environm.

Semiclassical resolvent estimates for Schrödinger matrix operators with eigenvalues crossing.

Thierry Jecko
IRMAR, Universit de Rennes I,
Campus Beaulieu,
F-35042 Rennes Cdex, France
jecko@maths.univ-rennes1.fr

09-11-01

Abstract

For semiclassical Schrödinger 2×2-matrix operators, the symbol of which has crossing eigenvalues, we investigate the semiclassical Mourre theory to derive bounds $O(h^{-1})$ (h being the semiclassical parameter) for the boundary values of the resolvent, viewed as bounded operator on weighted spaces. Under the non-trapping condition on the eigenvalues of the symbol and under a condition on its matricial structure, we obtain the desired bounds for codimension one crossings. For codimension two crossings, we show that a geometrical condition at the crossing must hold to get the existence of a global escape function, required by the usual semiclassical Mourre theory.

Keywords: Schrödinger matrix operators, eigenvalues crossing, semiclassical resolvent estimates, semiclassical Mourre method, global escape function.

1 Introduction.

In this paper, we consider semiclassical Schrödinger operators with 2×2-matrix potential. Under general assumptions, they are self-adjoint, have continuous spectrum on the positive real axis, and, away from the pure point spectrum, their resolvents admit boundary values on this half-axis, as bounded operators on suitable weighted spaces. Our purpose is to find sufficient conditions to show that these resolvents are $O(h^{-1})$, where h is the semiclassical parameter.

Our main motivation for this kind of estimates is the semiclassical scattering theory for molecules and, in particular, the question of the accuracy of the Born-Oppenheimer

approximation in this context. Matrix potentials are a convenient simplification of Born-Oppenheimer effective potentials, which are operator-valued (see [Jec]). Semiclassical estimates of relevant objects in scattering theory may be deduced from these resolvent estimates (see [W1, RT]).
Using the semiclassical Mourre commutator method (see [Mo]), these resolvent estimates follow from non-trapping conditions on associated classical dynamics in the scalar case (see [GM, Kl]), the bound $O(h^{-1})$ being in this case a signature for non-trapping dynamics (see [W2]), and in the present case when the modes, i.e. the eigenvalues of the symbol of the operators, cross nowhere (see [Jec]). Therefore we want to study crossing modes and it is natural to try to adapt Mourre's method.
As far as the modes' crossing is concerned, we do not want to cover all cases, but our choices, inspired by [Ha], are not too restrictive. The first one, that we call Codimension 1 crossings, is of particular interest for the Born-Oppenheimer approximation for diatomic molecules. In this case, we manage to derive the expected bounds from non-trapping assumptions on the modes (see Theorem 2.4), provided some condition on the spectral subspaces of the symbol holds true. In contrast to [Jec], the proof is more complicated here, because, roughly speaking, the two modes do not decouple and we had to solve a nonlinear problem related to this fact. The condition on the spectral subspaces, which is independent with the non-trapping condition on the modes, enables us to construct global solutions of the nonlinear problem. For our second type of crossings, we have a negative result: the usual Mourre method (see Section 3) cannot apply (even under the previous non-trapping conditions), if some geometrical condition at the crossing does not hold. Although it is only an obstruction to Mourre method, we have some reasons to believe, the latter being also a trapping phenomenon at the crossing (that cannot be expressed in terms of the dynamics of the modes since they may break down there), which excludes the desired resolvent estimates (see Remark 2.7). If a strengthed version of the geometrical condition hold, we show in some weak sense that this trapping phenomenon at the crossing does not occur (see Proposition 2.8), but we were not able to derive the resolvent estimates under the previous non-trapping assumptions.
It is interesting to compare our present work with a part of [Ha] (see Section 2) and with [FG], although the full evolution is not considered there. In a different way, the present paper is complementary to [Ne1, Ne2].
Before ending this introduction, we want to mention an interesting comment by C. Grard on the subject. He regrets that we did not use a flow directly constructed from the symbol of the operator (via its Liouvillean). We did try but could not overcome the problem of non-commutation of matrix symbols.
In Section 2, we precisely present the frame in which we shall work, the assumptions we need, and the announced results, followed by some comments. In Section 3, we review the general strategy known as semiclassical Mourre method, that we follow here. Then we focus on the problem of constructing a global escape function, a key point in our strategy. Codimension 1 crossings are treated in Section 4 while Codimension 2 ones are considered in Section 5. Finally, some useful facts are collected in the appendix.

Acknowledgment: the author thanks, for fruitful discussions and advices, V. Bach, Y. Colin de Verdire, C. Grard, G. Hagedorn, A. Joye, N. Lerner, A. Martinez, G. Mtivier,

and F. Nier.

