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RESONANT STATES FOR A THREE-BODY PROBLEM UNDER AN EXTERNAL FIELD

V. GRECCHI, H. KOVAŘÍK, A. MARTINEZ, A. SACCHETTI, AND V. SORDONI

ABSTRACT. Here we consider one of the basic models for many-body problems under an external field: the molecule ion H_2^+ under the effect of an external Stark-type potential. If we consider the vibrational energy levels of the first two electronic states of the molecule ion H_2^+ then, in the semiclassical limit and by means of a suitable modified Born-Oppenheimer method, we can prove that they switch to sharp resonances localized in the same interval of energy of the vibrational levels when an external Stark-type field, with the same direction of the nuclear axis, occurs.

In Memory of Pierre Duclos

1. INTRODUCTION

In this paper we consider the spectral problem of the Hamiltonian operator

$$H = -h^2 \Delta_{\mathbf{R}} + \frac{1}{R} + H_e \tag{1}$$

where $h^2 \ll 1$ is a semiclassical parameter, and H_e is the so-called *electronic Hamiltonian*, formally defined on $L^2(\mathbb{R}^3_r)$ as

$$H_e := H_e(\mathbf{R}) = -\Delta_{\mathbf{r}} - \frac{1}{|\mathbf{r} - \frac{1}{2}\mathbf{R}|} - \frac{1}{|\mathbf{r} + \frac{1}{2}\mathbf{R}|} + V, \qquad (2)$$

where V is an external potential. It is well known (see [HMS] and the references therein) that when V is a Stark potential then the spectrum of H is absolutely continuous. Here, we'll prove that the stable state of the unperturbed many-body problem turn into resonances when an external Stark-type potential is introduced. The Hamiltonian operator (1) is usually associated with the dynamics of the three particle system called molecule-ion H_2^+ , referred to its center of mass, and under the effect of an external homogeneous field; $h \ll 1$ is the effective semiclassical parameter given by the square root of the ratio between the light mass of the electron e and the heavy mass (when compared with the electron mass) of the hydrogen nuclei, **R** is the relative position of the two hydrogen nuclei of H_2^+ , and, for the sake of definiteness, we assume that the units are such that the electron charge is 1. The electronic Hamiltonian (2) describes the relative motion of the electron *e* referred to the *fixed* nuclei, and it actually depends on the nuclear distance R, where V is the potential of the external force. Up to now, this problem has been treated by many authors in a heuristic way in the coaxial case where the external field and the nuclear axis of the molecule have same direction [Ca, Hi, MPS]. This

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attitude is justified since, in such a case, the effect of the external field on the diatomic molecule is the strongest one. In fact, in this paper we adopt such an assumption (see Hyp. 1).

Because of the heavy mass of the nuclei, at a first stage it is possible to consider the position of the nuclei as fixed, in order to determine the electronic states. This approach is known as the Born-Oppenheimer's one [BoOp, KMSW]. The first two levels of the electron, $E_1(R)$ of the state $1\sigma_g$ and $E_2(R)$ of the state $1\sigma_u$, as functions of the nuclear distance R, contribute to the effective potentials used for the determination of the nuclear dynamics. Such behavior of the electronic levels are well known by the explicit asymptotic expansions for large R [Ci] and their distributional Borel sums [CGM, GG, LiSi] and it is a reasonable hypothesis that each effective potential function, $W_j(R) = (1/R) + E_j(R)$, j = 1, 2, has only one minimum point where a certain number of nucleonic states are trapped, identified with the first vibrational energy levels of the molecule.

The operator (1) acts on the Hilbert space of square integrable sections in the trivial fiber bundle

$$\mathcal{K} = L^2(\mathbb{R}^3_{\mathbf{R}}; L^2(\mathbb{R}^3_{\mathbf{r}})) \,.$$

In this picture the operator H decomposes into two terms. The first one, the nuclear kinetic energy, acts on the base space. The second one operates on the fiber only,

$$\tilde{H}_e = \int^{\oplus} H_e(\mathbf{R}) d\mathbf{R} \,,$$

where $H_e(\mathbf{R})$ is the electronic Hamiltonian for fixed \mathbf{R} . The small parameter h allows the use of semiclassical approximation. For our purposes, the second order is enough.

Under some reasonable assumptions on the problem, we prove (see Theorem 7.1) the existence of resonances. Resonances are defined as complex eigenvalues of a distorted Hamiltonian; it is worth pointing out that our definition of resonances includes, as a special case, the notion of embedded eigenvalues where the imaginary part is exactly zero (actually, with similar techniques it can be proved that the absolute value of the imaginary part of the resonances considered in this paper are exponentially small with respect to the semiclassical parameter h defined below). Finally, our result still holds true even in absence of the external field; in such a case we do not need to define the distorted Hamiltonian and we simply have discrete eigenvalues instead of resonances.

Let us also observe that H_e is not simply a multiplication operator, and for this reason we use the pseudo-differential calculus with operator valued symbols. In that way, by the so-called Grushin-Feshbach method, we can translate the eigenvalue problem for H into that of inverting a 2 × 2 matrix operator. This method has become a standard way for defining and computing a finite number of expected eigenvalues [KMSW]. Moreover we define the spectral projector $\Pi_e(\mathbf{R})$ of $H_e(\mathbf{R})$ up to a fixed value of the energy, so that,

$$\Pi = \int^{\oplus} \Pi_e(\mathbf{R}) d\mathbf{R} \,,$$

is a projector on the molecular space \mathcal{K} . The lower part of the spectrum of the compressed operator $\Pi H \Pi$ is expected near of part of the spectrum of H. The

eigenvalues are given by the generalized eigenvalues, $Q(E)\psi = E\psi$, where Q(E) is the Feshbach operator,

$$Q(E) = \Pi H \Pi - \Pi H (\Pi^{\perp} (H - E)^{-1}) \Pi^{\perp} H \Pi.$$

Furthermore, a smooth relationship, with respect to \mathbf{R} , is requested between the first eigenvectors of $H_e(\mathbf{R})$ and the corresponding final generalized eigenvectors of the Feshbach operator.

We also use the theory of the twisted pseudo-differential operators introduced in [MaSo]. The theory of pseudo-differential operators goes back to the quantization rule of Hermann Weyl and is now well established [Ro, Ma1]. The recent theory of twisted pseudo-differential operators [MaSo] is a formalization and extension of the method of regularization going back to Hunziker [Hu, KMSW]. This theory is able to regularize the Coulomb singularity of the nuclei-electrons potentials of the interaction.

The paper is organized as follows.

In Section 2 we introduce the model and we state our main assumptions.

In Section 3 we consider the analytic distortion and regularization of the operator. Analytic distortion is a standard way to define resonances [BCD]. Because of the singularity of the Coulomb potential we have to regularize our effective Hamiltonian. If we denote by \tilde{H}_{μ} (μ is the complex distortion constant) the regularized operator then we see (see Theorem 3.8) that part of its spectrum coincides with the spectrum of a reduced problem denoted by \tilde{P}_{μ} . The reduced problem consists of two coupled Schrödinger operator.

In Section 4 we study the spectrum of the reduced problem denoted by P^{\sharp}_{μ} , which coincides with \tilde{P}_{μ} up to a bounded operator with norm less that Ch^2 for some C > 0. We separately consider the spectrum associated to first level alone, and the part of the spectrum located in the bottom of the second level.

In Section 5 we compare the spectrum of the two operators P^{\sharp}_{μ} and \tilde{H}^{0}_{μ} , where \tilde{H}^{0}_{μ} is the restriction of the regularized and distorted operator on the eigenspace of the vibrational spectrum.

In Section 6 we compare the spectrum of the two operators \tilde{H}^0_{μ} and H^0_{μ} , where H^0_{μ} is the restriction of the distorted operator on the eigenspace of the vibrational spectrum.

In Section 7 we finally state our main results.

1.1. Notations. Here we list the main notations, meaning $j \in \{1, 2\}$:

- H denotes the Hamiltonian operator (1);
- H_e denotes the electronic Hamiltonian operator (2) with eigenvalues $\mathcal{E}_j(R)$ depending on R;
- $\mathcal{H}_0 = Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})$ where $\mathbf{L}_{\mathbf{R}}$ and $\mathbf{L}_{\mathbf{r}}$ respectively denote the angular momentum with respect to the variables \mathbf{R} and \mathbf{r} ;
- $W_j(R) = \frac{1}{R} + \mathcal{E}_j(R)$ denotes the effective potential;
- m_1 and m_2 respectively are the non degenerate minima of $W_1(R)$ and $W_2(R)$ at $R_{1,m}$ and $R_{2,m}$, M_1 is the non degenerate maximum of $W_1(R)$ at $R_{1,M}$ (see Remark 2.3);
- P_j is the operator formally defined by

$$-h^2\frac{d^2}{dR^2} + W_j(R)$$

on $L^2(\mathbb{R}, dR)$ with Dirichlet boundary conditions at R = 0;

- S_{μ} denotes the analytic distortion operator (14);
- H_{μ} and $H_{\mu,e}$ denote the distorted operators

$$H_{\mu} = \mathcal{S}_{\mu} H \mathcal{S}_{\mu}^{-1}$$
 and $H_{\mu,e} = \mathcal{S}_{\mu} H_e \mathcal{S}_{\mu}^{-1}$;

- $H_{\mu,e}$ is the regularization of $H_{\mu,e}$ as defined in Proposition 3.4;
- \widetilde{H}_{μ} is the regularization of H_{μ} as defined in Definition 3.5;
- H^0_μ and \widetilde{H}^0_μ respectively are the restriction of H_μ and \widetilde{H}_μ to the invariant subspace $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}});$
- P^{\sharp}_{μ} is the reduced problem defined by equation (30) on the Hilbert space

$$\mathcal{H}^{\sharp} = L^2\left([0, +\infty), dR\right) \oplus L^2\left([0, +\infty), dR\right)$$

with Dirichlet boundary conditions at R = 0;

- $P_{j,\mu}$ is the operator formally defined by

$$h^2 \mathcal{S}_\mu \mathrm{D}_R^2 \mathcal{S}_\mu^{-1} + W_{j,\mu}(R)$$

on $L^2(\mathbb{R}, dR)$ with Dirichlet boundary conditions at R = 0, where D_R and $W_{j,\mu}$ are defined at the beginning of §4;

- P_D^{\sharp} is the Dirichlet realization of P_0^{\sharp} on the interval $[0, R_{1,M}]$; $\widetilde{P}_{\mu}^{\sharp}$ and \widetilde{P}_j are respectively obtained by P_{μ}^{\sharp} and P_j by substituting \widetilde{W}_j to \dot{W}_j , that is we "fill the well";
- $\widetilde{P}^0_{\mu}(z)$ is the restriction of $\widetilde{P}_{\mu}(z)$, defined by equation (23), to $Ker(\mathbf{L}_{\mathbf{R}})$;
- when this fact does not cause misunderstanding $\|\cdot\|$ denotes the usual norm on the Hilbert space L^2 or the norm of linear operators defined on the Hilbert space L^2 .

2. The model

2.1. The three-body problem. The analysis of the three-body problem (1) is a very difficult task and we have to introduce here some suitable assumptions.

Hypothesis 1. We assume that the potential V only depends on the component of the vector \mathbf{r} along the direction \mathbf{R} ; that is

$$V(\mathbf{R}, \mathbf{r}) = \chi\left(\left\langle \frac{\mathbf{R}}{R}, \mathbf{r} \right\rangle\right), \quad R = |\mathbf{R}|, \quad (3)$$

where χ is a real-valued function bounded from below. The function χ admits an analytic extension in a complex strip containing the real axis.

That is, following [Hi, MuSh], we consider the case where the external field is a Stark-like field directed along the axes of the two nuclei and where, for instance, the function χ has the form

$$\chi(x) = \chi_d(x) = \nu \frac{x}{\sqrt{1 + (x/d)^2}} = \frac{d\nu}{\sqrt{1 + (d/x)^2}}$$
(4)

where d > 0 is a parameter much larger than the molecular diameter. Under Hypothesis 1 the Hamiltonian H commutes with the angular momentum $L_R + L_r$.

Remark 2.1. Given a rotation O in \mathbb{R}^3 , let us consider the unitary operators S_O and T_O on $L^2(\mathbb{R}^3_{\mathbf{R}})$ and $L^2(\mathbb{R}^3_{\mathbf{R}}) \otimes L^2(\mathbb{R}^3_{\mathbf{r}})$ respectively, given by,

$$S_O\phi(\mathbf{R}) = \phi(O\mathbf{R}), \quad \forall \phi \in L^2(\mathbb{R}^3_{\mathbf{R}})$$

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$$T_O := S_O \otimes S_O, \quad T_O \psi(\mathbf{R}, \mathbf{r}) = \psi(O\mathbf{R}, O\mathbf{r}), \quad \forall \psi \in L^2(\mathbb{R}^3_{\mathbf{R}}) \otimes L^2(\mathbb{R}^3_{\mathbf{r}})$$

Then H commutes with T_O , i.e. $T_OH = HT_O$ and therefore, the spectrum of the electronic Hamiltonian operator $H_e(\mathbf{R})$ depends only on $R := |\mathbf{R}|$.

Remark 2.2. Now, let us denote by L_R and L_r the angular momentum with respect to the variables R and r respectively. By the previous remark, we see that we have,

$$[H, \mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}] = 0. \tag{5}$$

In the sequel, we will be particularly interested on the eigenvalues and resonances of the restriction of H to the invariant subspace

$$\mathcal{H}_0 := Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}).$$

This somehow corresponds to fix to 0 the rotational energy of the molecule. As we will see, after the Born-Oppenheimer reduction to an effective Hamiltonian $P = P(\mathbf{R}, hD_{\mathbf{R}})$, this is equivalent to study the restriction of P to $Ker(\mathbf{L}_{\mathbf{R}})$. Therefore, this will also permit us to reduce the study to a one-dimensional operator.

2.2. Effective Potential. For any fixed $\mathbf{R} \in \mathbb{R}^3$, we denote by $\operatorname{Sp}(H_e(\mathbf{R}))$ the spectrum of the electronic Hamiltonian operator $H_e(\mathbf{R})$ defined on the Hilbert space $L^2(\mathbb{R}^3_r)$. This spectrum actually depends on R (see Remark 2.1) and we assume that

Hypothesis 2. The discrete spectrum of the electronic Hamiltonian operator $H_e(\mathbf{R})$ contains at least two eigenvalues, and the first two eigenvalues $\mathcal{E}_1(R)$ and $\mathcal{E}_2(R)$ are non degenerate, extend holomorphically to complex values of R in a domain of the form $\Gamma_{\delta} := \{R \in \mathbb{C} ; \operatorname{Re} R \geq \delta^{-1}, |\operatorname{Im} R| < \delta \operatorname{Re} R\}$ with $\delta > 0$ constant, and are such that,

$$\lim_{|R| \to +\infty, R \in \Gamma_{\delta}} \mathcal{E}_j(R) = \mathcal{E}_j^{\infty},\tag{6}$$

where,

$$\mathcal{E}_1^{\infty} < \mathcal{E}_2^{\infty} \,. \tag{7}$$

Furthermore, there is a gap between $\mathcal{E}_j(R)$, j = 1, 2, and the remainder of the spectrum:

$$\inf_{R>0} \operatorname{dist} \left[\left\{ \mathcal{E}_1(R), \mathcal{E}_2(R) \right\}, \mathcal{E}_3(R) \right] \ge C$$

for some positive constant C > 0, where

$$\mathcal{E}_3(R) = \{ \text{Sp}(H_e(\mathbf{R})) - \{ \mathcal{E}_1(R), \mathcal{E}_2(R) \} \},\$$

Remark 2.3.

We observe that, for any rotation O in \mathbb{R}^3 , one has (with obvious notations),

$$H_e(O\mathbf{R}, O\mathbf{r}, O^{-1}D_\mathbf{r}) = H_e(\mathbf{R}, \mathbf{r}, D_\mathbf{r}), \quad D_\mathbf{r} = -i\nabla_\mathbf{r}.$$

As a consequence, the first two normalized eigenfunctions

$$H_e(\mathbf{R})\,\psi_j(\mathbf{r},\mathbf{R}) = \mathcal{E}_j(R)\,\psi_j(\mathbf{r},\mathbf{R})\,,\ j = 1,2\,.$$
(8)

can be taken real-valued and verify $\psi_i(O\mathbf{R}, O\mathbf{r}) = \psi_i(\mathbf{R}, \mathbf{r})$, and thus

$$(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})\psi_j = 0. \tag{9}$$

We also denote by,

$$W_j(R) = \frac{1}{R} + \mathcal{E}_j(R), \ j = 1, 2,$$

the effective potential associated with the j-th eigenvalue. By Hypothesis 2 we observe that the effective potential satisfies to the following properties

- (1) The effective potentials $W_i(R)$, j = 1, 2, are analytic functions;
- (2) There exists a positive constant C > 0 such that

$$\inf_{R>0} [W_3(R) - W_2(R)] \ge C$$

where $W_3 = \frac{1}{R} + \inf [\mathcal{E}_3(R)].$ (3) The following limits hold true

$$\lim_{R \to 0^+} W_j(R) = +\infty, \ j = 1, 2$$

Here, we introduce the following assumptions on the effective potentials $W_1(R)$ and $W_2(R).$

Hypothesis 3. The effective potential W_1 has a single well shape, with local nondegenerate minimum value m_1 at some point $R_{1,m}$, with a barrier with local nondegenerate maximum value M_1 at some point $R_{1,M}$; beside, W_1 does not admit other critical points in the domain $W_1^{-1}([m_1, M_1])$. The effective potential W_2 has a single well shape, with local minimum value m_2 at some point $R_{2,m} > R_{1,m}$.

