 0. \tag{\textbf{H3}}$$

Now, at first glance, one would say there is no barrier. But classically one can see that for the energy $e_0 = (2n+1)\hbar$ (the n^{th} quantum state of H^2) the allowed momenta for H^1 and H^2 are separated by a gap of size $\sqrt{-\max V^1}$ for $\hbar$ small enough. This gap indicates a classically forbidden region for the hamiltonian H^d in the momentum space rather than in the configuration space. So we can speak of a *dynamical barrier* being present and of *dynamical tunneling* as the reason for the escape of the bound state (see [AD] for the same discussion in the case of the reflection over a potential barrier). However assumption (H3) is much stronger than necessary for this phenomenon to take place. Wilkinson [W] and Martinez [Ma2] have remarked that it is sufficient to require that the energy shells do not cross: $\{H^1_{cl}(q,p) = H^2_{cl}(q,p) = E\}$[1] $= \emptyset$ to get such an effect which they called respectively *tunneling in phase space* and *microlocal tunneling.*

The dynamical tunneling manifests itself in the so-called resonances of the quantum system. According to the standard machinery ([AgC, RS4]) these resonances are recognized as complex eigenvalues of H_θ which are the perturbed eigenvalues of H^d_θ. Notice that these eigenvalues do not depend on θ. Since the essential spectrum of H^1_θ has turned down in the complex energy plane, the eigenvalues of H^d_θ to be perturbed are now isolated provided H^1_θ does not have eigenvalues too close. This last requirement is achieved by imposing a nontrapping condition on V^1:

$$\exists S < 0, \quad \forall 0 \le \beta < \beta_0 \quad \mathrm{Im}\, e^{i2\beta} V^1_{i\beta} \le \beta S \tag{\textbf{H4}}$$

The perturbation W_θ being H^d_θ-bounded with relative bound zero our problem falls into the category of regular perturbation theory. Section 2 is devoted to this perturbation theory. Once the resonances are shown to exist we shall give for a restricted model the asymptotics of the Fermi rule contribution to their width in section 3 and finally estimate this width in section 4.

Such a model with $V^1 = -1$ and $V^{1,2} = V^{2,1} = \hbar^2$ has been proposed by J. Asch [A] as a simple model to understand the predissociation phenomenon in diatomic molecules. V^1 and V^2 play the role of the electronic curves, $\hbar^2$ the inverse of the nucleus mass. We have chosen, here, more realistic coupling terms. Reducing the complete molecular hamiltonian to a two by two matrix of this type is the purpose of the Born-Oppenheimer approximation, see e.g. [CDS] and [Ma1]. In these articles the basic algebraic tool is a method bearing numerous names: Brilloin-Wigner, Feshbach, Grushin, Schur... not to forget the Livsic Matrix [Ho]. However by

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[1] H^i_{cl} denotes the classical Hamiltonian funtion associated to H^i.

"putting" into H^1 all the electronic curves except the second one, it is conceivable to obtain the same result not using the energy dependent perturbation theory, see e.g. [DEŠ].

2 Perturbation Expansion of the Resonances

We first prove that under (H1,4) H^1_θ has no spectrum close to a given eigenvalue e_0 of H^2. It will be sufficient to have this property in the closed neighbourhood of e_0 bounded by the contour $\Gamma := \{z \in \mathbb{C}, |z - e_0| = \hbar\}$.

2.1 Nontrapping Estimates

Lemma 2. Under hypothesis (H1,4) one has:

$$\forall\, 0 < \beta < \beta_0,\ \exists\, c^1_\beta := \frac{-2}{\beta S},\ \forall\, 0 < \hbar < \frac{1}{c^1_\beta},\ \forall\, z \in \Gamma,\ \|R^1_{i\beta}(z)\| \le c^1_\beta.$$

Sketch of the proof: Such type of result is now rather standard (cf. [BCD1]). The condition on $\hbar$ (stronger than necessary), insures that

$$\Gamma \subset \nu := \{z \in \mathbb{C},\ \operatorname{Im} e^{i2\beta} z \ge \beta S\}.$$

ν is a set of complex energies that cannot be resonances of H^1 due to (H4). More precisely, since in the form sense on $\mathcal{D}(H^1)$ one has:

$$|H^1_{i\beta} - z| \ge \operatorname{Im} e^{i2\beta}(z - H^1_{i\beta}) = \operatorname{Im} e^{i2\beta}(z - V^1_{i\beta}) \ge \operatorname{Im} e^{i2\beta} z - \beta S \ge -\beta\frac{S}{2},$$

which yields the a priori estimate we need to bound $R^1_{i\beta}(z)$. In the last step we have explictely used that z belongs to Γ and the condition on $\hbar$. ■

2.2 Stability of the Resolvent Set of H^d_θ

The previous lemma gives sufficient conditions to insure that Γ is included in $\rho(H^1_\theta)$, the resolvent set of H^1_θ. Since it is well known (see e.g. [BCD2]) that the spectrum of H^2_θ is invariant with respect to θ as long as $|\operatorname{Im}\theta| < \frac{\pi}{4}$, we conclude that Γ is also in $\rho(H^d_\theta)$ under this extra condition on $\operatorname{Im}\theta$. Therefore, by standard perturbation theory, Γ will also be in $\rho(H_{i\beta})$ if in addition

$$\forall z \in \Gamma, \quad \|R^1_{i\beta}(z) V^{1,2}_{i\beta} R^2_{i\beta}(z) V^{2,1}_{i\beta}\| < 1.$$