Contents

2 Notation and results.

First of all, let us introduce the Schrödinger 2×2 matrix operator we want to study. For some integer $n \geq 2$, we consider the semiclassical operator

$$\hat{P} \;:=\; -h^2 \Delta_x \mathrm{I}_2 + M(x) \tag{1}$$

acting in $\mathrm{L}^2(\mathbb{R}^n; \mathbb{C}^2)$, where h is the semiclassical parameter ($h \in]0; h_0]$ for some $h_0 > 0$), Δ_x denotes the Laplacian in $\mathbb{R}^n$, I_2 is the 2×2 identity matrix, and where $M(x)$ is the multiplication operator by a real symetric 2×2 matrix $M(x)$. We require that M is C^∞ on $\mathbb{R}^n$ and that there exist some $\delta > 0$ and some real symetric matrix M_∞ such that

$$\forall \alpha \in \mathbb{N}^n \;, \; \forall x \in \mathbb{R}^n \;, \quad \Big\| \partial_x^\alpha \Big(M(x) - M_\infty \Big) \Big\| \;=\; O_\alpha \Big(\langle x \rangle^{-\delta - |\alpha|} \Big) \tag{2}$$

where $\| \cdot \|$ denotes the operator norm on the 2×2 matrices and $\langle x \rangle = (1 + |x|^2)^{1/2}$. It is well known that, under this assumption on M, the operator $\hat{P}$ is self-adjoint on the domain of the Laplacian (see [RS2] for instance). Its resolvent will be denoted by

$R(z) := (\hat{P}-z)^{-1}$, for z in the resolvent set of $\hat{P}$ (we omit the h-dependence). If, for $s \in \mathbb{R}$, we denote by $\mathrm{L}^2_s(\mathbb{R}^n;\mathbb{C}^2)$ the weighted L^2 space of mesurable, $\mathbb{C}^2$-valued functions f on $\mathbb{R}^n$ such that $x \mapsto \langle x\rangle^s f(x)$ belongs to $\mathrm{L}^2(\mathbb{R}^n;\mathbb{C}^2)$, then it follows from Mourre theory that this resolvent has boundary values $R(\lambda \pm i0)$ as bounded operators from $\mathrm{L}^2_s(\mathbb{R}^n;\mathbb{C}^2)$ to $\mathrm{L}^2_{-s}(\mathbb{R}^n;\mathbb{C}^2)$, for any $s > 1/2$ and λ outside the pure point spectrum of $\hat{P}$ (in fact, we partially prove here this property again).

The operator $\hat{P}$ is a h-pseudodifferential operateur obtained by Weyl quantization of the following symbol, defined on $T^*\mathbb{R}^n$ with values in the real symetric 2×2 matrices,

$$P(x,\xi) \;:=\; |\xi|^2\mathrm{I}_2 + M(x)\,. \tag{3}$$

Notice that $M(x) = u(x)\mathrm{I}_2 + V(x)$ where $u(x)$ is 1/2 times the trace of $M(x)$ and

$$V(x) \;:=\; \begin{pmatrix} v_1(x) & v_2(x) \\ v_2(x) & -v_1(x) \end{pmatrix}$$

for smooth real functions v_1 and v_2. The eigenvalues of $V(x)$ are $\pm\rho(x)$ with $\rho(x) = (v_1(x)^2 + v_2(x)^2)^{1/2} = (-\mathrm{det}V)^{1/2}$ ($\mathrm{det}V$ being the determinant of V) and we denote by $\Pi_\pm(x)$ the associated eigenprojectors. While $\Pi_\pm = \mathrm{I}_2$ if $\rho = 0$, we have, for $\rho \neq 0$, $\Pi_\pm = (\mathrm{I}_2 \pm V/\rho)/2$. Similarly we introduce the corresponding notation for M_∞, namely u_∞, V_∞, $v_{1,\infty}$, $v_{2,\infty}$, and ρ_∞. We also define the scalar function on the phase space $p(x,\xi) := |\xi|^2 + u(x)$, which is 1/2 times the trace of the symbol P. Then the eigenvalues of P are $p_\pm(x,\xi) := p(x,\xi) \pm \rho(x)$. Notice that $p_+(x,\xi) = p_-(x,\xi) \iff \rho(x) = 0$. We denote by $\mathcal{C}$ (resp. $\mathcal{C}^*$) the zero set of ρ (or V), viewed in $\mathbb{R}^n$ (resp. $T^*\mathbb{R}^n$), that is the crossing set of the eigenvalues of P. The functions $p_\pm$ and p are smooth functions at least on $T^*\mathbb{R}^n \setminus \mathcal{C}^*$ thus generate Hamilton flows on this set. For any Hamilton function q, we shall denote by H_q its Hamilton field and by ϕ^t_q its Hamilton flow at time t. The following non-trapping condition on Hamilton flows and connected notion of global escape function (see [DG]) will play an important rôle in this paper.