Remark 2.4. In absence of the external field the local maximum value M_1 disappears and we only have two local minimum values [Ci], in such a case $\mathcal{E}_1^{\infty} = \mathcal{E}_2^{\infty}$ and we could treat the spectral problem for eigenvalues belonging to the interval $[m_1, M_1]$, for any $M_1 < \mathcal{E}_1^{\infty}$. If the external field, with potential satisfying Hyp.1 and eq. (4), is small enough, but not zero, then we expect to observe a local maximum value such that $m_1 < m_2 < M_1$ and $R_{1,m} < R_{2,m} < R_{1,M}$ as in Fig. 1. For increasing external field, as considered by [MuSh], can happen to have $m_1 < M_1 < m_2.$

Remark 2.5. The asymptotic behavior for large R of the functions $W_i(R)$ is dominated by the Van der Waals force given by,

$$W_j(R) = -\frac{c_4}{R^4} + O(R^{-6}), \ W'_j(R) = 4\frac{c_4}{R^5} + O(R^{-7}), \ j = 1, 2,$$

for a constant $c_4 > 0$ (see the constant $E^{(4)}$ of [Ci]). The energy binding of the molecule, $\mathcal{E}_1^{\infty} - m_1 > 0$ is much smaller than the separation distance of the fundamental level of the atom $\mathcal{E}_3^{\infty} - \mathcal{E}_1^{\infty} > 0$.

2.3. Spectrum of the reduced operator. In polar coordinates, Hamiltonian (1) takes the form,

$$H = -h^2 \left[\frac{\partial^2}{\partial R^2} + \frac{2}{R} \frac{\partial}{\partial R} \right] - h^2 \frac{1}{R^2} \Lambda^2 + \frac{1}{R} + H_e(\mathbf{R})$$
(10)

where Λ^2 is the Legendrian operator,

$$\Lambda^2 = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2}.$$

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FIGURE 1. Graph of the effective potentials $W_1(R)$ and $W_2(R)$ with single well shapes. The effective potential $W_1(R)$ has a barrier and it does not admit other critical points in the domain $W_1^{-1}([m_1, M_1])$; where m_1 and M_1 are the values of the local maximum and minimum point of W_1 .

The operator $-h^2 \frac{1}{R^2} \Lambda^2$ has eigenvalues $h^2 \frac{1}{R^2} \ell(\ell+1)$, $\ell \in \{0, 1, 2, ...\}$. As a consequence, using Remark 2.2, a suitable choice of the rotation O makes the operator H take the form,

$$H = -h^2 \left[\frac{\partial^2}{\partial R^2} + \frac{2}{R} \frac{\partial}{\partial R} \right] + h^2 \frac{\ell(\ell+1)}{R^2} + \frac{1}{R} + H_e(R)$$

on $L^2(\mathbb{R}_+, R^2 dR; L^2(\mathbb{R}^3_{\mathbf{r}}))$. Finally, by taking $\ell = 0$, that is, by considering the restriction of H on $Ker(\mathbf{L}_{\mathbf{R}})$ (still denoted by H), and by performing the change $\psi(R, \mathbf{r}) \to R\psi(R, \mathbf{r})$, the Hamiltonian H takes the form,

$$H_0 = -h^2 \frac{\partial^2}{\partial R^2} + \frac{1}{R} + H_e(R)$$

on $L^2(\mathbb{R}_+, dR; L^2(\mathbb{R}^3_r))$ with Dirichlet boundary condition at R = 0. Let P_j , j = 1, 2, be the *reduced operator* formally defined by

$$P_j = -h^2 \frac{d^2}{dR^2} + W_j(R), \quad W_j(R) = \frac{1}{R} + \mathcal{E}_j(R), \tag{11}$$

on the Hilbert space $L^2(\mathbb{R}_+, dR)$ with Dirichlet boundary condition at R = 0. Then, it follows that for h small enough and for small external field, the discrete spectra of P_j in the interval $[m_j, \mathcal{E}_j^{\infty})$, j = 1, 2, is not empty (see, e.g., [La] in the case without the external field), and we denote it by

$$\operatorname{Sp}_{\mathrm{d}}(P_{j}) = \left\{ e_{k}^{j}, \ k \ge 1 \right\}, \ j = 1, 2.$$

In particular, in the case of non degenerate minima points m_1 and m_2 , combining results from [HeRo] and [HeSj1], we know that the gap $e_{k+1}^j - e_k^j$ between two consecutive eigenvalues of P_j (j = 1, 2) is of order h as $h \to 0_+$, in the sense that $c_jh \leq e_{k+1}^j - e_k^j \leq C_jh$ with $c_j, C_j > 0$ independent of h and $k = \mathcal{O}(h^{-1})$.

3. Analytic distortion and regularization of the operator

3.1. Analytic distortion. Let $s \in C^{\infty}(\mathbb{R})$, $0 \leq s \leq 1$ with s(x) = 0 in an arbitrarily large compact set containing 0, and s(x) = 1 if |x| is large enough. For μ real small enough, we set,

$$I_{\mu} : \mathbb{R}^3 \to \mathbb{R}^3, \quad I_{\mu}(\mathbf{R}) = \mathbf{R}(1 + \mu s(R))$$

$$(12)$$

$$J_{\mu} : \mathbb{R}^{6} \to \mathbb{R}^{3}, \quad J_{\mu}(\mathbf{R}, \mathbf{r}) = \mathbf{r} \left[1 + \mu s \left(\left\langle \frac{\mathbf{R}}{R}, \mathbf{r} \right\rangle \right) \right],$$
(13)

and we define the analytic distortion on the test function φ , by the formula,

$$(\mathcal{S}_{\mu}\varphi)(\mathbf{R},\mathbf{r}) = |J(\mathbf{R},\mathbf{r})|^{1/2}\varphi(I_{\mu}(\mathbf{R}),J_{\mu}(\mathbf{R},\mathbf{r})), \qquad (14)$$

where we have set $R = |\mathbf{R}|$, and $J(\mathbf{R}, \mathbf{r})$ is the Jacobian of the transformation F_{μ} given by,

$$F_{\mu}: \mathbb{R}^6 \to \mathbb{R}^6, F_{\mu}(\mathbf{R}, \mathbf{r}) = (I_{\mu}(\mathbf{R}), J_{\mu}(\mathbf{R}, \mathbf{r})).$$
(15)

We also set

$$\phi_{\mu}: \mathbb{R}_+ \to \mathbb{R}_+, \phi_{\mu}(R) = R(1 + \mu s(R)).$$

Then, the analytic distortion applied to the operator (1) defined on the Hilbert space \mathcal{K} takes the form,

$$H_{\mu} = \mathcal{S}_{\mu} H \mathcal{S}_{\mu}^{-1} = -h^2 \mathcal{S}_{\mu} \Delta_{\mathbf{R}} \mathcal{S}_{\mu}^{-1} + \frac{1}{\phi_{\mu}(R)} + H_{\mu,e}(\mathbf{R}), \qquad (16)$$

with $H_{\mu,e}(\mathbf{R})$ given by,

$$H_{\mu,e}(\mathbf{R}) = -\mathcal{S}_{\mu}\Delta_{\mathbf{r}}\mathcal{S}_{\mu}^{-1} - \frac{1}{|J_{\mu}(\mathbf{R},\mathbf{r}) - \frac{1}{2}I_{\mu}(\mathbf{R})|} - \frac{1}{|J_{\mu}(\mathbf{R},\mathbf{r}) + \frac{1}{2}I_{\mu}(\mathbf{R})|} + V^{\mu},$$

where the distorted external potential is given by,

$$V_{\mu}(\mathbf{R}, \mathbf{r}) = V\left[\left\langle \frac{\mathbf{R}}{R}, \mathbf{r} \right\rangle \left(1 + \mu s\left(\left\langle \frac{\mathbf{R}}{R}, \mathbf{r} \right\rangle\right)\right)\right]$$

Thus, $H_{\mu,e}(\mathbf{R})$ can be extended to small enough complex values of μ as an analytic family of type A.

Remark 3.1. We also observe that, if O is a rotation in \mathbb{R}^3 , then,

$$I_{\mu}(O\mathbf{R}) = OI_{\mu}(\mathbf{R}) \quad ; \quad J_{\mu}(O\mathbf{R}, O\mathbf{r}) = OJ_{\mu}(\mathbf{R}, \mathbf{r}) \,.$$

As a consequence,

$$[\mathcal{S}_{\mu}, \mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}] = 0, \qquad (17)$$

and,

$$H_{\mu,e}(O\mathbf{R}, O\mathbf{r}, O^{-1}D_{\mathbf{r}}) = H_{\mu,e}(\mathbf{R}, \mathbf{r}, D_{\mathbf{r}}).$$

We denote by $H_{\mu,0}$ the restriction of $H_{\mu,e}(\mathbf{R},\mathbf{r},D_{\mathbf{r}})$ to the invariant subspace $Ker(\mathbf{L}_{\mathbf{R}}+\mathbf{L}_{\mathbf{r}})$.

3.2. Regularization of H_{μ} . In this section, we want to regularize the operator H_{μ} with respect to the **R**-variable. Having in mind the representation (10) of the Laplacian in polar coordinates, we denote

$$\Omega(1/M) := \left\{ \mathbf{R} \in \mathbb{R}^3 : R > \frac{1}{M} \right\}, \quad \Omega_0(1/M) := \left\{ \mathbf{R} \in \mathbb{R}^3 : R < \frac{1}{M} \right\},$$

and S^2 is the unit sphere in $\mathbb{R}^3_{\mathbf{B}}$, and

$$L_0 := -\Delta_{\mathbf{r}} + C_0$$

with $C_0, M > 0$ large enough. We have the following preliminary technical lemma:

Lemma 3.2. Under the previous assumptions, there exists a finite family of conical open sets $(\Omega_{\ell})_{\ell=1}^{m}$ in \mathbb{R}^{3} , of the form $\Omega_{\ell} =]\frac{1}{M}, +\infty [\times \omega_{\ell} \text{ with } \omega_{\ell} \text{ bounded open set of}]$ S^2 , and a corresponding family of unitary operators $\mathcal{U}_{\ell}(\mathbf{R})$ $(\ell = 1, \cdots, m, \mathbf{R} \in \Omega_{\ell})$ on $L^2(\mathbb{R}^3_{\mathbf{r}})$, such that (denoting by U_{ℓ} the unitary operator on $L^2(\Omega_{\ell}; L^2(\mathbb{R}^3_{\mathbf{r}})) \simeq$ $L^2(\Omega_\ell) \otimes L^2(\mathbb{R}^3_{\mathbf{r}})$ induced by the action of $\mathcal{U}_\ell(\mathbf{R})$ on $L^2(\mathbb{R}^3_{\mathbf{r}})$, one has,

- Ω(1/M) = ∪_{ℓ=1}^mΩ_ℓ;
 For all ℓ = 1, · · · , m and **R** ∈ Ω_ℓ, U_ℓ(**R**) leaves H²(ℝ_r³) invariant;
 For all ℓ, the operator U_ℓ(-h²S_μΔ_{**R**}S_μ⁻¹)U_ℓ⁻¹ is a semiclassical differential operator with operator-valued symbols, of the form,

$$-h^2 \mathcal{S}_{\mu} \Delta_{\mathbf{R}} \mathcal{S}_{\mu}^{-1} + h \sum_{|\beta|=1} \omega_{\beta,\ell}(\mathbf{R}) (hD_{\mathbf{R}})^{\beta} + h^2 \omega_{0,\ell}(\mathbf{R}) , \ D_{\mathbf{R}} = -i \nabla_{\mathbf{R}}$$
(18)

where $\omega_{\beta,\ell} L_0^{\frac{|\beta|}{2}-1} \in C^{\infty}(\Omega_{\ell}; \mathcal{L}(L^2(\mathbb{R}^3_{\mathbf{r}})))$, and, for any $\gamma \in \mathbb{N}^3$, the quantity $\|\partial_x^{\gamma}\omega_{\beta,\ell}(x)L_0^{\frac{|\beta|}{2}-1}\|_{\mathcal{L}(L^2(\mathbb{R}^3_{\mathbf{r}}))}$ is bounded uniformly with respect to h small enough and locally uniformly with respect to $x \in \Omega_{\ell}$; (4) For all ℓ , the operators $\mathcal{U}_{\ell}H_{\mu,\epsilon}\mathcal{U}_{\ell}^{-1}$ are in $C^{\infty}(\Omega_{\ell}; \mathcal{L}(H^2(\mathbb{R}^3_{\mathbf{r}}), L^2(\mathbb{R}^3_{\mathbf{r}})))$.

Proof. At first, let us make a change of variables as in [MaMe], that localizes into a compact set the \mathbf{R} - dependent singularities appearing into the interaction potential. Let $\chi \in C^{\infty}(\mathbb{R}^+)$ satisfying $0 \leq \chi \leq 1, \chi' \leq 0$, such that,

$$\chi(s)=1, \quad \text{if } \ 0\leq s\leq 1, \qquad \chi(s)=0, \ \text{if } \ s\geq 2$$

For $\tau > 1/2M$ and t > 0, we consider the function,

$$p(\tau,t) = \frac{t}{\tau} \chi\left(\frac{t}{\tau}\right) + 2Mt\left(1 - \chi\left(\frac{t}{\tau}\right)\right).$$

Then, it is easy to check that

$$\begin{split} &\frac{\partial\rho}{\partial t} > 0 \ \text{ on } \ \bigg] \frac{1}{2M}, +\infty \bigg[\times \mathbb{R}_+, \\ &\rho \text{ is surjective onto } \mathbb{R}_+, \\ &\frac{\partial^k \rho}{\partial \tau^k} \text{ is uniformly bounded on } \big] \frac{1}{2M}, +\infty [\times \mathbb{R}_+, \forall k \geq 1] \end{split}$$

Therefore we can define α_{τ} as the inverse diffeomorphism on \mathbb{R}_+ of the function $t \to \rho(\tau, t)$. in particular, by construction we have,

$$\alpha_{\tau}(t) = \frac{t}{2M}$$
 if $t \ge 4M\tau$, $\alpha_{\tau}(t) = \tau t$ if $t \le 1$.

Now, for $\mathbf{R} \in \Omega(1/M)$, we define

$$\theta(\mathbf{R}, .) : \mathbb{R}^3 \to \mathbb{R}^3, \quad \theta(\mathbf{R}, \mathbf{r}) = \alpha_{R/2}(|\mathbf{r}|) \frac{\mathbf{r}}{|\mathbf{r}|}.$$

Then, for any $\mathbf{R} \in \Omega(1/M)$, the function $\theta(\mathbf{R}, .)$ is a diffeomorphism of \mathbb{R}^3 , it depends smoothly on \mathbf{R} , and is such that $\partial^{\alpha}_{\mathbf{R}}\theta(\mathbf{R}, \mathbf{r})$ is uniformly bounded on $\Omega(1/2M) \times \mathbb{R}^3$, for any $\alpha \in \mathbb{N}^3 \setminus \{0\}$ (see [MaMe], Lemma 3.1). Moreover

$$\begin{split} \theta\left(\mathbf{R}, \frac{\mathbf{R}}{R}\right) &= \frac{\mathbf{R}}{2},\\ \theta(\mathbf{R}, \mathbf{r}) &= \frac{\mathbf{r}}{2M} \quad \text{for } |\mathbf{r}| \ge 2MR,\\ \theta(\mathbf{R}, \mathbf{r}) &= \frac{R}{2}\mathbf{r} \quad \text{for } |\mathbf{r}| \le 1. \end{split}$$

For $R > \frac{1}{M}$, we consider the unitary transformation on $L^2(\mathbb{R}^3_{\mathbf{r}})$, given by,

$$(U(\mathbf{R})\phi)(\mathbf{r}) = \phi(\theta(\mathbf{R},\mathbf{r}))|\partial_{\mathbf{r}}\theta(\mathbf{R},\mathbf{r})|^{1/2}$$

The advantage of performing this change of variables is that the **R**-depending singularities of the potential are now localized in some compact subset of $\mathbb{R}^3_{\mathbf{r}}$. Now, following the arguments of [KMSW] and with the help of the previous change of variables, let us show that, by a patch and cut procedure, one can localize the singularities of the potential at some fixed (**R**-independent) points.

For any fixed $z_0 \in S^2$ (the unit sphere in \mathbb{R}^3), we choose a functions $f_{z_0} \in C_0^{\infty}(\mathbb{R}^3; \mathbb{R})$, such that,

$$f_{z_0}(z_0) = 1, \qquad f_{z_0}(-z_0) = 0$$

and, for z close enough to z_0 and $s \in \mathbb{R}^3$, we define

$$F_{z_0}(z,s) := s + (z - z_0)(f_{z_0}(s) - f_{z_0}(-s)) \in \mathbb{R}^3$$

For z in a smooth neighborhood ω_{z_0} of z_0 , the application $s \mapsto F_{z_0}(z,s)$ is a diffeomorphism of \mathbb{R}^3 , and we have,

$$F_{z_0}(z, z_0) = z, \quad F_{z_0}(z, -z_0) = -z.$$

Moreover, for any $\alpha \in \mathbb{R}^3$, there exists $C_\alpha > 0$ such that, for any $z \in \omega_{z_0}$, for any $s, s' \in \mathbb{R}^3$

$$\begin{aligned} &\frac{1}{C_0} |s - s'| \le |F_{z_0}(z, s) - F_{z_0}(z, s')| \le C_0 |s - s'| \\ &|\partial_x^{\alpha} F_{z_0}(z, s) - \partial_x^{\alpha} F_{z_0}(z, s')| \le C_\alpha |s - s'| \\ &|\partial_x^{\alpha} F_{z_0}(z, s)| \le C_0, \quad |\alpha| \ge 1 \end{aligned}$$

If $(\omega_{\ell})_{\ell=1}^m := (\omega_{z_{\ell}})_{\ell=1}^m$ is a family of such open sets that covers S^2 , we set $F_{\ell}(z, .) := F_{z_{\ell}}(z, .)$, and we define,

$$\Omega_{\ell} := \left] \frac{1}{M}, +\infty \right[\times \omega_{\ell}.$$

For $\mathbf{R} \in \Omega_{\ell}$, we also set,

$$(\widetilde{U}_{\ell}(\mathbf{R})\phi)(\mathbf{r}) = \left|\det(\partial_{\mathbf{r}}F_{\ell})\left(\frac{\mathbf{R}}{R},\mathbf{r}\right)\right|^{1/2}\phi\left(F_{\ell}\left(\frac{\mathbf{R}}{R},\mathbf{r}\right)\right),$$

and,

$$\mathcal{U}_{\ell}(\mathbf{R}) := \widetilde{U}_{\ell}(\mathbf{R})U(\mathbf{R});$$

$$(\mathcal{U}_{\ell}(\mathbf{R})\phi)(\mathbf{r})) = \phi(\gamma_{\ell}(\mathbf{R},\mathbf{r}))|\det(\partial_{\mathbf{r}}\gamma_{\ell})(\mathbf{R},\mathbf{r})|,$$

where

$$\gamma_\ell(\mathbf{R},\mathbf{r}) = \theta\left(\mathbf{R},F_\ell\left(\frac{\mathbf{R}}{R},\mathbf{r}\right)\right).$$

Then, it is easy to check (see [MaMe]) that \mathcal{U}_{ℓ} satisfy (1), (2), (3), and (4). This completes the proof of the lemma.