$R^1_{i\beta}(z)$ is already estimated by lemma 2. In the next lemma we shall estimate $V^{1,2}_{i\beta} R^2_{i\beta}(z) V^{2,1}_{i\beta}$ and other quantities needed in the sequel. As in Kato [Ka, Ch.II §2.1], we use the notation:

$$S^{2\,(k)}_{i\beta} := (\hat{R}^2_{i\beta}(e_0))^k, \text{ if } k \ge 1 \text{ and } S^{2\,(0)}_{i\beta} = -P^2_{i\beta}$$

where $\hat{R}^2_{i\beta}(e_0)$ is the reduced resolvent of $H^2_{i\beta}$ at e_0 and $P^2_{i\beta}$ the corresponding spectral projection.

Lemma 3. For any $0 < \beta < \hat{\beta}_0$ there exists c^2_β such that for any $\hbar > 0$,

$$\begin{aligned} \forall\, z \in \Gamma, \quad \|V^{1,2}_{i\beta} R^2_{i\beta}(z) V^{2,1}_{i\beta}\| &\leq c^2_\beta \hbar^2, \\ \forall\, k \geq 0, \quad \|V^{1,2}_{i\beta} S^{2(k)}_{i\beta} V^{2,1}_{i\beta}\| &\leq c^2_\beta \hbar^{3-k}. \end{aligned}$$

Sketch of proof: By the scaling $x \to \sqrt{\hbar} x \quad V^{1,2}_{i\beta} R^2_{i\beta}(z) V^{2,1}_{i\beta}$ is unitarily equivalent to:

$$\hbar^2 (t_{i\beta}(\hbar^{\frac{1}{2}} x)\partial_x + c.)(-e^{-i2\beta}\partial^2_x + e^{i2\beta}x^2 - \zeta)^{-1}(\partial_x t_{i\beta}(\hbar^{\frac{1}{2}} x) + c.)$$

where $c.$ means 'commutated term' and ζ belongs to the fixed compact set $\hbar^{-1}\Gamma := \{\zeta \in \mathbb{C}, |\zeta - (2n+1)| = 1\}$. The first statement follows easily by the continuity in ζ of the lhs of the formula above since $t_{i\beta}$ is bounded and ∂_x relatively bounded to $-e^{-i2\beta}\partial^2_x + e^{i2\beta}x^2$. For the derivation of the second statement we use the Cauchy formula and the same scaling trick. ∎

Thus we have obtained the stability of the resolvent set:

$$\left(0 < \beta < \hat{\beta}_0 \text{ and } 0 < \hbar < \frac{1}{c_\beta}\right) \Rightarrow \Gamma \subset \rho(H_{i\beta}), \quad c_\beta := \max\{c^1_\beta, c^2_\beta\}. \tag{1}$$

2.3 Stability of the Spectrum of H^2 and Existence of Resonances for H

The preceeding analysis proved that for $\hbar$ small enough $P_{i\beta}$, the eigenprojection of $H_{i\beta}$ associated to Γ, is well defined. This certainly remains true if one replaces W by αW with $0 \leq \alpha \leq 1$ thus defining a continuous family of projections interpolating between $P_{i\beta}\,(\alpha = 1)$ and $P^2_{i\beta}\,(\alpha = 0)$. Consequently

$$\forall\, 0 < \beta < \hat{\beta}_0,\ \forall\, 0 < \hbar < \frac{1}{c_\beta}, \quad \dim P_{i\beta} = 1.$$

Standard arguments on resonances ([RS4, Ch. XIII.10]) insure that the imaginary part of the eigenvalue associated to $P_{i\beta}$ cannot be positive. So we have proven the existence of a resonance of H close to each eigenvalue of H^2; however we cannot exclude a vanishing imaginary part of this resonance.

Remark 1. c^1_β depends only on β and S whereas c^2_β depends on β and the quantum number n of the eigenvalue e_0 of H^2. So the range of values of $\hbar$ for which the existence of the resonances is obtained depends on β, S and n.

2.4 Convergent Expansion of the Resonances

We denote by E the resonance obtained by perturbation of $e_0 = (2n+1)\hbar$. With the standard formula of regular perturbation theory [Ka, Ch.II§1] and noticing that W is off-diagonal we get:

$$E = \sum_{m=0}^{\infty} e_m, \tag{2}$$

$$
\begin{aligned}
e_m &= \frac{1}{2m}\sum_{l=0}^{m-1}\sum_{\sigma}\operatorname{tr} V^{2,1}(R^1)^{k_1}V^{1,2}(S^2)^{l_1}\dots V^{2,1}(R^1)^{k_m}V^{1,2}(S^2)^{l_m},\\
\sigma &= \{\sum l_i = l \wedge \sum k_i = 2m-1-l,\ l_i \geq 0,\ k_i \geq 1\},
\end{aligned}
$$