Definition 2.1. *A smooth, real function q defined on an open subset U^* of some cotangent bundle ($T^*\mathbb{R}^n$ or $T^*\mathcal{C}$) is said to be non-trapping on some set $U^*_1 \subset U^*$ at energy λ if, for any point $\alpha \in U^*_1 \cap q^{-1}(\lambda)$, the evolution of α, according to the Hamilton flow ϕ^t_q of q, in both time directions, leaves any compact subset of $U^* \cap q^{-1}(\lambda)$, that is*

$$\forall \alpha \in U^*_1 \cap q^{-1}(\lambda),\, \forall K \subset\subset U^* \cap q^{-1}(\lambda),\, \exists T > 0;\; |t| \geq T \implies \phi^t_q(\alpha) \notin K\,.$$

The largest open set U^*_1 satisfying the previous condition and $U^* \setminus U^*_1$ are respectively the non-trapping and trapping region of q at energy λ. A trajectory $\{\phi^t_q(\alpha), t \in \mathbb{R}\}$ of q is trapped if one of the sets $\{\phi^t_q(\alpha), t \in \mathbb{R}^+\}$ and $\{\phi^t_q(\alpha), t \in \mathbb{R}^-\}$ is bounded.
A smooth, real function a defined on some cotangent bundle ($T^*\mathbb{R}^n$ or $T^*\mathcal{C}$) is an escape function on U^*_1 for q at energy λ if there exists some $c > 0$ such that

$$\forall \alpha \in U^*_1 \cap q^{-1}(\lambda),\, \{q,a\}(\alpha) \;\geq c\,,$$

where $\{\cdot,\cdot\}$ denotes the usual Poisson bracket.
Notice that we can replace $q^{-1}(\lambda)$ by $q^{-1}(]\lambda-\epsilon_0;\lambda+\epsilon_0[)$ for $\epsilon_0 > 0$ small enough without

changing the above definitions.
If $U_1^* = U_1 \times \mathbb{R}^n$ for some subset U_1 of $\mathbb{R}^n$, we also say that q is non-trapping on U_1 and that a is an escape function on U_1. If $U_1^* = U^*$ or $U_1 = U$, we simply say that q is non-trapping at energy λ and that a is a global escape function for q at energy λ.

We shall indeed use such global escape function for scalar Hamilton functions like p but, to avoid difficulties at $\mathcal{C}^*$, we need a generalized version for the matricial symbol P, given in the following definition and suggested by A. Martinez.

Definition 2.2. *A smooth function A on $T^*\mathbb{R}^n$, valued in the 2×2 real symetric matrices, is an escape function for the matricial symbol P at energy λ on a subset U^* of $T^*\mathbb{R}^n$ (resp. on a subset U of $\mathbb{R}^n$) if there exist a function $\theta \in C_0^\infty(\mathbb{R};\mathbb{R})$, with $\theta = 1$ near λ, and some $c > 0$ such that, in the matrix sense of the order $\geq$, the "classical" Mourre estimate*

$$\theta(P)\,\{P, A\}\,\theta(P) \;\geq\; c\,\theta(P)^2 \tag{4}$$

holds true on U^* (resp. $U \times \mathbb{R}^n$), where $\{\cdot,\cdot\}$ denotes the Poisson bracket for matrix symbols (see (14)), and if the matricial commutator $[P, A]$ vanishes on $U^* \cap \operatorname{supp}\theta(P)$ (resp. $(U \times \mathbb{R}^n) \cap \operatorname{supp}\theta(P)$).
If $U^* = T^*\mathbb{R}^n$ or $U = \mathbb{R}^n$, we say that A is a global escape function for P at energy λ.

Let us precise the energy localization in Definition 2.2. It corresponds to the support of a matrix-valued function $\theta(P)$ (θ being as in Definition 2.2). By the functional calculus for real symetric matrices, this support is given by

$$\operatorname{supp}\,\theta(P) \;=\; \Big\{\alpha \in T^*\mathbb{R}^n;\ \exists\mu \in \operatorname{supp}\theta;\ \det\big(P(\alpha) - \mu \mathrm{I}_2\big) = 0\Big\}\,.$$