Now, let us consider the spectral projection $\Pi_0(\mathbf{R})$ associated to $\{\mathcal{E}_1(R), \mathcal{E}_2(R)\}$ of $H_e(\mathbf{R})$, where $\mathcal{E}_1(R)$ and $\mathcal{E}_2(R)$ are the first two (simple) eigenvalues of $H_e(\mathbf{R})$. If one denote by $\gamma(R)$ a continuous simple loop in \mathbb{C} enclosing $\{\mathcal{E}_1(R), \mathcal{E}_2(R)\}$ and having the rest of Sp $(H_e(\mathbf{R}))$ in its exterior, one can write $\Pi_0(\mathbf{R})$ as,

$$\Pi_0(\mathbf{R}) = \frac{1}{2\pi i} \int_{\gamma(R)} (H_e(\mathbf{R}) - z)^{-1} dz.$$

Moreover, for μ complex small enough, one can define the projector,

$$\Pi_{\mu,0}(\mathbf{R}) = \frac{1}{2\pi i} \int_{\gamma(R)} (H_{\mu,e}(\mathbf{R}) - z)^{-1} dz$$

satisfying $(\Pi_{\mu,0})^* = \Pi_{\bar{\mu},0}$. We have the following

Lemma 3.3. There exist two functions,

$$w_1^{\mu}(\mathbf{R},\mathbf{r}), w_2^{\mu}(\mathbf{R},\mathbf{r}) \in C^0(\mathbb{R}^3_{\mathbf{R}}; H^2(\mathbb{R}^3_{\mathbf{r}}))$$

depending analytically on μ , and real-valued for μ real, such that,

- i. $\langle w_{l}^{\mu}(\mathbf{R},\mathbf{r}), w_{l}^{\bar{\mu}}(\mathbf{R},\mathbf{r}) \rangle_{L^{2}(\mathbb{R}^{3}_{\mathbf{r}})} = \delta_{k,l}, \quad k, l = 1, 2;$ ii. $w_{j}^{\mu} \in C^{\infty}(\Omega_{0}(2/M); H^{2}(\mathbb{R}^{3}_{\mathbf{r}})), j = 1, 2, \text{ and, for } \mathbf{R} \in \Omega(3/M), w_{1}^{\mu}(\mathbf{R},\mathbf{r}) \text{ and}$ $w_2^{\mu}(\mathbf{R},\mathbf{r})$ form a basis of Ran $\Pi_{\mu,0}$;
- iii. For $\mathbf{R} \in \Omega(3/M)$, $w_1^{\mu}(\mathbf{R},\mathbf{r})$ and $w_2^{\mu}(\mathbf{R},\mathbf{r})$ are eigenfunctions of $H_{\mu,e}(\mathbf{R})$ associated to $\mathcal{E}_1(\phi_\mu(R))$ and $\mathcal{E}_2(\phi_\mu(R))$ respectively;
- iv. For all $\ell = 1, \ldots, m$, one has $\mathcal{U}_{\ell}(\mathbf{R}) w_{j}^{\mu}(\mathbf{R}, \mathbf{r}) \in C_{b}^{\infty}(\Omega_{\ell}(M), H^{2}(\mathbb{R}^{3}_{\mathbf{r}})), j =$ 1, 2.
- v. w_1^{μ} and w_2^{μ} can be chosen in such a way that, $(\mathbf{L_R} + \mathbf{L_r})w_1^{\mu} = (\mathbf{L_R} + \mathbf{L_r})w_2^{\mu} = 0.$

Proof. Taking into account that (see (7)),

$$\lim_{R\mapsto+\infty}\mathcal{E}_1(R)\neq\lim_{R\mapsto+\infty}\mathcal{E}_2(R),$$

the points (i)-(iv) follow from Lemma 3.1 of [MaSo] and from the arguments of Proposition 5.1 in [MaMe]. Moreover, since $\mathcal{E}_1(R)$ and $\mathcal{E}_2(R)$ are non degenerate, the last point (v) follows from [KMSW], Theorem 2.1, and from (17). \square

Thanks to the previous lemma, we see that the family $(U_{\ell}, \Omega_{\ell})_{\ell=0,m}$ (with Ω_0 = $\Omega_0(2/M), \mathcal{U}_0 = \mathbb{I}$ and $\Omega_\ell, \mathcal{U}_\ell$ defined in Lemma 3.2 and Lemma 3.3), is a regular unitary covering of $L^2(\mathbb{R}^3_{\mathbf{R}}; L^2(\mathbb{R}^3_{\mathbf{r}}))$ in the sense of [MaSo], Definition 4.1. We set,

$$\widetilde{\Pi}_{\mu,0}(\mathbf{R}) = \langle \cdot, w_1^{\mu}(\mathbf{R}) \rangle_{L^2(\mathbb{R}^3_*)} w_1^{\mu}(\mathbf{R}) + \langle \cdot, w_2^{\mu}(\mathbf{R}) \rangle_{L^2(\mathbb{R}^3_*)} w_2^{\mu}(\mathbf{R})$$

so that $\Pi_{\mu,0}(R)$ coincides with $\Pi_{\mu,0}(R)$ for $\mathbf{R} \in \Omega(3/M)$, and verify,

$$\mathcal{U}_{\ell}(\mathbf{R})\Pi_{\mu,0}(\mathbf{R})\mathcal{U}_{\ell}(\mathbf{R})^{-1} \in C^{\infty}(\Omega_{\ell},\mathcal{L}(L^{2}(\mathbb{R}^{3}_{\mathbf{r}}))).$$

for all $\ell = 0, \ldots, m$. Also observe that, for any rotation O,

$$T_O \Pi_{\mu,0}(\mathbf{R}) = \Pi_{\mu,0}(\mathbf{R}) T_O$$

or, equivalently, $[\Pi_{\mu,0}(\mathbf{R}), \mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}] = 0.$

We also denote by $\Pi_0(\mathbf{R})$ the value of $\Pi_{\mu,0}(\mathbf{R})$ for $\mu = 0$.

Now, with the help of $\Pi_{\mu,0}(\mathbf{R})$, we modify $H_{\mu,e}(\mathbf{R})$ outside a neighborhood of $\Omega(5/M)$ as follows (see Proposition 3.2 in [MaSo]).

Proposition 3.4. We choose a function $\zeta \in C^{\infty}(\mathbb{R}_+; [0, 1])$, such that $\zeta = 1$ for $R \geq 3/M$ and $\operatorname{supp} \zeta \subseteq]2/M, +\infty[$. Then, for all $\mathbf{R} \in \mathbb{R}^3$, and μ complex small enough, there exists an operator $\widetilde{H}_{\mu,e}(\mathbf{R})$ on $L^2(\mathbb{R}^3_{\mathbf{r}})$, with domain $H^2(\mathbb{R}^3_{\mathbf{r}})$, depending analytically on μ , such that,

$$\begin{split} \widetilde{H}_{\mu,e}(\mathbf{R}) &= H_{\mu,e}(\mathbf{R}) \quad \text{if } \mathbf{R} \in \Omega(4/M); \\ [\widetilde{H}_{\mu,e}(\mathbf{R}), \widetilde{\Pi}_{\mu,0}(\mathbf{R})] &= 0 \quad \text{for all } \mathbf{R} \in \mathbb{R}^3 \end{split}$$

and the application $\mathbf{R} \mapsto \mathcal{U}_{\ell}(\mathbf{R}) \widetilde{H}_{\mu,e}(\mathbf{R}) \mathcal{U}_{\ell}(\mathbf{R})^{-1}$ is in $C^{\infty}(\Omega_{\ell}; \mathcal{L}(H^2(\mathbb{R}^3_{\mathbf{r}}), L^2(\mathbb{R}^3_{\mathbf{r}})))$ for all $\ell = 0, \ldots, m$. Moreover, $\widetilde{H}_{\mu,e}(\mathbf{R})$ commutes with $\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}$, in the sense that, for any $\varphi \in C_0^{\infty}(\mathbb{R}^6)$, one has,

$$(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})\widetilde{H}_{\mu,e}(\mathbf{R})\varphi = \widetilde{H}_{\mu,e}(\mathbf{R})(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})\varphi.$$

Hence, the spectrum of $H_{\mu,e}(\mathbf{R})$ actually depends only on $R \in \mathbb{R}_+$. Moreover, for μ real, $\widetilde{H}_{\mu,e}(\mathbf{R})$ is self-adjoint, uniformly semibounded from below, and the bottom of its spectrum consists in two eigenvalues,

$$\widetilde{\mathcal{E}}_{j}^{\mu}(R) = \widetilde{\mathcal{E}}_{j}(\phi_{\mu}(R)), \ j = 1, 2,$$

where

$$\widetilde{\mathcal{E}}_j(R) = \zeta(R)\mathcal{E}_j(R).$$

Furthermore, $\widetilde{H}_{\mu,e}(\mathbf{R})$ admits a global gap in its spectrum, in the sense that,

$$\inf_{R \in \mathbb{R}_+} \operatorname{dist}(\{\widetilde{\mathcal{E}}_1^{\mu}(R), \widetilde{\mathcal{E}}_2^{\mu}(R)\}, \widetilde{\mathcal{E}}_3^{\mu}(R)) > 0.$$

where we set

1

$$\widetilde{\mathcal{E}}_{3}^{\mu}(R) = \operatorname{Sp}(\widetilde{H}_{\mu,e}(\mathbf{R})) \setminus \{\widetilde{\mathcal{E}}_{1}^{\mu}(R), \widetilde{\mathcal{E}}_{2}^{\mu}(R)\}$$

Proof. The proof is similar to that of Proposition 3.2 in [MaSo], and we write it for $\mu = 0$ only (the general case is obtained by just substituting $H_{\mu,e}$ to H_e and $\widetilde{\Pi}_{\mu,0}$ to $\widetilde{\Pi}_0$). We set $\widetilde{\Pi}_0^{\perp}(\mathbf{R}) = 1 - \widetilde{\Pi}_0(\mathbf{R})$ and

$$\widetilde{H}_e(\mathbf{R}) = \zeta(R)H_e(\mathbf{R}) + (1-\zeta(R))\widetilde{\Pi}_0^{\perp}(\mathbf{R})(-\Delta_{\mathbf{r}} + C_0)\widetilde{\Pi}_0^{\perp}(\mathbf{R}).$$

with $C_0 > 0$ large enough and such that $C_0 > \overline{\mathcal{E}}_3$, where

$$\bar{\mathcal{E}}_3 := \inf_R \mathcal{E}_3(R) \,. \tag{19}$$

Since $\widetilde{\Pi}_0(\mathbf{R}) = \Pi_0(\mathbf{R})$ on $\operatorname{Supp}\zeta$, we see that $\widetilde{\Pi}_0(\mathbf{R})$ commutes with $\widetilde{H}_e(\mathbf{R})$, and it is also clear that $\widetilde{H}_e(\mathbf{R})$ is self-adjoint with domain $H^2(\mathbb{R}^3)$. Moreover,

$$\Pi_0(\mathbf{R})H_e(\mathbf{R})\Pi_0(\mathbf{R}) = \zeta(\mathbf{R})\Pi_0(\mathbf{R})H_e(\mathbf{R})\Pi_0(\mathbf{R})$$

and,

$$\widetilde{\Pi}_{0}^{\perp}(\mathbf{R})\widetilde{H}_{e}(\mathbf{R})\widetilde{\Pi}_{0}^{\perp}(\mathbf{R}) \geq (\zeta(R)\mathcal{E}_{3}(R) + (1-\zeta(R))C_{0})\widetilde{\Pi}_{0}^{\perp}(\mathbf{R}) \geq \bar{\mathcal{E}}_{3}\widetilde{\Pi}_{0}^{\perp}(\mathbf{R}).$$
(20)

In particular, the bottom of the spectrum of $\widetilde{H}_e(\mathbf{R})$ consists in two eigenvalues $\widetilde{\mathcal{E}}_j(R) = \zeta(R)\mathcal{E}_j(R)$ with associated eigenvectors $\widetilde{\Pi}_0(\mathbf{R})\psi_j$, j = 1, 2, where \mathcal{E}_j and ψ_j are the first two eigenvalues and eigenvectors of (8). Furthermore, one has

$$\inf_{R>2/M} \operatorname{dist}(\tilde{\mathcal{E}}_{3}(R), \{\tilde{\mathcal{E}}_{1}(R), \tilde{\mathcal{E}}_{2}(R)\}) \\ \geq \inf_{R>2/M} \left(\zeta(R)(\inf [\mathcal{E}_{3}(R)] - \mathcal{E}_{2}(R)) + (1 - \zeta(R))C_{0}\right) > 0,$$

and

$$\inf_{0< R\leq 2/M} \operatorname{dist}(\widetilde{\mathcal{E}}_3(R), \{\widetilde{\mathcal{E}}_1(R), \widetilde{\mathcal{E}}_2(R)\}) \geq C_0.$$

In particular, $\widetilde{H}_e(\mathbf{R})$ admits a fix global gap in its spectrum as stated in the proposition. Finally, we see that $\widetilde{H}_e(\mathbf{R})$ commutes with $\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}$, and $\mathcal{U}_{\ell}\widetilde{H}_e(\mathbf{R})\mathcal{U}_{\ell}^{-1}$ depends smoothly on \mathbf{R} in Ω_{ℓ} for all $\ell = 0, \ldots, m$.

3.3. Regularization of the operator.

Definition 3.5 (Regularization of H_{μ}). Let S_{μ} be the analytic distortion defined in (14) for μ in some small complex neighborhood of zero, and let $\tilde{H}_{\mu,e}(\mathbf{R})$ and $\zeta(R)$ be defined as in Proposition 3.4. Then, we define the regularization of H_{μ} as,

$$\widetilde{H}_{\mu} = -h^2 \mathcal{S}_{\mu} \Delta_{\mathbf{R}} \mathcal{S}_{\mu}^{-1} + \widetilde{H}_{\mu,e}(\mathbf{R}) + \frac{\zeta(R)}{\phi_{\mu}(R)} + \frac{M}{3} (1 - \zeta(R)).$$
(21)

Taking into account Definition 4.4 in [MaSo], we see that Lemma 3.2, Proposition 3.4 and (17) imply,

Lemma 3.6. The operator \widetilde{H}_{μ} is a twisted PDO (of degree 2) on $L^2(\mathbb{R}^3_{\mathbf{R}}, L^2(\mathbb{R}^3_{\mathbf{r}}))$ (in the sense of Definition 5.1 in [MaSo]), associated with the regular unitary covering $(\mathcal{U}_{\ell}, \Omega_{\ell})_{\ell=0,...,m}$. Moreover, it commutes with $\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}$.

Now, we define

$$Z^+_{\mu}: L^2(\mathbb{R}^6) \to L^2(\mathbb{R}^3_{\mathbf{R}}) \oplus L^2(\mathbb{R}^3_{\mathbf{R}})$$

by the formula,

$$\left(Z_{\mu}^{+}\psi\right)(\mathbf{R}) = \langle\psi(\mathbf{R},\cdot), w_{1}^{\bar{\mu}}(\mathbf{R},\cdot)\rangle_{L^{2}(\mathbb{R}^{3}_{\mathbf{r}})} \oplus \langle\psi(\mathbf{R},\cdot), w_{2}^{\bar{\mu}}(\mathbf{R},\cdot)\rangle_{L^{2}(\mathbb{R}^{3}_{\mathbf{r}})},$$

and,

$$Z^{-}_{\mu} = (Z^{+}_{\bar{\mu}})^{*} : L^{2}(\mathbb{R}^{3}_{\mathbf{R}}) \oplus L^{2}(\mathbb{R}^{3}_{\mathbf{R}}) \to L^{2}(\mathbb{R}^{6}),$$

by

$$\left(Z_{\mu}^{-}(u_{1}\oplus u_{2})\right)(\mathbf{R},\mathbf{r})=u_{1}(\mathbf{R})w_{1}^{\mu}(\mathbf{R},\mathbf{r})+u_{2}(\mathbf{R})w_{2}^{\mu}(\mathbf{R},\mathbf{r}).$$

Following [MaMe], we consider the Grushin problem,

$$\widetilde{\mathcal{G}}_{\mu}(z) = \left(\begin{array}{cc} \widetilde{H}_{\mu} - z & Z_{\mu}^{-} \\ Z_{\mu}^{+} & 0 \end{array} \right),$$

that sends $H^2(\mathbb{R}^6) \oplus (L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3))$ into $L^2(\mathbb{R}^6) \oplus (H^2(\mathbb{R}^3) \oplus H^2(\mathbb{R}^3))$. Thanks to Lemma 3.3 and Lemma 3.6, we see that $\widetilde{\mathcal{G}}_{\mu}(z)$ is a twisted PDO (of degree 2) on $L^2(\mathbb{R}^3_{\mathbf{R}}; L^2(\mathbb{R}^3_{\mathbf{r}}) \oplus \mathbb{C} \oplus \mathbb{C})$, associated with the regular unitary covering $(\mathcal{V}_{\ell}, \Omega_{\ell})_{\ell=0,\ldots,m}$, where we have set

$$\mathcal{V}_{\ell} := \left(\begin{array}{cc} \mathcal{U}_{\ell} & 0 \\ 0 & 1_2 \end{array} \right).$$

We also have,

Lemma 3.7. For all $\mu \in \mathbb{C}$ small enough and $z \in \mathbb{C}$, the operator $\widetilde{\mathcal{G}}_{\mu}(z)$ commutes with $\mathcal{L} := \begin{pmatrix} L_{\mathbf{R}} + L_{\mathbf{r}} & 0 \\ 0 & L_{\mathbf{R}} \end{pmatrix}$.