where we have dropped the indices $i\beta$; all the resolvents in the above formula are evaluated at $z = e_0$. Straightforward combinatorics, lemmas 2 and 3, the definition (1) of c_β and the extra condition $\hbar c_\beta < 1$ to simplify the analysis yield

$$
|e_m| \leq \frac{1}{mc_\beta}\binom{3m-2}{m-1}(c_\beta\hbar)^{2m+1}.
$$

Using the d'Alembert criterium we arrive at

theorem 4. Under hypothesis (H1,4) and for $\hbar$ small enough each eigenvalue of H^2 gives rise to a resonance of H of multiplicity one. Furthermore for all β in $(0,\hat{\beta}_0)$ let c_β be defined by (1). If $\hbar$ is in $(0,\hbar_0)$, where $\hbar_0 := \frac{2}{3\sqrt{3}}c_\beta{}^{-1}$, then the series (2) converges to this resonance.

2.5 Discussion

The method of this section follows tightly [DEŠ] with extra niceties due to the simple form of H and the fact that the perturbation is off diagonal. Also we have been able to give a critical value of $\hbar$ below which the convergence of the perturbation series is assured. c^1_β is easily estimated in terms of V^1 but for c^2_β we have only an existence result since we do not yet know how to estimate the resolvent of the harmonic oscillator scaled with a complex parameter θ and for a spectral parameter in the numerical range. Thus this critical value of $\hbar$ is for the moment merely theoretical. We stress that we do not give here expansions of the resonances in $\hbar$; Martinez [Ma1] has shown that such expansions are asymptotic, see also [CDS].

3 Fermi-Rule Contribution to the Width of the Resonance

3.1 Asymptotics of $\operatorname{Im} e_1$ as $\hbar$ Tends to Zero

Heuristic arguments [LL, §90] lead to the conclusion that the width of the resonances of H which we found in section 2 are in fact exponentially small as $\hbar$ tends to zero. As an indication of this property we compute below the asymptotics of the imaginary part of the first order coefficient in the expansion (2).

Definition 1. Each point x in $\sum_{\beta_0,\eta_0}$ which is a root of $V^1(x) = V^2(x)$ is called a *transition point*.

We shall only consider here the restricted model

$$
V^1 = v_\infty, \quad v_\infty < 0. \tag{H5}
$$

We then conclude immediately that there are two transition points

$$
x_\star := i\sqrt{-v_\infty} \quad \text{and} \quad -x_\star.
$$

The other important points are the singularities of $V^{1,2}$ or equivalently of t. We suppose

$\eta_0 > |x_\star|$ *which means that* t *is analytic beyond the transition points.* **(H6)**

Theorem 5. Under (H1,5,6) and for the resonance associated to $e_0 := (2n+1)\hbar,\ n \in I\!N$ one has

$$\operatorname{Im} e_1 = -\frac{2\sqrt{2\pi}}{n! e^{2n+1}}\hbar^2 \left(\frac{4d_\star}{\hbar}\right)^{n+\frac{1}{2}} \exp(-\frac{2d_\star}{\hbar})\{|t(x_\star)|^2 + \mathcal{O}(\hbar)\} \tag{3}$$

where

$$d_\star := \frac{-v_\infty}{2} = |\operatorname{Im} \int_0^{x_\star} \sqrt{-V^2(y)}dy|.$$

Proof: Under (H5) H^1 obviously has a pair of generalized eigenvectors at energy e_0

$$H^1\varphi^{1,\nu} = e_0\varphi^{1,\nu}, \nu = \pm 1, \quad \varphi^{1,\nu} := (2\pi\hbar)^{-\frac{1}{2}} e^{\nu i \frac{k}{\hbar}x}, k := \sqrt{e_0 - v_\infty}.$$

e_1 which is constant with respect to θ may be computed for $\theta = 0$ using the boundary value of R^1 at $e_0 + i0$. We get [RS4, XII.6]

$$\operatorname{Im} e_1 = -\frac{\pi}{2k}\sum_{\nu=\pm 1} |(V^{2,1}\varphi^{1,\nu}, \varphi^2)|^2,$$

where

$$\varphi^2(x) := \frac{C_n}{\hbar^{\frac{1}{4}}}\mathcal{P}_n(\frac{x}{\sqrt{\hbar}})e^{-\frac{x^2}{2\hbar}}, \quad C_n := \pi^{-\frac{1}{4}}(2^n n!)^{-\frac{1}{2}},$$

$\mathcal{P}_n$ being the n^{th} Hermite polynomial. One derives easily

$$(V^{2,1}\varphi^{1,\nu}, \varphi^2) = -\hbar(f\varphi^{1,\nu}, \varphi^2), \quad f := 2\nu k t + \frac{\hbar}{i}t'.$$

Since by (H6) $I\!R + i\nu k$ is in $\sum_{\beta_0,\eta_0}$, we may take it as the "contour" of integration:

$$(V^{2,1}\varphi^{1,\nu}, \varphi^2) = -\frac{C_n}{\sqrt{2\pi}}\hbar^{\frac{1}{4}} e^{-\frac{k^2}{2\hbar}} \int_{I\!R} f(x + \nu i k)\mathcal{P}_n(\frac{x + \nu i k}{\sqrt{\hbar}})e^{-\frac{x^2}{2\hbar}}.$$