It is thus natural to consider the open set

$$E(\lambda, \epsilon_0) \;:=\; \bigcup_{\mu \in]\lambda-\epsilon_0;\lambda+\epsilon_0[} \Big\{\alpha \in T^*\mathbb{R}^n;\ \det\big(P(\alpha) - \mu \mathrm{I}_2\big) = 0\Big\}\,, \tag{5}$$

for some $\epsilon_0 > 0$, as an energy localization near λ. The energy shell of P of energy λ is defined as $E(\lambda) := \{\alpha \in T^*\mathbb{R}^n;\ \det\big(P(\alpha) - \lambda \mathrm{I}_2\big) = 0\}$.
Notice that $[P, A](\alpha) \neq 0$ implies $[P, A](\alpha)$ has a negative eigenvalue, since its trace is 0. Since we want to derive some positivity of $[\hat{P}, \hat{A}]$ by the sharp Gårding inequality, we require $[P, A] = 0$ on $\operatorname{supp}\theta(P)$.
It is straighforward to verify that, under (2) and for $\lambda > \|M_\infty\|$, the "classical" Mourre estimate (4) holds true for the scalar function A_∞ defined by

$$\forall (x, \xi) \in T^*\mathbb{R}^n,\ A_\infty(x, \xi) \;:=\; a_\infty(x, \xi)\,\mathrm{I}_2 \;:=\; x \cdot \xi\,\mathrm{I}_2\ , \tag{6}$$

provided $|x|$ is large enough. If $\lambda > \|M_\infty\|$ is large enough, this function is even a global escape function for P at energy λ.
To use the semiclassical Mourre method, we demand that the global escape function belongs to some class of semiclassical symbols. In fact, it suffices to require (see [GM], [Jec]) that, for $|x|$ large enough, the global escape function coincides with A_∞. In Section 3, we shall derive (almost as in the scalar case) the following

Theorem 2.3. *Assume that the symbol P satisfies (2) and let λ be some real number such that there exists some global escape function for P at energy λ, which is equal to A_∞ (cf. (6)) for $|x|$ large enough, then, for any $s > 1/2$, the boundary values of the resolvent satisfy the estimates $R(\lambda \pm i0) = O_s(h^{-1})$ as bounded operators from $\mathrm{L}^2_s(\mathbb{R}^n; \mathbb{C}^2)$ to $\mathrm{L}^2_{-s}(\mathbb{R}^n; \mathbb{C}^2)$.*

In the scalar case (cf. [GM]) (resp. the matricial case without crossing (cf. [Jec])), these resolvent estimates hold true under a non-trapping condition at energy λ on the symbol P of the operator (resp. the eigenvalues of P). Furthermore, it is also known, in the scalar case, that this non-trapping condition is necessary (cf. [W2]). What we are trying to understand in this paper is: under which condition can we apply Theorem 2.3 to P, if its eigenvalues cross somewhere?

We refer to [Ha] for the description of the different types of crossing that may appear and focus here on two important ones. In each case, we demand that $\mathcal{C}$ is a smooth submanifold of $\mathbb{R}^n$, while its codimension in $\mathbb{R}^n$ depends on the type. Since the results will be different for these two types, we shall present them together with the corresponding result concerning the existence of a global escape function.

<u>Codimension 1 crossing</u>: We assume that $\mathcal{C}$ is a submanifold of $\mathbb{R}^n$ of codimension one. More precisely, we demand that there exists some scalar C^∞ function τ and some C^∞ function $\widetilde{V}$, valued in the traceless, real, symetric matrices (i.e. like V), such that $V = \tau\widetilde{V}$ in some vicinity of $\mathcal{C}$, that $\widetilde{\rho} := (-\det\widetilde{V})^{1/2}$ and the gradient of τ does not vanish on the zero set of τ, which is $\mathcal{C}$. Finally, in view of (2), we require that there exist $\epsilon, C_0 > 0$ and some real symetric matrix $\widetilde{V}_\infty$, with $\widetilde{\rho}_\infty := (-\det\widetilde{V}_\infty)^{1/2} > 0$, such that

$$\forall \alpha \in \mathbb{N}^n, \forall x \in \mathbb{R}^n,\ \rho(x) < \epsilon \implies |\partial_x^\alpha \tau(x)| + \left\| \partial_x^\alpha (\widetilde{V}(x) - \widetilde{V}_\infty) \right\| \ = \ O_\alpha\Big(\langle x \rangle^{-\delta - |\alpha|}\Big) . \quad (7)$$

We point out that (7) is in fact an assumption at infinity near $\mathcal{C}$, since it holds automatically true, if $\mathcal{C}$ is compact, under the previous assumptions. If $\mathcal{C}$ is not compact, then V tend to 0 at infinity by (2), so this assumption says that, near the crossing, the convergence of V to 0 is due to the convergence of τ to zero, while the matrix structure of V tends to some invertible matrix $\widetilde{V}_\infty$. Notice further that the difference $\widetilde{\rho} - \widetilde{\rho}_\infty$ also satisfies the estimates (7).

Among the Codimension 1 crossings, there is the following radial situation, which contains the case of Born-Oppenheimer diatomic molecules with crossing.

