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THOMAS NORMAND

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Spectral analysis of a semiclassical random walk associated to a general confining potential (*)

Thomas Normand (1)

Abstract. — We consider a semiclassical random walk with respect to a probability measure associated to a potential with a finite number of critical points. We recover the spectral results from [1] on the corresponding operator in a more general setting and with improved accuracy. In particular we do not make any assumption on the distribution of the critical points of the potential, in the spirit of [14]. Our approach consists in adapting the ideas from [14] to the recent *gaussian quasimodes* framework which appears to be more robust than the usual methods, especially when dealing with non local operators.

Résumé. — On considère une marche aléatoire semiclassique définie à l'aide d'une mesure de probabilité associée à un potentiel présentant un nombre fini de points critiques. On retrouve les résultats de [1] sur le spectre de l'opérateur associé dans un contexte plus général et avec une précision améliorée. On ne formule en particulier aucune hypothèse sur la distribution des points critiques du potentiel, dans l'esprit de [14]. Notre approche consiste à adapter les idées de [14] aux récentes techniques de *quasimodes guassiens* qui s'avèrent être plus robustes que les méthodes usuelles, en particulier pour l'étude d'opérateurs non locaux.

1. Introduction

1.1. Motivation

Let $W : \mathbb{R}^d \to \mathbb{R}$ a smooth function, $h > 0$ a small parameter and Z_h a normalization factor such that

$$\mathrm{d}\mu_h(x) = Z_h \mathrm{e}^{-W(x)/h} \mathrm{d}x$$

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(1) CERMICS, École des Ponts ParisTech, 77455 Marne la Vallée Cedex 2, France — thomas.normand@enpc.fr
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is a probability measure on $\mathbb{R}^d$. Consider the random walk with step h associated to μ_h : if at time $n \in \mathbb{N}$ the walk is in x_n, then the point x_{n+1} is chosen in the small ball $B(x_n, h)$ uniformly at random with respect to the measure

$$t_h(x, \mathrm{d}y) = \frac{1}{\mu_h(B(x,h))} \mathbf{1}_{|x-y|<h} \mathrm{d}\mu_h(y).$$

It is clear that t_h is a Markov kernel and the associated random walk operator is

$$\mathbf{T}_h f(x) = \int_{\mathbb{R}^d} f(y) t_h(x, \mathrm{d}y) = \frac{1}{\mu_h(B(x,h))} \int_{|x-y|<h} f(y) \mathrm{d}\mu_h(y) \qquad (1.1)$$

which acts on continuous functions. The evolution of the walk is dictated by $\mathbf{T}_h^*$ (acting on Borel measures) as follows : if the starting point x_0 of the random walk is distributed according to $\mathrm{d}\nu$, then x_n is distributed according to $(\mathbf{T}_h^*)^n(\mathrm{d}\nu)$. Our goal will then be to study the behavior of the sequence $(\mathbf{T}_h^*)^n(\mathrm{d}\nu)$ as $n \to \infty$. One can easily check that $\mathbf{T}_h^*$ admits the invariant measure

$$\mathrm{d}\nu_{h,\infty} = \widetilde{Z}_h \mu_h(B(x,h)) \mathrm{d}\mu_h(x)$$

where $\widetilde{Z}_h$ is a normalization factor. We will therefore be more precisely interested in the convergence of $(\mathbf{T}_h^*)^n(\mathrm{d}\nu)$ towards $\mathrm{d}\nu_{h,\infty}$. This type of study is in particular motivated by applications such as probability sampling or Monte-Carlo methods (see [13]). Some first results for discrete time processes on continuous state space were obtained in [5, 6, 8, 12]. In these papers, the spectral gap of the studied operators is of order h^2 as the probability $\mathrm{d}\mu_h$ does not depend on h. In our case, the h-dependence of μ_h leads us to deal with an exponentially small spectral gap for the operator $\mathbf{T}_h^*$.

The random walk operator $\mathbf{T}_h$ defined in (1.1) was studied in [1] where the authors showed the convergence of $(\mathbf{T}_h^*)^n(\mathrm{d}\nu)$ towards $\mathrm{d}\nu_{h,\infty}$ when $n \to \infty$ and gave some precise information on the speed of convergence. More precisely, they showed by an interpolation argument that $\mathbf{T}_h^*$ extends as a bounded self-adjoint operator on $L^2(\mathrm{d}\nu_{h,\infty})$ with norm 1 and gave an accurate description of its spectrum near 1. It enables the authors to state in [1, Corollary 1.4] the existence of metastable states, in the spirit for instance of the works [3, 4]. This indicates in particular that a very large number of iterations is required to make sure that the system returns to equilibrium.

The precise asymptotics of the exponentially small spectral gap and more generally of the eigenvalues exponentially close to 1 were also obtained in [1] thanks to the exhibition of a supersymmetric-type structure for the operator, allowing to see it as a Hodge–Witten Laplacian on 0-forms for some pseudo-differential metric. The idea is then to study both the associated derivative acting from 0-forms into 1-forms and its adjoint with the help of basic quasimodes. This used to be a common method to study the small spectrum of semiclassical operators (see for instance [9, 10]). However, our goal here will be to give precise spectral asymptotics for the operator $\mathbf{T}_h^*$ through a more recent approach developed for the study of Fokker–Planck type differential operators in [2, 18] and adapted to a non local framework in [16]. This approach consists in directly constructing a family of accurate quasimodes for our operator that we call *gaussian quasimodes*.

The results from [1] are established under a generic *non degeneracy* assumption on the associated potential (see [1, Hypothesis 2]). This type of hypothesis is very common in the literature about the spectrum of semiclassical operators associated to some potential (see also for instance [2, Assumption (Gener)] or [16, Hypothesis 3.11]). Our goal in this paper will be to retrieve the spectral results on $\mathbf{T}_h^*$ from [1] (and actually slightly improve their accuracy thanks to our sharp quasimodes) but for a very general confining Morse potential W not necessarily satisfying any non degeneracy assumption (see Hypothesis 1.1 below). To do so, we will use the ideas from [14] where the author was able to study the Witten Laplacian associated to such a general potential. We will thus have to adapt these ideas to our non local framework and to the use of gaussian quasimodes as those do not appear in [14].

1.2. Setting

Before we can state the properties of the potential W and the associated operator, let us introduce a few notations of semiclassical microlocal analysis which will be used in all this paper. These are mainly extracted from [19, Chapter 4]. We will denote $\xi \in \mathbb{R}^d$ the dual variable of x and consider the space of semiclassical symbols

$$S^0\Big(\langle x\rangle^k\langle\xi_m\rangle^{k'}\langle\xi_p\rangle^{k'}\Big) = \left\{a^h \in \mathcal{C}^\infty(\mathbb{R}^{2d});\ \begin{array}{c}\forall\, \alpha \in \mathbb{N}^{2d}, \exists\, C_\alpha > 0 \textit{ such that}\\ \big|\partial^\alpha a^h(x,\xi)\big| \leqslant C_\alpha\langle x\rangle^k\langle\xi_m\rangle^{k'}\langle\xi_p\rangle^{k'}\end{array}\right\}$$

where $m, p \in [\![1, d]\!]$ and $k, k' \in \mathbb{R}$. Given a symbol $a^h \in S^0(\langle x\rangle^k\langle\xi_m\rangle^{k'}\langle\xi_p\rangle^{k'})$, we define the associated semiclassical pseudo-differential operator for the Weyl quantization acting on functions $u \in \mathcal{S}(\mathbb{R}^d)$ by

$$\mathrm{Op}_h(a^h)u(x) = (2\pi h)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \mathrm{e}^{\frac{i}{h}(x-x')\cdot\xi} a^h\left(\frac{x+x'}{2},\xi\right)u(x')\mathrm{d}x'\mathrm{d}\xi$$

where the integrals may have to be interpreted as oscillating integrals.

Our only hypothesis on the potential W is the following.

Hypothesis 1.1. — *The potential W is a smooth Morse function with values in $\mathbb{R}$ such that*

$$\mathrm{e}^{-W/h} \in L^2(\mathbb{R}^d), \qquad \lim_{|x|\to+\infty} W(x) = +\infty \quad \text{and} \quad W \in S^0(\langle x\rangle^\eta)$$

for some $\eta \in \mathbb{N}$. Moreover, for every $0 \leqslant k \leqslant d$, the set of critical points of index k of W that we denote $\mathcal{U}^{(k)}$ is finite and we set

$$n_0 = \#\mathcal{U}^{(0)}.$$

Finally, we will suppose that $n_0 \geqslant 2$.

For the operator $\mathbf{T}_h^*$ acting on $L^2(\mathrm{d}\nu_{h,\infty})$, as it is more convenient to work with the standard Lebesgue measure, and since we want to study its spectrum near 1, we choose to consider the operator

$$P_h = \mathrm{Id} - \mathcal{M}_h^{1/2} \circ \mathbf{T}_h^* \circ \mathcal{M}_h^{-1/2} \tag{1.2}$$

instead, where $\mathcal{M}_h^{1/2}$ stands for both the square root of the function

$$\mathcal{M}_h(x) = \widetilde{Z_h} Z_h \mu_h(B(x,h)) \mathrm{e}^{-W(x)/h}$$

and the associated unitary operator from $L^2(\mathrm{d}\nu_{h,\infty})$ to $L^2(\mathbb{R}^d)$. Our goal is now to give a sharp description of the small spectrum of P_h acting on $L^2(\mathbb{R}^d)$. We will actually be able to treat the case of some slightly more general operators P_h than the one given by (1.2). In order to focus the difficulties mainly on the topology of the potential W, we will consider some operators P_h which still present some nice properties, even though it makes no doubt that we could adopt an even more general setting.

More precisely, let us introduce some notions of expansions of symbols: we will say that

$$a^h \sim \sum_{j\geqslant 0} h^j a_j \quad \text{ in } S^0(1)$$

if $(a_j)_{j\geqslant 0} \subset S^0(1)$ is a family of symbols independent of h and such that for all $N \in \mathbb{N}$,

$$a^h - \sum_{j=0}^{N-1} h^j a_j = O_{S^0(1)}(h^N).$$

We also need to introduce the notion of analytic symbols.

Definition 1.2. — *For $\kappa > 0$, let us introduce the set*

$$\Sigma_\kappa = \{z \in \mathbb{C}; |\mathrm{Im}\ z| < \kappa\}^d \subset \mathbb{C}^d.$$

We denote $S^0_\kappa(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'})$ the space of symbols

$$a^h \in S^0\Big(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}\Big)$$

such that:

(i) *For all* $x \in \mathbb{R}^d$, $a^h(x,\cdot)$ *is analytic on* Σ_κ.
(ii) *For all* $\beta \in \mathbb{N}^d$, *there exists* $C_\beta > 0$ *such that*

$$\left|\partial_x^\beta a^h\right| \leqslant C_\beta \langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'} \qquad \text{on } \mathbb{R}^d \times \Sigma_\kappa.$$

We will also use the notation $a^h = O_{S^0_\kappa(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'})}(h^N)$ *to say that for all* $\alpha \in \mathbb{N}^{2d}$, *there exists* $C_{\alpha,N}$ *such that* $|\partial^\alpha a^h| \leqslant C_{\alpha,N} h^N \langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}$ *on* $\mathbb{R}^d \times \Sigma_\kappa$.

Using the Cauchy–Riemann equations, we see that Definition 1.2 (i) implies that for all $\beta \in \mathbb{N}^d$ and $x \in \mathbb{R}^d$, the functions $\partial_x^\beta a^h(x,\cdot)$ are also analytic on Σ_κ. Besides, the Cauchy formula implies that for any $\widetilde{\kappa} < \kappa$, $\alpha \in \mathbb{N}^d$ and $\beta \in \mathbb{N}^d$, there exists $C_{\alpha,\beta}$ such that

$$\left|\partial_\xi^\alpha \partial_x^\beta a^h\right| \leqslant C_{\alpha,\beta} \langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'} \qquad \text{on } \mathbb{R}^d \times \Sigma_{\widetilde{\kappa}}$$

i.e up to taking κ smaller, Definition 1.2 (ii) can be extended to $\beta \in \mathbb{N}^{2d}$. When dealing with analytic symbols, our notion of expansion becomes

$$a^h \sim \sum_{j\geqslant 0} h^j a_j \quad \text{ in } S^0_\kappa\Big(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}\Big)$$

if $(a_j)_{j\geqslant 0} \subset S^0_\kappa(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'})$ is a family of symbols independent of h and such that for all $N \in \mathbb{N}$,

$$a^h - \sum_{j=0}^{N-1} h^j a_j = O_{S^0_\kappa\left(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}\right)}(h^N).$$

We now extend these notions to matrix valued symbols: if n_1, $n_2 \in [\![1,d]\!]$ and

$$q^h = (q_{m,p})_{\substack{1\leqslant m\leqslant n_1\\ 1\leqslant p\leqslant n_2}}$$

is a matrix of functions such that each $q_{m,p} \in S^0_\kappa(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'})$, we say that $q^h \in \mathcal{M}_{n_1,n_2}(S^0_\kappa(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}))$ and we denote

$$\mathrm{Op}_h(q^h) = \Big(\mathrm{Op}_h(q_{m,p})\Big)_{\substack{1\leqslant m\leqslant n_1\\ 1\leqslant p\leqslant n_2}}.$$

Even though it does not appear in the notations, the function $q_{m,p}$ may also depend on h. The notation

$$q^h = O_{\mathcal{M}_{n_1,n_2}\left(S^0_\kappa\left(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}\right)\right)}\big(h^N\big)$$

means that for all $(m,p) \in [\![1,n_1]\!] \times [\![1,n_2]\!]$, the symbol $q_{m,p}$ is

$$O_{S^0_\kappa\left(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}\right)}(h^N).$$

Furthermore, the notion of expansion

$$q \sim \sum_{n \geqslant 0} h^n q_n \text{ in } \mathcal{M}_{n_1,n_2}\Big(S^0_\kappa\Big(\langle x\rangle^k \langle \xi_m\rangle^{k'} \langle \xi_p\rangle^{k'}\Big)\Big)$$

is a straightforward adaptation of the one for scalar symbols.

These notions enable us to introduce the class of operators that we will consider. Let us denote d_W the twisted derivative

$$\mathrm{d}_W = h\nabla + \nabla W.$$

We also use the standard notation $\mathcal{M}_d(\mathbb{R})$ for the set of all d-by-d real matrices.

Hypothesis 1.3. — *We assume that P_h is a bounded operator such that*

$$P_h = a^h \circ \widetilde{P}_h \circ a^h$$

with

$$\widetilde{P}_h = \mathrm{d}_W^* \circ \widehat{Q} \circ \mathrm{d}_W$$

where $\widehat{Q} = \mathrm{Op}_h(q^h)$ is a self-adjoint, non negative pseudo-differential operator and $a^h \sim \sum_{j \geqslant 0} h^j a_j$ in $S^0(1)$ is a positive symbol such that $(a^h)^{-1} \in S^0(1)$ and $a_0(x) = 1$ as soon as x is a critical point of W. Moreover,

(a) *P_h admits 0 as a simple eigenvalue.*
(b) *There exist $c > 0$ and $h_0 > 0$ such that for all $0 < h \leqslant h_0$, we have that $\mathrm{Spec}(P_h) \cap [0, ch]$ consists of exactly n_0 eigenvalues (counted with algebraic multiplicity) that are exponentialy small with respect to $1/h$.*
(c) *For all x, $\xi \in \mathbb{R}^d$, we have $q^h(x, -\xi) = q^h(x, \xi)$.*
(d) *The symbol q^h is analytic in the variable ξ. More precisely, there exists $\kappa > 0$ such that*

$$q^h \sim \sum_{n \geqslant 0} h^n q_n$$

in the space of analytic symbols $\mathcal{M}_d(S^0_\kappa(\langle \xi_m\rangle^{-1} \langle \xi_p\rangle^{-1}))$.

(e) *There exists a constant $\varrho > 0$ such that for every saddle point $\mathbf{s}$ (i.e a critical point with index 1) of W, we have $q_0(\mathbf{s}, 0) = \varrho\, \mathrm{Id}$.*

In particular, the resolvent estimate

$$(z - P_h)^{-1} = O\big(h^{-1}\big) \tag{1.3}$$

is satisfied on $|z| = ch$.

Throughout the paper, we will work under Hypothesis 1.3.