It is now easy to compute the asymptotics of the last integral by first scaling x by $\sqrt{\hbar}$, then expanding

$$f(\nu ik + \sqrt{\hbar}x)\mathcal{P}_n(\frac{\nu ik}{\sqrt{\hbar}} + x) = \Big(f(\nu ik) + f'(\nu ik)\sqrt{\hbar}x\Big)\Big(\mathcal{P}_n(\frac{\nu ik}{\sqrt{\hbar}}) + \mathcal{P}_n'(\frac{\nu ik}{\sqrt{\hbar}})x\Big)$$
$$+\mathcal{O}\left(\hbar^{-\frac{n}{2}+1}(1 + |x|^{n+2})\right) \text{ (as } \hbar \to 0 \text{ and uniformly in } x),$$

and finally integrating with $e^{-\frac{x^2}{2}}$.■

3.2 Discussion

The idea of looking at the imaginary part of the first non real coefficient of the perturbation expansion (2) has a long history, see e.g. [RS4, Ya, GMS, DEŠ] not to mention the physics litterature. Methods to compute the aymptotics of $\operatorname{Im} e_1$ using the analyticity of the potential are all based more or less on the stationary phase or steepest descent methods.

However since it is expected that all coefficients of (2) will contribute to the imaginary part of the resonance E with the same exponential behavior, the prefactor of (3) has not the right asymptotics for $\operatorname{Im} E$. Such a phenomenon is discussed for example in [Be]. Below we give a classical interpretation of $d_\star$.

3.2.1 Exponential Decay of $\mathrm{Im}\, E$ and Classical Action of Instantons

The following interpretation of $d_\star$ is a well known heuristic fact (see [LL]); we would like to illustrate it in detail with our simple model.

On the complex phase space $\mathbb{C} \times \mathbb{C}$ we consider the two energy shells

$$\Sigma^{(i)}(e_0) := \{(q,p) \in \mathbb{C}, \quad H^i_{cl}(q,p) = e_0\}, \quad i = 1,2,$$

and their trace on the real phase space $\Sigma^{(i)}_{\mathbb{R}}, i = 1,2$. The two real energy shells do not intersect, but the complex ones do:

$$\begin{cases} p^2 + v_\infty &= e_0 \\ p^2 + q^2 &= e_0 \end{cases} \Longleftrightarrow \begin{cases} p &= \pm\sqrt{e_0 - v_\infty} = \pm k \\ q &= \pm i\sqrt{-v_\infty} = \pm x_\star \end{cases}$$

These points will also be called *transition points*.

We want to endow the union of the two complex energy shells $\Sigma(e_0) := \Sigma^{(1)}(e_0) \cup \Sigma^{(2)}(e_0)$ with a (pseudo-) distance δ as follows. Let A and B be two points of $\Sigma(e_0)$, then

$$A, B \in \Sigma^{(i)}(e_0) \quad \Longrightarrow \quad \delta(A,B) := |\mathrm{Im}\, s(A,B)|,$$

where $s(A,B)$ is the minimal (complex) action to join A and B by a (complex) trajectory on the energy shell $\Sigma^{(i)}(e_0)$:

$$s(A,B) := \int_{A \to B} p dq = \int_{A \to B} \sqrt{e_0 - V^i(q)} dq.$$

Such a complex trajectory is usually called an *instanton*. Otherwise,

$$\begin{aligned} & A \in \Sigma^{(i)}(e_0), \; B \in \Sigma^{(j)}(e_0), \; i \neq j, \quad \Longrightarrow \\ \delta(A,B) &:= \min\{|\mathrm{Im}\, s(A,T_\star) + \mathrm{Im}\, s(T_\star, B)|, \; T_\star \in \Sigma^{(1)}(e_0) \cap \Sigma^{(2)}(e_0)\}. \end{aligned}$$

In other words the distance $\delta(A,B)$ is the minimal imaginary part of the action of all instantons joining A and B.

We want to compute the distance between the two real energy shells: $\delta(\Sigma^{(1)}_{\mathbb{R}}(e_0), \Sigma^{(2)}_{\mathbb{R}}(e_0))$. We remark that the distance between two points of the same connected component of $\Sigma^{(i)}_{\mathbb{R}}(e_0), i = 1,2$, of course vanishes. As consequence we may take any point in each one and compute their distance. So let $A = (0,k)$ be in $\Sigma^{(1)}_{\mathbb{R}}(e_0)$ and $B = (0, \sqrt{e_o})$ be in $\Sigma^{(2)}_{\mathbb{R}}(e_0)$. We choose $T_\star = (x_\star, k)$ among the transition points. Then we have:

$$\begin{aligned} s(A,T_\star) + s(T_\star, B) &= \int_0^{x_\star} k dq + \int_{x_\star}^0 \sqrt{e_0 - q^2} dq \\ &= k x_\star + \frac{1}{2}\left[q\sqrt{e_0 - q^2} + e_0 \arcsin(\frac{q}{\sqrt{e_0}})\right]_{x_\star}^0 \\ &= i d_\star + \mathcal{O}(\hbar \ln \hbar) \end{aligned}$$