<u>Radial potential with crossing</u>: We assume that M is a radial function (depending only on $|x|$) and that $\mathcal{C}$ is the sphere of $\mathbb{R}^n$ centered at 0 with radius $r_0 > 0$. We demand further that the gradients of v_1 and v_2 do not vanish on $\mathcal{C}$.

Using a Taylor expansion with rest integral near r_0, we see that this is a Codimension 1 crossing, if we choose $\tau(x) = |x| - r_0$ near $\mathcal{C}$. Notice that $\mathcal{C}$ could be a finite union of spheres centered at 0.

Let us return to general Codimension 1 crossings. Notice that, at $\mathcal{C}^*$, the eigenvalues $p_\pm = p \pm |\tau|\widetilde{\rho}$ and their associated eigenprojectors are not smooth. But one can easily regularize the situation (cf. [K]). Denoting by $\mathcal{C}^*_\pm$ the regions of $T^*\mathbb{R}^n$ where $\pm\tau > 0$, we define two new functions $\tilde{p}_\pm$ on $T^*\mathbb{R}^n$ by $\tilde{p}_\pm = p_\pm$ on $\mathcal{C}^*_+$, $\tilde{p}_\pm = p_\mp$ on $\mathcal{C}^*_-$, and $\tilde{p}_\pm = p$ on $\mathcal{C}^*$. Similarly, we set $\tilde{\Pi}_\pm(x) = \Pi_\pm(x)$ on $\mathcal{C}^*_+$ and $\tilde{\Pi}_\pm(x) = \Pi_\mp(x)$ on $\mathcal{C}^*_-$. Since $\tilde{p}_\pm = p \pm \tau\tilde{\rho}$ and $\tilde{\Pi}_\pm = (\mathrm{I}_2 \pm \widetilde{V}/\tilde{\rho})/2$ near $\mathcal{C}^*$, these functions are smooth everywhere and, by (7),

$$\forall \alpha \in \mathbb{N}^n, \forall x \in \mathbb{R}^n,\ \rho(x) < \epsilon \implies \left\| \partial_x^\alpha (\tilde{\Pi}_\pm(x) - \tilde{\Pi}_{\pm,\infty}) \right\| \ = \ O_\alpha\Big(\langle x\rangle^{-\delta-|\alpha|}\Big)\,, \tag{8}$$

where $\tilde{\Pi}_{\pm,\infty} = (\mathrm{I}_2 \pm \widetilde{V}_\infty/\tilde{\rho}_\infty)/2$. We just have changed the numbering of the eigenvalues in order to get smooth ones and smooth eigenprojectors. For convenience, we may assume that, for $\rho(x) \geq \epsilon$ and $\pm\tau(x) > 0$, $\tau(x) = \pm\rho(x)$ and $\tau(x)\widetilde{V}(x) = V(x)$. Our first main result, proved in Section 4, is the following

Theorem 2.4. *Assume that the symbol P satisfies (2) and let $\lambda > \|M_\infty\|$, the operator norm of M_∞. Assume that the Hamilton functions $\tilde{p}_\pm$ are non-trapping at energy λ. Then there exists $\kappa > 0$ such that, if $\|\langle x\rangle^{1+\delta}(\nabla_x\tilde{\Pi}_+)(x)\| \leq \kappa$ for all $x \in \mathbb{R}^n$, then there exists a global escape function for P at energy λ (cf. Definition 2.2) which equals A_∞, defined in (6), for $|x|$ large. In particular, Theorem 2.3 applies.*

At first sight, one could argue that this result should be clear, even without any condition on $\nabla_x\tilde{\Pi}_+$, since one can smoothly diagonalize P and probably decouple the two levels. This is not true and, already in [Ha] where the propagation of coherent states is studied, one can see that the two levels do interact, however not at the leading order. In Section 4, we shall explain why we cannot simply adapt the proof of [Jec] to the present case.
In contrast to Codimension 2 crossings (see below), the geometrical formulation of the problem at the crossing does not predict any local obstruction to the existence of escape function there. We really have the two degrees of freedom allowed by the commutation condition in Definition 2.2. Fixing appropriatly one of them, attached to $\tilde{p}_+$ for instance, we demand that the other satisfies a nonlinear, scalar p.d.e, which reduces to an ordinary differential equation along the flow of $\tilde{p}_-$. Thanks to the condition on $\nabla_x\tilde{\Pi}_+$ (see Remark 4.2), which does not depend on $\tilde{p}_\pm$, the resolution of this p.d.e furnishes the second part of the desired global escape function. The size of κ may be estimated in terms of the time needed by the flow of $\tilde{p}_-$ to leave some compact region (see the proof of Theorem 2.4 in Section 4).
Notice that, if $V = \tau\widetilde{V}$ everywhere with constant $\widetilde{V}$, we can simplify the proof considerably (see Remark 4.4) since the two levels decouple in this case.
Are the non-trapping conditions necessary to get the resolvent estimates ? If the crossing is empty, we believe that the arguments by [W2] may be adapted successfully. This could be probably extended to the present case for constant $\widetilde{V}$ near $\mathcal{C}$, that is for a fixed matricial structure near the crossing. It seems impossible to remove the condition on $\nabla_x\tilde{\Pi}_+$ in Theorem 2.4 if we follow the present Mourre method (see Section 4). Another method could perhaps do it, but a relevant non-trapping condition on the symbol might also be more complicated than ours.