It is shown in [1, Theorem 1.1 as well as Corollary 3.1] that the random walk operator (1.2) studied in this reference is an example of a non local operator satisfying Hypothesis 1.3 with $\varrho = (2d+4)^{-1}$. We could for instance easily treat the case where the identity matrix is replaced by a positive definite matrix in Hypoythesis 1.3 (e) (as it is done in [16]), but our real interest here are the considerations brought by the potential W.

The main result of this paper is Theorem 8.4 in which we give a sharp description of the small eigenvalues of P_h. As we have not yet introduced all the technical objects involved in this statement, let us for the moment give a rather vague version of this result.

Theorem 1.4. — *Under Hypothesis 1.3, there exist $p \in \mathbb{N}$ and a finite set $\mathcal{A}$ both explicit as well as some positive definite matrices $(\mathcal{M}_h^{\alpha,j})_{1\leqslant j\leqslant p;\alpha\in\mathcal{A}}$ depending on ϱ from Hypothesis 1.3 and admitting a classical expansion whose first term is given in Theorem 8.4 such that*

$$\Big(\mathrm{Spec}(P_h)\cap[0,ch]\Big) \subset h\bigcup_{\alpha\in\mathcal{A}}\bigcup_{j=1}^{p}\mathrm{e}^{-2\hat{S}_j/h}\Big(\mathrm{Spec}\Big(\mathcal{M}_h^{\alpha,j}+D\big(0,O(h^\infty)\big)\Big)\Big)$$

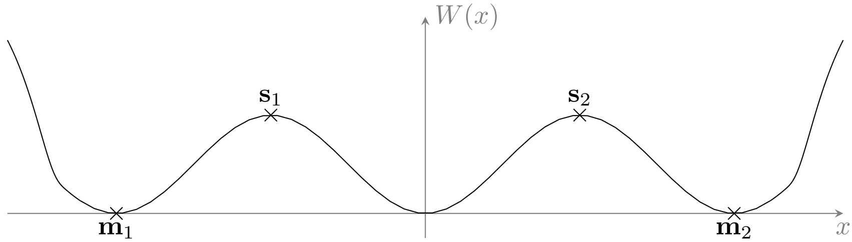
where $\{\widehat{S}_1<\cdots<\widehat{S}_p\}$ are the finite values taken by the map S introduced in Definition 2.3.

In particular, when P_h is given by (1.2)*, we have*

$$\begin{aligned}\Big(\mathrm{Spec}(\mathbf{T}_h^*)\cap[1-ch,1]\Big)&\\ \subset\left(1-h\bigcup_{\alpha\in\mathcal{A}}\bigcup_{j=1}^{p}\mathrm{e}^{-2\hat{S}_j/h}\Big(\mathrm{Spec}\Big(\mathcal{M}_h^{\alpha,j}+D\big(0,O(h^\infty)\big)\Big)\Big)\right)&\end{aligned}$$

with $\varrho = (2d+4)^{-1}$.

It is an improvement of the result of [1] in two ways: first, we treat in the spirit of [14] the case of general potentials satisfying only Hypothesis 1.1 instead of [1, Hypotheses 1 and 2]. Here is the picture of an example in dimension $d=1$ of potential satisfying Hypothesis 1.1 but not [1, Hypothesis 2]: here we clearly see that $W(\mathbf{s}_1)-W(\mathbf{m}_1)=W(\mathbf{s}_2)-W(\mathbf{m}_2)$. Actually, this potential does not even satisfy the more general framework of [11] mentioned below [1, Hypothesis 2] as it admits 3 global minima.



Moreover, we establish complete asymptotic expansions of the small eigenvalues, i.e the remainder terms in the prefactors are of order h^∞ and not of order h as in [1]. This work can also be seen as an adaptation of the considerations from [14] to a non local framework and to the gaussian quasimodes approach, as there exist some operators for which it is the only known approach to succeed (see for instance the Boltzmann operators from [16, 17]).

The strategy of proof is the following: we aim at constructing a family F of quasimodes (in bijection with the minima of W) satisfying

$$F \text{ is (almost) orthonormal} \tag{1.4}$$

as well as

$$\|P_h f\|^2 = O(h^\infty \langle P_h f, f\rangle) \quad \text{for all } f \in F. \tag{1.5}$$

We will then be able to show that the spectrum of P_h in $[0, ch]$ is essentially the spectrum of the so-called *interaction matrix* $(\langle P_h f, g\rangle)_{f,g\in F}$. To obtain such a family, we will use the *gaussian quasimodes* constructions introduced in [18] and also used in [2, 16]. However, these references do not treat the case of a Morse potential whose critical points are distributed in a completely general fashion as we attempt to do here; in particular it becomes unclear in our framework how to guarantee the orthogonality of the family F. This is where we will rely on the sharp topological considerations on the potential developed in [14]. Even though the quasimodes from [14] are not gaussian and do not satisfy (1.5), we will still be able to use these ideas in order to choose the support of our *gaussian* quasimodes to recover some orthogonality and finally obtain a family F satisfying both (1.4) and (1.5).

More precisely, in Section 2, we introduce the necessary material related to the topology of W in the spirit of [11] with the improvements from [14]. This will in particular enable us to describe on which wells of W each of our quasimodes will have to be supported. The heaviness and the technicalities of this section come from the fact that we consider a general Morse potential. We start Section 3 by recalling the profile of a usual gaussian quasimode on one well as can be found in [2, 16], allowing us to then give a precise definition of the family F, which will be composed of some well chosen sums of gaussian quasimodes supported on some (also well chosen) wells of W. In Section 4, we prove that the newly defined family F is almost orthonormal (i.e it satisfies (1.4)). Section 5 is devoted to the computation of $P_h f$ for $f \in F$. This is a first step towards showing that (1.5) holds true. The second step, achieved in Section 6, is to use this computation of $P_h f$ to optimize the choice of the remaining parameters in the definition of f (namely the auxiliary functions $\ell^{\mathbf{s},\mathbf{m}}$ introduced in p. 1270 and appearing in (3.2)) in order to minimize $\|P_h f\|$. This part of the analysis is already known from [16] and here we only recall the procedure. Finally, Sections 7 and 8 consist in computing the coefficients of the interaction matrix, showing thanks to the optimization made in Section 6 that (1.5) also holds true and finally providing the proof of Theorem 8.4.

Acknowledgments

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2. General labeling of the potential minima

Before we can construct our quasimodes, we need to recall the general labeling of the minima which originates from [9] and was generalized in [11], as well as the topological constructions that go with it. Here we only introduce the essential objects and omit the proofs. For more details, we refer to [14, 16]. Recall that we denote

$$\mathcal{U}^{(k)} \text{ the critical points of } W \text{ of index } k. \tag{2.1}$$

For shortness, we will write "CC" instead of "connected component". The constructions rely on the following fundamental observation which is an easy consequence of the Morse Lemma (see for instance [16, Lemma 3.1] for a proof):

Lemma 2.1. — *If $x \in \mathcal{U}^{(1)}$, then there exists $r_0 > 0$ such that for all $0 < r < r_0$, x has a connected neighborhood $\mathcal{O}_r$ in $B(x, r)$ such that $\mathcal{O}_r \cap \{W < W(x)\}$ has exactly 2 CCs.*

It motivates the following definition:

Definition 2.2.

(1) *We say that* $x \in \mathcal{U}^{(1)}$ *is a separating saddle point and we denote* $x \in \mathcal{V}^{(1)}$ *if for every* $r > 0$ *small enough, the two CCs of* $\mathcal{O}_r \cap \{W < W(x)\}$ *are contained in different CCs of* $\{W < W(x)\}$*.*
(2) *We say that* $\sigma \in \mathbb{R}$ *is a separating saddle value if* $\sigma \in W(\mathcal{V}^{(1)})$*.*

It is known (see for instance [16, Lemma 3.4]) that $\mathcal{V}^{(1)} \neq \emptyset$. Let us then denote $\sigma_2 > \cdots > \sigma_N$ where $N \geqslant 2$ the different separating saddle values of W and for convenience we set $\sigma_1 = +\infty$. For $\sigma \in \mathbb{R} \cup \{+\infty\}$, let us denote $\mathcal{C}_\sigma$ the set of all the CCs of $\{W < \sigma\}$. We call *labeling* of the minima of W any injection $\mathcal{U}^{(0)} \to [\![1, N]\!] \times \mathbb{N}^*$ which we denote for shortness $(\mathbf{m}_{k,j})_{k,j}$. Given a labeling $(\mathbf{m}_{k,j})_{k,j}$ of the minima of W, we denote for $k \in [\![1, N]\!]$

$$\mathtt{U}_k^{(0)} = \left\{\mathbf{m}_{k',j} ; 1 \leqslant k' \leqslant k, j \in \mathbb{N}^*\right\} \cap \left\{W < \sigma_k\right\}$$

and we say that the labeling is *adapted* to the separating saddle values if for all $k \in [\![1, N]\!]$, each $\mathbf{m}_{k,j}$ is a global minimum of W restricted to some CC of $\{W < \sigma_k\}$ and the map

$$T_k : \mathtt{U}_k^{(0)} \longrightarrow \mathcal{C}_{\sigma_k} \tag{2.2}$$

sending $\mathbf{m} \in \mathtt{U}_k^{(0)}$ on the element of $\mathcal{C}_{\sigma_k}$ to which it belongs is bijective. In particular, it implies that each $\mathbf{m}_{k,j}$ belongs to $\mathtt{U}_k^{(0)}$. Such labelings exist, one can for instance easily check that the usual labeling procedure presented in [11] is adapted to the separating saddle values. From now on, we fix a labeling $(\mathbf{m}_{k,j})_{k,j}$ adapted to the separating saddle values of W.

Definition 2.3. — *Recall the notation* (2.1) *and Definition 2.2. We define the following mappings:*

- $\begin{aligned} E : \mathcal{U}^{(0)} &\longrightarrow \mathcal{P}(\mathbb{R}^d) \\ \mathbf{m}_{k,j} &\longmapsto T_k(\mathbf{m}_{k,j}) \end{aligned}$ *where* T_k *is the map defined in* (2.2)*.*
- $\mathbf{j} : \mathcal{U}^{(0)} \to \mathcal{P}(\mathcal{V}^{(1)} \cup \{\mathbf{s}_1\})$ *given by* $\mathbf{j}(\mathbf{m}_{1,1}) = \{\mathbf{s}_1\}$ *where* $\mathbf{s}_1$ *is a fictive saddle point such that* $W(\mathbf{s}_1) = \sigma_1 = +\infty$*; and for* $2 \leqslant k \leqslant N$*,* $\mathbf{j}(\mathbf{m}_{k,j}) = \partial E(\mathbf{m}_{k,j}) \cap \mathcal{V}^{(1)}$ *which is not empty (see for instance* [16, Lemma 3.5]*) and included in* $\{W = \sigma_k\}$*.*
- $\begin{aligned} \boldsymbol{\sigma} : \mathcal{U}^{(0)} &\longrightarrow W(\mathcal{V}^{(1)}) \cup \{\sigma_1\} \\ \mathbf{m} &\longmapsto W(\mathbf{j}(\mathbf{m})) \end{aligned}$ *where we allow ourselves to identify the set* $W(\mathbf{j}(\mathbf{m}))$ *and its unique element in* $W(\mathcal{V}^{(1)}) \cup \{\sigma_1\}$*.*
- $\begin{aligned} S : \mathcal{U}^{(0)} &\longrightarrow \,]0, +\infty] \\ \mathbf{m} &\longmapsto \boldsymbol{\sigma}(\mathbf{m}) - W(\mathbf{m}). \end{aligned}$

We refer to [14, Figure 4] for a nice depiction of the above notations on a concrete example. We now introduce some material originating from [14].

Let us denote

$$\underline{\mathbf{m}} = \mathbf{m}_{1,1} \quad \text{and} \quad \underline{\mathcal{U}}^{(0)} = \mathcal{U}^{(0)} \backslash \{\underline{\mathbf{m}}\}$$

and define for $\mathbf{m} = \mathbf{m}_{k,j} \in \underline{\mathcal{U}}^{(0)}$

$$\widehat{\mathbf{m}} = T_{k-1}^{-1}\big(E_-(\mathbf{m})\big)$$

where $E_-(\mathbf{m})$ is the element of $\mathcal{C}_{\sigma_{k-1}}$ containing $\mathbf{m}$. Since $\widehat{\mathbf{m}}$ and $\mathbf{m}$ both belong to $E_-(\mathbf{m})$, we have $W(\widehat{\mathbf{m}}) \leqslant W(\mathbf{m})$ and $\widehat{\mathbf{m}} \in \mathtt{U}_k^{(0)}$.

Definition 2.4.

- *A minimum* $\mathbf{m} \in \underline{\mathcal{U}}^{(0)}$ *is said to be of type I if* $W(\widehat{\mathbf{m}}) < W(\mathbf{m})$. *Otherwise (i.e when* $W(\widehat{\mathbf{m}}) = W(\mathbf{m})$*), we say that* $\mathbf{m}$ *is of type II.*
- *We define an equivalence relation* $\mathcal{R}$ *on* $\underline{\mathcal{U}}^{(0)}$ *by* $\mathbf{m}\mathcal{R}\mathbf{m}'$ *if and only if the two following conditions are satisfied:*
  - (i) $\boldsymbol{\sigma}(\mathbf{m}) = \boldsymbol{\sigma}(\mathbf{m}') = \sigma_k$
  - (ii) *There exist some minima* $\mathbf{m}^1, \dots, \mathbf{m}^K$ *such that* $\mathbf{m}^1 = \mathbf{m}$, $\mathbf{m}^K = \mathbf{m}'$ *and for all* $1 \leqslant n \leqslant K-1$, *we have* $\overline{T_k(\mathbf{m}^n)} \cap \overline{T_k(\mathbf{m}^{n+1})} \neq \emptyset$ *with*

$$\mathbf{m}^n \in \{\mathbf{m}_{k,j}; j \in \mathbb{N}^*\} \cup \big\{\widehat{\mathbf{m}}_{k,j}; j \in \mathbb{N}^* \text{ and } \mathbf{m}_{k,j} \text{ is of type II}\big\}.$$

We denote the associated equivalence classes $(\mathcal{U}_\alpha^{(0)})_{\alpha\in\mathcal{A}}$, where $\mathcal{A}$ is a finite set. Once again, we refer to [14, Figures 5-8] for some illustrations of these notions. It is shown in [14, Proposition 2.6] that for $\mathbf{m}\mathcal{R}\mathbf{m}'$, we have $\boldsymbol{\sigma}(\mathbf{m}) = \boldsymbol{\sigma}(\mathbf{m}')$ and $\widehat{\mathbf{m}} = \widehat{\mathbf{m}}'$. Finally, for $\mathbf{m} \in \mathcal{U}_\alpha^{(0)}$, we put

$$\boldsymbol{\sigma}(\alpha) = \boldsymbol{\sigma}(\mathbf{m}) \qquad \text{and} \qquad \widehat{\mathcal{U}}_\alpha^{(0)} = \mathcal{U}_\alpha^{(0)} \cup \{\widehat{\mathbf{m}}\}$$

which do not depend on the choice of $\mathbf{m} \in \mathcal{U}_\alpha^{(0)}$, as well as

$$E^\alpha(\mathbf{m}) = T_{k(\alpha)}(\mathbf{m}) \qquad \text{and} \qquad \mathbf{j}^\alpha(\mathbf{m}) = \partial E^\alpha(\mathbf{m}) \cap \mathcal{V}^{(1)}$$

for $\mathbf{m} \in \widehat{\mathcal{U}}_\alpha^{(0)}$, where $k(\alpha)$ is such that $\boldsymbol{\sigma}(\alpha) = \sigma_{k(\alpha)}$. When $\mathbf{m} \in \mathcal{U}_\alpha^{(0)}$, we have $E^\alpha(\mathbf{m}) = E(\mathbf{m})$ but for $\widehat{\mathbf{m}} \in \widehat{\mathcal{U}}_\alpha^{(0)} \cap \mathcal{U}_{\alpha'}^{(0)}$, we have $E(\widehat{\mathbf{m}}) = E^{\alpha'}(\widehat{\mathbf{m}}) \neq E^\alpha(\widehat{\mathbf{m}})$.

3. Gaussian quasimodes

This section aims at giving a precise definition of our family of quasimodes. We will first recall the general profile of a usual gaussian quasimode on one well (in (3.2) and below) as can be found in [2, 16], and use it together with the material from Section 2 and Lemma 3.1 to define our quasimodes in (3.6) and (3.10).