Performing the analoguous calculations for the other transition points, we see that the above result gives indeed the minimal contribution to the definition of $\delta(A,B)$. This shows that the distance between the two real energy shells is $d_\star$ in the limit $\hbar$ tending to zero. But on the other hand this is nothing else than the rate of exponential decay of the width of the resonance due to quantum dynamical tunneling between the two real energy shells. This tunneling takes place through

3.2.2 The Dynamical Barrier.

Looking at the two real energy shells in the real phase space we see three curves. $\Sigma^{(2)}_{I\!R}(e_0)$ is the circle centered at the origin with radius $\sqrt{e_0}$ and $\Sigma^{(1)}_{I\!R}(e_0)$ consists of the two straight lines $p = \pm k$. As already mentioned the curves do not intersect. More precisely their projections in the configuration space do intersect but not their projection in the momentum space. The latter are the classically allowed regions in the momentum space: $\{\pm k\}$ for H^1_{cl} and $[-\sqrt{e_0}, \sqrt{e_0}]$ for H^2_{cl}. They are separated by the classically forbidden region: $(-k, -\sqrt{e_0}) \cup (\sqrt{e_0}, k)$. In analogy with tunneling in the configuration space we would like to say that associated to this classically forbidden region there is a *dynamical barrier*. And through this barrier the bound state of H^2 has to tunnel to become a scattering state of H^1. The strength of this tunneling, as in the configuration space, depends on the diameters of the dynamical barriers. These are measured by the length of each component of the classically forbidden region in the *instanton metric*:

$$\Big((V^2)^{-1}(p^2 - e_0)\Big)^2_+ dp^2 = (p^2 - e_0)_+ dp^2. \tag{4}$$

Computing this diameter for the barrier of the positive momenta we obtain

$$\int_{\sqrt{e_0}}^{k} \sqrt{(p^2 - e_0)_+}dp = d_\star + \mathcal{O}(\hbar \ln \hbar)$$

which is in agreement with the result of theorem 5. The reason why V^1 does not enter in formula (4) is due to the fact that the instanton joining A and $T_\star$ has a constant velocity.

4 Exponential Bounds on the Resonance Width

We recall that in section 2 we proved that H possesses a resonance E in the vicinity of each eigenvalue e_0 of H^2 for small enough $\hbar$. In section 3, for the restricted model $V^1 = v_\infty$ (see H5), we have shown that the imaginary part of the first term e_1 of the perturbation expansion (2) of $E - e_0$ is actually exponentially small as $\hbar$ tends to zero. The purpose of this section is to show that this exponential behavior is also true for the full width of the resonance E.

For technical reasons we have to require the following additional condition on the coupling term $V^{1,2}$:

$$\exists \varepsilon > 0, \quad t(z) = \mathcal{O}(|z|^{-\varepsilon}) \textit{ as } z \textit{ tends to infinity in } \textstyle\sum_{\beta_0,\eta_0}, \tag{\textbf{H7}}$$

to state our main

theorem 6. Assume (H1,5,6,7). Then each eigenvalue e_0 of H^2 gives rise for $\hbar$ small enough to a resonance E of H and:

$$\forall 1 \geq \xi > 0, \quad 0 \geq \operatorname{Im} E = \mathcal{O}(\xi^{-2}\hbar \exp(-\frac{2d_\xi}{\hbar})) \quad \text{as } \hbar \to 0,$$

where

$$d_\xi := \int_0^{|x_\star|} \sqrt{(V^2(y) - e_0 - \hbar\xi)_+}dy.$$

Remark 2. Since the lifetime τ_E of the resonance E is defined as $\frac{2}{\operatorname{Im} E}$, the above theorem provides a lower bound on τ_E.

One can check easily that

$$\xi^{-2}\hbar e^{-2\hbar^{-1}d_\xi} = \mathcal{O}(\xi^{-2}\hbar^{-n+(1-\xi)/2}e^{-2\hbar^{-1}d_\star}).$$

This shows that the exponential behaviour of the bound of theorem 6 is the same as the one of $\operatorname{Im} e_1$ (see (3)). However the exponent in the prefactor differs by the quantity $-1-\frac{\xi}{2}$. We do not know yet whether the $\hbar$ behavior of the prefactor of $\operatorname{Im} e_1$ differs from the one of $\operatorname{Im} E$ or if our upper bound is not optimal.

Since the proof is rather involved we only give a synopsis of it. The details of the proof will appear somewhere else together with a more general analysis including non constant V^1's.

4.1 Passing to the Fourier Image

As we explained in §3.2, the exponential behaviour of the width of the resonance E is due to tunneling through the barrier of classically forbidden momenta between the two energy shells $\Sigma_{I\!R}^{(1)}(e_0)$ and $\Sigma_{I\!R}^{(2)}(e_0)$.

A Fourier transformation of H causes the exchange of q and p in the classical picture. Consequently the tunneling takes now place in the configuration space, a situation we are more familiar with. We denote below by the same symbols the Fourier image of $H^i, i=1,2$ and $V^{1,2}$:

$$H^1 = x^2 + v_\infty, \quad H^2 = D^2 + x^2, \quad V^{1,2} = \hbar(t(D)x + xt(D)).$$

The price to pay is that we have to deal with non local operators as, e.g. $t(D)$ (see §4.5 below). We emphasize that this transformation is only for convenience and in principle not necessary.