We come now to our second type of crossing, namely

Codimension 2 crossing: We assume that $\mathcal{C}$ is a submanifold of $\mathbb{R}^n$ of codimension two.

More precisely, we demand that the gradients of v_1 and v_2 are linearly independent on $\mathcal{C}$, the intersection of their zero set.

The eigenvalues $p_\pm$ and their associated eigenprojectors are not smooth at $\mathcal{C}^*$, in general, and the previous regularization does not work. It turns out that the cotangent space $T^*\mathcal{C}$ of $\mathcal{C}$ will be important. Its fiber over some $x \in \mathcal{C}$ is defined by

$$T_x^*\mathcal{C} \;:=\; \left\{\xi \in T_x^*\mathbb{R}^n;\, \xi \in \Big(\mathrm{Vect}(\nabla v_1(x), \nabla v_2(x))\Big)^\perp\right\}, \tag{9}$$

where $\mathcal{V}(x) := \mathrm{Vect}(\nabla v_1(x), \nabla v_2(x))$ is the vector space spanned by the vectors $\nabla v_1(x)$ and $\nabla v_2(x)$, and where $\mathcal{V}(x)^\perp$ is the space of linear forms vanishing on $\mathcal{V}(x)$. Here, we do not view it in an intrinsic way but as a submanifold of $T^*\mathbb{R}^n$. Its importance comes from the identity (see Appendix B)

$$T^*\mathcal{C} \;=\; \{\alpha \in \mathcal{C}^*,\, H_p(\alpha) \in T_\alpha \mathcal{C}^*\}\,. \tag{10}$$

Furthermore, we have a special, geometrical configuration (see Appendix B). For $\alpha \in T^*\mathcal{C}$, $T_\alpha\mathcal{C}^* = \mathrm{Vect}(H_{v_1}, H_{v_2}) \oplus T_\alpha T^*\mathcal{C}$. According to this decomposition,

$$\forall \alpha \in T^*\mathcal{C},\, H_p(\alpha) \;=\; \Big(\mu_1(\alpha) H_{v_1}(\alpha) + \mu_2(\alpha) H_{v_2}(\alpha)\Big) \;+\; H_{p'}(\alpha)\,, \tag{11}$$

for some real coefficients $\mu_1(\alpha), \mu_2(\alpha)$, where p' denotes the restriction of p to $T^*\mathcal{C}$.

The experience of the scalar case, the matrix case without crossing, and the matrix case with codimension 1 crossing, says us that the Hamilton functions $p_\pm$ should be non-trapping at the considered energy. But, assuming this, in the sense given in Definition 2.1, is it sufficient? As discussed in Section 3, where we compare the present situation with the one without crossing, we have to understand what happens at the crossing. To this end, we express the problem of the existence of an escape function near the crossing in geometrical terms. The previous geometrical situation reveals a local obstruction for Codimension 2 crossings. To describe this obstruction, we need the following

Definition 2.5. *Let $\lambda \in \mathbb{R}$ and $\alpha \in T^*\mathcal{C}$. We say that the crossing is confining at α for P at energy λ if α belongs to the energy shell $E(\lambda)$ of P and if $\mu_1(\alpha)^2 + \mu_2(\alpha)^2 \leq 1$, these coefficients being defined in (11).*

This leads to the following, negative result, proved in Section 5.

Theorem 2.6. *If the crossing is confining for P at energy λ on some region in $T^*\mathcal{C}$, which contains a trapped trajectory for p' (at energy λ), then there exists no global escape function for P at energy λ.*

The assumptions of Theorem 2.6 imply that P cannot have a scalar escape function near $T^*\mathcal{C}$ and this also works for Codimension 1 crossings (see Appendix B). But, for Codimension 2 crossings, the existence of a global escape function for P implies the existence of a scalar one near $T^*\mathcal{C}$ (see Appendix D), yielding Theorem 2.6.
The condition of Definition 2.5 roughly says that the component of H_p in $\mathrm{Vect}(H_{v_1}, H_{v_2})$