Proof. By Lemma 3.6, we only need to study the commutation rules between Z^{\pm}_{μ} and the operators $L_{\mathbf{R}}$ and $L_{\mathbf{r}}$. But, using Lemma 3.3, v., plus the fact that the formal adjoint of $L_{\mathbf{r}}$ is $-L_{\mathbf{r}}$, we immediately obtain,

$$(L_{\mathbf{R}} + L_{\mathbf{r}})Z_{\mu}^{-} = Z_{\mu}^{-}L_{\mathbf{R}} \quad ; \quad L_{\mathbf{R}}Z_{\mu}^{+} = Z_{\mu}^{+}(L_{\mathbf{R}} + L_{\mathbf{r}}),$$

and the result follows.

Moreover, we see as in [MaMe], Section 5, that, for $z \in \mathbb{C}$ with $\operatorname{Re} z < \inf_R \widetilde{\mathcal{E}}_3(R)$ and $\operatorname{Im} z$ sufficiently small, the operator $\widetilde{\mathcal{G}}_{\mu}(z)$ is invertible, and its inverse $\widetilde{\mathcal{G}}_{\mu}(z)^{-1}$ is such that the operators,

$$\begin{pmatrix} 1 & 0 \\ 0 & \langle -\Delta_{\mathbf{R}} \rangle^{-1} \end{pmatrix} \widetilde{\mathcal{G}}_{\mu}(z)^{-1}, \quad \widetilde{\mathcal{G}}_{\mu}(z)^{-1} \begin{pmatrix} 1 & 0 \\ 0 & \langle -\Delta_{\mathbf{R}} \rangle^{-1} \end{pmatrix}$$

are twisted (bounded) *h*-admissible operators associated with the regular unitary covering $(\mathcal{V}_{\ell}, \Omega_{\ell})_{\ell=0,...,m}$. As a consequence, $\widetilde{\mathcal{G}}_{\mu}(z)^{-1}$ can be written as,

$$\widetilde{\mathcal{G}}_{\mu}(z)^{-1} = \begin{pmatrix} E_{\mu}(z) & E_{\mu}^{+}(z) \\ E_{\mu}^{-}(z) & z - \widetilde{P}_{\mu}(z) \end{pmatrix},$$

where $\widetilde{P}_{\mu}(z)$ is an unbounded *h*-admissible operator on $L^{2}(\mathbb{R}^{3}_{\mathbf{R}}) \oplus L^{2}(\mathbb{R}^{3}_{\mathbf{R}})$ with domain $H^{2}(\mathbb{R}^{3}_{\mathbf{R}}) \oplus H^{2}(\mathbb{R}^{3}_{\mathbf{R}})$, and $E_{\mu}(z)$, $E_{\mu}^{\pm}(z)$ are (bounded) twisted *h*-admissible operators (all depending in a holomorphic way on *z*).

More precisely, it results from [MaMe], formula (2.11), that the operator $\hat{P}_{\mu}(z)$ is given by the formula,

$$\widetilde{P}_{\mu}(z) = Z_{\mu}^{+} \widetilde{H}_{\mu} Z_{\mu}^{-} - Z_{\mu}^{+} [h^{2} \mathcal{S}_{\mu} \Delta_{\mathbf{R}} \mathcal{S}_{\mu}^{-1}, \widetilde{\Pi}_{\mu,0}] (\widetilde{H}_{\mu}^{\prime} - z)^{-1} [\widetilde{\Pi}_{\mu,0}, h^{2} \mathcal{S}_{\mu} \Delta_{\mathbf{R}} \mathcal{S}_{\mu}^{-1}] Z_{\mu}^{-},$$
(22)

where $\tilde{\Pi}_{\mu,0}$ stands for the projection on $L^2(\mathbb{R}^6)$ induced by the action of $\tilde{\Pi}_{\mu,0}(\mathbf{R})$ on $L^2(\mathbb{R}^3_{\mathbf{r}})$, and \tilde{H}'_{μ} is the restriction of $(1 - \tilde{\Pi}_{\mu,0})\tilde{H}_{\mu}(1 - \tilde{\Pi}_{\mu,0})$ to the range of $1 - \tilde{\Pi}_{\mu,0}$. In particular, $\tilde{H}'_{\mu} - z$ is invertible in virtue of (20), and $\tilde{\Pi}_{\mu,0}$ is a twisted *h*-admissible operator on $L^2(\mathbb{R}^3_{\mathbf{R}}, L^2(\mathbb{R}^3_{\mathbf{r}}))$ (in the sense of Definition 4.4 in [MaSo]), associated with the regular unitary covering $(\mathcal{U}_{\ell}, \Omega_{\ell})_{\ell=0,...,m}$.

By Lemma 3.7, we also know that $\tilde{P}_{\mu}(z)$ commutes with $L_{\mathbf{R}}$, and thus, gathering all the previous information on $\tilde{P}_{\mu}(z)$, we finally obtain that it can be written as,

$$\widetilde{P}_{\mu}(z) = -h^2 \mathcal{S}_{\mu} \Delta_{\mathbf{R}} \mathcal{S}_{\mu}^{-1} + \mathcal{M}_{\mu}(R) + h \mathcal{A}_{\mu}(\mathbf{R}, h \mathbf{D}_{\mathbf{R}}) + h^2 \mathcal{B}_{\mu}(\mathbf{R}, h \mathbf{D}_{\mathbf{R}}; z, h)$$
(23)

where, for any $R > \frac{3}{M}$, \mathcal{M}_{μ} is given by,

$$\mathcal{M}_{\mu}(R) = \begin{pmatrix} W_1(\phi_{\mu}(R)) & 0\\ 0 & W_2(\phi_{\mu}(R)) \end{pmatrix}, W_j(R) = \mathcal{E}_j(R) + \frac{1}{R}, \quad (24)$$

and, for $R \leq \frac{3}{M}$ and μ sufficiently small, it satisfies,

$$\operatorname{Re}\mathcal{M}_{\mu}(R) \ge \frac{M}{4} + \inf_{R}\mathcal{E}_{1}(R).$$
(25)

Here, M is the same as in Proposition 3.4 and Definition 3.5, and it can be chosen arbitrarily large.

Moreover $\mathcal{A}_{\mu}(\mathbf{R}, h\mathbf{D}_{\mathbf{R}})$ is of the form,

$$\mathcal{A}_{\mu} = \begin{pmatrix} 0 & a_{\mu}(\mathbf{R}) \cdot h \mathbf{D}_{\mathbf{R}} \\ h \mathbf{D}_{\mathbf{R}} \cdot \overline{a_{\mu}}(\mathbf{R}) & 0 \end{pmatrix},$$
(26)

for some smooth bounded (together with its derivatives) function $a_{\mu}(\mathbf{R})$ independent of z. Finally, $\mathcal{B}_{\mu}(\mathbf{R}, hD_{\mathbf{R}}; z, h)$ is an *h*-admissible pseudo-differential operator depending analytically on z, with Weyl symbol $b_{\mu}(\mathbf{R}, \mathbf{R}^*; z, h)$ holomorphic with respect to R^* in a complex strip of the form $\{|\Im R^*| < \delta\}$ (with $\delta > 0$ independent of z and μ), such that, for any multi-index α ,

$$\partial^{\alpha} b_{\mu}(\mathbf{R}, \mathbf{R}^*; z, h) = \mathcal{O}(1) \tag{27}$$

uniformly with respect to $(\mathbf{R}, \mathbf{R}^*) \in \mathbb{R}^3 \times \mathbb{R}^3$, h > 0 small enough, and z close enough to some fix $\lambda_0 \in \mathbb{C}$ such that $\operatorname{Re}\lambda_0 < \inf_R \widetilde{\mathcal{E}}_3(R)$ and $\operatorname{Im}\lambda_0$ sufficiently small.

Finally, the operators \mathcal{A}_{μ} and $\mathcal{B}_{\mu}(\mathbf{R}, h\mathbf{D}_{\mathbf{R}}; z, h)$ commute with $L_{\mathbf{R}}$, and one has the Feshbach identities,

$$(\widetilde{H}_{\mu} - z)^{-1} = E_{\mu}(z) + E_{\mu}^{+}(z)(\widetilde{P}_{\mu}(z) - z)^{-1}E_{\mu}^{-}(z), \qquad (28)$$
$$(\widetilde{P}_{\mu}(z) - z)^{-1} = Z_{\mu}^{+}(\widetilde{H}_{\mu} - z)^{-1}Z_{\mu}^{-}.$$

Summing up, we have proved,

Theorem 3.8. Let $\widetilde{\mathcal{E}}_3(R)$ be defined as in Proposition 3.4 and let $\lambda_0 \in \mathbb{C}$ with $\operatorname{Re}(\lambda_0) < \inf_R \widetilde{\mathcal{E}}_3(R)$ and $\operatorname{Im}(\lambda_0)$ sufficiently small. Under the previous assumptions, there exists a complex neighborhood D_{λ_0} of λ_0 such that, for any $z \in D_{\lambda_0}$, one has the equivalence,

$$z \in \operatorname{Sp}(H_{\mu}) \iff z \in \operatorname{Sp}(P_{\mu}(z)),$$

where $\widetilde{P}_{\mu}(z)$ is as in (23) with (24)-(27).

Now, taking advantage of Lemma 3.7, we can consider the restriction of the Grushin problem $\widetilde{\mathcal{G}}_{\mu}(z)$ on $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}) \oplus Ker(\mathbf{L}_{\mathbf{R}}) \oplus Ker(\mathbf{L}_{\mathbf{R}})$, and we also immediately obtain,

Corollary 3.9. Denote by \widetilde{H}^0_{μ} the restriction of \widetilde{H}_{μ} on the invariant subspace $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})$, and by $\widetilde{P}^0_{\mu}(z)$ the restriction of $\widetilde{P}_{\mu}(z)$ on the invariant subspace $Ker(\mathbf{L}_{\mathbf{R}})$. Then, for any $\lambda_0 \in \mathbb{C}$ with $\operatorname{Re}(\lambda_0) < \inf_R \widetilde{\mathcal{E}}_3(R)$ and $\operatorname{Im}(\lambda_0)$ sufficiently small, there exists a complex neighborhood D_{λ_0} of λ_0 such that, for any $z \in D_{\lambda_0}$, one has the equivalence,

$$z \in \operatorname{Sp}(\widetilde{H}^0_{\mu}) \iff z \in \operatorname{Sp}(\widetilde{P}^0_{\mu}(z)).$$

In the sequel, we also denote by H^0_{μ} the restriction of H_{μ} on the invariant subspace $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})$.

4. Reduced problem

Let us introduce the following shortcut notation,

$$\mathbf{D} = h\mathbf{D}_R, \ \mathbf{D}_R = -i\frac{d}{dR}.$$

For all R > 0, we define,

$$W_{j,\mu}(R) := \zeta(R)W_j(\phi_\mu(R)) + \frac{M}{3}(1-\zeta(R)),$$

where ζ is as in Proposition 3.4, and M is taken large enough. In particular, $W_{j,\mu}$ is bounded and depends analytically on μ .

Then, we set,

$$\mathcal{M}^{0}_{\mu}(R) := \left(\begin{array}{cc} W_{\mu,1}(R) & 0 \\ 0 & W_{\mu,2}(R) \end{array} \right),$$

and we denote by $\mathcal{A}^0_{\mu}(R, hD_R)$ the restriction of the differential operator (actually, vector-field) $\mathcal{A}_{\mu}(\mathbf{R}, h \mathbf{D}_{\mathbf{R}})$ on the space $Ker(\mathbf{L}_{\mathbf{R}})$. In particular, since $[\mathcal{A}_{\mu}, \mathbf{L}_{\mathbf{R}}] = 0$ then \mathcal{A}^{0}_{μ} can be represented as a differential operator in the variable $R = |\mathbf{R}|$, and it can be written as,

$$\mathcal{A}^0_\mu = \mathcal{A}^0_\mu(R,h\mathrm{D}_R) = \left(egin{array}{cc} 0 & a^0_\mu(R)h\mathrm{D}_R \ h\mathrm{D}_R\cdot\overline{a^0_\mu}(R) & 0 \end{array}
ight),$$

where the function a^0_{μ} is smooth and bounded together with all its derivatives on $(0, +\infty).$

In this section, we look for the solutions to the eigenvalue equation,

$$P^{\sharp}_{\mu}\varphi = \lambda\varphi, \quad \lambda \in \mathbb{C}, \ \varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}, \tag{29}$$

where P_{μ}^{\sharp} is the differential operator formally defined as,

$$P^{\sharp}_{\mu} = h^2 \mathcal{S}_{\mu} \mathcal{D}^2_R \mathcal{S}^{-1}_{\mu} + \mathcal{M}^0_{\mu}(R) + h \mathcal{A}^0_{\mu}(R, h \mathcal{D}_R)$$
(30)

acting on the Hilbert space,

$$\mathcal{H}^{\sharp} = L^2 \left([0, +\infty), dR \right) \oplus L^2 \left([0, +\infty), dR \right),$$
(31)

with zero Dirichlet boundary condition at R = 0, and where now, with abuse of notation, we denote,

$$(\mathcal{S}_{\mu}\varphi)(R) = |I'(R)|^{1/2}\varphi[I(R)], \ I(R) = R [1 + \mu s(R)].$$
(32)

If we set,

$$P_{j,\mu} = h^2 \mathcal{S}_{\mu} \mathcal{D}_R^2 \mathcal{S}_{\mu}^{-1} + W_{j,\mu}(R) \,,$$

then equation (29) turns into

$$(P_{1,\mu} - \lambda)\varphi_1 = -hA^0_\mu\varphi_2; \tag{33}$$

$$(P_{1,\mu} - \lambda) \varphi_1 = -h A^0_{\mu} \varphi_2;$$
(33)
$$(P_{2,\mu} - \lambda) \varphi_2 = -h A^{0*}_{\mu} \varphi_1,$$
(34)

where

$$A^0_\mu = ha^0_\mu(R)\mathbf{D}_R.$$

Let us also observe that, by the Weyl theorem, the essential spectrum of P^{\sharp}_{μ} is given by,

$$\operatorname{Sp}_{ess}(P^{\sharp}_{\mu}) = \mathcal{E}_{1}^{\infty} + (1+\mu)^{-2}[0,+\infty).$$

As before, m_j is the local minima of W_j and M^1 is the local maximum of W^1 , as defined in Remark 2.3. Now, for the sake of definiteness, we consider the case where

$$\mathcal{E}_1^{\infty} < m_1 < m_2 < M_1 \tag{35}$$

In the case where $\mathcal{E}_1^{\infty} < m_1 < M_1 < m_2$ then we can apply the same argument to the interval $[m_1, M_1]$.

Remark 4.1. By construction, we have $\operatorname{Sp}(H_{\mu,e}(\mathbf{R})) = \operatorname{Sp}(H_e(I_{\mu}(\mathbf{R})))$. Therefore, if the function s(x) used in the distortion vanishes in a sufficiently compact set (and since $W_{j,\mu}$ and W_j coincide on this set), a continuity argument shows that, for $\mu \in \mathbb{C}$ small enough, the critical points of $\operatorname{Re} W_{j,\mu}$ and W_j coincide and remain non-degenerate.

As a consequence, for any $\lambda \in [m_1, m_2 + \alpha]$ (with $\alpha > 0$ small enough), the function $W_1(R) - \lambda$ presents the shape of a *well in an island* in the sense of [HeSj2]. Moreover, since we are in dimension one, the complementary of the island (that is, the non compact component of $\{W_1 \leq \lambda\}$) is automatically non-trapping, and we can adopt the general strategy used in [Ma2] (see also [CMR, FLM]), that consists in taking $\mu = 2ih \ln \frac{1}{h}$ in the definition of the analytic distortion. The function *s* used in (12)-(13) can also be assumed to be 0 on a neighborhood of the "greatest" island, defined by $\{R > 0; W_1(R) \geq m_1\}$. Then, following [FLM], Theorem 2.2 (see also [HeSj2], Proposition 9.6), we first show that the eigenvalues of P^{\sharp}_{μ} with their real part in $[m_1, m_2 + \alpha]$, coincide, up to an exponentially small error term, with eigenvalues of the Dirichlet realization P^{\sharp}_{D} of P^{\sharp}_{0} on the interval $[0, R_{1,M}]$.

Proposition 4.2. Let $\alpha > 0$ small enough, and let $\mathcal{J} \subset (0, 1]$, with $0 \in \overline{\mathcal{J}}$, such that there exists a function a(h) > 0 defined for $h \in \mathcal{J}$ and verifying,

For all
$$\varepsilon > 0$$
, $a(h) \ge \frac{1}{C_{\varepsilon}} e^{-\varepsilon/h}$ for $h \in \mathcal{J}$ small enough; (36)

$$\operatorname{Sp}(P_D^{\sharp}) \cap [m_2 + \alpha - 2a(h), m_2 + \alpha + 2a(h)] = \emptyset.$$
(37)

Set,

$$\Omega(h) := \{ z \in \mathbb{C} ; \operatorname{dist}(\operatorname{Re} z, [m_1, m_2 + \alpha]) < a(h), |\operatorname{Im} z| < C^{-1}h \ln \frac{1}{h} \},\$$

with C > 0 a large enough constant. Then, there exists $\delta_0 > 0$ and a bijection,

$$b : \operatorname{Sp}(P_D^{\sharp}) \cap [m_1, m_2 + \alpha] \to \operatorname{Sp}(P_{\mu}^{\sharp}) \cap \Omega(h),$$

such that,

$$b(\lambda) - \lambda = \mathcal{O}(e^{-\delta_0/h}),$$

uniformly for $h \in \mathcal{J}$.