Throughout the paper, for $d' \in \mathbb{N}^*$, $\Omega \subseteq \mathbb{R}^{d'}$ and $a \in \mathcal{C}^\infty(\Omega)$ a function depending on h and such that for all $\beta \in \mathbb{N}^{d'}$ we have $\partial^\beta a = O_{L^\infty}(1)$, we will say that $a \in \mathcal{C}^\infty(\Omega)$ admits a classical expansion on Ω and denote $a \sim \sum_{j \geqslant 0} h^j a_j$, where $(a_j)_{j\geqslant 0} \subset \mathcal{C}^\infty(\Omega)$ are independent of h, provided that for all $\beta \in \mathbb{N}^{d'}$ and $N \in \mathbb{N}$, there exists $C_{\beta,N}$ such that

$$\left\| \partial^\beta \left(a - \sum_{j=0}^{N-1} h^j a_j \right) \right\|_{\infty,\Omega} \leqslant C_{\beta,N} h^N.$$

It implies in particular that $\partial^\beta a_j = O_{L^\infty}(1)$. From now on, the letter r will denote a small universal positive constant whose value may decrease as we progress in this paper (one can think of r as $1/C$).

We are now going to introduce some quasimodes for the operator P_h. With the notations from Hypothesis 1.3, our approach consists in constructing some gaussian quasimodes for the factorised operator $\widetilde{P}_h$ in the spirit of [2, 16] and multiply those by $(a^h)^{-1}$.

Let $\alpha \in \mathcal{A}$ and $\mathbf{m} \in \widehat{\mathcal{U}}_\alpha^{(0)}$. For each $\mathbf{s} \in \mathbf{j}^\alpha(\mathbf{m})$ we introduce a function $\ell^{\mathbf{s},\mathbf{m}}$ that will appear in our quasimodes. Note that thanks to Lemma 2.1, there are at most two functions $\ell^{\mathbf{s},\mathbf{m}}$ and $\ell^{\mathbf{s},\mathbf{m}'}$ associated to a saddle point $\mathbf{s} \in \mathcal{V}^{(1)}$. Our goal will be to find some functions $\ell^{\mathbf{s},\mathbf{m}}$ such that our quasimodes are the most accurate possible. In order to begin the computations that will yield the equations that the function $\ell^{\mathbf{s},\mathbf{m}}$ should satisfy, we will for the moment assume that it satisfies the following:

(a) $\ell^{\mathbf{s},\mathbf{m}}$ is a smooth real valued function on $\mathbb{R}^d$ whose support is contained in $B(\mathbf{s}, 3r)$.
(b) $\ell^{\mathbf{s},\mathbf{m}}$ admits a classical expansion $\ell^{\mathbf{s},\mathbf{m}} \sim \sum h^j \ell_j^{\mathbf{s},\mathbf{m}}$ on $B(\mathbf{s}, 2r)$.
(c) $\ell_0^{\mathbf{s},\mathbf{m}}$ vanishes at $\mathbf{s}$.
(d) $\mathbf{s}$ is a local minimum of the function $W + (\ell_0^{\mathbf{s},\mathbf{m}})^2/2$ which is non degenerate.
(e) The functions $\theta^\alpha_{\mathbf{m},h}$ (which depends on $\ell^{\mathbf{s},\mathbf{m}}$) and χ_α that we will introduce in (3.2)–(3.4) are such that $\theta^\alpha_{\mathbf{m},h}$ is smooth on a neighborhood of supp χ_α.

Once we will have found the desired function $\ell^{\mathbf{s},\mathbf{m}}$, we will see in Proposition 6.8 that these assumptions are actually satisfied. Denote $\zeta \in \mathcal{C}_c^\infty(\mathbb{R}, [0,1])$ an even cut-off function supported in $[-\gamma, \gamma]$ that is equal to 1 on $[-\gamma/2, \gamma/2]$ where $\gamma > 0$ is a parameter to be fixed later and

$$A_h = \frac{1}{2} \int_{\mathbb{R}} \zeta(s) \mathrm{e}^{-\frac{s^2}{2h}} \mathrm{d}s = \int_0^\gamma \zeta(s) \mathrm{e}^{-\frac{s^2}{2h}} \mathrm{d}s = \frac{\sqrt{\pi h}}{\sqrt{2}} \Big(1 + O\Big(\mathrm{e}^{-c/h}\Big)\Big) \tag{3.1}$$

for some $c > 0$. We now define for each $\mathbf{m} \in \widehat{\mathcal{U}}_\alpha^{(0)}$ a function $\theta^\alpha_{\mathbf{m},h}$ as follows: if $x \in B(\mathbf{s}, r) \cap \{|\ell_0^{\mathbf{s},\mathbf{m}}| \leqslant 2\gamma\}$ for some $\mathbf{s} \in \mathbf{j}^\alpha(\mathbf{m})$,

$$\theta^\alpha_{\mathbf{m},h}(x) = \frac{1}{2}\left(1 + A_h^{-1}\int_0^{\ell^{\mathbf{s},\mathbf{m}}(x)} \zeta(s)\mathrm{e}^{-s^2/2h}\mathrm{d}s\right) \tag{3.2}$$

whereas we set

$$\theta^\alpha_{\mathbf{m},h} = 1 \quad \text{on } \Big(E^\alpha(\mathbf{m}) + B(0,\varepsilon)\Big)\Bigg\backslash\left(\bigsqcup_{\mathbf{s}\in\mathbf{j}^\alpha(\mathbf{m})} \big(B(\mathbf{s},r) \cap \big\{|\ell_0^{\mathbf{s},\mathbf{m}}| \leqslant 2\gamma\big\}\big)\right)$$

with $\varepsilon(r) > 0$ to be fixed later and

$$\theta_{\mathbf{m},h} = 0 \quad \text{everywhere else.}$$

Note that $\theta^\alpha_{\mathbf{m},h}$ takes values in $[0,1]$ and that we have

$$\operatorname{supp}\theta^\alpha_{\mathbf{m},h} \subseteq E^\alpha(\mathbf{m}) + B(0,\varepsilon') \tag{3.3}$$

where $\varepsilon' = \max(\varepsilon, r)$. Denote now Ω_α the CC of $\{W \leqslant \boldsymbol{\sigma}(\alpha)\}$ containing $\widehat{\mathcal{U}}_\alpha^{(0)}$. The CCs of $\{W \leqslant \boldsymbol{\sigma}(\alpha)\}$ are separated so for $\varepsilon > 0$ small enough, there exists $\widetilde{\varepsilon} > 0$ such that

$$\min\big\{W(x); \mathrm{d}\big(x, \Omega_\alpha\big) = \varepsilon\big\} = \boldsymbol{\sigma}(\alpha) + 2\widetilde{\varepsilon}.$$

Thus the distance between $\{W \leqslant \boldsymbol{\sigma}(\alpha) + \widetilde{\varepsilon}\} \cap (\Omega_\alpha + B(0,\varepsilon))$ and $\partial(\Omega_\alpha + B(0,\varepsilon))$ is positive and we can consider a cut-off function

$$\chi_\alpha \in \mathcal{C}_c^\infty\big(\mathbb{R}^d, [0,1]\big) \tag{3.4}$$

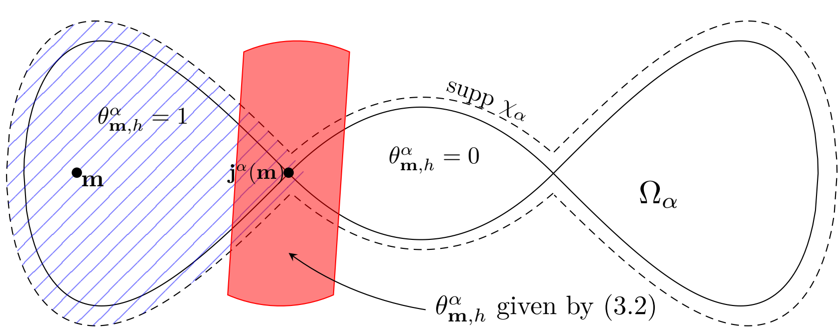
such that

$$\chi_\alpha = 1 \text{ on } \{W \leqslant \boldsymbol{\sigma}(\alpha) + \widetilde{\varepsilon}\} \cap \big(\Omega_\alpha + B(0,\varepsilon)\big)$$

and

$$\operatorname{supp}\chi_\alpha \subset \big(\Omega_\alpha + B(0,\varepsilon)\big).$$

To sum up, we have the following picture, which is essentially (up to the α's) extracted from [16, Section 3.1]:



We also denote
$$W_{\mathbf{m}}(x) = W(x) - W(\mathbf{m})$$
and it is clear that
$$W_{\mathbf{m}} \geqslant S(\mathbf{m}) + \widetilde{\varepsilon} \quad \text{on the support of } \nabla\chi_\alpha \text{ as soon as } \mathbf{m} \in \mathcal{U}_\alpha^{(0)}. \tag{3.5}$$
Recalling the function a^h from Hypothesis 1.3, the global quasimode associated to the eigenvalue 0 is
$$f_{\underline{\mathbf{m}},h}(x) = (a^h)^{-1} h^{-d/4} c_h(\underline{\mathbf{m}}) \mathrm{e}^{-W_{\underline{\mathbf{m}}}(x)/h} \in \operatorname{Ker} P_h \tag{3.6}$$
which is an exact one, while for $\mathbf{m} \in \mathcal{U}_\alpha^{(0)}$, our quasimodes will be linear combinations of the functions
$$(a^h)^{-1} h^{-d/4} c_h^\alpha(\widetilde{\mathbf{m}}) \chi_\alpha(x) \theta^\alpha_{\widetilde{\mathbf{m}},h}(x) \mathrm{e}^{-W_{\widetilde{\mathbf{m}}}(x)/h}$$
where $\widetilde{\mathbf{m}} \in \widehat{\mathcal{U}}_\alpha^{(0)}$. Here $c_h^\alpha(\mathbf{m})$ and $c_h(\underline{\mathbf{m}})$ are normalization factors assuring that
$$\begin{aligned} \left\|(a^h)^{-1} h^{-d/4} c_h^\alpha(\widetilde{\mathbf{m}}) \chi_\alpha(x) \theta^\alpha_{\widetilde{\mathbf{m}},h}(x) \mathrm{e}^{-W_{\widetilde{\mathbf{m}}}(x)/h}\right\| &= 1 \\ \text{and} \qquad \left\|(a^h)^{-1} h^{-d/4} c_h(\underline{\mathbf{m}}) \mathrm{e}^{-W_{\underline{\mathbf{m}}}(x)/h}\right\| &= 1. \end{aligned} \tag{3.7}$$
In particular, thanks to Hypothesis 1.3 we have that for all $\mathbf{m} \in \widehat{\mathcal{U}}_\alpha^{(0)}$, the constant $c_h^\alpha(\mathbf{m})$ (resp. the constant $c_h(\underline{\mathbf{m}})$) admits an asymptotic expansion whose first term is
$$\pi^{-d/4}\left(\sum_{\widetilde{\mathbf{m}} \in H^\alpha(\mathbf{m})} \det \mathcal{W}_{\widetilde{\mathbf{m}}}^{-1/2}\right)^{-1/2} \qquad \text{resp.} \quad \pi^{-d/4}\left(\sum_{\widetilde{\mathbf{m}} \in H(\underline{\mathbf{m}})} \det \mathcal{W}_{\widetilde{\mathbf{m}}}^{-1/2}\right)^{-1/2} \tag{3.8}$$
with
$$\begin{aligned} H^\alpha(\mathbf{m}) &= \left\{\widetilde{\mathbf{m}} \in \mathcal{U}^{(0)} \cap E^\alpha(\mathbf{m}); W(\widetilde{\mathbf{m}}) = W(\mathbf{m})\right\}, \\ H(\underline{\mathbf{m}}) &= \left\{\widetilde{\mathbf{m}} \in \mathcal{U}^{(0)}; W(\widetilde{\mathbf{m}}) = W(\underline{\mathbf{m}})\right\} \end{aligned}$$
and
$$\mathcal{W}_x \text{ is the Hessian of } W \text{ at } x. \tag{3.9}$$
Let us introduce the coefficients that we will use to define our quasimodes, in the spirit of [14]. We denote $\mathcal{F}_\alpha$ the finite-dimensional vector space of functions from $\widehat{\mathcal{U}}_\alpha^{(0)}$ into $\mathbb{R}$ endowed with the natural euclidian structure
$$\langle \varphi, \varphi' \rangle_{\mathcal{F}_\alpha} = \sum_{\widetilde{\mathbf{m}} \in \widehat{\mathcal{U}}_\alpha^{(0)}} \varphi(\widetilde{\mathbf{m}}) \varphi'(\widetilde{\mathbf{m}}).$$

Denoting also

$$\mathcal{U}_\alpha^{(0),I} \text{ the elements of } \mathcal{U}_\alpha^{(0)} \text{ of type I}$$

and using (3.8), the following lemma is established in [14, Section 3] (see below the statement for more details).

Lemma 3.1. — *Recall the notation* (3.9)*. One can construct an h-dependent orthonormal family $(\varphi_{\mathbf{m}}^\alpha)_{\mathbf{m}\in\widehat{\mathcal{U}}_\alpha^{(0)}} \subset \mathcal{F}_\alpha$ such that*

(a) $\varphi_{\widehat{\mathbf{m}}}^\alpha(\widetilde{\mathbf{m}}) = \widehat{c}_h c_h^\alpha(\widetilde{\mathbf{m}})^{-1}\mathbf{1}_{\widehat{\mathcal{U}}_\alpha^{(0)}\setminus\mathcal{U}_\alpha^{(0),I}}(\widetilde{\mathbf{m}})$ *where $\widehat{c}_h$ is a normalization constant such that $\|\varphi_{\widehat{\mathbf{m}}}^\alpha\|_{\mathcal{F}_\alpha} = 1$.*
(b) *If $\{\mathbf{m},\widetilde{\mathbf{m}}\}\cap\mathcal{U}_\alpha^{(0),I} \neq \emptyset$, then $\varphi_{\mathbf{m}}^\alpha(\widetilde{\mathbf{m}}) = \delta_{\mathbf{m},\widetilde{\mathbf{m}}}$.*
(c) *If $\varphi_{\mathbf{m}}^\alpha(\widetilde{\mathbf{m}}) \neq 0$, then $W(\mathbf{m}) = W(\widetilde{\mathbf{m}})$.*
(d) *Each $\varphi_{\mathbf{m}}^\alpha$ admits an asymptotic expansion. The leading term of $\varphi_{\widehat{\mathbf{m}}}^\alpha$ is given by*

$$\begin{aligned}\varphi_{\widehat{\mathbf{m}}}^{\alpha,0}(\widetilde{\mathbf{m}}) &= \widehat{c}_0 c_0^\alpha(\widetilde{\mathbf{m}})^{-1}\mathbf{1}_{\widehat{\mathcal{U}}_\alpha^{(0)}\setminus\mathcal{U}_\alpha^{(0),I}}(\widetilde{\mathbf{m}}) \\ &= \left(\frac{\sum_{\mathring{\mathbf{m}}\in H^\alpha(\widetilde{\mathbf{m}})}\det\mathcal{W}_{\mathring{\mathbf{m}}}^{-1/2}}{\sum_{\mathbf{m}'\in\widehat{\mathcal{U}}_\alpha^{(0)}\setminus\mathcal{U}^{(0),I}}\sum_{\mathring{\mathbf{m}}\in H^\alpha(\mathbf{m}')}\det\mathcal{W}_{\mathring{\mathbf{m}}}^{-1/2}}\right)^{1/2}\mathbf{1}_{\widehat{\mathcal{U}}_\alpha^{(0)}\setminus\mathcal{U}_\alpha^{(0),I}}(\widetilde{\mathbf{m}}).\end{aligned}$$

Finally, for all $\mathbf{m}\in\mathcal{U}_\alpha^{(0)}$, the leading term of $\varphi_{\mathbf{m}}^\alpha$ can be computed explicitly and is orthogonal to the one of $\varphi_{\widehat{\mathbf{m}}}^\alpha$.

Actually, (a) is a consequence of [14, (3.11) and (3.16)] (be careful that the notation θ^α from [14] becomes φ^α in our framework); (b) is a consequence of [14, (3.16)]; (c) is a consequence of (b) and the definition of a type II minimum; while item (d) is a consequence of [14, Lemma 3.6 (ii) and (3.16)]. Finally, the family $(\varphi_{\mathbf{m}}^\alpha)_{\mathbf{m}\in\widehat{\mathcal{U}}_\alpha^{(0)}} \subset \mathcal{F}_\alpha$ is orthonormal thanks to [14, Lemma 3.6 (i) and (3.16)].