has a small size. Since it forbids to "escape" in the conormal direction to the crossing near $T^*\mathcal{C}$ (see the proof), it may be seen as a kind of confining condition in that direction on the crossing w.r.t. p at the considered energy. Here we are thinking of quantum evolution constrained to (a neighborhood of) a submanifold as in [FH], for instance. The assumptions in Theorem 2.6 seem to describe a (quantum) capture phenomenon, that cannot be expressed in terms of the classical Hamilton functions p_+ and p_-, thus to be independent with non-trapping properties of p_+ and p_-.
It is not surprising that $T^*\mathcal{C}$ plays a central rôle for the existence of a global escape function if we consider the work [Ha] by Hagedorn, where the evolution of coherent states through eigenvalues crossing, with transversal impuls at the crossing, does not reveal any capture phenomenon. He had to avoid the non-generic situation of a tangent impuls that we have to take into account here, since we work on the full resolvent, and that precisely corresponds to considering a point in $T^*\mathcal{C}$.

Remark 2.7. *In the situation of Theorem 2.6, we do not know if the resolvent estimates of Theorem 2.3 hold. However we would not be surprised if they would not hold and that resonances would run rapidly (faster than h) to the real axis as h goes to 0. A corresponding resonant state could be essentially a tensor product of a microlocally confined state in the conormal direction to the crossing and of an eigenstate on $T^*\mathcal{C}$ (under some kind of Bohr-Sommerfeld quantization condition). Technics from [GS] and [FH] may be useful to deal with this question. At least, there is a positive answer by [Ne1]. Notice that [Ne2] predicts the presence of resonances near λ in the present situation but does not describe semiclassically their width.*

Now it is natural to ask what happens when the obstruction does not occur. Is there a global escape function, if we assume further that p_+ and p_- are non-trapping at the considered energy? Unfortunately, we did not succeed in finding a complete answer to this question. However, our previous geometrical analysis allows us to exhibit sufficient conditions (almost converse to the assumptions of Theorem 2.6), under which there are (scalar) escape functions near the crossing (see Proposition 2.8 below). Maybe these conditions, together with the non-trapping condition on p_+ and p_-, are sufficient to construct a global escape function. We could not prove this using Proposition 2.8, since it is rather difficult to transform an escape function on some quite arbitrary region into a global one.

Proposition 2.8. *Assume that the symbol P satisfies (2) and let $\lambda > \|M_\infty\|$, the operator norm of M_∞. If one of the following two conditions*

1. *the restriction p' of the half-trace p of P to $T^*\mathcal{C}$ is non-trapping at energy λ,*
2. *there is no $\alpha \in T^*\mathcal{C}$ at which the crossing is confining for P at energy λ,*

holds true then there exists a smooth, scalar function A, which is an escape function for P at energy λ on $\mathcal{C}^*$ and which equals A_∞, for $|x|$ large.

In fact, we first show that there is an escape function near $T^*\mathcal{C}$ and then add appropriately some function to get an escape function near $\mathcal{C}^*$.

Assumption 1 in Proposition 2.8 allows us to construct a global escape function for p' on $T^*\mathcal{C}$ (as in [GM]), that we extend to an escape function for P near $T^*\mathcal{C}$. Notice that this assumption implies that $\mathcal{C}$ is not compact.
Under Assumption 2 in Proposition 2.8, we can construct explicitly an escape function and really use conormal directions to $\mathcal{C}^*$ to "escape".
It is interesting to compare this result with the case where λ is very large, for which we have a global escape function, namely A_∞. If $\mathcal{C}$ is given by $\{x_1 = x_2 = 0\}$ in $\mathbb{R}^3$, the kinetic energy is concentrated "along the crossing" so that 1 is true and 2 is false if u is constant on $\mathcal{C}$. Now, if $\mathcal{C}$ is a circle in $\mathbb{R}^3$, then 1 cannot be true but one can verify that 2 holds true.
In order to exhibit clearly the relevant properties on which this result is based, we did not really optimize the assumptions. In fact, if $\mathcal{C}$ is not compact, we can relax them as shown in Remark 2.9 below. This comes from the fact that we have roughly two independent escape directions, one cotangent the crossing and one conormal to the crossing. If one is not practicable somewhere, we can follow the other. This leads to the following refinement of Proposition 2.8, proved in Section 5.

Remark 2.9. *Assume that the symbol P satisfies (2) and let $\lambda > \|M_\infty\|$. If the crossing is not confining for P at energy λ on some vicinity of the (closed) trapping region of p' at energy λ then there exists some scalar escape function for P at energy λ on $\mathcal{C}^*$, which equals A_∞ for $|x|$ large.*

3 Semiclassical Mourre method.

In this section, we describe the semiclassical Mourre method which leads to a proof of Theorem 2.3. We also review semiclassical resolvent estimates in the scalar case (cf. [GM, W2]) and in the matrix case without crossing (cf. [Jec]). A new proof of the latter case will be sketched to enlighten the present situation.