Remark 4.3. In our situation, it is well known (see, e.g., [HeRo]) that the distance between two consecutive eigenvalues of the Dirichlet realizations of P_1 and P_2 on $(0, R_{1,M})$, behaves like h as $h \to 0_+$. Then, by slightly moving the parameter α , it is not difficult to deduce that the previous proposition actually gives a complete description of the spectrum of P_{μ}^{\sharp} in a neighborhood of $[m_1, m_2 + \alpha]$, for all sufficiently small values of h > 0. *Proof.* At first, we fix a function $F = F(R) \in C_0^{\infty}((0, R_{1,M}); \mathbb{R}_+)$, such that,

$$\inf_{(0,R_{1,M}]} (W_1 + F) > m_2 + \alpha_2$$

and we denote by $p_{j,\mu} = p_{j,\mu}(R, R^*)$ the principal symbol of the operator $P_{j,\mu}$. We also denote by $\tilde{p}_{j,\mu}$ an almost analytic extension of $p_{j,\mu}$ (see, e.g., [MeSj]).

Then, using the fact that the whole interval of energy $[m_1, m_2 + \alpha]$ is non-trapping for the operator $P_1 + F$, we can construct as in [CMR] Section 7 (or [Ma2] Section 4), a real valued function $f_0 = f_0(R, R^*) \in C_0^{\infty}((\mathbb{R}_+ \setminus \text{Supp } F) \times \mathbb{R})$, such that, on the set $\{F(R) + \text{Re } p_{1,\mu}(R, R^*) \in [m_1 - \delta, m_2 + \alpha + \delta]\}$ (with $\delta > 0$ small enough), one has,

$$-\operatorname{Im}\widetilde{p}_{1,\mu}\left(R-h\ln\frac{1}{h}\left(\partial_{R}f_{0}+i\partial_{R^{*}}f_{0}\right),R^{*}-h\ln\frac{1}{h}\left(\partial_{R^{*}}f_{0}-i\partial_{R}f_{0}\right)\right)\geq\delta h\ln\frac{1}{h}.$$

As a consequence (see, e.g., [CMR] Section 7), if $z \in \mathbb{C}$ is such that $\operatorname{dist}(z, [m_1, m_2 + \alpha]) << h \ln(1/h)$, then, the operator $P_{1,\mu} + F - z$ is invertible on $L^2(\mathbb{R}_+)$, and its inverse satisfies,

$$\|h^{-f_0}T(P_{1,\mu}+F-z)^{-1}u\|_{L^2(\mathbb{R}^2)} \le C|h\ln h|^{-1}\|h^{-f_0}Tu\|_{L^2(\mathbb{R}^2)},\tag{38}$$

where C > 0 is a constant, and $T : L^2(\mathbb{R}_+) \to L^2(\mathbb{R}^2)$ is the Bargmann transform, defined by,

$$Tu(R,R^*) := \frac{1}{2\pi h} \int_{R'>0} e^{i(R-R')R^*/h - (R-R')^2/2h} u(R')dR'.$$

Indeed, for any $v \in C_0^{\infty}(\mathbb{R}_+)$ we have,

$$\|h^{-f_0}Tv\|_{L^2(\mathbb{R}^2)} \le \frac{C}{|h\ln h|} \|h^{-f_0}T(P_{1,\mu} + F - z)v\|_{L^2(\mathbb{R}^2)},$$
(39)

and, by means of a density argument, we can extend such an estimate to any $v \in H^2 \cap H^1_0(\mathbb{R}_+)$. Then, inequality (38) holds true for the function $u = (P_{1,\mu} + F - z)v$, which belongs to the space $L^2(\mathbb{R}_+)$ and satisfies the Dirichlet condition at R = 0. This means that the operator $(P_{1,\mu} + F - z)^{-1}$ has a norm $\mathcal{O}(|h \ln h|^{-1})$ if we consider it as acting on the space $\mathcal{H} = L^2(\mathbb{R}_+)$ endowed with the norm given by: $\|u\|_{\mathcal{H}} := \|h^{-f_0}Tu\|_{L^2(\mathbb{R}^2)}$.

On the other hand, by construction, the operator $P_{2,\mu} + F$ has a real part greater than $m_2 + \alpha$, and thus, if $\operatorname{Re} z \leq m_2 + \alpha$, we also see that the operator $(P_{2,\mu} + F - z)^{-1}$ has a uniformly bounded norm when acting on \mathcal{H} .

Then, proceeding as in [HeSj2], Section 9 (see also [FLM], Section 2), we pick up two functions $\chi_1, \chi_2 \in C_0^{\infty}((0, R_{1,M}); [0, 1])$, such that $\chi_1 = 1$ in a neighborhood of Supp χ_2 , and $\chi_2 = 1$ in a neighborhood of SuppF. Setting,

$$Q^{\sharp}_{\mu} := P^{\sharp}_{\mu} + F \quad ; \quad R^{\sharp}_{\mu}(z) := \chi_1 (P^{\sharp}_D - z)^{-1} \chi_2 + (Q^{\sharp}_{\mu} - z)^{-1} (1 - \chi_2), \tag{40}$$

we see that, if $dist(z, Sp(P_D^{\sharp})) \ge a(h)$, then ([HeSj2], Formula (9.39) and Proposition 9.8),

$$(P^{\sharp}_{\mu} - z)R^{\sharp}_{\mu}(z) = I + K_{\mu}(z)$$
 with $||K_{\mu}(z)||_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(e^{-2\delta/h}),$

where $\delta > 0$ is some constant. Therefore, for such values of z and for h small enough, we have,

$$(P^{\sharp}_{\mu} - z)^{-1} = R^{\sharp}_{\mu}(z) \sum_{j \ge 0} (-K_{\mu}(z))^{j}, \qquad (41)$$

and since $||R_{\mu}^{\sharp}(z)||_{\mathcal{H}} = \mathcal{O}(h^{-C})$ for some constant C > 0, we deduce that, if γ is a simple oriented loop around $\operatorname{Sp}(P_D^{\sharp}) \cap [m_1, m_2 + \alpha]$ such that $\operatorname{dist}(\gamma, \operatorname{Sp}(P_D^{\sharp})) \geq a(h)$ and $\operatorname{dist}(\gamma, [m_1, m_2 + \alpha]) << |h \ln h|$, then,

$$\Pi^{\sharp}_{\mu} := \frac{1}{2i\pi} \int_{\gamma} (z - P^{\sharp}_{\mu})^{-1} dz = -\frac{1}{2i\pi} \int_{\gamma} R^{\sharp}_{\mu}(z) + \mathcal{O}(e^{-\delta/h}) \\ = \frac{1}{2i\pi} \int_{\gamma} \chi_1 (z - P^{\sharp}_D)^{-1} \chi_2 dz + \mathcal{O}(e^{-\delta/h}).$$
(42)

Here, we have also used the fact that $z \mapsto (Q_{\mu}^{\sharp} - z)^{-1}$ is holomorphic in the interior of γ , that can be taken equal to $\Omega(h)$.

Now, since Π^{\sharp}_{μ} is the spectral projector of P^{\sharp}_{μ} associated with $\Omega(h)$, the corresponding resonances of P^{\sharp} are nothing but the eigenvalues of $P^{\sharp}_{\mu}\Pi^{\sharp}_{\mu}$ restricted to the range of Π^{\sharp}_{μ} . Moreover, if we set $\{\mu_1, \ldots, \mu_m\} := \operatorname{Sp}(P^{\sharp}_D) \cap [m_1, m_2 + \alpha]$, and if we denote by $\varphi_1, \ldots, \varphi_m$ an orthonormal basis of $\bigoplus_{j=1}^m \operatorname{Ker}(P^{\sharp}_D - \mu_j)$, then, by Agmon estimates, we see on (42) (see also [HeSj2], Theorem 9.9 and Corollary 9.10) that the functions $\Pi^{\sharp}_{\mu}\chi_1\varphi_j$ ($j=1,\ldots,m$) form a basis of $\operatorname{Ran}\Pi^{\sharp}_{\mu}$, and the matrix of $P^{\sharp}_{\mu}\Big|_{\operatorname{Ran}\Pi^{\sharp}_{\mu}}$ in this basis, is of the form diag $(\mu_1,\ldots,\mu_m) + \mathcal{O}(e^{-\delta/h})$. Then, the result follows from standard arguments on the eigenvalues of finite matrices (plus the fact that $m = \mathcal{O}(h^{-N_0})$ for some $N_0 \geq 1$ constant).

Now, exploiting the fact that both $W_1(R_{1,M})$ and $W_2(R_{1,M})$ are (strictly) greater than m_2 , we consider two functions $\widetilde{W}_j \in C^{\infty}(\mathbb{R}_+; \mathbb{R})$ (j = 1, 2), such that,

 $\widetilde{W}_j = W_j \text{ on } [0, R_{1,M}] \, ; \, \widetilde{W}_j \text{ is constant on } [2R_1^M, +\infty) \, ; \quad \inf_{[R_{1,M}, +\infty)} \widetilde{W}_j > m_2,$

and we set,

$$\widetilde{\mathcal{M}}_0(R) := \begin{pmatrix} \widetilde{W}_1(R) & 0\\ 0 & \widetilde{W}_2(R) \end{pmatrix},$$
$$\widetilde{P}^{\sharp} := h^2 \mathcal{D}_R^2 + \widetilde{\mathcal{M}}_0(R) + h\mathcal{A}_0(R, h\mathcal{D}_R),$$

acting on the space \mathcal{H}^{\sharp} . That is, \widetilde{P}^{\sharp} is obtained form P^{\sharp} by substituting $\widetilde{W}_1, \widetilde{W}_2$ to W_1, W_2 . Then, the same arguments used in Proposition 4.2 (and actually simpler, since both operators are self-adjoints) show that, under the same conditions, the spectrum of P_D^{\sharp} and the spectrum of \widetilde{P}^{\sharp} coincide in $[m_1, m_1 + \alpha + a(h)]$, up to some exponentially small error-terms. Therefore, in order to know the resonances of P^{\sharp} in $\Omega(h)$ (up to those exponentially small error-terms), it is sufficient to study the eigenvalues λ of the self-adjoint \widetilde{P}^{\sharp} in $[m_1, m_1 + \alpha + a(h)]$. For j = 1, 2, we set,

$$\widetilde{P}_j := h^2 D_R^2 + \widetilde{W}_j$$

acting on $L^2(\mathbb{R}^+; dR)$ with Dirichlet condition at R = 0, and we consider separately two different cases.

4.1. Case 1: $\lambda \leq (m_2 - \alpha)$. In that case, the operator $\widetilde{P}_2 - \lambda$ is invertible, with a uniformly bounded inverse, and the equation,

$$\widetilde{P}^{\sharp}\varphi = \lambda\varphi, \quad \varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix},$$
(43)

can be re-written as,

$$\varphi_2 = -h(\widetilde{P}_2 - \lambda)^{-1} A_0^* \varphi_1;$$
$$\left[\widetilde{P}_1 - h^2 A_0 (\widetilde{P}_2 - \lambda)^{-1} A_0^*\right] \varphi_1 = \lambda \varphi_1$$

Thus, the eigenvalues λ are given by the equation,

$$\lambda = f_k(\lambda),\tag{44}$$

where the $\tilde{f}_k(\lambda)$'s are the eigenvalues of $\hat{P}_1(\lambda) := \tilde{P}_1 - h^2 A_0 (\tilde{P}_2 - \lambda)^{-1} A_0^*$. Writing,

$$\hat{P}_1(\lambda) - z = (1 - h^2 A_0 (\widetilde{P}_2 - \lambda)^{-1} A_0^* (\widetilde{P}_1 - z)^{-1}) (\widetilde{P}_1 - z),$$

and observing that, for $z \notin \operatorname{Sp}(\widetilde{P}_1)$, $A_0^*(\widetilde{P}_1 - z)^{-1}$ is bounded and has a norm $\mathcal{O}(\operatorname{dist}(z, \operatorname{Sp}(\widetilde{P}_1))^{-1})$, we conclude that, if dist $(z, \operatorname{Sp}(\widetilde{P}_1)) >> h^2$, then $\hat{P}_1(\lambda) - z$ is invertible, and its inverse satisfies,

$$(\hat{P}_1(\lambda) - z)^{-1} = (\widetilde{P}_1 - z)^{-1} (1 + \mathcal{O}(h^2/\text{dist}(z, \text{Sp}(\widetilde{P}_1))))$$

Differentiating with respect to λ , we also obtain,

$$\frac{d}{d\lambda}(\hat{P}_1(\lambda)-z)^{-1} = (\widetilde{P}_1-z)^{-1}\mathcal{O}(h^2/\text{dist}(z,\operatorname{Sp}(\widetilde{P}_1))) = \mathcal{O}(h^2/\text{dist}(z,\operatorname{Sp}(\widetilde{P}_1))^2).$$

Then, using the fact that, under the non degenerate condition discussed in Remark 4.1, the eigenvalues $E_{1,k}$ $(k \ge 1)$ of \tilde{P}_1 are distant at least of order h between each other, for each of them we can define the projection,

$$\hat{\Pi}_1(\lambda) := \frac{1}{2i\pi} \int_{\gamma_k} (z - \hat{P}_1(\lambda))^{-1} dz,$$

where γ_k is a complex oriented simple circle centered at E_k^1 of radius δh with $\delta > 0$ small enough. Applying standard regular perturbation theory, we easily conclude that the k-th eigenvalue of $\tilde{f}_k(\lambda)$ of $\hat{P}_1(\lambda)$ satisfies,

$$f_k(\lambda) = E_{1,k} + \mathcal{O}(h^2) \quad ; \quad \frac{df_k}{d\lambda}(\lambda) = \mathcal{O}(h),$$
 (45)

uniformly with respect to h small enough, $k \ge 1$ such that $E_k^1 \le m_2 - \frac{1}{2}\alpha$, and $\lambda \le m_2 - \alpha$.

By the implicit function theorem, it follows that the k-th eigenvalue λ_k of P^{\sharp} satisfies,

$$\lambda_k = E_{1,k} + \mathcal{O}(h^2)$$

uniformly with respect to h > 0 small enough and to $k = \mathcal{O}(h^{-1})$, such that $E_{1,k} \leq m_2 - \frac{1}{2}\alpha$.

4.2. Case 2: $\lambda \in [m_2 - \alpha, m_2 + \alpha]$ with $\alpha > 0$ small enough. We denote by ϕ_1, \ldots, ϕ_n an orthonormal family of eigenfunctions of \widetilde{P}_1 with eigenvalues in the interval $[m_2 - 2\alpha, m_2 + 2\alpha]$ and by ψ_1, \ldots, ψ_m an orthonormal family of eigenfunctions of \widetilde{P}_2 with eigenvalues in the interval $[m_2, m_2 + 2\alpha]$ (in particular, we have $n, m = \mathcal{O}(h^{-1})$).

For $\alpha \oplus \beta \in \mathbb{C}^n \oplus \mathbb{C}^m$, we set,

$$R_{-}(\alpha \oplus \beta) := \alpha \cdot \phi \oplus \beta \cdot \psi \in \mathcal{H}^{\sharp},$$

where we have used the notation,

$$\alpha \cdot \phi := \sum_{k=1}^n \alpha_k \phi_k \quad ; \quad \beta \cdot \psi := \sum_{\ell=1}^m \beta_\ell \psi_\ell.$$

We also denote by R_+ the adjoint of R_- , given by,

$$R_+(u\oplus v) = (\langle u, \phi_k \rangle)_{1 \le k \le n} \oplus (\langle v, \psi_\ell \rangle)_{1 \le \ell \le m}.$$

Then, we consider the operator valued matrix,

$$G(\lambda) = \left(\begin{array}{cc} \widetilde{P}^{\sharp} - \lambda & R_{-} \\ R_{+} & 0 \end{array}\right),$$

on

$$\mathcal{H}^{\sharp} \oplus \mathbb{C}^n \oplus \mathbb{C}^m,$$

with domain $(H^2 \cap H^1_0)(\mathbb{R}_+) \oplus (H^2 \cap H^1_0)(\mathbb{R}_+) \oplus \mathbb{C}^n \oplus \mathbb{C}^m$, and we want to know whether $G(\lambda)$ is invertible.

We denote by Π_1 and Π_2 the orthogonal projections on the subspaces S_n and S_m of $L^2(\mathbb{R}_+)$ spanned by the eigenfunctions ϕ_1, \ldots, ϕ_n and ψ_1, \ldots, ψ_m respectively, and we set,

$$\Pi := \begin{pmatrix} \Pi_1 & 0 \\ 0 & \Pi_2 \end{pmatrix}; \ \Pi^{\perp} = \begin{pmatrix} \Pi_1^{\perp} & 0 \\ 0 & \Pi_2^{\perp} \end{pmatrix} := \begin{pmatrix} 1 - \Pi_1 & 0 \\ 0 & 1 - \Pi_2 \end{pmatrix}.$$

We first prove,

Lemma 4.4. For $\lambda \in [m_2 - \alpha, m_2 + \alpha]$, the operator $\Pi^{\perp} \tilde{P}^{\sharp} \Pi^{\perp} - \lambda =: \tilde{P}^{\sharp}_{\perp} - \lambda$ is invertible on the range Ran Π^{\perp} of Π^{\perp} , and its inverse $(\tilde{P}^{\sharp}_{\perp} - \lambda)^{-1}$ is uniformly bounded.