For $\mathbf{m}\in\mathcal{U}_\alpha^{(0)}$, our quasimodes will be the functions

$$f_{\mathbf{m},h}(x) = (a^h)^{-1}h^{-d/4}\chi_\alpha(x) \times\left(\sum_{\widetilde{\mathbf{m}}\in\widehat{\mathcal{U}}_\alpha^{(0)}}\varphi_{\mathbf{m}}^\alpha(\widetilde{\mathbf{m}})c_h^\alpha(\widetilde{\mathbf{m}})\theta_{\widetilde{\mathbf{m}},h}^\alpha(x)\right)\mathrm{e}^{-W_{\mathbf{m}}(x)/h}. \quad (3.10)$$

Note that $f_{\mathbf{m},h}$ belongs to $\mathcal{C}_c^\infty(\mathbb{R}^d)$ thanks to (e) from hypothesis in p. 1270 and that

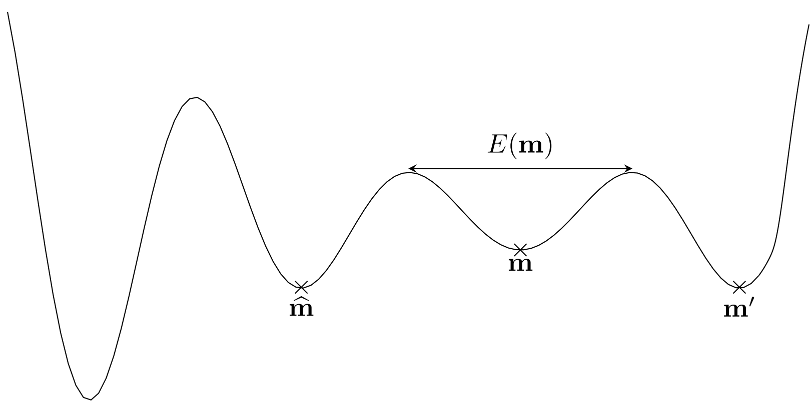
$$\operatorname{supp} f_{\mathbf{m},h} \subseteq E_-(\mathbf{m}) \quad (3.11)$$

thanks to (3.3).

4. Orthogonality

The goal of this section is to show that the family of quasimodes that we introduced in (3.10) and (3.6) is almost orthonormal. This result was already established in [2] in the case where W has no type II minimum (see [2, Remark 6.3]). Therefore, we will consider $\mathbf{m} \in \mathcal{U}_{\alpha}^{(0)}$, $\mathbf{m}' \in \mathcal{U}_{\alpha'}^{(0)}$ and we will study here the orthogonality of the quasimodes $f_{\mathbf{m},h}$ and $f_{\mathbf{m}',h}$ with $\mathbf{m}$ or $\mathbf{m}'$ (or both) a type II minimum. We follow the spirit of [14, Proposition 3.10] and adapt it to the gaussian quasimodes framework.

The case where $\mathbf{m}\mathcal{R}\mathbf{m}'$ *and one of them is of type I, say* $\mathbf{m}$ *(in particular* $\mathbf{m} \neq \mathbf{m}'$ *because of our assumption:*



In that case, Lemma 3.1 (b) implies $\varphi_{\mathbf{m}}(\widetilde{\mathbf{m}}) = \delta_{\mathbf{m},\tilde{\mathbf{m}}}$ for all $\widetilde{\mathbf{m}} \in \widehat{\mathcal{U}}_{\alpha}^{(0)}$ and $\varphi_{\mathbf{m}'}(\mathbf{m}) = 0$ so by (3.3), we have

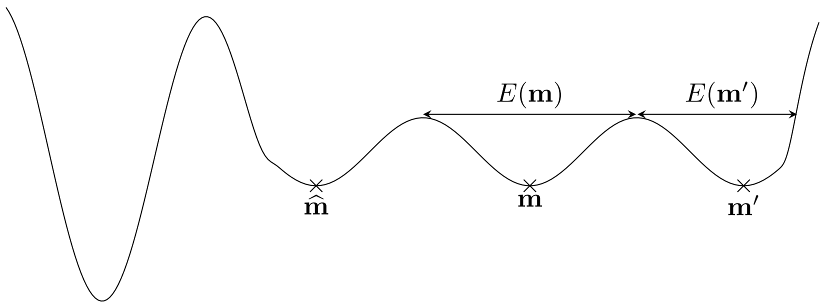
$$\operatorname{supp} f_{\mathbf{m},h} \subseteq E(\mathbf{m}) + B(0,\varepsilon') \quad \text{and} \quad \operatorname{supp} f_{\mathbf{m}',h} \subseteq \big(\mathbb{R}^d \backslash E(\mathbf{m})\big) + B(0,\varepsilon')$$

and hence

$$\operatorname{supp} f_{\mathbf{m},h} \cap \operatorname{supp} f_{\mathbf{m}',h} \subseteq \big\{2W - W(\mathbf{m}) - W(\mathbf{m}') \geqslant c > 0\big\}.$$

Consequently, $\langle f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle = O(\mathrm{e}^{-c/h})$.

The case where $\mathbf{m}\mathcal{R}\mathbf{m}'$ *(i.e* $\alpha = \alpha'$*) and both minima are of type II:*



In that case, start by noticing that because of (3.3), if $\tilde{\mathbf{m}}$, $\tilde{\mathbf{m}}' \in \widehat{\mathcal{U}}_\alpha^{(0)}$ with $\tilde{\mathbf{m}} \neq \tilde{\mathbf{m}}'$, we have

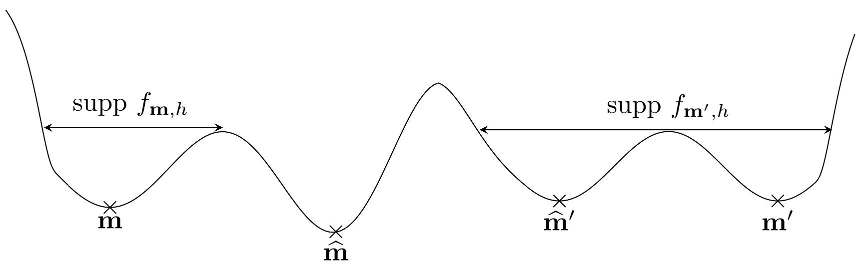
$$\operatorname{supp} \theta^\alpha_{\tilde{\mathbf{m}},h} \cap \operatorname{supp} \theta^\alpha_{\tilde{\mathbf{m}}',h} \subseteq \{W_{\tilde{\mathbf{m}}} \geqslant c > 0\}.$$

Therefore, using the definitions of our quasimodes (3.10) as well as Lemma 3.1 (c) and (3.7), we compute

$$\begin{aligned}
&\langle f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle + O\left(\mathrm{e}^{-c/h}\right) \\
&= (a^h)^{-2} h^{-d/2} \sum_{\tilde{\mathbf{m}} \in \widehat{\mathcal{U}}_\alpha^{(0)}} \varphi^\alpha_{\mathbf{m}}(\tilde{\mathbf{m}}) \varphi^\alpha_{\mathbf{m}'}(\tilde{\mathbf{m}}) c^\alpha_h(\tilde{\mathbf{m}})^2 \int_{\mathbb{R}^d} \chi^2_\alpha (\theta^\alpha_{\tilde{\mathbf{m}},h})^2 \mathrm{e}^{-2W_{\tilde{\mathbf{m}}}/h} \mathrm{d}x \\
&= \langle \varphi^\alpha_{\mathbf{m}}, \varphi^\alpha_{\mathbf{m}'}\rangle_{\mathcal{F}_\alpha} \\
&= \delta_{\mathbf{m},\mathbf{m}'}
\end{aligned}$$

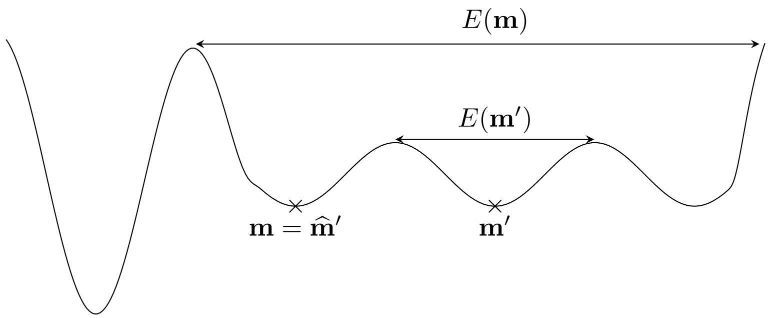
by Lemma 3.1.

The case where $\mathbf{m}\not\mathcal{R}\mathbf{m}'$ *and* $\boldsymbol{\sigma}(\mathbf{m}) = \boldsymbol{\sigma}(\mathbf{m}')$*:*



In that case, it follows from the support properties of our quasimodes and the result of [14, Proposition 3.8] that ε' can be chosen small enough so that the supports of $f_{\mathbf{m},h}$ and $f_{\mathbf{m}',h}$ do not intersect. Thus, $\langle f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle = 0$.

The case where $\mathbf{m}\not\mathcal{R}\mathbf{m}'$, $\boldsymbol{\sigma}(\mathbf{m}) > \boldsymbol{\sigma}(\mathbf{m}')$ *and* $W(\mathbf{m}) = W(\mathbf{m}')$*:*



In that situation, thanks to (3.10), (3.11) and (3.3) we can suppose that

$$f_{\mathbf{m},h} = (a^h)^{-1}\widetilde{c}_h(\mathbf{m})h^{-d/4}\mathrm{e}^{-W_{\mathbf{m}}/h} \qquad \text{on the support of } f_{\mathbf{m}',h}, \tag{4.1}$$

with $\widetilde{c}_h(\mathbf{m}) = O(1)$ (otherwise the supports of $f_{\mathbf{m},h}$ and $f_{\mathbf{m}',h}$ are disjoint and the result is obvious) and consequently $\mathbf{m}'$ is of type II. Hence, using a standard Laplace method, we can write

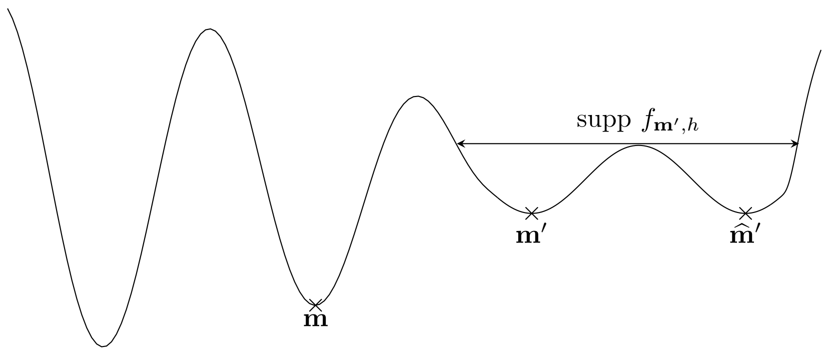
$$\begin{aligned}
\langle f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle &= (a^h)^{-2}h^{-d/2}\widetilde{c}_h(\mathbf{m}) \sum_{\tilde{\mathbf{m}}'\in\widehat{\mathcal{U}}^{(0)}_{\alpha'}} \varphi^{\alpha'}_{\mathbf{m}'}(\widetilde{\mathbf{m}}')c^{\alpha'}_h(\widetilde{\mathbf{m}}') \\
&\qquad \times \int_{\mathbb{R}^d} \chi_{\alpha'}\theta^{\alpha'}_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-2W_{\mathbf{m}}/h}\mathrm{d}x \\
&= (a^h)^{-2}h^{-d/2}\widetilde{c}_h(\mathbf{m}) \sum_{\tilde{\mathbf{m}}'\in\widehat{\mathcal{U}}^{(0)}_{\alpha'}} \varphi^{\alpha'}_{\mathbf{m}'}(\widetilde{\mathbf{m}}')c^{\alpha'}_h(\widetilde{\mathbf{m}}') \\
&\qquad \times \int_{\mathbb{R}^d} \chi^2_{\alpha'}(\theta^{\alpha'}_{\tilde{\mathbf{m}}',h})^2\mathrm{e}^{-2W_{\mathbf{m}}/h}\mathrm{d}x + O(\mathrm{e}^{-c/h}) \\
&= \widetilde{c}_h(\mathbf{m}) \sum_{\tilde{\mathbf{m}}'\in\widehat{\mathcal{U}}^{(0)}_{\alpha'}} \varphi^{\alpha'}_{\mathbf{m}'}(\widetilde{\mathbf{m}}')c^{\alpha'}_h(\widetilde{\mathbf{m}}')^{-1} + O(\mathrm{e}^{-c/h})
\end{aligned}$$

by (3.7). Now, using successively (b) and (a) from Lemma 3.1, we obtain

$$\begin{aligned}
\langle f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle &= \widetilde{c}_h(\mathbf{m}) \sum_{\tilde{\mathbf{m}}'\in\widehat{\mathcal{U}}^{(0)}_{\alpha'}\setminus\mathcal{U}^{(0),I}_{\alpha'}} \varphi^{\alpha'}_{\mathbf{m}'}(\widetilde{\mathbf{m}}')c^{\alpha'}_h(\widetilde{\mathbf{m}}')^{-1} + O(\mathrm{e}^{-c/h}) \\
&= \frac{\widetilde{c}_h(\mathbf{m})}{\widehat{c}_h}\Big\langle \varphi^{\alpha'}_{\mathbf{m}'}, \varphi^{\alpha'}_{\widehat{\mathbf{m}}'}\Big\rangle_{\mathcal{F}_{\alpha'}} + O(\mathrm{e}^{-c/h}) \\
&= O(\mathrm{e}^{-c/h})
\end{aligned}$$

thanks to the orthogonality of the family $(\varphi_{\mathbf{m}})_{\mathbf{m}\in\widehat{\mathcal{U}}^{(0)}_{\alpha'}}$.

The case where $\mathbf{m}\not{\mathcal{R}}\mathbf{m}'$, $\boldsymbol{\sigma}(\mathbf{m}) > \boldsymbol{\sigma}(\mathbf{m}')$ *and* $W(\mathbf{m}) \neq W(\mathbf{m}')$*:*



Here again we can suppose that (4.1) holds true so $W(\mathbf{m}) < W(\mathbf{m}')$. By Lemma 3.1 (c), we have $W \geqslant W(\mathbf{m}')$ on the support of $f_{\mathbf{m}',h}$. Therefore, $W_{\mathbf{m}} \geqslant c > 0$ on the support of $f_{\mathbf{m}',h}$ and since $f_{\mathbf{m}',h} = O_{L^\infty}(h^{-d/4})$, we get $\langle f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle = O(\mathrm{e}^{-c/h})$.

As a result of the above discussion, we obtain the following statement.

Proposition 4.1. — *The family of quasimodes* $(f_{\mathbf{m},h})_{\mathbf{m}\in\mathcal{U}^{(0)}}$ *introduced in* (3.10) *and* (3.6) *is almost orthonormal:*

$$\langle f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle = \delta_{\mathbf{m},\mathbf{m}'} + O\Big(\mathrm{e}^{-c/h}\Big).$$

5. Action of the operator P_h

In order to eventually establish (1.5), this section is devoted to providing a computation of $P_h f_{\mathbf{m},h}$.

Let us fix $\mathbf{m} \in \mathcal{U}_\alpha^{(0)}$. For $\tilde{\mathbf{m}} \in \widehat{\mathcal{U}}_\alpha^{(0)}$ we will denote

$$\widetilde{W}_{\tilde{\mathbf{m}},h} = W_{\mathbf{m}} + \sum_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})} (\ell^{\mathbf{s},\tilde{\mathbf{m}}})^2/2 \tag{5.1}$$

and

$$\psi^{\tilde{\mathbf{m}},h}(x,y) = \int_0^1 \nabla\widetilde{W}_{\tilde{\mathbf{m}},h}(y + t(x-y))\mathrm{d}t. \tag{5.2}$$

Remark 5.1. — Using Hypotheses 1.1 and 1.3 as well as symbolic calculus, one gets $\mathrm{d}_W^* \operatorname{Op}_h(q^h) = \operatorname{Op}_h(g^h)$, with $g^h \sim \sum_n h^n g_n$ in $\mathcal{M}_{1,d}(S^0_\kappa(\langle x\rangle^\eta))$ given by

$$g_0(x,\xi) = \big(-i\xi^t + \nabla W^t\big)q_0(x,\xi) \tag{5.3}$$

and

$$g_n(x,\xi) = \left(-i\xi^t + \nabla W^t\right)q_n(x,\xi) - \nabla_x^t q_{n-1}(x,\xi) \\ + \sum_{k=0}^{n} i^k \sum_{\substack{\beta\in\mathbb{N}^d;\\ |\beta|=k}} c_{k,\beta}(x)\partial_\xi^\beta(q_{n-k})(x,\xi) \quad (5.4)$$

for some $c_{k,\beta} \in S^0(\langle x\rangle^\eta)$ taking values in $\mathbb{R}^d$.