4.2 Why Exterior Scaling?

Consider now (E, ϕ_θ) a resonance and the corresponding resonance function: $H_\theta\phi_\theta = E\phi_\theta$. By a simple algebraic manipulation one also has

$$(H_\theta^2 - B_\theta)\phi_\theta^2 = E\phi_\theta^2, \quad B_\theta := V_\theta^{2,1}R_\theta^1(E)V_\theta^{1,2},$$

where ϕ_θ^i denotes the i^{th} component of ϕ_θ. Thus

$$\operatorname{Im} E\|\phi_\theta^2\|^2 = (\operatorname{Im}(H_\theta^2 - B_\theta)\phi_\theta^2, \phi_\theta^2). \tag{5}$$

In section 2 we have seen that ϕ_θ and therefore ϕ_θ^2 "converge" in norm to φ_θ^2, the corresponding eigenfunction of H_θ^2. The latter is of course known to decay exponentially as x goes to infinity and/or $\hbar$ tending to zero. So suppose that the operator $\operatorname{Im}(H_\theta^2 - B_\theta)$ is localized on Ω_e where

$$\Omega_i := (-\omega, \omega), \quad \Omega_e := I\!R \setminus \overline{\Omega}_i, \quad \omega^2 = -v_\infty,$$

we would obtain that $\operatorname{Im} E$ is roughly $\|\chi_e\phi_\theta^2\|^2 \sim e^{-\hbar^{-1}\omega^2}$ which is more or less what we are looking for. χ_a will denote the sharp characteristic function of $\Omega_a, a = i, e$. Ω_i is nothing but the dynamical barrier for $\hbar = 0$ (see §3.2.2). With the usual complex scaling $\operatorname{Im}(H_\theta^2 - B_\theta)$ is certainly not localized in Ω_e, whereas $\operatorname{Im} H_\theta^2$ would be with the exterior scaling

$$s_\theta(x) := \begin{cases} x & \text{if } \ x \in \Omega_i \\ \pm\omega + e^\theta(x \mp \omega) & \text{if } \ \pm x > \omega. \end{cases} \tag{6}$$

Thus in this section we choose the above complex exterior scaling to deform all our operators; a subscript θ will now mean the image under (6).

It is well known that the resonances of H do not depend on the choice of the complex deformation (see e.g. [Hu]). Here they will be considered as eigenvalues of H_θ for a certain complex θ where, as announced above, H_θ is now obtained by (6). Making sense out of all our scaled objects is rather standard (see e.g [CDKS]) except for the non local terms $V_\theta^{1,2}$ and B_θ. We shall explain briefly in §4.5 how we proceed. We have in particular the analogue of theorem 1:

theorem 7. $H_\theta^i, i = 1, 2$ and H_θ are selfadjoint analytic families for all θ such that $|\mathrm{Im}\,\theta| < \hat{\beta}_0$. H_θ^1 is of type A with domain $\mathcal{D}(H_\theta^1) = \mathcal{D}(x^2)$. The domain of H_θ^2 is given by

$$u \in \mathcal{D}(H_\theta^2) \iff \begin{array}{l} u \in \mathcal{H}^2(\Omega_i) \oplus \mathcal{H}^2(\Omega_e) \text{ and} \\ u(\pm\omega \pm 0) = e^{\theta/2} u(\pm\omega \mp 0) \\ u'(\pm\omega \pm 0) = e^{3\theta/2} u'(\pm\omega \mp 0). \end{array}$$

4.3 Spectral Stability Again

We shall need in the sequel information on the spectrum of H_θ^d and some bounds on its resolvent. Since H_θ^1 is a multiplication operator its spectrum is nothing but the range of the function $x \mapsto v_\infty + s_\theta^2(x)$. There are two facts to remark here. First the spectrum of H_θ^1 consists of the union of the interval $[v_\infty, 0]$ and a curve starting from zero, contained in the sector $\{|\mathrm{Im}\,\theta| < \mathrm{sgn}(\mathrm{Im}\,\theta) \arg(z) < 2|\mathrm{Im}\,\theta|\}$; secondly the essential spectrum of H^1 above zero turns up in the upper half plane, if $\mathrm{Im}\,\theta > 0$. In order to work with the resonances which have a negative imaginary part we shall from now on take only θ with negative imaginary part. The spectrum of H_θ^2 remains $(2\mathbb{N} + 1)\hbar$ by standard arguments. So for small enough $\hbar$ the same contour Γ as in §2 is contained in the resolvent set of H_θ^d. To prove that it lies also in $\rho(H_\theta)$ we need the

lemma 8. For any $0 < |\beta| < \hat{\beta}_0$ and for any z on Γ one has
i) $\|V_{i\beta}^{1,2} R_{i\beta}^2(z) V_{i\beta}^{2,1}\| = \mathcal{O}(\hbar^2)$.
ii) $\|R_{i\beta}^1(z)\|, \|x R_{i\beta}^1(z)\|, \|x R_{i\beta}^1(z) x\|$ are all $\mathcal{O}(\hbar^{-1})$; this is also valid for z inside Γ.