Proof. We have,

$$\Pi^{\perp}(\widetilde{P}^{\sharp} - \lambda)\Pi^{\perp} = \begin{pmatrix} \Pi_{1}^{\perp}(\widetilde{P}_{1} - \lambda)\Pi_{1}^{\perp} & h\Pi_{1}^{\perp}A_{0}\Pi_{2}^{\perp} \\ h\Pi_{2}^{\perp}A_{0}^{*}\Pi_{1}^{\perp} & \Pi_{2}^{\perp}(\widetilde{P}_{2} - \lambda)\Pi_{2}^{\perp} \end{pmatrix},$$

and, denoting by $\widetilde{P}_{j}^{\perp}$ the restriction of \widetilde{P}_{j} to Ran Π_{j}^{\perp} , we know that $\widetilde{P}_{j}^{\perp} - \lambda$ is invertible, and it is standard to show that its inverse is uniformly bounded from Ran Π_{j}^{\perp} to Ran $\Pi_{j}^{\perp} \cap (H^{2} \cap H_{1}^{0})(\mathbb{R}_{+})$, if one takes the *h*-dependent norm on $H^{2}(\mathbb{R}_{+})$ defined by: $\|u\|_{H^{2}}^{2} := \|h^{2}\Delta u\|_{L^{2}}^{2} + \|u\|_{L^{2}}^{2}$. As a consequence, $A_{0}\Pi_{2}^{\perp}(\widetilde{P}_{2}^{\perp} - \lambda)^{-1}\Pi_{2}^{\perp}$ and $A_{0}\Pi_{1}^{\perp}(\widetilde{P}_{1}^{\perp} - \lambda)^{-1}\Pi_{1}^{\perp}$ are uniformly bounded on $L^{2}(\mathbb{R}_{+})$ (together with their adjoint), and we find,

$$\Pi^{\perp}(\widetilde{P}^{\sharp}-\lambda)\Pi^{\perp}\begin{pmatrix} (\widetilde{P}_{1}^{\perp}-\lambda)^{-1} & 0\\ 0 & (\widetilde{P}_{2}^{\perp}-\lambda)^{-1} \end{pmatrix}\Pi^{\perp}=\Pi^{\perp}(1+\mathcal{O}(h))\Pi^{\perp};$$

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$$\Pi^{\perp} \begin{pmatrix} (\widetilde{P}_1^{\perp} - \lambda)^{-1} & 0\\ 0 & (\widetilde{P}_2^{\perp} - \lambda)^{-1} \end{pmatrix} \Pi^{\perp} (\widetilde{P}^{\sharp} - \lambda) \Pi^{\perp} = \Pi^{\perp} (1 + \mathcal{O}(h)) \Pi^{\perp}.$$

Thus, the result follows by taking the restriction to Ran Π^{\perp} , and by using the Neumann series in order to inverse $\Pi^{\perp}(1+\mathcal{O}(h))\Pi^{\perp}|_{\operatorname{Ran} \Pi^{\perp}} = (1+\Pi^{\perp}\mathcal{O}(h))|_{\operatorname{Ran} \Pi^{\perp}}$.

Using the previous lemma, it is easy to show that $G(\lambda)$ is invertible, and to check that its inverse is given by,

$$G(\lambda)^{-1} = \begin{pmatrix} \Pi^{\perp} (\widetilde{P}_{\perp}^{\sharp} - \lambda)^{-1} \Pi^{\perp} & (1 - \Pi^{\perp} (\widetilde{P}_{\perp}^{\sharp} - \lambda)^{-1} \Pi^{\perp} \widetilde{P}^{\sharp}) R_{-} \\ R_{+} (1 - \widetilde{P}^{\sharp} \Pi^{\perp} (\widetilde{P}_{\perp}^{\sharp} - \lambda)^{-1} \Pi^{\perp}) & \lambda - Q(\lambda) \end{pmatrix}$$

with,

$$Q(\lambda) := R_{+} \widetilde{P}^{\sharp} (1 - \Pi^{\perp} (\widetilde{P}_{\perp}^{\sharp} - \lambda)^{-1} \Pi^{\perp} \widetilde{P}^{\sharp}) R_{-}.$$

$$\tag{46}$$

In particular, $Q(\lambda)$ is an $(n+m) \times (n+m)$ matrix with $n, m = \mathcal{O}(h^{-1})$.

Proposition 4.5. The matrix $Q(\lambda)$ satisfies,

 $Q(\lambda) = \text{diag} (E_{1,1}, \dots, E_{1,n}, E_{2,1}, \dots, E_{2,m}) + S(\lambda),$

where $E_{1,j}, E_{2,k} \in [m_2 - 2\alpha, m_2 + 2\alpha]$ are the eigenvalues associated with ϕ_j and ψ_k , respectively, and with,

$$||S(\lambda)|| + ||\frac{d}{d\lambda}S(\lambda)|| = \mathcal{O}(h^2),$$

in the sense of the norm of operators on \mathbb{C}^{n+m} , and uniformly with respect to h > 0 small enough and $n, m = \mathcal{O}(h^{-1})$.

Proof. Since $R_{+}\Pi^{\perp} = 0$ and $\Pi^{\perp}R_{-} = 0$, by (46), we have,

$$Q(\lambda) = R_{+} \widetilde{P}^{\sharp} R_{-} - R_{+} \Pi \widetilde{P}^{\sharp} \Pi^{\perp} (\widetilde{P}_{\perp}^{\sharp} - \lambda)^{-1} \Pi^{\perp} \widetilde{P}^{\sharp} \Pi R_{-},$$
(47)

$$\frac{d}{d\lambda}Q(\lambda) = R_{+}\Pi\widetilde{P}^{\sharp}\Pi^{\perp}(\widetilde{P}_{\perp}^{\sharp} - \lambda)^{-2}\Pi^{\perp}\widetilde{P}^{\sharp}\Pi R_{-}, \qquad (48)$$

and, since $\Pi_j \widetilde{P}_j \Pi_j^{\perp} = 0 \ (j = 1, 2),$

$$\Pi \widetilde{P}^{\sharp} \Pi^{\perp} = \begin{pmatrix} 0 & h \Pi_1 A_0 \Pi_2^{\perp} \\ h \Pi_2 A_0^* \Pi_1^{\perp} & 0 \end{pmatrix}.$$

$$\tag{49}$$

Moreover, using that $\|\widetilde{P}_{j}\Pi_{j}\|_{\mathcal{L}(L^{2})} \leq |m_{2}| + 2\alpha$ and the ellipticity of \widetilde{P}_{j} , it is easy to see that both $A_{0}^{*}\Pi_{1}$ and $A_{0}\Pi_{2}$ are uniformly bounded, thus so are their adjoints $\Pi_{1}A_{0}$ and $\Pi_{2}A_{0}^{*}$, and we deduce from (47)-(49) (plus the fact that $\|R_{\pm}\| \leq 1$),

$$Q(\lambda) = R_{+} \widetilde{P}^{\sharp} R_{-} + \mathcal{O}(h^{2}) \quad ; \quad \frac{d}{d\lambda} Q(\lambda) = \mathcal{O}(h^{2}).$$
(50)

Therefore, in order to complete the proof of Proposition 4.5, it is enough to show,

Lemma 4.6. For all $N \ge 0$, there exists a constant $C_N > 0$ such that, for all $j \in \{1, ..., n\}$ and $k \in \{1, ..., m\}$, one has,

$$|\langle A_0\phi_j,\psi_k\rangle| + |\langle A_0\psi_k,\phi_j\rangle| \le C_N h^N.$$

Proof. We use the equations,

$$(\tilde{P}_1 - E_{1,j})\phi_j = 0 \quad ; \quad (\tilde{P}_2 - E_{2,k})\psi_k = 0.$$
 (51)

At first, we observe that, for R close enough to 0 (say, $0 < R < r_0$), and R large enough (say, $R > R_0$), both $W_1(R) - E_{1,j}$ and $W_2(R) - E_{2,k}$ remain greater than some fix constant C > 0. Therefore, by standard Agmon estimates (see, e.g., [Ma1], Chapter 3, exercise 8), it is easy to show that, for h small enough,

$$\|\phi_j\|_{H^s((0,r_0)\cup(R_0,+\infty))} + \|\psi_k\|_{H^s((0,r_0)\cup(R_0,+\infty))} \le e^{-c_0/h},\tag{52}$$

where the positive constant c_0 does not depend on $j, k = \mathcal{O}(h^{-1})$, and $s \ge 0$ is arbitrary.

For $\ell = 1, 2$, we set,

$$\Sigma_{\ell} := \{ (R, R^*) \in \mathbb{R}_+ \times \mathbb{R} \, ; \, \widetilde{p}_{\ell}(R, R^*) \in [m_2 - 2\alpha, m_2 + 2\alpha] \}$$

(where we have used the notation $\widetilde{p}_{\ell}(R, R^*) := (R^*)^2 + \widetilde{W}_{\ell}(R)$), and we chose $\chi_{\ell} \in C_0^{\infty}((\frac{1}{2}r_0, 2R_0) \times \mathbb{R})$, supported near Σ_{ℓ} , such that $\chi_{\ell} = 1$ in a neighborhood of Σ_{ℓ} . We also fix $\chi_0 = \chi_0(R) \in C_0^{\infty}(\frac{1}{2}r_0, 2R_0)$, such that $\chi_0 = 1$ near $[r_0, R_0]$.

Then, using standard pseudo-differential calculus, for any $E \in [m_2 - 2\alpha, m_2 + 2\alpha]$ one can construct a symbol $q_{\ell}(E) = q_{\ell}(E, R, R^*; h) \in S(\langle R^* \rangle^{-2})$, supported in $(\frac{1}{2}r_0, 2R_0) \times \mathbb{R}$ and depending smoothly on E, such that,

$$q_{\ell}(E) \# (\widetilde{p}_{\ell} - E)(R, R^*) \sim \chi_0(R)(1 - \chi_{\ell}(R, R^*)).$$
(53)

Here, # stands for the Weyl-composition of symbols, and the asymptotic equivalence holds in S(1), uniformly with respect to $E \in [m_2 - 2\alpha, m_2 + 2\alpha]$ (see, e.g., [Ma1]). Then, first multiplying (51) by χ_0 , then, commuting χ_0 and \tilde{P}_j , and finally applying the usual Weyl-quantization of $q_\ell(E)$ (with $E = E_{1,j}, E_{2,k}$, respectively), we deduce from (51), (52) and (53),

$$\|(1 - \chi_1(R, hD_R))\chi_0\phi_j\|_{H^s} = \mathcal{O}(h^\infty);$$
(54)

$$\|(1 - \chi_2(R, hD_R))\chi_0\psi_k\|_{H^s} = \mathcal{O}(h^\infty)$$
(55)

uniformly with respect to j, k (here, $\chi_{\ell}(R, hD_R)$ stands for the Weyl-quantization of χ_{ℓ}).

Now, if α is taken sufficiently small, the sets Σ_1 and Σ_2 are disjoints, and thus the supports of χ_1 and χ_2 can be taken disjoints, too. Since they are also disjoints from Supp $(1 - \chi_0)$, one can find $\chi_3 \in C^{\infty}(\mathbb{R}_+ \times \mathbb{R}; [0, 1])$, supported in $(\frac{1}{2}r_0, 2R_0) \times \mathbb{R}$, such that the family $\{\chi_1, \chi_2, \chi_3\}$ forms a partition of unity on Supp $\chi_0 \times \mathbb{R}$. In particular, on $L^2(\mathbb{R}_+)$, one has,

$$1 - \chi_0(R) + \sum_{\ell=1}^{3} \chi_\ell(R, hD_R)\chi_0(R) = I,$$

and now, it is clear that, inserting this microlocal partition of unity in the products $\langle A_0\phi_j,\psi_k\rangle$ and $\langle A_0\psi_k,\phi_j\rangle$, the estimates (52), (54) and (55) give the required result.

Remark 4.7. Actually, following more precisely the construction of \widetilde{H}_e^{μ} made in Section 4, one can prove that the functions \widetilde{W}_j (j = 1, 2) and a_0 depend in an analytic way of R in a neighborhood of the relevant classically allowed region $\{\widetilde{W}_1(R) \leq m_2 + 2\alpha\}$. As a consequence, one can use the standard microlocal analytic techniques in this region (see, e.g., [Sj, Ma1]), and obtain the existence of a constant $c_0 > 0$ (independent of j, k), such that,

$$|\langle A_0\phi_j,\psi_k\rangle| + |\langle A_0\psi_k,\phi_j\rangle| \le e^{-c_0/h}.$$

Completion of the proof of the proposition: Since the matrix,

$$R_{+}\widetilde{P}^{\sharp}R_{-} - \operatorname{diag}\left(E_{1,1}, \dots, E_{2,m}\right) = \left(\begin{array}{cc} 0 & \left(\langle A_{0}\psi_{k}, \phi_{j}\right) \\ \left(\langle A_{0}^{*}\phi_{j}, \psi_{k}\rangle\right) & 0 \end{array}\right)$$

is of size $\mathcal{O}(h^{-1})$, Lemma 4.6 implies that it has a norm $\mathcal{O}(h^{\infty})$ on \mathbb{C}^{n+m} , uniformly with respect to n, m. Thus, Proposition 4.5 is a consequence of (50).

By the Min-Max principle, it results from Proposition 4.5 that, for $\lambda \in [m_2 - \alpha, m_2 + \alpha]$, the eigenvalues $g_1(\lambda), \ldots, g_{m+n}(\lambda)$ of $Q(\lambda)$ satisfy,

$$\{g_1(\lambda), \dots, g_{m+n}(\lambda)\} = \{E_{1,1}, \dots, E_{1,n}, E_{2,1}, \dots, E_{2,m}\} + \mathcal{O}(h^2);$$

$$\lambda \mapsto g_\ell(\lambda) \text{ is Lipschitz continuous } (\ell = 1, \dots, n+m);$$

$$\left|\frac{dg_\ell}{d\lambda}\right| = \mathcal{O}(h^2) \ a.e. \ (k = 1, \dots, n+m).$$
(56)

Note that the values $E_{1,1}, \ldots, E_{1,n}$ are at a distance of order h from each other, and the same is true for the values $E_{2,1}, \ldots, E_{2,m}$. So the only problem that may appear in the computation of $g_{\ell}(\lambda)$ is when, along some sequence $h = h_j \to 0_+$, two values $E_{1,j}$ and $E_{2,k}$ become closer than $\mathcal{O}(h^2)$. But, in that case, the two corresponding values of $g_{\ell}(\lambda)$ are given by,

$$g_{\ell}(\lambda) = \frac{1}{2} \left(E_{1,j} + E_{2,k} + h^2 r_1 \pm \sqrt{(E_{1,j} - E_{2,k} + h^2 r_2)^2 + h^4 r_3^2} \right), \tag{57}$$

with $r_t = r_t(\lambda)$ smooth, $r_t = \mathcal{O}(1)$, $dr_t/d\lambda = \mathcal{O}(1)$ (t = 1, 2, 3). Thus, actually, a correct (*h*-depending) indexing of the g_ℓ 's make them smooth functions of λ , and then (56) becomes true everywhere.

Anyway, (56) is enough to insure that all the values of $\lambda \in [m_2 - \alpha, m_2 + \alpha]$ such that $\lambda \in \text{Sp } Q(\lambda)$ verify,

dist
$$(\lambda, \{E_{1,1}, \ldots, E_{1,n}, E_{2,1}, \ldots, E_{2,m}\}) = \mathcal{O}(h^2),$$

and, conversely, at any $E \in \{E_{1,1}, \ldots, E_{1,n}, E_{2,1}, \ldots, E_{2,m}\} \cap [m_2 - \alpha + Ch^2, m_2 + \alpha - Ch^2]$ (C > 0 large enough), can be associated a unique $\lambda \in [m_2 - \alpha, m_2 + \alpha]$ such that $\lambda \in \text{Sp } Q(\lambda)$.

Finally, using the fact that, by construction, the eigenvalues of \hat{P}^{\sharp} that lie in $[m_2 - \alpha, m_2 + \alpha]$ coincide with the solutions there of $\lambda \in \text{Sp } Q(\lambda)$, and summing up with the results of Subsection 4.1 and Proposition 4.2, we finally obtain,

Theorem 4.8. For h > 0 small enough the resonances of P^{\sharp} with real part in $[m_1, m_2 + \alpha]$ and with imaginary part $\langle |h \ln h|$, coincide, up to $\mathcal{O}(h^2)$ errorterms, with eigenvalues of the Dirichlet realizations of P_1 and P_2 on $(0, R_{1,M})$, where $R_{1,M} > 0$ is the point where W_1 admits a local maximum with value greater than m_2 . RESONANT STATES FOR A THREE-BODY PROBLEM UNDER AN EXTERNAL FIELD 25

5. Comparison between the spectrum of the operators P^{\sharp}_{μ} and \hat{H}^{0}_{μ}

Here we prove,

Proposition 5.1. Let $\alpha > 0$ fixed small enough, and let $\mathcal{J} \subset (0, 1]$, with $0 \in \overline{\mathcal{J}}$, such that there exists $\delta > 0$ such that,

$$\operatorname{Sp}(P_D^{\sharp}) \cap [m_2 + \alpha - 2\delta h, m_2 + \alpha + 2\delta h] = \emptyset.$$
(58)

Set,

$$\Omega(h) := \{ z \in \mathbb{C} ; \operatorname{dist}(\operatorname{Re} z, [m_1, m_2 + \alpha]) < \delta h, |\operatorname{Im} z| < C^{-1} h \ln \frac{1}{h} \},\$$

with C > 0 a large enough constant. Then, there exists a bijection,

$$b : \operatorname{Sp}(P^{\sharp}_{\mu}) \cap \Omega(h) \to \operatorname{Sp}(\widetilde{H}^{0}_{\mu}) \cap \Omega(h),$$

 $such\ that,$

$$b(\lambda) - \lambda = \mathcal{O}(h^2),$$

uniformly for $h \in \mathcal{J}$.

Remark 5.2. As before, by slightly moving the parameter α , one can actually reach all the values of h > 0 small enough.