Lemma 5.2. — *The operator* $\mathrm{Op}_h(g^h) = \mathrm{d}_W^* \circ \widehat{Q}$ *introduced in Remark 5.1 is bounded on* $L^2(\mathbb{R}^d)$.

Proof. — Since $\widehat{Q}$ is self-adjoint, it is sufficient to prove that $\widehat{Q}\circ \mathrm{d}_W$ is bounded. Thanks to the facts that $\widehat{Q}$ is bounded and non negative, we can simply write for $u \in L^2(\mathbb{R}^d)$

$$\begin{aligned}\left\|\widehat{Q}\mathrm{d}_W u\right\|^2 &\leqslant C\left\|\widehat{Q}^{1/2}\mathrm{d}_W u\right\|^2\\ &\leqslant C\left\langle \widehat{Q}\mathrm{d}_W u, \mathrm{d}_W u\right\rangle\\ &\leqslant C\langle P_h u, u\rangle\\ &\leqslant C\|u\|^2\end{aligned}$$

according to Hypothesis 1.3, and the statement is proven. □

Proposition 5.3. — *Let* $f_{\mathbf{m},h}$ *be the quasimode defined in* (3.10). *With the notations introduced in* (3.1) *and* (5.1), *one has*

$$P_h f_{\mathbf{m},h} = a^h \frac{h^{1-d/4}}{2} A_h^{-1} \sum_{\tilde{\mathbf{m}}\in\widehat{\mathcal{U}}_\alpha^{(0)}} \varphi_{\mathbf{m}}^\alpha(\tilde{\mathbf{m}}) c_h^\alpha(\tilde{\mathbf{m}}) \omega^{\tilde{\mathbf{m}},\alpha} \mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}}{h}} \mathbf{1}_{\mathbf{j}^\alpha(\tilde{\mathbf{m}})+B(0,2r)} \\ + O_{L^2}\left(h^\infty \mathrm{e}^{-\frac{S(\mathbf{m})}{h}}\right)$$

where $\omega^{\tilde{\mathbf{m}},\alpha}$ *is a function bounded uniformly in* h *and defined for* $x \in \mathbf{j}^\alpha(\tilde{\mathbf{m}}) + B(0,2r)$ *by*

$$\omega^{\tilde{\mathbf{m}},\alpha}(x) = \sum_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})} (2\pi h)^{-d} \int_{\mathbb{R}^d} \int_{|y-\mathbf{s}|\leqslant 2r} \mathrm{e}^{\frac{i}{h}\xi\cdot(x-y)} \\ \times g^h\left(\frac{x+y}{2}, \xi + i\psi^{\tilde{\mathbf{m}},h}(x,y)\right) \nabla \ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\mathrm{d}y\mathrm{d}\xi.$$

Proof. — In order to lighten the notations, we will drop some of the exponents and indexes $\mathbf{m}$, $\mathbf{s}$, α and h in the proof. Let $\tilde{\mathbf{m}} \in \widehat{\mathcal{U}}_\alpha^{(0)}$. By hypotheses p. 1270, we have on the support of χ that $\theta_{\tilde{\mathbf{m}}}^\alpha$ is smooth and since it is constant outside of $B(\mathbf{s},r)$, we have

$$\nabla\theta^\alpha_{\tilde{\mathbf{m}}} = \frac{A_h^{-1}}{2}\sum_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})} \mathrm{e}^{-\left(\ell^{\mathbf{s},\tilde{\mathbf{m}}}\right)^2/2h}\zeta\left(\ell^{\mathbf{s},\tilde{\mathbf{m}}}\right)\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}\mathbf{1}_{B(\mathbf{s},r)}. \tag{5.5}$$

We can then use Remark 5.1 to write

$$\begin{aligned}
P_h(f) &= a^h h^{1-d/4}\sum_{\tilde{\mathbf{m}}\in\widehat{\mathcal{U}}_\alpha^{(0)}} \varphi^\alpha_{\mathbf{m}}(\widetilde{\mathbf{m}})c^\alpha_h(\widetilde{\mathbf{m}}) \\
&\qquad\times \mathrm{Op}_h(g)\left(\nabla\theta^\alpha_{\tilde{\mathbf{m}}}\chi\mathrm{e}^{-W_{\mathbf{m}}/h}+\nabla\chi\theta^\alpha_{\tilde{\mathbf{m}}}\mathrm{e}^{-W_{\mathbf{m}}/h}\right)\\
&= O\left(h\mathrm{e}^{-\frac{S(\mathbf{m})+\tilde{\varepsilon}}{h}}\right) + a^h\frac{h^{1-d/4}}{2}A_h^{-1}\sum_{\tilde{\mathbf{m}}\in\widehat{\mathcal{U}}_\alpha^{(0)}} \varphi^\alpha_{\mathbf{m}}(\widetilde{\mathbf{m}})c^\alpha_h(\widetilde{\mathbf{m}})\\
&\qquad\times\sum_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})}\mathrm{Op}_h(g)\left(\zeta(\ell^{\mathbf{s},\tilde{\mathbf{m}}})\chi\mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}}{h}}\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}\mathbf{1}_{B(\mathbf{s},r)}\right)
\end{aligned}\tag{5.6}$$

where we used (3.5) and Lemma 5.2. Now we have for $\mathbf{s}\in\mathbf{j}^\alpha(\widetilde{\mathbf{m}})$

$$\begin{aligned}
(2\pi h)^d\,\mathrm{Op}_h(g)&\left(\zeta(\ell^{\mathbf{s},\tilde{\mathbf{m}}})\chi\mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}}{h}}\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}\mathbf{1}_{B(\mathbf{s},r)}\right)(x)\\
&= \int_{\mathbb{R}^d}\int_{|y-\mathbf{s}|\leqslant r}\mathrm{e}^{\frac{i}{h}\xi\cdot(x-y)}g\left(\frac{x+y}{2},\xi\right)\\
&\qquad\qquad \chi(y)\zeta\left(\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\right)\mathrm{e}^{-\tilde{W}_{\tilde{\mathbf{m}}}(y)/h}\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\,\mathrm{d}y\mathrm{d}\xi.
\end{aligned}\tag{5.7}$$

Let us now treat separately the cases $|x-\mathbf{s}|\geqslant 2r$ and $|x-\mathbf{s}|<2r$. When $|x-\mathbf{s}|\geqslant 2r$, we have $|x-y|\geqslant r$ as soon as $|y-\mathbf{s}|\leqslant r$ so we can apply the non stationary phase method to the integral in ξ to get that for all $N\geqslant 1$, there exists $C_N>0$ such that

$$\begin{aligned}
\left|\int_{\mathbb{R}^d}\int_{|y-\mathbf{s}|\leqslant r}\mathrm{e}^{\frac{i}{h}\xi\cdot(x-y)}g\left(\frac{x+y}{2},\xi\right)\chi(y)\zeta\left(\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\right)\mathrm{e}^{-\tilde{W}_{\tilde{\mathbf{m}}}(y)/h}\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\,\mathrm{d}y\mathrm{d}\xi\right|\\
\leqslant C_N h^N|x-\mathbf{s}|^{\eta-N}\mathrm{e}^{-\frac{S(\mathbf{m})}{h}}
\end{aligned}$$

where we used (d) p. 1270, the fact that $W_{\mathbf{m}}(\mathbf{s})+(\ell_0^{\mathbf{s},\tilde{\mathbf{m}}})^2(\mathbf{s})/2=S(\mathbf{m})$ and the estimate $|x-y|\geqslant|x-\mathbf{s}|/2$. Hence we have shown that

$$P_hf\mathbf{1}_{\left\{\mathrm{dist}\left(\cdot,\bigcup_{\tilde{\mathbf{m}}\in\hat{\mathcal{U}}_\alpha^{(0)}}\mathbf{j}^\alpha(\tilde{\mathbf{m}})\right)\geqslant 2r\right\}} = O\left(h^\infty\mathrm{e}^{-\frac{S(\mathbf{m})}{h}}\right). \tag{5.8}$$

Now for the case $|x-\mathbf{s}|<2r$, let us denote $J_1^{\mathbf{s},\tilde{\mathbf{m}}}(x)$ the RHS of (5.7). Proceeding as in [15, Section 3] in order to take the $\mathrm{e}^{-\tilde{W}_{\tilde{\mathbf{m}}}(y)/h}$ in front of the oscillatory integral, we get that

$$J_1^{\mathbf{s},\tilde{\mathbf{m}}}(x)=\mathrm{e}^{-\tilde{W}_{\tilde{\mathbf{m}}}(x)/h}J_2^{\mathbf{s},\tilde{\mathbf{m}}}(x) \tag{5.9}$$

where

$$J_2^{\mathbf{s},\tilde{\mathbf{m}}}(x) = \int_{\mathbb{R}^d}\int_{|y-\mathbf{s}|\leqslant r} \mathrm{e}^{\frac{i}{h}(\xi - i\psi(x,y))\cdot(x-y)} g\Big(\frac{x+y}{2},\xi\Big) \\ \times \chi(y)\zeta\big(\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\big)\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\,\mathrm{d}y\mathrm{d}\xi$$

and ψ is the function defined in (5.2). Note that up to taking r smaller, we can suppose that $|\psi| < 1$ (and thus $\xi + i\psi$ lies in the analyticity strip of g) on $B(\mathbf{s},2r)\times\{|y-\mathbf{s}|<r\}$. Applying the Cauchy formula as in [16, proof of Proposition 3.13], one gets $J_2^{\mathbf{s},\tilde{\mathbf{m}}} = J_3^{\mathbf{s},\tilde{\mathbf{m}}}$ where

$$J_3^{\mathbf{s},\tilde{\mathbf{m}}}(x) = \int_{\mathbb{R}^d}\int_{|y-\mathbf{s}|\leqslant r} \mathrm{e}^{\frac{i}{h}\xi\cdot(x-y)} g\bigg(\frac{x+y}{2},\xi + i\psi(x,y)\bigg) \\ \times \chi(y)\zeta\big(\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\big)\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}(y)\,\mathrm{d}y\mathrm{d}\xi$$

Combined with (5.7) and (5.9), this yields for $|x-\mathbf{s}|<2r$

$$(2\pi h)^d\,\mathrm{Op}_h(g)\bigg(\zeta(\ell^{\mathbf{s},\tilde{\mathbf{m}}})\chi\mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}}{h}}\nabla\ell^{\mathbf{s},\tilde{\mathbf{m}}}\mathbf{1}_{B(\mathbf{s},r)}\bigg)(x) \\ = \mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}(x)}{h}} J_3^{\mathbf{s},\tilde{\mathbf{m}}}(x). \quad (5.10)$$

Therefore, setting on $\mathbf{j}^\alpha(\widetilde{\mathbf{m}}) + B(0,2r)$

$$\widetilde{\omega}^{\tilde{\mathbf{m}},\alpha} = (2\pi h)^{-d}\sum_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})} J_3^{\mathbf{s},\tilde{\mathbf{m}}}(x),$$

we have according to (5.6), (5.8) and (5.10)

$$P_h f = a^h\frac{h^{1-d/4}}{2}A_h^{-1}\sum_{\tilde{\mathbf{m}}\in\widehat{\mathcal{U}}_\alpha^{(0)}} \varphi_{\mathbf{m}}^\alpha(\widetilde{\mathbf{m}})c_h^\alpha(\widetilde{\mathbf{m}})\widetilde{\omega}^{\tilde{\mathbf{m}},\alpha}\mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}}{h}}\mathbf{1}_{\mathbf{j}^\alpha(\tilde{\mathbf{m}})+B(0,2r)} \\ + O\Big(h^\infty\mathrm{e}^{-\frac{S(\mathbf{m})}{h}}\Big).$$

Hence it is sufficient to check that on $\mathbf{j}^\alpha(\widetilde{\mathbf{m}}) + B(0,2r)$

$$\big(\widetilde{\omega}^{\tilde{\mathbf{m}},\alpha} - \omega^{\tilde{\mathbf{m}},\alpha}\big)\mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}}{h}} = O\Big(h^\infty\mathrm{e}^{-\frac{S(\mathbf{m})}{h}}\Big).$$

This can be done easily using again the non stationary phase method with x in an h-independent neighborhood of $\mathbf{s}$ on which $\chi\zeta(\ell)-1$ vanishes since (d) p. 1270 implies that

$$\mathrm{e}^{\frac{-\tilde{W}_{\tilde{\mathbf{m}},h}}{h}} = O\Big(\mathrm{e}^{-(S(\mathbf{m})+\delta)/h}\Big)$$

outside of this neighborhood for some $\delta > 0$. □

6. Choice of $\ell^{\mathbf{s},\tilde{\mathbf{m}}}$

Now that we have computed $P_h f_{\mathbf{m},h}$, the next step towards establishing (1.5) is to optimize the choice of the functions $\ell^{\mathbf{s},\mathbf{m}}$ in order to minimize $\|P_h f_{\mathbf{m},h}\|$. This part of the analysis is the point of this section. The results presented here are already known from [16] and we only recall the main arguments.

From now on, we also fix $\widetilde{\mathbf{m}} \in \widehat{\mathcal{U}}_\alpha^{(0)}$ and $\mathbf{s} \in \mathbf{j}^\alpha(\widetilde{\mathbf{m}})$. We write for shortness $\ell^{\mathbf{s}}$ instead of $\ell^{\mathbf{s},\tilde{\mathbf{m}}}$.

Lemma 6.1. — *The function $\omega^{\tilde{\mathbf{m}},\alpha}$ admits the classical expansion $\omega^{\tilde{\mathbf{m}},\alpha} \sim \sum_{j\geqslant 0} h^j \omega_j^{\tilde{\mathbf{m}},\alpha}$ on $B(\mathbf{s},2r)$ where*

$$\omega_0^{\tilde{\mathbf{m}},\alpha} = q_0\Big(x, i\big(\nabla W + \ell_0^{\mathbf{s}}\nabla\ell_0^{\mathbf{s}}\big)\Big)\big(2\nabla W + \ell_0^{\mathbf{s}}\nabla\ell_0^{\mathbf{s}}\big)\cdot\nabla\ell_0^{\mathbf{s}}$$

and for $j \geqslant 1$,

$$\begin{aligned}\omega_j^{\tilde{\mathbf{m}},\alpha} &= 2q_0\Big(x, i\big(\nabla W + \ell_0^{\mathbf{s}}\nabla\ell_0^{\mathbf{s}}\big)\Big)\big(\nabla W + \ell_0^{\mathbf{s}}\nabla\ell_0^{\mathbf{s}}\big)\cdot\nabla\ell_j^{\mathbf{s}}\\ &\quad + i\ell_0^{\mathbf{s}}\big(2\,\nabla W^t + \ell_0^{\mathbf{s}}(\nabla\ell_0^{\mathbf{s}})^t\big)D_\xi q_0\big(x, i(\nabla W + \ell_0^{\mathbf{s}}\nabla\ell_0^{\mathbf{s}})\big)\big(\nabla\ell_j^{\mathbf{s}}\big)\nabla\ell_0^{\mathbf{s}}\\ &\quad + q_0\Big(x, i\big(\nabla W + \ell_0^{\mathbf{s}}\nabla\ell_0^{\mathbf{s}}\big)\Big)\nabla\ell_0^{\mathbf{s}}\cdot\nabla\ell_0^{\mathbf{s}}\ell_j^{\mathbf{s}}\\ &\quad + i\big(2\nabla W^t + \ell_0^{\mathbf{s}}\big(\nabla\ell_0^{\mathbf{s}}\big)^t\big)D_\xi q_0\big(x, i(\nabla W + \ell_0^{\mathbf{s}}\nabla\ell_0^{\mathbf{s}})\big)\big(\nabla\ell_0^{\mathbf{s}}\big)\nabla\ell_0^{\mathbf{s}}\ell_j^{\mathbf{s}}\\ &\quad + R_j\big(\ell_0^{\mathbf{s}},\dots,\ell_{j-1}^{\mathbf{s}}\big) \qquad (6.1)\end{aligned}$$

where $R_j : (\mathcal{C}^\infty(B(\mathbf{s},2r)))^j \to \mathcal{C}^\infty(B(\mathbf{s},2r))$ and D_ξ denotes the partial differential with respect to the variable ξ.