Thus stability of e_0 is assured for $\hbar$ small enough.

4.4 Estimate of $(\mathrm{Im}\,(H_\theta^2 \phi_\theta^2, \phi_\theta^2)$

We want to show that $(\mathrm{Im}\,(H_\theta^2 \phi_\theta^2, \phi_\theta^2)$ is exponentially small using the decay properties of ϕ_θ^2 and the localisation of $\mathrm{Im}\,H_\theta^2$. The following estimate is adapted from [Agm]. However there is a novelty with respect to the standard situation: the operator $H_\theta^2 - B_\theta$ contains the non local energy dependent "potential term" B_θ. Let $\exp(-\hbar^{-1}\rho)$ be the expected decay behavior and let $\phi_{\theta,\rho}^2 := \exp(\hbar^{-1}\rho)\phi_\theta^2$ be the boosted eigenfunction; more generally we denote all objects boosted by $\exp(\hbar^{-1}\rho)$ with the subscript ρ. $\phi_{\theta,\rho}^2$ is a solution of $(H_{\theta,\rho}^2 - B_{\theta,\rho} - E)\phi_{\theta,\rho}^2 = 0$ and therefore

$$\mathrm{Re}\,((H_{\theta,\rho}^2 - B_{\theta,\rho} - E)\phi_{\theta,\rho}^2, \phi_{\theta,\rho}^2) = 0.$$

To cope with the $B_{\theta,\rho}$ problem we use the following property

lemma 9. Assume (H6), then there exists $a, b > 0$ such that for any $0 < |\mathrm{Im}\,\theta| < \hat{\beta}_0$ and any real Lifschitz function ρ one has:

$$\rho'^2 \leq \omega^2 \chi_i \quad \Longrightarrow \quad -\mathrm{Re}\, B_{\theta,\rho} \geq -a\hbar \mathrm{Re}\, x_\theta^2 - b\hbar^3.$$

¿From this result we deduce that

$$\hbar^2 \| s_\theta'^{-\frac{1}{2}} \partial_x \phi^2_{\theta,\rho} \|^2 + \Big(((1-a\hbar)\mathrm{Re}\, x_\theta^2 - b\hbar^3 - \mathrm{Re}\, E - \rho'^2) \phi^2_{\theta,\rho}, \phi^2_{\theta,\rho} \Big) \leq 0.$$

This motivates the choice of ρ:

$$\rho'^2 := \Big((1-a\hbar)x^2 - b\hbar^3 - \mathrm{Re}\, E - \hbar\xi \Big)_+ \chi_i, \quad \xi > 0,$$

and we obtain the

lemma 10. For any $0 < |\mathrm{Im}\,\theta| < \hat{\beta}_0$ one has as $\hbar$ tends to zero and for any $0 < \xi \leq 1$:

$$\|\phi^2_{\theta,\rho}\| = \mathcal{O}(\xi^{-\frac{1}{2}}), \quad \|\chi_e x \phi^2_{\theta,\rho}\| = \mathcal{O}(\hbar^{\frac{1}{2}}), \quad \hbar \|\chi_e \partial_x \phi^2_{\theta,\rho}\| = \mathcal{O}(\hbar^{\frac{1}{2}}).$$

We can now estimate $\mathrm{Im}\,(H^2_\theta \phi^2_\theta, \phi^2_\theta)$:

$$\begin{aligned}
\mathrm{Im}\,(H^2_\theta \phi^2_\theta, \phi^2_\theta) &= \mathrm{Im}\,(e^{-\hbar^{-1}\rho} H^2_\theta e^{-\hbar^{-1}\rho} \phi^2_{\theta,\rho}, \phi^2_{\theta,\rho}) \\
&= e^{-2\hbar^{-1}\rho(\omega)} (\mathrm{Im}\, H^2_\theta \phi^2_{\theta,\rho}, \phi^2_{\theta,\rho}) = \mathcal{O}(\hbar e^{-2\hbar^{-1}\rho(\omega)}).
\end{aligned}$$

An elementary calculus shows that $e^{-2\hbar^{-1}\rho(\omega)} = \mathcal{O}(e^{-2\hbar^{-1}d_\xi})$ so that this term has the announced behavior. It remains to do the

4.5 Estimate of $\mathrm{Im}\,(B_\theta \phi^2_\theta, \phi^2_\theta)$.

We start by explaining how we make sense out of B_θ. We may write formally

$$B_\theta = -\hbar^2 (2t(D_\theta)x_\theta + i\hbar t'(D_\theta)) R^1_\theta(E) (2x_\theta t(D_\theta) - i\hbar t'(D_\theta)).$$