Proof. By Corollary 3.9, it is enough to prove that, for any $z \in \Omega(h)$, there exists a bijection

$$b_z : \operatorname{Sp}(P^{\sharp}_{\mu}) \cap \Omega(h) \to \operatorname{Sp}(\widetilde{P}^0_{\mu}(z)) \cap \Omega(h)$$

such that,

$$b_z(\lambda) - \lambda = \mathcal{O}(h^2),$$

uniformly for $h \in \mathcal{J}$ and $z \in \Omega(h)$. By (23) we have,

$$\widetilde{P}^{0}_{\mu}(z) = Q^{0}_{\mu} + h^{2} \mathcal{B}^{0}_{\mu},$$
(59)

where B^0_{μ} stands for the restriction of $\mathcal{B}_{\mu}(\mathbf{R}, h\mathbf{D}_{\mathbf{R}}; z, h)$ to $Ker(\mathbf{L}_R)$, and where we have set,

$$Q^{0}_{\mu} := Q_{\mu} |_{Ker(\mathbf{L}_{R})} ,$$
$$Q_{\mu} := -h^{2} \mathcal{S}_{\mu} \Delta_{\mathbf{R}} \mathcal{S}_{\mu}^{-1} + \mathcal{M}_{\mu}(R) + h \mathcal{A}_{\mu}(\mathbf{R}, h \mathcal{D}_{\mathbf{R}}).$$

By passing in polar coordinates, and by conjugating Q_{μ} with the transform

$$L^{2}(\mathbb{R}_{+}; R^{2}dR) \otimes L^{2}(S^{2}) \ni \psi \mapsto R\psi \in L^{2}(\mathbb{R}_{+}; dR) \otimes L^{2}(S^{2}),$$

we see that Q^0_{μ} is unitarily equivalent to,

$$\widetilde{Q}^0_{\mu} := h^2 \mathcal{S}_{\mu} \mathrm{D}^2_R \mathcal{S}^{-1}_{\mu} + \mathcal{M}_{\mu}(R) + h \mathcal{A}^0_{\mu}(R, h \mathrm{D}_R)$$

on $L^2(\mathbb{R}_+; dR)$ with Dirichlet boundary condition at R = 0 (the notations are those of the previous section, in particular (32)). We first have,

Lemma 5.3. There exist $\delta_0 > 0$ and a bijection,

$$b_0 : \operatorname{Sp}(P^{\sharp}_{\mu}) \cap \Omega(h) \to \operatorname{Sp}(Q^0_{\mu}) \cap \Omega(h),$$

such that,

$$b_0(\lambda) - \lambda = \mathcal{O}(e^{-\delta_0/h}),$$

uniformly for $h \in \mathcal{J}$.

Proof. This is just a slight modification of the proof of Proposition 4.2. Indeed, using (25), we see that the proof can be repeated exactly in the same way by substituting \tilde{Q}^0_{μ} to P^{\sharp}_{μ} . Thus, both the spectra of \tilde{Q}^0_{μ} and P^{\sharp}_{μ} are close to that of P^{\sharp}_{D} up to exponentially small error terms, and since \tilde{Q}^0_{μ} and Q^0_{μ} have the same spectrum, the result follows.

Therefore, it only remains to compare the spectra of $\widetilde{P}^0_{\mu}(z)$ and Q^0_{μ} .

For any fixed integer $k \geq 1$, let us denote by $E_k = E_k(h)$ the k-th eigenvalue of P_2 . By the previous lemma and Remark 4.3, we see that, if we fix $\delta > 0$ sufficiently small, then, the disc $\{\lambda \in \mathbb{C} ; |\lambda - E_k(h)| \leq \delta h\}$ contains at most two eigenvalues of Q^0_{μ} (for h > 0 small enough) and, on the set \mathcal{J}_k of those values of h for which it contains two eigenvalues, the domain $\{\lambda \in \mathbb{C} ; \delta h < |\lambda - E_k(h)| \leq 2\delta h\}$ does not meet $\operatorname{Sp}(Q^0_{\mu})$.

Then, for $k \ge 1$ we define,

$$\gamma_k(h) = \begin{cases} \{\lambda \in \mathbb{C} ; |\lambda - E_k(h)| = 3\delta h/2\} \text{ if } h \in \mathcal{J}_k; \\ \{\lambda \in \mathbb{C} ; |\lambda - E_k(h)| = \delta h/2\} \text{ if } h \in \mathcal{J} \setminus \mathcal{J}_k. \end{cases}$$
(60)

In the same way, the set $\{\lambda \in \mathbb{C} ; |\lambda - m_2| \leq \delta h\}$ contains at most one eigenvalue of Q^0_{μ} , and on the set \mathcal{J}_0 of those values of h for which it contains one eigenvalue, the domain $\{\lambda \in \mathbb{C} ; \delta h < |\lambda - m_2| \leq 2\delta h\}$ does not meet $\operatorname{Sp}(Q^0_{\mu})$. Then, we set,

$$\gamma_0(h) = \begin{cases} \{\lambda \in \mathbb{C} ; \operatorname{dist}(\lambda, [m_1, m_2]) = 3\delta h/2 \} & \text{if } h \in \mathcal{J}_0; \\ \{\lambda \in \mathbb{C} ; \operatorname{dist}(\lambda, [m_1, m_2]) = \delta h/2 \} & \text{if } h \in \mathcal{J} \setminus \mathcal{J}_0. \end{cases}$$

When $\lambda \in \gamma_k(h)$ $(k \ge 0)$, we see as in the proof of Proposition 4.2 (see (41)) that the inverse of $\widetilde{Q}^0_{\mu} - \lambda$ can be written as,

$$(\widetilde{Q}^0_{\mu} - \lambda)^{-1} = \chi_1 (\widetilde{Q}_D - \lambda)^{-1} \chi_2 + \mathcal{R}(\lambda),$$

where \widetilde{Q}_D is the Dirichlet realization of \widetilde{Q}^0_{μ} on $[0, R_{1,M}]$, χ_1, χ_2 are as in (40), and $\mathcal{R}(\lambda)$ satisfies,

$$\|\mathcal{R}(\lambda)\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(|h\ln h|^{-1})$$

as in (39). Here, \mathcal{H} is the space introduced in the proof of Proposition 4.2. In particular, we obtain,

$$\|(\widetilde{Q}^0_{\mu} - \lambda)^{-1}\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(h^{-1}).$$

and thus, if we denote by \mathcal{K}_0 the space $Ker(L_{\mathbf{R}})$ endowed with the norm

$$\|\psi\|_{\mathcal{K}_0} := \|R\psi(R\omega)\|_{\mathcal{H}\otimes L^2(S^2)},$$

we have,

$$\|(Q^0_{\mu} - \lambda)^{-1}\|_{\mathcal{L}(\mathcal{K}_0)} = \mathcal{O}(h^{-1}).$$
(61)

On the other hand, thanks to (27), and by using the Calderon-Vaillancourt theorem (see, e.g., [Ma1]), it is not difficult to show that the operator \mathcal{B}^0_{μ} is uniformly bounded on \mathcal{K}_0 (for instance, one can start by working on $C_0^{\infty}(\mathbb{R}^3 \setminus 0)$ with the so-called right-quantization, in order to be able to pass in polar coordinates without problem, and then use a density argument and the fact that the polynomial weight used in the definition of \mathcal{H} becomes trivial near R = 0).

Therefore, we see on (59) that, for h > 0 small enough and $\lambda \in \bigcup_{k \ge 0} \gamma_k(h)$, the operator $\widetilde{P}^0_{\mu}(z) - \lambda$ is invertible, and its inverse can be written as,

$$(\widetilde{P}^{0}_{\mu}(z) - \lambda)^{-1} = (Q^{0}_{\mu} - \lambda)^{-1} \left(I - h^{2} \mathcal{B}^{0}_{\mu} (Q^{0}_{\mu} - \lambda)^{-1} + \mathcal{O}(h^{2}) \right),$$
(62)

in $\mathcal{L}(\mathcal{K}_0)$. For $k \ge 0$, we set,

$$\Pi_{P,k}(h) := \frac{1}{2i\pi} \oint_{\gamma_k(h)} (\lambda - \widetilde{P}^0_\mu(z))^{-1} d\lambda;$$
$$\Pi_{Q,k}(h) := \frac{1}{2i\pi} \oint_{\gamma_k(h)} (\lambda - Q^0_\mu)^{-1} d\lambda.$$

In particular, for $k \geq 1$, the rank of $\Pi_{Q,k}(h)$ is 1 or 2, depending if $h \in \mathcal{J}_k$ or not. In both cases, (61)-(62) show that the ranks of $\Pi_{P,k}(h)$ and $\Pi_{Q,k}(h)$ are identical, and that the eigenvalues of $\widetilde{P}^0_{\mu}(z)$ inside $\gamma_k(h)$ coincide to those of Q^0_{μ} up to $\mathcal{O}(h^2)$ (the computation is similar to that of (57)).

For k = 0, the situation is even simpler, because we know that the eigenvalues of Q^0_{μ} that lie inside $\gamma_0(h)$ are simple and separated by a distance of order h, and the same result holds.

Finally, for $\lambda \in \Omega(h)$ in the exterior of all the $\gamma_k(h)$'s, the estimate (61) is still valid, and thus so is (62). Therefore, the spectral projector of $\tilde{P}^0_{\mu}(z)$ on $\Omega(h)$ can be split into a finite sum of the $\Pi_{P,k}(h)$ (with a number of k's that is $\mathcal{O}(h^{-1})$), and the previous arguments show that the eigenvalues of $\tilde{P}^0_{\mu}(z)$ in $\Omega(h)$ coincide with those of Q^0_{μ} up to $\mathcal{O}(h^2)$.

6. Comparison between the spectrum of the operators \widetilde{H}^0_μ and H^0_μ

We have,

Proposition 6.1. Let $\alpha > 0$ fixed small enough, and let $\mathcal{J} \subset (0, 1]$, with $0 \in \overline{\mathcal{J}}$, such that there exists $\delta > 0$ such that,

$$\operatorname{Sp}(P_D^{\sharp}) \cap [m_2 + \alpha - 2\delta h, m_2 + \alpha + 2\delta h] = \emptyset.$$
(63)

Set,

$$\Omega(h) := \{ z \in \mathbb{C} ; \operatorname{dist}(\operatorname{Re} z, [m_1, m_2 + \alpha]) < \delta h, |\operatorname{Im} z| < C^{-1}h \ln \frac{1}{h} \},\$$

with C > 0 a large enough constant. Then, there exists $\delta_0 > 0$ and a bijection,

$$b : \operatorname{Sp}(\widetilde{H}^0_{\mu}) \cap \Omega(h) \to \operatorname{Sp}(H^0_{\mu}) \cap \Omega(h),$$

such that,

$$b(\lambda) - \lambda = \mathcal{O}(e^{-\delta_0/h}),$$

uniformly for $h \in \mathcal{J}$.

Proof. To prove this result, we use the arguments of Proposition 6.1 in [MaMe]. In particular we have to check that condition (6.6) in [MaMe] holds true. We consider the oriented loop,

$$\gamma(h) := \{ z \in \mathbb{C} ; \operatorname{dist}(z, [m_1, m_2 + \alpha]) = \delta h/2 \}.$$

By (28) and the results of the previous section (in particular (61)-(62)), we already know that there exists some constant C > 0 such that,

$$\sup_{z\in\gamma(h)} \|(z-\widetilde{H}^0_{\mu})^{-1}\|_{\mathcal{L}(Ker(\mathbf{L}_{\mathbf{R}}+\mathbf{L}_{\mathbf{r}}))} = \mathcal{O}(h^{-C}).$$

We set,

$$\widetilde{\Pi}_{\mu} := \frac{1}{2i\pi} \oint_{\gamma(h)} (z - \widetilde{H}^0_{\mu})^{-1} dz,$$

and we denote by $F = F(R) \in C_0^{\infty}((\frac{4}{M}, R_{1,M}); \mathbb{R}_+)$ a function that 'fills the wells', in the same sense as in the proof of Proposition 4.2, that is,

$$\inf_{(0,R_{1,M}]} (W_1 + F) > m_2 + \alpha.$$
(64)

Then, we set,

$$\widehat{H}^{0}_{\mu} = H^{0}_{\mu} + F(R), \tag{65}$$

and we first prove,

Lemma 6.2. Let $\Gamma(h)$ be the closure of the complex domain surrounded by $\gamma(h)$. Then, there exists a constant C > 0 such that, for all $z \in \Gamma(h)$, one has,

$$\left\| (\widehat{H}^0_{\mu} - z)^{-1} \right\|_{\mathcal{L}(Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}}))} = \mathcal{O}(h^{-C}),$$

uniformly for h > 0 small enough.

Proof. We use a standard method of localization that consists in decoupling the effects of the barrier from those of the remaining part of the operator (see, e.g., [BCD]).

We fix a, b > 0 such that $\frac{3}{M} < a < b < \frac{4}{M}$, and we denote by $J_I, J_E \in C^{\infty}(\mathbb{R}_+; [0, 1])$ two functions satisfying,

$$\operatorname{Supp} J_I \subset [0, b]; \operatorname{Supp} J_E \subset (a, +\infty);$$
(66)

$$J_I = 1$$
 on $[0, a]; J_E = 1$ on $[b, +\infty);$ (67)

$$J_I^2 + J_E^2 = 1. ag{68}$$

Next we denote by \mathcal{H}_I the space $\{u \mid_{\{|\mathbf{R}| \leq b\}}; u \in Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})\}$ endowed with the standard L^2 -norm, and \mathcal{H}_E the space $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})$ endowed with the norm,

$$\|u\|_{\mathcal{H}_E} := \|Ru(R\omega, \mathbf{r})\|_{\mathcal{H}\otimes L^2(S^2_{\omega})\otimes L^2(\mathbb{R}^3_{\mathbf{r}})}.$$

We also define $\widetilde{\mathcal{H}}$ as the space $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})$ endowed with the norm,

$$||u||_{\widetilde{\mathcal{H}}} := \left(||J_I u||_{L^2}^2 + ||J_E u||_{\mathcal{H}_E}^2 \right)^{\frac{1}{2}}.$$

All these norms are clearly equivalent to the standard L^2 -norms, with constants of equivalence of order $h^{\pm C}$ with C > 0 constant, that is

$$h^{C} \|u\|_{L^{2}} \le \|u\|_{\mathcal{H}_{E}} \le h^{-C} \|u\|_{L^{2}}.$$

In particular, it is enough to prove the result with $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})$ substituted by $\widetilde{\mathcal{H}}$.

Moreover, we have the so-called identifying operators,

$$J: \begin{array}{cccc} \mathcal{H}_{I} \oplus \mathcal{H}_{E} & \to & \widetilde{\mathcal{H}} \\ & u \oplus v & \mapsto & J_{I}u + J_{E}v \\ \widetilde{J}: & \widetilde{\mathcal{H}} & \to & \mathcal{H}_{I} \oplus \mathcal{H}_{E} \\ & w & \mapsto & J_{I}w \oplus J_{E}w \end{array}$$

that satisfy $J\widetilde{J} = \mathbf{1}_{\widetilde{\mathcal{H}}}$, $\|\widetilde{J}\| = 1$ (actually, \widetilde{J} is an isometry, and is nothing but the adjoint of J for the standard L^2 -scalar product). By standard estimates on the transform T (see, e.g., [Ma1]), one can also easily see that $\|J\| = \mathcal{O}(1)$ uniformly as $h \to 0$.

Observing that the operator \widehat{H}^0_{μ} is differential with respect to **R** (with operatorvalued coefficients acting on $L^2(\mathbb{R}^3_{\mathbf{r}})$), we can consider the zero Dirichlet boundary condition at $|\mathbf{R}| = b$ realizations H_I of \widehat{H}^0_{μ} on \mathcal{H}_I (note that it is nothing else but the restriction to $Ker(\mathbf{L}_{\mathbf{R}} + \mathbf{L}_{\mathbf{r}})$ of the Dirichlet realizations of $H_{\mu} + F$ on $L^2(|\mathbf{R}| < b)$). Finally, we set

$$H_E := \widetilde{H}^0_\mu + F_z$$

acting on \mathcal{H}_E , and we define,

$$H_A := H_I \oplus H_E$$

as an operator acting on $\mathcal{H}_I \oplus \mathcal{H}_E$. Then, setting, $\Theta := \widehat{H}^0_{\mu} J - J H_A,$

it is elementary to check the identity,

$$(\widehat{H}^0_{\mu} - z)^{-1} = J(H_A - z)^{-1}\widetilde{J} - (\widehat{H}^0_{\mu} - z)^{-1}\Theta(H_A - z)^{-1}\widetilde{J}.$$
(69)

Using (28) and proceeding as in the proof of Proposition 4.2 and in Section 5, we immediately obtain,

$$\|(H_E - z)^{-1}\|_{\mathcal{L}(\mathcal{H}_E)} = \mathcal{O}(|h\ln h|^{-1}).$$
(70)

On the other hand, since b < 4/M, by (24)-(25) we have,

$$\operatorname{Re} H_I \ge \frac{M}{4} + \inf_R \mathcal{E}_1(R) \ge m_2 + \alpha + 1,$$

if $M \ge 1$ has been chosen sufficiently large. As a consequence, for $z \in \Gamma(h)$, we have,

$$\|(H_I - z)^{-1}\|_{\mathcal{L}(\mathcal{H}_I)} = \mathcal{O}(1), \tag{71}$$

uniformly. From (70)-(71), we deduce,

 $\|\langle l$

$$\|(H_A-z)^{-1}\|_{\mathcal{L}(\mathcal{H}_I\oplus\mathcal{H}_E)}=\mathcal{O}(|h\ln h|^{-1}),$$

and thus also, by standard estimates on the Laplacian,

$$n\nabla_{\mathbf{R}}\rangle(H_A - z)^{-1}\|_{\mathcal{L}(\mathcal{H}_I \oplus \mathcal{H}_E)} = \mathcal{O}(|h\ln h|^{-1}).$$
(72)

Now, we compute,

$$\begin{aligned} \Theta(u \oplus v) &= -h^2[\Delta_{\mathbf{R}}, J_I]u - h^2[\Delta_{\mathbf{R}}, J_E]v \\ &= -h^2(2(\nabla_{\mathbf{R}}J_I)\nabla_{\mathbf{R}} + (\Delta_{\mathbf{R}}J_I))u - h^2(2(\nabla_{\mathbf{R}}J_E)\nabla_{\mathbf{R}} + (\Delta_{\mathbf{R}}J_E))v. \end{aligned}$$

Therefore, we deduce from (72) that we have,

$$\|\Theta(H_A - z)^{-1}\widetilde{J}\|_{\mathcal{L}(\widetilde{\mathcal{H}})} = \mathcal{O}(|\ln h|^{-1}).$$

FIGURE 2. Construction of the cut-off functions χ_1 and χ_2 .