Proof. — Once again, we drop some of the exponents and indexes $\widetilde{\mathbf{m}}$, $\mathbf{s}$, α and h in the proof. Denote $B_\infty(\mathbf{s},2r) = \{(y,\xi)\in\mathbb{R}^{2d};\max(|y-\mathbf{s}|,|\xi|) < 2r\}$. We need to get an expansion of $g(x/2+y/2,\xi+i\psi(x,y))$ that we will then be able to combine with the stationary phase method to get an expansion of ω. Let us start with an expansion of ψ : the expansion of ℓ yields

$$\nabla\widetilde{W} - \nabla W \sim \sum_{j\geqslant 0} h^j \sum_{k=0}^{j} \ell_k \nabla\ell_{j-k} \quad \text{on } B(\mathbf{s},2r)$$

so using (5.2), we get

$$\psi \sim \sum_{j\geqslant 0} h^j\psi_j \quad \text{on } B(\mathbf{s},2r)\times\{|y|\leqslant 2r\}$$

where

$$\psi_0(x,y) = \int_0^1 \big(\nabla W + \ell_0\nabla\ell_0\big)(y + t(x-y))\mathrm{d}t \qquad (6.2)$$

and for $j \geqslant 1$,

$$\psi_j(x,y) = \int_0^1 \sum_{k=0}^{j} \big(\ell_k \nabla \ell_{j-k}\big)(y+t(x-y))\mathrm{d}t. \tag{6.3}$$

Proceeding as in [16, proof of Lemma 4.1], we then get thanks to Remark 5.1 that

$$g\bigg(\frac{x+y}{2}, \xi + i\psi(x,y)\bigg) \sim \sum_{j\geqslant 0} h^j \sum_{n=0}^{j} g_{n,j-n}(x,y,\xi) \tag{6.4}$$

on $B(\mathbf{s},2r)\times B_\infty(\mathbf{s},2r)$; with

$$g_{n,0}(x,y,\xi) = g_n\bigg(\frac{x+y}{2}, \xi + i\psi_0(x,y)\bigg) \tag{6.5}$$

and for $j-n \geqslant 1$

$$\begin{aligned} g_{n,j-n}(x,y,\xi) = iD_\xi g_n\bigg(\frac{x+y}{2}, \xi + i\psi_0(x,y)\bigg)\big(\psi_{j-n}(x,y)\big) \\ + R^1_{j-n}(\ell_0,\dots,\ell_{j-n-1}) \end{aligned} \tag{6.6}$$

where $R^1_{j-n} : (\mathcal{C}^\infty(B(\mathbf{s},2r)))^{j-n} \to \mathcal{C}^\infty(B(\mathbf{s},2r))$. Thus, using the expansion (6.4) that we just got, the one of $\nabla\ell$, and the one for an oscillatory integral given by the stationary phase method (see for instance [19, Theorem 3.17]) as well as [16, Proposition C.3], we finally get

$$\omega \sim \sum_{j\geqslant 0} h^j \omega_j \quad \text{on } B(\mathbf{s},2r),$$

where

$$\omega_j(x) = \sum_{n_1+n_2+n_3+n_4=j} \frac{1}{i^{n_1} n_1!} \big(\partial_y\cdot\partial_\xi\big)^{n_1} \Big(g_{n_2,n_3}(x,y,\xi)\nabla\ell_{n_4}(y)\Big)\Big|_{\substack{y=x\\ \xi=0}}.$$

We can already use (6.5) to deduce the expression of ω_0 by noticing that according to (6.2), $\psi_0(x,x) = (\nabla W + \ell_0\nabla\ell_0)(x)$. For $j \geqslant 1$, the terms of ω_j in which the function ℓ_j appears are obviously the one given by $n_4 = j$, but also the one given by $n_3 = j$ according to (6.6). Indeed, in that case, we have using (6.3) that

$$\begin{aligned} g_{0,j}(x,x,0) = i\ell_0 D_\xi g_0\big(x, i(\nabla W + \ell_0\nabla\ell_0)\big)\big(\nabla\ell_j\big) \\ + iD_\xi g_0\big(x, i(\nabla W + \ell_0\nabla\ell_0)\big)\big(\nabla\ell_0\big)\ell_j + R^2_j(\ell_0,\dots,\ell_{j-1}) \end{aligned}$$

where $R_j^2 : (\mathcal{C}^\infty(B(\mathbf{s},2r)))^j \to \mathcal{C}^\infty(B(\mathbf{s},2r))$. We can now conclude as for any $X \in \mathbb{R}^d$,

$$\begin{aligned} D_\xi g_0\big(x, i(\nabla W + \ell_0 \nabla \ell_0)\big)(X) \\ &= -iX^t q_0\big(x, i(\nabla W + \ell_0\nabla\ell_0)\big) \\ &\quad + \big(2\nabla W^t + \ell_0(\nabla \ell_0)^t\big) D_\xi q_0\big(x, i(\nabla W + \ell_0\nabla\ell_0)\big)(X) \end{aligned}$$

according to (5.3). □

Denote $(q^n_{m,p})_{m,p}$ the entries of the matrix q_n from Hypothesis 1.3. Since we have for $X \in \mathbb{R}^d$

$$D_\xi q_0\big(x, i(\nabla W + \ell_0\nabla\ell_0)\big)(X) = \Big(\partial_\xi q^0_{m,p}\big(x, i(\nabla W + \ell_0\nabla\ell_0)\big)\cdot X\Big)_{1\leqslant m,p\leqslant d}$$

we get by putting

$$\begin{aligned} U(x) &= q_0\Big(x, i\big(\nabla W + \ell_0\nabla\ell_0\big)\Big)\nabla\ell_0 \\ &+ \sum_{1\leqslant m,p\leqslant d} (2\partial x_m W + \ell_0 \partial_{x_m}\ell_0) i \partial_\xi q^0_{m,p}\Big(x, i\big(\nabla W + \ell_0\nabla\ell_0\big)\Big)\partial_{x_p}\ell_0 \end{aligned} \tag{6.7}$$

that equation (6.1) reads

$$\begin{aligned} \omega_j = \bigg(q_0\Big(x, i\big(\nabla W + \ell_0\nabla\ell_0\big)\Big)(2\nabla W + \ell_0\nabla\ell_0) + \ell_0 U\bigg)\cdot\nabla\ell_j + U\cdot\nabla\ell_0\ell_j \\ + R_j(\ell_0,\dots,\ell_{j-1}). \end{aligned}$$

Lemma 6.2. — *Let x, $y \in B(\mathbf{s},2r)$. For any $n\in\mathbb{N}$, $\beta\in\mathbb{N}^d$ and $1\leqslant m,p\leqslant d$, we have*

$$\partial_\xi^\beta q^n_{m,p}\left(\frac{x+y}{2}, i\psi_0^{\tilde{\mathbf{m}},h}(x,y)\right) \in i^{|\beta|}\mathbb{R}$$

and

$$\partial_\xi^\beta g_n\left(\frac{x+y}{2}, i\psi_0^{\tilde{\mathbf{m}},h}(x,y)\right) \in i^{|\beta|}\mathbb{R}^d.$$

In particular, U defined in (6.7) *sends $B(\mathbf{s},2r)$ in $\mathbb{R}^d$.*

Proof. — Since ℓ_0 vanishes at $\mathbf{s}$, we can suppose that r is such that $i\psi_0(x,y)$ is in

$$D(0,1)^d = \{z\in\mathbb{C}; |z|<1\}^d$$

so by analyticity and using the parity of $q^n_{m,p}$, we have

$$\partial_\xi^\beta q^n_{m,p}\left(\frac{x+y}{2}, i\psi_0(x,y)\right) = \sum_{\substack{\gamma\in\mathbb{N}^d;\\ |\gamma|+|\beta|\in 2\mathbb{N}}} i^{|\gamma|}\frac{\partial_\xi^{\gamma+\beta} q^n_{m,p}\left(\frac{x+y}{2},0\right)}{\gamma!}\psi_0(x,y)^\gamma \in i^{|\beta|}\mathbb{R}.$$

The result for g_n follows easily using (5.3) and (5.4). $\square$

Using this Lemma, we also get the following result (see [16, Appendix D] for a proof).

Lemma 6.3. — *The term $R_j(\ell_0^{\mathbf{s},\tilde{\mathbf{m}}},\dots,\ell_{j-1}^{\mathbf{s},\tilde{\mathbf{m}}})$ from Lemma 6.1 is real valued. Moreover, it satisfies*

$$R_j\left(\ell_0^{\mathbf{s},\tilde{\mathbf{m}}},\dots,\ell_{j-1}^{\mathbf{s},\tilde{\mathbf{m}}}\right) = -R_j\left(-\ell_0^{\mathbf{s},\tilde{\mathbf{m}}},\dots,-\ell_{j-1}^{\mathbf{s},\tilde{\mathbf{m}}}\right).$$

In view of the results from Proposition 5.3 and Lemma 6.1, we want to find $\ell^{\mathbf{s},\tilde{\mathbf{m}}}$ such that on $B(\mathbf{s},2r)$,

$$q_0\Big(x, i\big(\nabla W+\ell_0\nabla\ell_0\big)\Big)\big(2\nabla W+\ell_0\nabla\ell_0\big)\cdot\nabla\ell_0 = 0 \tag{6.8}$$

and for $j\geqslant 1$

$$\Big(q_0\Big(x,i\big(\nabla W+\ell_0\nabla\ell_0\big)\Big)(2\nabla W+\ell_0\nabla\ell_0)+\ell_0 U\Big)\cdot\nabla\ell_j + U\cdot\nabla\ell_0\ell_j + R_j(\ell_0,\dots,\ell_{j-1}) = 0 \tag{6.9}$$

where U was introduced in (6.7). Note that Lemmas 6.2 and 6.3 ensure that the fact that the $(\ell_j)_{j\geqslant 0}$ are real valued is compatible with equations (6.9).

6.1. Solving for $\ell_0^{\mathbf{s},\tilde{\mathbf{m}}}$

Denote

$$\begin{aligned} p(x,\xi) &= \big(-i\xi^t+\nabla W^t\big)q_0(x,\xi)(i\xi+\nabla W)\\ &= q_0(x,\xi)\xi\cdot\xi + q_0(x,\xi)\nabla W\cdot\nabla W \end{aligned}$$

the principal symbol of the whole operator P_h and $\widetilde{p}\,(x,\xi) = -p(x,i\xi)$ its complexification. Notice that thanks to Hypothesis 1.3 (e), the quadratic approximation of $\widetilde{p}$ at $(\mathbf{s},0)$ coincides with the one of the complexification of the symbol of the Schrödinger operator $-h^2 \mathrm{d}\delta + |\nabla W|^2$ (up to a factor ϱ). Hence, we get all the results from [7, Chapter 3]. In particular, denoting

$$\Lambda_\pm = \left\{ (x,\xi); \lim_{t\to\mp\infty} \mathrm{e}^{tH_{\tilde p}}(x,\xi) = (\mathbf{s},0) \right\}$$

the stable manifolds associated to the Hamiltonian of $\widetilde{p}$ near $(\mathbf{s},0)$, we obtain the following.

Lemma 6.4. — *There exist $\phi_\pm \in \mathcal{C}^\infty(B(\mathbf{s},2r),\mathbb{R})$ vanishing together with their gradients at* $\mathbf{s}$ *and such that*

$$\Lambda_\pm = \left\{ \big(x, \nabla\phi_\pm(x)\big); x \in B(\mathbf{s},2r) \right\}.$$

Moreover, the Hessian matrix of $\pm\phi_\pm$ at $\mathbf{s}$ *is positive definite.*

At this point, one can proceed as in [2, Lemmas 3.2 and 3.3] to establish the following Proposition after matching the notations. More precisely, using (3.9), the matrix $\Lambda(\mathbf{s})$ introduced in [2, Lemma 3.3] should be replaced by $2\varrho\mathcal{W}_s$, the matrix A^0 (resp. the vector field b^0) introduced in [2, (1.8) and below] should be replaced by $\varrho\,\mathrm{Id}$ (resp. by 0) and the matrix $B(\mathbf{s})$ introduced in [2, beginning of Section 2] should be replaced by 0.

Proposition 6.5. — *Recall the notation* (3.9)*. There exists*

$$\ell_0^{\mathbf{s},\tilde{\mathbf{m}}} \in \mathcal{C}^\infty(B(\mathbf{s},2r),\mathbb{R})$$

such that

- *For $x \in B(\mathbf{s},2r)$,*

$$\phi_+(x) = W(x) - W(\mathbf{s}) + \frac{\ell_0^{\mathbf{s},\tilde{\mathbf{m}}}(x)^2}{2}.$$

  In particular, $\ell_0^{\mathbf{s},\tilde{\mathbf{m}}}$ vanishes at $\mathbf{s}$.
- *The function $\ell_0^{\mathbf{s},\tilde{\mathbf{m}}}$ is a solution of* (6.8) *in $B(\mathbf{s},2r)$.*
- *The vector $\nabla\ell_0^{\mathbf{s},\tilde{\mathbf{m}}}(\mathbf{s})$ that we denote $\nu^{\mathbf{s},\tilde{\mathbf{m}}}$ is not 0 and satisfies*

$$2\mathcal{W}_s\nu^{\mathbf{s},\tilde{\mathbf{m}}} = -\left|\nu^{\mathbf{s},\tilde{\mathbf{m}}}\right|^2 \nu^{\mathbf{s},\tilde{\mathbf{m}}}.$$

- *Finally,*

$$\det\left(\mathrm{Hess}_{\mathbf{s}}\left(W + \frac{\left(\ell_0^{\mathbf{s},\tilde{\mathbf{m}}}\right)^2}{2}\right)\right) = \left|\det \mathcal{W}_{\mathbf{s}}\right|.$$

6.2. Solving for $(\ell_j^{\mathbf{s},\tilde{\mathbf{m}}})_{j\geqslant 1}$

Once again we drop some exponents $\mathbf{s}$ and $\tilde{\mathbf{m}}$ for shortness. Now that ℓ_0 is given by Proposition 6.5, we can solve the transport equations (6.9) by induction, so we suppose that $\ell_0,\dots,\ell_{j-1}$ are given and we want to find a solution ℓ_j to (6.9). Denote

$$\widetilde{U}=q_0\Big(x,i\big(\nabla W+\ell_0\nabla\ell_0\big)\Big)(2\nabla W+\ell_0\nabla\ell_0)+\ell_0 U\in\mathcal{C}^\infty(B(\mathbf{s},2r))$$

and

$$\tau=\nabla\ell_0\cdot U\in\mathcal{C}^\infty(B(\mathbf{s},2r))$$

where U was introduced in (6.7). The function ℓ_j must satisfy $(\widetilde{U}\cdot\nabla+\tau)\ell_j=-R_j(\ell_0,\dots,\ell_{j-1})$ so we are interested in the operator $\mathcal{L}=\widetilde{U}\cdot\nabla+\tau$ that we decompose as $\mathcal{L}=\mathcal{L}_0^{\mathbf{s}}+\mathcal{L}_>$ with

$$\mathcal{L}_0^{\mathbf{s}}=\widetilde{U}_0^{\mathbf{s}}\big(x-\mathbf{s}\big)\cdot\nabla+\tau_0^{\mathbf{s}}$$

where $\widetilde{U}_0^{\mathbf{s}}$ is the differential of $\widetilde{U}$ at $\mathbf{s}$ and $\tau_0^{\mathbf{s}}=\tau(\mathbf{s})$, that is with (3.9)

$$\widetilde{U}_0^{\mathbf{s}}=2\varrho\big(\mathcal{W}_s+\nu\nu^t\big)\quad\text{and}\quad\tau_0^{\mathbf{s}}=\varrho\big|\nu^{\mathbf{s},\tilde{\mathbf{m}}}\big|^2.$$

As usual, we will often omit the exponents $\mathbf{s}$ in the notations. Notice that if we denote $\mathcal{P}^n_{\mathrm{hom}}$ the space of homogeneous polynomials of degree n in the variables $(x-\mathbf{s})$, we have $\mathcal{L}_0\in\mathscr{L}(\mathcal{P}^n_{\mathrm{hom}})$ and for $P\in\mathcal{P}^n_{\mathrm{hom}}$, $\mathcal{L}_>P(x)=O((x-\mathbf{s})^{n+1})$ near $\mathbf{s}$. Using Proposition 6.5, it is easy to check that the spectrum of $\widetilde{U}_0^{\mathbf{s}}$ is exactly the spectrum of $2\varrho\mathcal{W}_s$ except that the negative eigenvalue $-\tau_0^{\mathbf{s}}$ is replaced by $\tau_0^{\mathbf{s}}$. We can then apply [2, Lemma A.1] to get that $\mathcal{L}_0^{\mathbf{s}}$ is invertible on $\mathcal{P}^n_{\mathrm{hom}}$. Thanks to this fact, one can proceed as in [2, Section 3.3] (see also [7, Chapter 3]), i.e find an approximate solution of (6.9) using formal power series and then refine it into an actual solution using the characteristic method. This gives the following result.