The operator x_θ is controlled by $R^1_\theta(E)$ (see lemma 8) so it is sufficient to show that $t(D_\theta)$ and $t'(D_\theta)$ are bounded operators. D_θ is the image of D under our exterior scaling for which we know the

theorem 11. $\{D_\theta, \theta \in \mathbb{C}\}$ is a selfadjoint analytic family of operators and:
i) the domain of D_θ is defined by

$$\mathcal{D}(D_\theta) \ni u \iff \begin{array}{l} u \in \mathcal{H}^1(\Omega_i) \oplus \mathcal{H}^1(\Omega_e) \text{ and} \\ u(\pm\omega \pm 0) = e^{\theta/2} u(\pm\omega \mp 0); \end{array}$$

ii) the spectrum of D_θ is just: $\sigma(D_\theta) = e^{-\theta}\mathbb{R}$.
iii) The following resolvent estimate holds: let $\nu := \{z \in \mathbb{C},\ \mathrm{Im}\, s'_\theta z > 0 \text{ or } \mathrm{Im}\, s'_\theta z < 0\}$; then for every z in ν, one has

$$\|(D_\theta - z)^{-1}\| \leq |\mathrm{Im}\, s'_\theta z|^{-1} = \mathrm{dist}(z, \mathbb{C} \setminus \nu)^{-1}.$$

To define $t(D_\theta)$ we use the Dunford-Taylor integral

$$t(D_\theta) := \frac{1}{2\pi i} \int_C t(\lambda)(D_\theta - \lambda)^{-1} d\lambda, \quad |\mathrm{Im}\,\theta| < \hat{\beta}_0$$

where the contour C is taken in $\nu \cap \sum_{\beta_0,\eta_0}$ enclosing $\sigma(D_\theta)$ and such that $\mathrm{dist}(C,\nu)^{-1} = \mathcal{O}(\lambda^{-1})$ as $|\lambda|$ tends to infinity. The convergence of the above integral is due to (H7) and lemma 11 iii). Furthermore we know that

lemma 12. $t(D_\theta), t'(D_\theta)$ are bounded selfadjoint analytic families as long as $|\mathrm{Im}\,\theta| < \hat{\beta}_0$.

We now explain how one can define $B_{\theta,\rho}$. Using the same strategy as for B_θ and the fact that the boost $e^{\hbar^{-1}\rho}$ commutes with x_θ and $R^1_\theta(E)$, it suffices to show that $t(D_{\theta,\rho})$ and $t'(D_{\theta,\rho})$ are bounded. One can show the analogue of theorem 11 and lemma 12 for them. Moreover $t(D_{\theta,\rho})$ and $t'(D_{\theta,\rho})$ are uniformly bounded with respect to ρ as long as ρ obeys: $\rho'^2 \leq \omega^2\chi_i$. Here one must use assumption (H6). By a straightforward though rather involved algebraic calculus one gets a reformulation of (5)

$$\mathrm{Im}\,E(\|\phi_\theta\|^2 + (1 - e^{-2\hbar^{-1}\rho(\omega)})\|\phi^1_{\theta,\rho}\|^2) = e^{-2\hbar^{-1}\rho(\omega)}\mathrm{Im}\,((H^2_\theta - B_{\theta,\rho})\phi^2_{\theta,\rho}, \phi^2_{\theta,\rho}). \tag{7}$$

One has the estimate

$$\|\phi^1_{\theta,\rho}\|^2 = \|R^1_\theta(E)V^{1,2}_{\theta,\rho}\phi^2_{\theta,\rho}\|^2 = \mathcal{O}(\xi^{-1}),$$

(use lemma 8, 12 and 10). Finally one also has

$$(B_{\theta,\rho}\phi^2_{\theta,\rho}, \phi^2_{\theta,\rho}) = \mathcal{O}(\hbar\xi^{-1}).$$

Inserting this estimate and the one of §4.4 in (7) completes the proof of theorem 6.

4.6 Discussion

The use of a complex deformation in the momentum space leaving invariant $\Omega_{i,\varepsilon} := \{p \in I\!R, |p| < \omega - \varepsilon\}, \varepsilon$ small, i.e. a region which contains approximately the dynamical barrier (see §3.2.2), was brought to our attention by M. Rouleux. In his notes [Ro] he combines this idea with the Green's formula

$$2\ \mathrm{Im}\,E \int_{\Omega_{i,\varepsilon}} |\phi(x)|^2 dx = -\hbar^2 \mathrm{Im}\,\phi'\overline{\phi}\Big|_{\partial\Omega_{i,\varepsilon}}; \tag{8}$$

as above ϕ stands here for the Fourier image of the original ϕ.

The last ingredient to get the asymptotics of $\mathrm{Im}\,E$ would be the knowledge of the behavior of the r.h.s. of (8) since obviously the norm of ϕ on $\Omega_{i,\varepsilon}$ is $1 + o(1)$ as $\hbar$ tends to zero.

The idea of using the Green's formula can be traced back to Herring [Her] through e.g. [HeSj, AsHa, W].

The first idea, the exterior complex deformation, is now rather standard when translated to the shape resonance framework (see e.g. [CDKS, HeSj]).

The choice of $\Omega_{i,\varepsilon}$ with a non zero ε is a consequence of the use of a smooth exterior distortion. Here we hope to get immediately the right exponential decay rate by employing an exterior scaling (§4.2).

Also instead of the Green's formula (8) we use a full L^2 calculus (5). With (5) we need only L^2-exponential decay estimates on ϕ (see §4.4,5) which are simpler to derive than the pointwise estimates needed in (8). However by using this L^2 approach we are forced to loose a little bit of the exponential decay rate; the correct one being given by d_ξ with $\xi = 0$ (see theorem 6).

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