In particular, for h small enough we obtain $\|\Theta(H_A - z)^{-1}\widetilde{J}\|_{\mathcal{L}(\widetilde{\mathcal{H}})} \leq 1/2$, and then, by using (69) and, again, (72), we finally deduce,

$$\|(\widehat{H}^0_{\mu} - z)^{-1}\|_{\mathcal{L}(\widetilde{\mathcal{H}})} = \mathcal{O}(|h\ln h|^{-1}),$$

and the result follows.

Now, let (see Fig. 2)

$$\begin{split} R_1 &:= \inf\{R > 0 \ ; \ W_1(R) = m_2 + \alpha, \ W_1'(R) > 0\};\\ R_2 &:= \inf\{R > R_1 \ ; \ W_1(R) = m_2 + \alpha, \ W_1'(R) < 0\}.\\ \text{Let also } \chi_1(R), \chi_2(R) \in C_0^\infty([0, R_2]), \text{ and } R_3 \in (R_1, R_2), \text{ such that,} \end{split}$$

 $\chi_1 = \chi_2 = 1 \text{ near } [0, R_1] \quad ; \quad \text{supp}\chi_2 \subset [0, R_3] \subset \{\chi_1 = 1\}.$

We can also assume that the function F(R) used in (64) is such that $\chi_1 = \chi_2 = 1$ in a neighborhood of SuppF, too.

Then, following [HeSj2], we set,

$$\mathcal{R}_1(z) = \chi_1 (H_D - z)^{-1} \chi_2 + (\widehat{H}^0_\mu - z)^{-1} (1 - \chi_2),$$

where H_D is the Dirichlet realization of H^0_{μ} on $L^2(\{|\mathbf{R}| \leq R_3\} \times \mathbb{R}^3)$. Actually, H_D does not depend on μ since $S_{\mu} \equiv 1$ for $|\mathbf{R}| < R_3$. Since $\chi_1 \chi_2 = \chi_2$, it follows from this definition (recalling that $H^0_{\mu} = \hat{H}^0_{\mu} - F(R)$), that we have,

$$(H^0_{\mu} - z)\mathcal{R}_1(z) = [h^2 D^2_R, \chi_1](H_D - z)^{-1}\chi_2 + \chi_2 + (H^0_{\mu} - z)(\hat{H}^0_{\mu} - z)^{-1}(1 - \chi_2)$$

= $[h^2 D^2_R, \chi_1](H_D - z)^{-1}\chi_2 + 1 - F(R)(\hat{H}^0_{\mu} - z)^{-1}(1 - \chi_2)$
= $1 + K_1(z) + K_2(z),$

where we have set,

$$K_1(z) := [h^2 D_R^2, \chi_1] (H_D - z)^{-1} \chi_2$$

$$K_2(z) := -F(R) (\hat{H}^0_\mu - z)^{-1} (1 - \chi_2)$$

Here, we observe that,

$$\operatorname{Supp}(D_R\chi_1) \cap \operatorname{Supp}(\chi_2) = \emptyset = \operatorname{Supp} F \cap \operatorname{Supp}(1-\chi_2)$$

Moreover, introducing the notations,

$$H_D = -h^2 \Delta_{\mathbf{R}} + P(R);$$

$$\hat{H}^0_\mu = -h^2 \mathcal{S}_\mu \Delta_{\mathbf{R}} \mathcal{S}^{-1}_\mu + Q(R)$$

(where the two R-dependent operators P(R) and Q(R) act on the electronic variables only), we also have,

$$\operatorname{Supp}(D_R\chi_1) \subset \{P(R) > m_2 + \alpha\} \quad ; \quad \operatorname{Supp} F \subset \{\operatorname{Re} Q(R) > m_2 + \alpha\}.$$

Therefore, proceeding as in [HeSj2], Section 9 (see also [HeSj1]), by performing Agmon estimates, we deduce the existence of some constant $\delta > 0$, such that,

$$||K_1(z)|| + ||K_2(z)|| = \mathcal{O}(e^{-\delta/h}), \tag{73}$$

uniformly for $z \in \gamma(h)$ and h > 0 small enough. In the same way, setting,

$$\mathcal{R}_2(z) = \chi_2(H_D - z)^{-1}\chi_1 + (1 - \chi_2)(\hat{H}^0_\mu - z)^{-1},$$

we also have,

$$\mathcal{R}_2(z)(H^0_\mu - z) = 1 + \mathcal{O}(e^{-\delta'/h}),$$

with $\delta' > 0$ constant. As a consequence, we deduce that $H^0_{\mu} - z$ is invertible, and its inverse is given by,

$$(H^0_{\mu} - z)^{-1} = \mathcal{R}_1(z)(1 + K_1 + K_2)^{-1}.$$
(74)

In particular, using Lemma 6.2 and the fact that H_D is self-adjoint, and defining $\gamma_k(h)$ as in (60), we conclude that, for all $z \in \gamma_k(h)$, we have,

$$\|(H^0_{\mu} - z)^{-1}\| = \mathcal{O}(h^{-C}) \tag{75}$$

where C > 0 is a constant.

Now, we set,

$$\Pi_{\mu,k} := \frac{1}{2i\pi} \oint_{\gamma_k(h)} (H^0_\mu - z)^{-1} dz;$$
$$A_k := \frac{1}{2i\pi} \chi_1 \oint_{\gamma_k(h)} (H_D - z)^{-1} \chi_2 dz$$

(Note that, by construction, $||A_k|| = O(h^{-1})$ and A_k is of rank at most 2.) From (73)-(74) and Lemma 6.2 (plus the fact that $(\hat{H}^0_{\mu} - z)^{-1}$ is holomorphic inside $\gamma(h)$), we obtain,

$$\Pi_{\mu,k} = A_k + \mathcal{O}(e^{-\delta/h}). \tag{76}$$

In particular, since $\Pi^2_{\mu,k} = \Pi_{\mu,k}$ and $\|\Pi_{\mu,k}\| = \mathcal{O}(h^{-C})$, we deduce,

$$A_k^2 = A_k + \mathcal{O}(e^{-\delta/2h}),\tag{77}$$

and thus, for any $\zeta \in \mathbb{C}$,

$$(A_k - \zeta)(A_k + \zeta - 1) = -\zeta(\zeta - 1) + R_k, \ \|R_k\| = \mathcal{O}(e^{-\delta/2h}).$$
(78)

As a consequence, if $\zeta \neq 0, 1$ is fixed, then $(A_k - \zeta)$ is invertible, and we can consider the projection,

$$\Pi_{A_k} := \frac{1}{2i\pi} \oint_{|\zeta - 1| = 1/2} (\zeta - A_k)^{-1} d\zeta.$$

Then, we prove,

Lemma 6.3. One has,

$$\|A_k - \Pi_{A_k}\| = \mathcal{O}(e^{-\delta/4h}).$$

uniformly for h > 0 small enough.

Proof. We write,

$$\Pi_{A_k} - A_k = \frac{1}{2\pi i} \oint_{|\zeta - 1| = 1/2} \left[(\zeta - A_k)^{-1} - (\zeta - 1)^{-1} A_k \right] d\zeta$$

and,

$$(\zeta - A_k)^{-1} - (\zeta - 1)^{-1}A_k = (\zeta - A_k)^{-1} \left(1 - A_k + (\zeta - 1)^{-1} (A_k - A_k^2) \right).$$

Moreover, by (78), we also have,

$$(A_k - \zeta)^{-1} = (A_k + \zeta - 1) \left[\zeta (1 - \zeta) + R_k \right]^{-1}$$
(79)

In particular, $||(A_k - \zeta)^{-1}|| = \mathcal{O}(h^{-1})$ uniformly on $\{|\zeta - 1| = 1/2\}$, and thus, using (77), we obtain,

$$\Pi_{A_k} - A_k = \Pi_{A_k} (1 - A_k) + \mathcal{O}(e^{-\delta/3h}).$$
(80)

On the other hand, using (79) (and the fact that $R_k = A_k^2 - A_k$ commutes with A_k), we have,

$$\begin{aligned} \Pi_{A_k}(1-A_k) &= \frac{1}{2i\pi} \oint_{|\zeta-1|=1/2} (A_k-\zeta)^{-1} (\zeta-1) d\zeta \\ &= \frac{1}{2i\pi} \oint_{|\zeta-1|=1/2} (\zeta-1) (A_k+\zeta-1) \left[\zeta(1-\zeta) + R_k \right]^{-1} d\zeta \\ &= \frac{1}{2i\pi} \oint_{|\zeta-1|=1/2} \left(\zeta - 1 - \frac{1}{\zeta} R_k \right) (\zeta(1-\zeta) + R_k)^{-1} (A_k+\zeta-1) dz \\ &+ \frac{1}{2i\pi} \oint_{|\zeta-1|=1/2} \zeta^{-1} R_k \left(\zeta(1-\zeta) + R_k \right)^{-1} (A_k+\zeta-1) d\zeta \\ &= \frac{1}{2i\pi} \oint_{|\zeta-1|=1/2} \zeta^{-1} R_k \left(\zeta(1-\zeta) + R_k \right)^{-1} (A_k+\zeta-1) d\zeta \\ &= \mathcal{O}(e^{-\delta/4h}), \end{aligned}$$

where we have used the fact that,

$$\oint_{|\zeta-1|=1/2} \left(\zeta - 1 - \frac{1}{\zeta} R_k \right) \left(\zeta (1-\zeta) + R_k \right)^{-1} (A_k + \zeta - 1) d\zeta$$
$$= \oint_{|\zeta-1|=1/2} -\zeta^{-1} (A_k + \zeta - 1) d\zeta = 0,$$

because the function inside the integral is analytic in the disc $\{|\zeta - 1| \le 1/2\}$. \Box

We deduce from Lemma 6.3 and (76) that we have,

$$\Pi_{\mu,k} = \Pi_{A_k} + \mathcal{O}(e^{-\delta/4h}). \tag{81}$$

Moreover, still by Lemma 6.3, we see that the restriction,

$$A_k \Big|_{\operatorname{Im}(\Pi_{A_k})} : \operatorname{Im}(\Pi_{A_k}) \to \operatorname{Im}(\Pi_{A_k})$$

is invertible, and thus, since the rank of A_k is at most 2, we deduce,

$$\operatorname{Rank}(\Pi_{A_k}) \leq 2.$$

As a consequence, by (81), we obtain,

$$\operatorname{Rank}(\Pi_{\mu,k}) \leq 2.$$

Then, we are exactly in the situation of [MaMe] Proposition 6.1, (i)-(ii), and, setting,

$$\widetilde{\Pi}_{\mu,k} := \frac{1}{2i\pi} \oint_{\gamma_k(h)} (z - \widetilde{H}^0_\mu)^{-1} dz,$$

we conclude that we have,

$$\|\Pi_{\mu,k} - \widetilde{\Pi}_{\mu,k}\| = \mathcal{O}(e^{-\delta''/h}),\tag{82}$$

with $\delta'' > 0$ constant. As before, the result on the interior of $\gamma_k(h)$ $(k \ge 1)$ follows in a standard way, and one obtains the required comparison of the spectra of H^0_μ and \tilde{H}^0_μ on

$$\mathcal{B} = \{ \operatorname{Re} z \in [m_2, m_2 + \alpha], |\operatorname{Im} z| < C^{-1} |h \ln h| \}.$$

As before, the same arguments can be performed on $\{Rez \in [m_1, m_2], |\operatorname{Im} z| < C^{-1}|h \ln h|\}$ (in a simpler way, since the eigenvalues of H_D are separated by a distance of order $\sim h$), and Proposition 6.1 follows.

Remark 6.4. The same argument, using (75), also show that the spectrum of H^0_{μ} and H_D on \mathcal{B} coincides up to an exponentially small term. In particular, the eigenvalues of H_D are real and then the resonances of H^0_{μ} have exponentially small part.

7. MAIN RESULT

Here, by collecting the Propositions 5.1 and 6.1, and Theorem 4.8 it turns out our main result.

Theorem 7.1. Let $\alpha > 0$ fixed small enough, and let $\mathcal{J} \subset (0, 1]$, with $0 \in \overline{\mathcal{J}}$, such that there exists $\delta > 0$ such that,

$$\operatorname{Sp}(P_D^{\sharp}) \cap [m_2 + \alpha - 2\delta h, m_2 + \alpha + 2\delta h] = \emptyset.$$

Set,

$$\Omega(h) := \{ z \in \mathbb{C} ; \operatorname{dist}(\operatorname{Re} z, [m_1, m_2 + \alpha]) < \delta h, |\operatorname{Im} z| < C^{-1} h \ln \frac{1}{h} \},\$$

with C > 0 a large enough constant. For h > 0 small enough then the resonances of H^0_{μ} in $\Omega(h)$ coincide up to $\mathcal{O}(h^2)$ error-terms, with eigenvalues of the Dirichlet realizations of P_1 and P_2 on $(0, R_{1,M})$, where $R_{1,M} > 0$ is the point where W_1 admits a local maximum with value greater than m_2 .

Remark 7.2. As done in §5, by slightly moving the parameter α one can actually reach all the values of h > 0 small enough.

Remark 7.3. We would point out that this result still holds true even in absence of the external field; in such a case we don't have resonances for H^0_{μ} , but real eigenvalues. In fact, in such a case we don't need to perform the analytical distortion and we may apply the same strategy as in §sub511.

References

- [BoOp] BORN, M., OPPENHEIMER, R., Zur Quantentheorie der Molekeln, Ann. Phys. 84, 457 (1927).
- [BCD] BRIET, P., COMBES, J.-M., DUCLOS, P., On the location of resonances for Schrödinger operators in the semiclassical limit II, Comm. Part. Diff. Eq., 12(2) (1987), 201–222.
- [CGM] CALICETI, E., GRECCHI, V., MAIOLI, M., Double Wells: Nevanlinna Analyticity, Distributional Borel Sum and Asymptotics, Commun. Math. Phys. 176 (1996), 1–22.
- [Ca] CARRINGTON, A., MCNAB, I. R., AND MONTGOMERIE, C. A., Spectroscopy of the hydrogen molecular ion, J. Phys. B 22 (1989), 3551–3586.
- [Ci] CIZEK, J., et al, 1/R expansion for H⁺₂: Calculation of exponentially small terms and asymptotics, Phys. Rev. A 33 (1986), 12–54.
- [CMR] CANCELIER, C., MARTINEZ, A., RAMOND, T., Quantum resonances without analyticity, Asymptot. Anal. 44 (2005), 47–74.
- [FLM] FUJHE, S., LAHMAR-BENBERNOU, A., MARTINEZ, A., Width of shape resonances for non globally analytic potentials, Preprint arXiv: 0811.0734 (2008).
- [GG] GIACHETTI, R., GRECCHI, V., Perturbation theory for metastable states of the Dirac equation with quadratic vector interaction, Phys. Rev. A 80 (2009), 032107.
- [HeRo] HELFFER, B., ROBERT, D., Puits de potentiel généralisés et asymptotique semi-classique, Ann. Inst. Henri Poincaré, section Physique Théorique, 41(3) (1984), 291–331.

- [HeSj1] HELFFER, B., SJÖSTRAND, J., Puits Multiple wells in the semiclassical limit I, Commun. Part. Diff. Eq. 9(4) (1984), 337–408.
- [HeSj2] HELFFER, B., SJÖSTRAND, J., Resonances en limite semi-classique, Bull. Soc. Math. France, Mémoire 24/25, (1986).
- [HMS] HERBST, I., MØLLER, J.S., SKIBSTED, E., Spectral analysis of N-boby Stark Hamiltonian, Commun. Math. Phys. 174 (1995), 261–294.
- [Hi] HISKES, J.R., Dissociation of molecular ions by electric and magnetic fields, Phys. Rev. 122 (1961), 1207–1217.
- [MPS] MULYUKOV Z., PONT M. AND SHAKESHAFT R., Ionization, dissociation, and level shifts of H⁺₂ in a strong dc or low frequency ac field Phys. Rev. A, 54, (1996) 4299-4308.
- [Hu] HUNZIKER, W., Distortion analycity and molecular resonance curve, Ann. Inst. H. Poincaré 45 (1986), 339–358
- [KMSW] M. KLEIN, A. MARTINEZ, R. SEILER, X.P. WANG, On the Born-Oppenheimer Expansion for Polyatomic Molecules, Commun. Math. Phys. 143(3) (1992), 607–639.
- [La] LIFSHITZ, E.M., LANDAU, L.D., Quantum Mechanics: Non-Relativistic Theory, (Butterworth-Heinemann) (1981).
- [LiSi] LIEB, E., SIMON, B., Monotonicity of the electronic contribution to the Born-Oppenheimer energy, J. Phys. B 11, No. 18 (1978), L537–L542.
- [Ma1] MARTINEZ, A., An Introduction to Semiclassical and Microlocal Analysis, Springer-Verlag New-York, UTX Series, ISBN: 0-387-95344-2 (2002).
- [Ma2] MARTINEZ, A., Resonance Free Domains for Non Globally Analytic Potentials, Ann. Henri Poincaré 4 (2002), 739–756 [Erratum: Ann. Henri Poincaré 8 (2007), 1425–1431]
- [MaMe] MARTINEZ, A., MESSERDI, B., Resonances of diatomic molecules in the Born-Oppenheimer approximation, Comm. Part. Diff. Eq. 19 (1994), 1139–1162.
- [MaSo] MARTINEZ, A., SORDONI, V., Twisted pseudo-differential calculus and application to the quantum evolution of molecules, Memoirs of the American Mathematical Society 200(936) (2009).
- [MeSj] MELIN, A., SJÖSTRAND, J., Fourier integral operators with complex valued phase functions, Springer Lecture Notes in Math. 459 (1974), 120–223.
- [MuSh] MULYUKOV, Z., SHAKESHAFT, R., Breakup of H⁺₂ by one photon in the presence of a strong dc field, Phys. Rev. A 63 (2001), 053404:1-10.
- [Ro] ROBERT, D., Autour de l'Approximation Semi-Classique, Progress in Mathematics, Volume 68, Birkhäuser, 1987
- [Sj] SJÖSTRAND, J., Singularités analytiques microlocales, Soc. Math. France, Astérisque 95 (1982), 1–166.

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