Proposition 6.6. — *For all $j\geqslant 1$, there exists $\ell_j^{\mathbf{s},\tilde{\mathbf{m}}}\in\mathcal{C}^\infty(B(\mathbf{s},2r))$ solving* (6.9)*. Moreover, $\ell_j^{\mathbf{s},\tilde{\mathbf{m}}}$ is real valued in view of Lemmas 6.2 and 6.3.*

6.3. Construction of $\ell^{\mathbf{s},\tilde{\mathbf{m}}}$

Now that we have found $(\ell_j)_{j\geqslant 0}\subset\mathcal{C}^\infty(B(\mathbf{s},2r),\mathbb{R})$ solving (6.8) and (6.9) with ℓ_0 vanishing at $\mathbf{s}$, we can use a Borel procedure to construct $\ell\in\mathcal{C}^\infty(\mathbb{R}^d,\mathbb{R})$ supported in $B(\mathbf{s},3r)$ and satisfying $\ell\sim\sum_{j\geqslant 0}h^j\ell_j$ on $B(\mathbf{s},2r)$.

Remark 6.7. — The properties (a)–(d) p. 1270 are satisfied by both the functions $\ell^{\mathbf{s},\tilde{\mathbf{m}}}$ and $-\ell^{\mathbf{s},\tilde{\mathbf{m}}}$. Moreover, by Lemma 6.3, $(-\ell_j^{\mathbf{s},\tilde{\mathbf{m}}})_{j\geqslant 0}$ also solve (6.8) and (6.9).

At this point, a straightforward adaptation of the proof of [16, Proposition 5.2] yields the following result which states that all the properties from p. 1270 are satisfied.

Proposition 6.8. — *We can choose the signs of the functions*

$$(\ell^{\mathbf{s},\tilde{\mathbf{m}}})_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})}$$

such that hypotheses p. 1270 holds true and the coefficients from the classical expansion of $\ell^{\mathbf{s},\tilde{\mathbf{m}}}$ *solve* (6.8) *and* (6.9).

We end this section with the following observation from [2, Lemma 6.4].

Lemma 6.9. — *If* $\mathbf{s}\in\mathbf{j}^\alpha(\mathbf{m})\cap\mathbf{j}^{\alpha'}(\mathbf{m}')$ *with* $\mathbf{m}\neq\mathbf{m}'$, *we can suppose (up to a modification by* $O(h^\infty)$*) that*

$$\ell^{\mathbf{s},\mathbf{m}} = -\ell^{\mathbf{s},\mathbf{m}'}$$

and consequently,

$$\theta^\alpha_{\mathbf{m},h} = 1-\theta^{\alpha'}_{\mathbf{m}',h} \quad \text{on } B(\mathbf{s},r)\cap\Big(\operatorname{supp}\theta^\alpha_{\mathbf{m},h}\cup\operatorname{supp}\theta^{\alpha'}_{\mathbf{m}',h}\Big).$$

7. Interaction between two wells

One of the final steps of proof is to compute the coefficients of the interaction matrix $(\langle P_h f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle)_{\mathbf{m},\mathbf{m}'\in\mathcal{U}^{(0)}}$ (in particular to prove that (1.5) holds true). It appears that the main contributions in the expression of $\langle P_h f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle$ are given near the saddle points separating two wells on which $f_{\mathbf{m},h}$ and $f_{\mathbf{m}',h}$ are supported. In view of (3.10), we are then first going to compute the interaction only between two wells, namely

$$\Big\langle P_h\Big((a^h)^{-1}\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big),\quad (a^h)^{-1}\chi_{\alpha'}\theta^{\alpha'}_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\Big\rangle.$$

Recall that the equivalence classes of $\mathcal{R}$ are denoted $(\mathcal{U}^{(0)}_\alpha)_{\alpha\in\mathcal{A}}$ (with $\mathcal{A}$ a finite set) and let α, $\alpha'\in\mathcal{A}$ as well as $\mathbf{m}\in\mathcal{U}^{(0)}_\alpha$ and $\mathbf{m}'\in\mathcal{U}^{(0)}_{\alpha'}$.

Lemma 7.1. — *For all* $\widetilde{\mathbf{m}}\in\widehat{\mathcal{U}}^{(0)}_\alpha$ *and* $\widetilde{\mathbf{m}}'\in\widehat{\mathcal{U}}^{(0)}_{\alpha'}$ *such that* $\mathbf{j}^\alpha(\widetilde{\mathbf{m}})\cap\mathbf{j}^{\alpha'}(\widetilde{\mathbf{m}}')\neq\emptyset$, *the following holds:*

$$\alpha=\alpha' \quad \text{or} \quad \varphi^\alpha_{\mathbf{m}}(\widetilde{\mathbf{m}})\varphi^{\alpha'}_{\mathbf{m}'}(\widetilde{\mathbf{m}}')=0.$$

Proof. — First, notice that since $\widehat{\mathcal{U}}^{(0)}_\alpha\subset E_-(\mathbf{m})$ and $\widehat{\mathcal{U}}^{(0)}_{\alpha'}\subset E_-(\mathbf{m}')$, our hypothesis implies that $E_-(\mathbf{m})=E_-(\mathbf{m}')$. In particular, $\widehat{\mathbf{m}}'=\widehat{\mathbf{m}}$. If $\widehat{\mathbf{m}}\notin\{\widetilde{\mathbf{m}},\widetilde{\mathbf{m}}'\}$, we easily have $\widetilde{\mathbf{m}}\mathcal{R}\widetilde{\mathbf{m}}'$ and $\alpha=\alpha'$. Let us now suppose that

$$\widehat{\mathbf{m}}\in\{\widetilde{\mathbf{m}},\widetilde{\mathbf{m}}'\}. \tag{7.1}$$

According to [16, Lemma 3.4], $\mathbf{m}$ and $\mathbf{m}'$ are in the same CC of $\{W \leqslant \boldsymbol{\sigma}(\mathbf{m})\}$ that we denote $E_{\leqslant}$. By uniqueness of $\widehat{\mathbf{m}}$ in $E_-(\mathbf{m})$, each CC of $\{W < \boldsymbol{\sigma}(\mathbf{m})\} \cap E_{\leqslant}$ contains exactly one element from $\boldsymbol{\sigma}^{-1}(\{\boldsymbol{\sigma}(\mathbf{m})\}) \cup \{\widehat{\mathbf{m}}\}$. If $\mathbf{m}$ or $\mathbf{m}'$ is of type II, we get by definition of $\mathcal{R}$ that $\alpha = \alpha'$. Otherwise, (7.1) combined with Lemma 3.1 (b) yield $\varphi^{\alpha}_{\mathbf{m}}(\widetilde{\mathbf{m}})\varphi^{\alpha'}_{\mathbf{m}'}(\widetilde{\mathbf{m}}') = 0$. $\square$

With the notations from Section 3, let us denote for $\widetilde{\mathbf{m}} \in \widehat{\mathcal{U}}^{(0)}_{\alpha}$ and $\widetilde{\mathbf{m}}' \in \widehat{\mathcal{U}}^{(0)}_{\alpha'}$

$$\mathcal{N}^{\alpha,\alpha'}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'} = h^{-d/2} c^{\alpha}_h(\widetilde{\mathbf{m}}) c^{\alpha'}_h(\widetilde{\mathbf{m}}') \mathrm{e}^{\frac{W(\tilde{\mathbf{m}})+W(\tilde{\mathbf{m}}')}{h}} \\ \times \left\langle P_h\Big((a^h)^{-1}\chi_{\alpha}\theta^{\alpha}_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big), \quad (a^h)^{-1}\chi_{\alpha'}\theta^{\alpha'}_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\right\rangle.$$

When $\alpha = \alpha'$, we denote for shortness $\mathcal{N}^{\alpha,\alpha}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'} = \mathcal{N}^{\alpha}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}$.

Lemma 7.2. — *Let $\widetilde{\mathbf{m}} \in \widehat{\mathcal{U}}^{(0)}_{\alpha}$ and $\widetilde{\mathbf{m}}' \in \widehat{\mathcal{U}}^{(0)}_{\alpha'}$.*

- *If $\mathbf{j}^{\alpha}(\widetilde{\mathbf{m}}) \cap \mathbf{j}^{\alpha'}(\widetilde{\mathbf{m}}') = \emptyset$, we have*

$$\mathcal{N}^{\alpha,\alpha'}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'} = O\bigg(h^{\infty}\mathrm{e}^{-\frac{\boldsymbol{\sigma}(\alpha)+\boldsymbol{\sigma}(\alpha')-W(\tilde{\mathbf{m}})-W(\tilde{\mathbf{m}}')}{h}}\bigg).$$

- *When $\alpha = \alpha'$, we have*

$$\mathcal{N}^{\alpha}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'} = h\mathrm{e}^{-\frac{2\boldsymbol{\sigma}(\alpha)-W(\tilde{\mathbf{m}})-W(\tilde{\mathbf{m}}')}{h}} N^{\alpha}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}$$

with $N^{\alpha}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}$ admitting an asymptotic expansion whose first term is

$$N^{\alpha,0}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'} = \frac{(-1)^{1-\delta_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}}}{2\pi}\left(\sum_{\mathbf{m}\in H^{\alpha}(\tilde{\mathbf{m}})} \det \mathcal{W}_{\mathbf{m}}^{-1/2}\right)^{-1/2} \\ \times \left(\sum_{\mathbf{m}'\in H^{\alpha}(\tilde{\mathbf{m}}')} \det \mathcal{W}_{\mathbf{m}'}^{-1/2}\right)^{-1/2} \sum_{\mathbf{s}\in \mathbf{j}^{\alpha}(\tilde{\mathbf{m}})\cap \mathbf{j}^{\alpha}(\tilde{\mathbf{m}}')} |\det \mathcal{W}_{\mathbf{s}}|^{-1/2}\tau^{\mathbf{s}}_0$$

where we recall the notation (3.9) *and that $-\tau^{\mathbf{s}}_0$ is the negative eigenvalue of $2\varrho\mathcal{W}_{\mathbf{s}}$.*

Proof. — First, notice that by Hypothesis 1.3, we have

$$\left\langle P_h\Big((a^h)^{-1}\chi_{\alpha}\theta^{\alpha}_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big), \quad (a^h)^{-1}\chi_{\alpha'}\theta^{\alpha'}_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\right\rangle \\ = \left\langle \widetilde{P}_h\Big(\chi_{\alpha}\theta^{\alpha}_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big), \quad \chi_{\alpha'}\theta^{\alpha'}_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\right\rangle.$$

We will use the following localizations and estimates obtained thanks to (3.5) and (5.5):

$$\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big)\mathbf{1}_{\left\{\mathrm{dist}\left(\cdot,\mathbf{j}^\alpha\left(\widehat{\mathcal{U}}^{(0)}_\alpha\right)\right)\geqslant r\right\}} = O\Big(h^\infty\mathrm{e}^{-\frac{\boldsymbol{\sigma}(\alpha)}{h}}\Big); \tag{7.2}$$

$$\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big) = O\Big(h^{\frac{2+d}{4}}\mathrm{e}^{-\frac{\boldsymbol{\sigma}(\alpha)}{h}}\Big) \tag{7.3}$$

and by the non stationary phase method applied as for (5.8)

$$\mathrm{Op}_h(q^h)\Big(\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big)\Big)\mathbf{1}_{\left\{\mathrm{dist}(\cdot,\mathbf{j}^\alpha(\widehat{\mathcal{U}}^{(0)}_\alpha))\geqslant 2r\right\}} = O\Big(h^\infty\mathrm{e}^{-\frac{\boldsymbol{\sigma}(\alpha)}{h}}\Big). \tag{7.4}$$

Using the fact that

$$\widetilde{P}_h = \mathrm{d}_W^*\circ\widehat{Q}\circ\mathrm{d}_W,$$

the boundedness of $\mathrm{Op}_h(q^h)$ as well as (7.2), (7.3) and (7.4), we can write that

$$\begin{aligned}&\Big\langle\widetilde{P}_h\big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\big),\chi_{\alpha'}\theta^{\alpha'}_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\Big\rangle + O\Big(h^\infty\mathrm{e}^{-\frac{\boldsymbol{\sigma}(\alpha)+\boldsymbol{\sigma}(\alpha')}{h}}\Big)\\ &\quad= \sum_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})\cap\mathbf{j}^{\alpha'}(\tilde{\mathbf{m}}')}\Big\langle\mathrm{Op}_h(q^h)\big(\mathrm{d}_W\big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\big)\big),\mathrm{d}_W\big(\chi_{\alpha'}\theta^{\alpha'}_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\big)\Big\rangle_{\mathbf{s}}\end{aligned} \tag{7.5}$$

where $\langle\cdot,\cdot\rangle_{\mathbf{s}}$ denotes the inner product on $L^2(B(\mathbf{s},r))$. This already proves the first statement. Now when $\alpha=\alpha'$, thanks to the fact that $\mathrm{e}^{-W/h}\in\mathrm{Ker}\ \mathrm{d}_W$ and by Lemma 6.9, we have for $\mathbf{s}\in\mathbf{j}^\alpha(\widetilde{\mathbf{m}})\cap\mathbf{j}^\alpha(\widetilde{\mathbf{m}}')$

$$\begin{aligned}\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big) &= \mathrm{d}_W\Big(\big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}-1\big)\mathrm{e}^{-W/h}\Big)\\ &= \mathrm{d}_W\Big(\chi_\alpha\big(\theta^\alpha_{\tilde{\mathbf{m}},h}-1\big)\mathrm{e}^{-W/h}\Big) + O\Big(h^\infty\mathrm{e}^{-\frac{\boldsymbol{\sigma}(\alpha)}{h}}\Big)\\ &= (-1)^{1-\delta_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}}\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\Big) + O\Big(h^\infty\mathrm{e}^{-\frac{\boldsymbol{\sigma}(\alpha)}{h}}\Big)\end{aligned}$$

on $B(\mathbf{s},r)$. Thus, (7.5) becomes

$$\begin{aligned}&\Big\langle\widetilde{P}_h\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big),\ \chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}}',h}\mathrm{e}^{-W/h}\Big\rangle + O\Big(h^\infty\mathrm{e}^{-\frac{2\boldsymbol{\sigma}(\alpha)}{h}}\Big)\\ &\quad= (-1)^{1-\delta_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}}\\ &\qquad\times\sum_{\mathbf{s}\in\mathbf{j}^\alpha(\tilde{\mathbf{m}})\cap\mathbf{j}^\alpha(\tilde{\mathbf{m}}')}\Big\langle\mathrm{Op}_h(q^h)\Big(\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big)\Big),\ \mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big)\Big\rangle_{\mathbf{s}}.\end{aligned}$$

We can now work as in [16, proof of Lemma 5.3], to get that

$$\begin{aligned}\Big\langle\mathrm{Op}_h(q^h)\Big(\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big)\Big),\quad\mathrm{d}_W\Big(\chi_\alpha\theta^\alpha_{\tilde{\mathbf{m}},h}\mathrm{e}^{-W/h}\Big)\Big\rangle_{\mathbf{s}}&\\ = \frac{h}{2\pi}(\pi h)^{d/2}\mathrm{e}^{-\frac{2\boldsymbol{\sigma}(\alpha)}{h}}\vartheta^{\mathbf{s},h}&\end{aligned}$$

with $\vartheta^{\mathbf{s},h}$ admitting a classical expansion whose first term is $|\det\mathcal{W}_{\mathbf{s}}|^{-1/2}\tau_0^{\mathbf{s}}$. Combining this with (3.8), we get the announced result. ☐

8. Interaction between two quasimodes

In this section, we finish the computation of the interaction matrix that we started in Section 7. It will in particular yield that (1.5) holds true (see (8.1) and Lemma 8.1). We will then be able to provide the proof of Theorem 8.4 which is the main result of the paper.

By (3.10), we have for $\mathbf{m} \in \mathcal{U}_{\alpha}^{(0)}$ and $\mathbf{m}' \in \mathcal{U}_{\alpha'}^{(0)}$

$$\begin{aligned}
&\langle P_h f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle \\
&\qquad = h^{-d/2} \sum_{\tilde{\mathbf{m}} \in \widehat{\mathcal{U}}_{\alpha}^{(0)}} \sum_{\tilde{\mathbf{m}}' \in \widehat{\mathcal{U}}_{\alpha'}^{(0)}} \varphi_{\mathbf{m}}^{\alpha}(\widetilde{\mathbf{m}}) \varphi_{\mathbf{m}'}^{\alpha'}(\widetilde{\mathbf{m}}') c_h^{\alpha}(\widetilde{\mathbf{m}}) c_h^{\alpha'}(\widetilde{\mathbf{m}}') \\
&\qquad\qquad \times \left\langle P_h\Big((a^h)^{-1}\chi_{\alpha}\theta_{\tilde{\mathbf{m}},h}^{\alpha} \mathrm{e}^{-W_{\mathbf{m}}/h}\Big), (a^h)^{-1}\chi_{\alpha'}\theta_{\tilde{\mathbf{m}}',h}^{\alpha'}\mathrm{e}^{-W_{\mathbf{m}'}/h}\right\rangle \\
&\qquad = \sum_{\tilde{\mathbf{m}} \in \widehat{\mathcal{U}}_{\alpha}^{(0)}} \sum_{\tilde{\mathbf{m}}' \in \widehat{\mathcal{U}}_{\alpha'}^{(0)}} \varphi_{\mathbf{m}}^{\alpha}(\widetilde{\mathbf{m}}) \varphi_{\mathbf{m}'}^{\alpha'}(\widetilde{\mathbf{m}}') \mathcal{N}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}^{\alpha,\alpha'} \\
&\qquad = \sum_{\substack{\tilde{\mathbf{m}} \in \widehat{\mathcal{U}}_{\alpha}^{(0)};\\ W(\tilde{\mathbf{m}})=W(\mathbf{m})}} \sum_{\substack{\tilde{\mathbf{m}}' \in \widehat{\mathcal{U}}_{\alpha'}^{(0)};\\ W(\tilde{\mathbf{m}}')=W(\mathbf{m}')}} \varphi_{\mathbf{m}}^{\alpha}(\widetilde{\mathbf{m}}) \varphi_{\mathbf{m}'}^{\alpha'}(\widetilde{\mathbf{m}}') \mathcal{N}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}^{\alpha,\alpha'}
\end{aligned}$$

by Lemma 3.1 (c). According to Lemma 7.2, the leading terms in the previous sum are the ones for which $\widetilde{\mathbf{m}}$, $\widetilde{\mathbf{m}}'$ are such that $\mathbf{j}^{\alpha}(\widetilde{\mathbf{m}}) \cap \mathbf{j}^{\alpha'}(\widetilde{\mathbf{m}}') \neq \emptyset$. Combined with Lemma 7.1, we get

$$\begin{aligned}
&\langle P_h f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle \\
&\qquad = \delta_{\alpha,\alpha'} \sum_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}' \in \widehat{\mathcal{U}}_{\alpha}^{(0)}} \varphi_{\mathbf{m}}^{\alpha}(\widetilde{\mathbf{m}}) \varphi_{\mathbf{m}'}^{\alpha}(\widetilde{\mathbf{m}}') \mathcal{N}_{\tilde{\mathbf{m}},\tilde{\mathbf{m}}'}^{\alpha} + O\Big(h^{\infty}\mathrm{e}^{-\frac{S(\mathbf{m})+S(\mathbf{m}')}{h}}\Big). \qquad (8.1)
\end{aligned}$$

We now want to go from quasimodes to actual eigenfunctions. This is where the optimization on the choice of the functions $\ell^{\mathbf{s},\mathbf{m}}$ will enable us to have the correct error terms. Here we briefly remind the procedure and give the main arguments. We refer to [18, Lemma 4.9, Proposition 4.12] for more details. First, combining Proposition 5.3, (d) p. 1270, Proposition 6.8, and a standard Laplace method, we obtain the following fundamental estimate.

Lemma 8.1. — *Let $\mathbf{m} \in \underline{\mathcal{U}}^{(0)}$. We have*

$$\|P_h f_{\mathbf{m},h}\| = O\Big(h^{\infty}\mathrm{e}^{-\frac{S(\mathbf{m})}{h}}\Big).$$

Now, considering the orthogonal projector on the generalized eigenspace associated to the small eigenvalues of P_h given by

$$\Pi_0 = \frac{1}{2i\pi}\int_{|z|=ch}(z-P_h)^{-1}\mathrm{d}z \tag{8.2}$$

and writing

$$(1-\Pi_0)f_{\mathbf{m},h} = \frac{-1}{2i\pi}\int_{|z|=ch} z^{-1}(z-P_h)^{-1}P_h f_{\mathbf{m},h}\mathrm{d}z,$$

Lemma 8.1 together with the resolvent estimate (1.3) give that for any $\mathbf{m}\in\mathcal{U}^{(0)}$, we have

$$\|(1-\Pi_0)f_{\mathbf{m},h}\| = O\Big(h^\infty \mathrm{e}^{-\frac{S(\mathbf{m})}{h}}\Big).$$

Proceeding as in [18, Proposition 4.10], one can then establish the following thanks to Proposition 4.1.

Lemma 8.2. — *Recall the notation* (8.2)*. The family* $(\Pi_0 f_{\mathbf{m},h})_{\mathbf{m}\in\mathcal{U}^{(0)}}$ *is almost orthonormal: there exists* $c>0$ *such that*

$$\langle \Pi_0 f_{\mathbf{m},h}, \Pi_0 f_{\mathbf{m}',h}\rangle = \delta_{\mathbf{m},\mathbf{m}'} + O\Big(\mathrm{e}^{-c/h}\Big).$$

In particular, it is a basis of the space $H=\operatorname{Ran}\Pi_0$*. Moreover, we have*

$$\langle P_h\Pi_0 f_{\mathbf{m},h}, \Pi_0 f_{\mathbf{m}',h}\rangle = \langle P_h f_{\mathbf{m},h}, f_{\mathbf{m}',h}\rangle + O\Big(h^\infty \mathrm{e}^{-\frac{S(\mathbf{m})+S(\mathbf{m}')}{h}}\Big).$$

Let us re-label the local minima $\mathbf{m}_1,\dots,\mathbf{m}_{n_0}$ so that $(S(\mathbf{m}_j))_{j=1,\dots,n_0}$ is non increasing in j. For shortness, we will now denote

$$f_j = f_{\mathbf{m}_j,h}$$

which still depends on h. We also denote $(\widetilde{u}_j)_{j=1,\dots,n_0}$ the orthogonalization by the Gram–Schmidt procedure of the family $(\Pi_0 f_j)_{j=1,\dots,n_0}$ and

$$u_j = \frac{\widetilde{u}_j}{\|\widetilde{u}_j\|}.$$

In this setting and with our previous results, we get the following (see [18, Proposition 4.12] for a proof).

Lemma 8.3. — *For all* $1\leqslant j,k\leqslant n_0$*, it holds*

$$\langle P_h u_j, u_k\rangle = \langle P_h f_j, f_k\rangle + O\Big(h^\infty \mathrm{e}^{-\frac{S(\mathbf{m}_j)+S(\mathbf{m}_k)}{h}}\Big).$$

In order to compute the small eigenvalues of P_h, let us now consider the restriction $P_h|_H : H\to H$. We denote $\widehat{u}_j = u_{n_0-j+1}$ and $\mathcal{M}$ the matrix of $P_h|_H$ in the orthonormal basis $(\widehat{u}_1,\dots,\widehat{u}_{n_0})$. Since $\widehat{u}_{n_0}=u_1=f_1$, we have

$$\mathcal{M} = \begin{pmatrix}\mathcal{M}' & 0\\ 0 & 0\end{pmatrix} \qquad \text{where} \qquad \mathcal{M}' = (\langle P_h\widehat{u}_j,\widehat{u}_k\rangle)_{1\leqslant j,k\leqslant n_0-1}$$

and it is sufficient to study the spectrum of $\mathcal{M}'$. We will also denote $\{\widehat{S}_1 < \cdots < \widehat{S}_p\}$ the set $\{S(\mathbf{m}_j); 2 \leqslant j \leqslant n_0\}$ and for $1 \leqslant k \leqslant p$, E_k the subspace of $L^2(\mathbb{R}^d)$ generated by $\{\widehat{u}_r; S(\mathbf{m}_r) = \widehat{S}_k\}$. Finally, we set $\varpi_k = \mathrm{e}^{-(\hat{S}_k - \hat{S}_{k-1})/h}$ for $2 \leqslant k \leqslant p$ and $\varepsilon_j(\varpi) = \prod_{k=2}^{j} \varpi_k = \mathrm{e}^{-(\hat{S}_j - \hat{S}_1)/h}$ for $2 \leqslant j \leqslant p$ (with the convention $\varepsilon_1(\varpi) = 1$).

For a given class $\alpha \in \mathcal{A}$, let us denote $n_\alpha = |\mathcal{U}_\alpha^{(0)}|$ and also label its elements $\mathbf{m}_1^\alpha, \dots, \mathbf{m}_{n_\alpha}^\alpha$ so that $(S(\mathbf{m}_j^\alpha))_{j=1,\dots,n_\alpha}$ is non decreasing in j. We also set $\mathbf{m}_{n_\alpha+1}^\alpha = \widehat{\mathbf{m}}$ for some $\mathbf{m} \in \mathcal{U}_\alpha^{(0)}$. We will consider the matrix

$$M_h^\alpha = \Big(N^\alpha \varphi_{\mathbf{m}_j^\alpha}^\alpha \cdot \varphi_{\mathbf{m}_k^\alpha}^\alpha\Big)_{1 \leqslant j,k \leqslant n_\alpha} = \mathcal{T}_\alpha^* N^\alpha \mathcal{T}_\alpha$$

where N^α is the matrix whose entries were introduced in Lemma 7.2 and

$$\mathcal{T}_\alpha = \Big(\varphi_{\mathbf{m}_k^\alpha}^\alpha(\mathbf{m}_j^\alpha)\Big)_{\substack{1 \leqslant j \leqslant n_\alpha+1 \\ 1 \leqslant k \leqslant n_\alpha}}.$$

Before we can state our main result, we need to introduce some material from [2, Section 6.3]. For the finite dimensional vector space $E = E_1 \oplus \cdots \oplus E_p$, and $j \in \{1, \dots, p\}$, let us write a general matrix $M \in \mathcal{M}(E)$ by blocks

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in \mathscr{L}\Big((E_1 \oplus \cdots \oplus E_{j-1}) \oplus (E_j \oplus \cdots \oplus E_p)\Big). \tag{8.3}$$

If $A \in \mathcal{M}(E_1 \oplus \cdots \oplus E_{j-1})$ is invertible, the Schur matrix of M (with respect to the vector space $E_1 \oplus \cdots \oplus E_{j-1}$) is the matrix on $E_j \oplus \cdots \oplus E_p$ defined by

$$\mathcal{R}_j(M) = D - CA^{-1}B,$$

where by convention $\mathcal{R}_1(M) = M$. By the Schur complement method, M is invertible if and only if $\mathcal{R}_j(M)$ is invertible. We will also denote by $\mathcal{J} : \mathcal{M}(\oplus_{k=j,\dots,p} E_k) \to \mathcal{M}(E_j)$ the restriction map to the first vector space E_j of $\oplus_{k=j,\dots,p} E_k$. More precisely, with the notations of (8.3), we will write $\mathcal{J}(M) = A$ when $j = 1$. Of course, the map $\mathcal{J}$ depends on $j \in \{1, \dots, p\}$, but we omit this dependence since the set on which $\mathcal{J}$ is acting will be obvious in the sequel. We will also use the convention

$$\operatorname{Spec}(\mathcal{J} \circ \mathcal{R}_j(M_h^\alpha)) = \emptyset \quad \text{if} \quad \widehat{S}_j \notin \{S(\mathbf{m}_k^\alpha); k = 1, \dots, n_\alpha\}.$$

Theorem 8.4. — *With the notations introduced above, we have*

$$\operatorname{Spec}(\mathcal{M}') \subset h\mathrm{e}^{-2\hat{S}_1/h} \bigcup_{\alpha \in \mathcal{A}} \bigcup_{j=1}^{p} \varepsilon_j(\varpi)^2 \Big(\operatorname{Spec}\big(\mathcal{J} \circ \mathcal{R}_j(M_h^\alpha)\big) + D\big(0, O(h^\infty)\big)\Big)$$

with M_h^α admitting an asymptotic expansion whose first term is $\mathcal{T}_0^* N^{\alpha,0} \mathcal{T}_0$ where $N^{\alpha,0}$ is defined in Lemma 7.2 and $\mathcal{T}_0$ is the leading term of the matrix $\mathcal{T}_\alpha$, so that $\mathcal{T}_0$ is given by Lemma 3.1.

Proof. — Consider the symmetric matrix $M_h^{\#} \in \mathcal{M}_{n_0-1}(\mathbb{R})$ defined by

$$\big(M_h^{\#}\big)_{j,k} = \begin{cases} N^\alpha \varphi^\alpha_{\mathbf{m}_{n_0-j+1}} \cdot \varphi^\alpha_{\mathbf{m}_{n_0-k+1}} & \text{if } \mathbf{m}_{n_0-j+1}, \mathbf{m}_{n_0-k+1} \in \mathcal{U}_\alpha^{(0)} \\ 0 & \text{otherwise} \end{cases}$$

and notice that in view of Lemma 8.3 and (8.1), we have

$$h^{-1} e^{2\hat{S}_1/h} \mathcal{M}' = \Omega(\varpi)\big(M_h^{\#} + O(h^\infty)\big)\Omega(\varpi)$$

where $\Omega(\varpi) = \operatorname{diag}(\varepsilon_1(\varpi) \operatorname{Id}_{E_1}, \dots, \varepsilon_p(\varpi) \operatorname{Id}_{E_p})$. Clearly, M_h^α is the restriction to α of the matrix $M_h^{\#}$ which is permutation similar to the block-diagonal matrix $\operatorname{diag}(M_h^\alpha; \alpha \in \mathcal{A})$. In particular, $M_h^{\#}$ admits an asymptotic expansion thanks to Lemmas 3.1 and 7.2. Moreover, it is positive definite as each M_h^α appears to be positive definite. Indeed, $\mathcal{T}_0$ is clearly injective as the family $(\varphi^\alpha_{\mathbf{m}})_{\mathbf{m} \in \mathcal{U}_\alpha^{(0)}}$ is orthonormal and it is shown in [2, Proposition 6.8], that $N^{\alpha,0} = L_\alpha^* L_\alpha$ where L_α is an injective matrix, so M_0^α is positive definite. In the words of [2, Definition 6.7], we obtain that $h^{-1} e^{2\hat{S}_1/h} \mathcal{M}'$ is a classical graded symmetric matrix so we can apply [2, Theorem 4] to get

$$\operatorname{Spec}(\mathcal{M}') \subset h e^{-2\hat{S}_1/h} \bigcup_{j=1}^{p} \varepsilon_j(\varpi)^2 \Big(\operatorname{Spec}\big(\mathcal{J} \circ \mathcal{R}_j\big(M_h^{\#}\big)\big) + D\big(0, O(h^\infty)\big)\Big).$$

We can then conclude as

$$\operatorname{Spec}\big(\mathcal{J} \circ \mathcal{R}_j\big(M_h^{\#}\big)\big) = \bigcup_{\alpha \in \mathcal{A}} \operatorname{Spec}\big(\mathcal{J} \circ \mathcal{R}_j(M_h^\alpha)\big)$$

(see [2, Theorem 6] and above for details). □

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