The semiclassical Mourre method for the operator $\hat{P}$ (defined in (1)) consists in seeking a so called conjugate operator which will be a h-pseudodifferential operator $\hat{A}$ (the Weyl h-quantization of some symbol A) that "coincide" with the generator of dilations (i.e. $A = A_\infty$), for $|x|$ large, and satisfies two conditions. Firstly, we should have, for the energy λ that we consider, the existence of some function $\theta \in C_0^\infty(\mathbb{R};\mathbb{R})$, with $\theta = 1$ near λ, and some $c > 0$ such that,

$$\theta(\hat{P})\, i[\hat{P}, \hat{A}]\, \theta(\hat{P}) \;\geq\; c \cdot h \cdot \theta(\hat{P})^2 \,. \tag{12}$$

Here $[\cdot,\cdot]$ denotes the commutator of (unbounded) operators. Secondly, we need that the double commutator $[[\hat{P}, \hat{A}], \hat{A}]$ is $\hat{P}$-bounded and that

$$\Big[\theta(\hat{P})[\hat{P}, \hat{A}]\theta(\hat{P}), \hat{A}\Big]\, (\hat{P} + i)^{-1} \;=\; O(h) \,. \tag{13}$$

A bound $O(h^2)$ is usually required (see [Jec]) since it directly holds in the scalar case. But in the matrix case, we do not expect in general such a bound because of commutation

problems. Fortunately, if we carefully follow Mourre's arguments (cf. [Mo]), the bound in (13) suffices (see [W2]) to get the desired semiclassical resolvent estimates.
To get (12), we can use the sharp Gårding inequality, as usual, since it works for matricial symbols, as pointed out in [H]. For convenience, we sketch a proof in Appendix A, which is the matricial version of an elegant proof indicated to us by A. Martinez.
By the functional calculus of B.Helffer and J.Sjöstrand (see [HS, DG]), the energy localization operator $\theta(\hat{P})$ is a h-pseudodifferential operator with principal symbol $\theta(P)$. Therefore, the principal symbol of the r.h.s. of (12) is $\theta(P)[P,A]\theta(P)$ ($[\cdot,\cdot]$ denoting here the matricial commutator), according to the composition formula for h-pseudodifferential operators (see [Ro]). Since $[P,A]$ is traceless, it has opposite eigenvalues, thus $[P,A]\geq 0$ implies $[P,A]=0$. This explains the commutation condition required in Definition 2.2 (which is trivially realized in the scalar case), that we also use to get (13). Under this condition, the principal symbol of $ih^{-1}[\hat{P},\hat{A}]$ is, using the previous composition rule,

$$\begin{aligned}\{P,A\} &:= \frac{1}{2}\Big((\nabla_\xi P\cdot\nabla_x A-\nabla_\xi A\cdot\nabla_x P)-(\nabla_x P\cdot\nabla_\xi A-\nabla_x A\cdot\nabla_\xi P)\Big)\,, \qquad (14)\\ &= \frac{1}{2}\Big((\nabla_\xi P\cdot\nabla_x A-\nabla_x P\cdot\nabla_\xi A)+(\nabla_x A\cdot\nabla_\xi P-\nabla_\xi A\cdot\nabla_x P)\Big)\,.\end{aligned}$$

In the scalar case, we recognize the usual Poisson bracket.

Proof of Theorem 2.3: As conjugate operator we choose the Weyl h-quantization $\hat{A}$ (see Appendix A) of the global escape function A (here we use the fact that $A=A_\infty$ for large enough $|x|$). Let $\theta,\theta'\in C_0^\infty(\mathbb{R};\mathbb{R})$ with $\theta'=\theta=1$ near λ and satisfying $\theta\theta'=\theta$, and assume the properties of Definition 2.2 for θ'. Thanks to $[P,A]=0$ on $\operatorname{supp}\theta'(P)$, the principal symbol of $\theta'(\hat{P})ih^{-1}[\hat{P},\hat{A}]\theta'(\hat{P})$ is $\theta'(P)\{P,A\}\theta'(P)$. By (4), this matricial symbol is bounded below by $c'\theta'(P)^2$, for some $c'>0$. Now, by the sharp Gårding inequality for the bounded, non-negative symbol $\theta'(P)\{P,A\}\theta'(P)-c'\theta'(P)^2$,

$$\theta'(\hat{P})\,ih^{-1}[\hat{P},\hat{A}]\,\theta'(\hat{P})\;\geq\;c'\cdot\theta'(\hat{P})^2\;-\;O(h)\,,$$

which, after left and right multiplication by $\theta(\hat{P})$, yields the Mourre estimate (12) for $c=c'/2>0$ and h small enough. The double commutator is seen to be $\hat{P}$-bounded thanks to assumption (2) and, since P and A commute on $\operatorname{supp}\theta(P)$, (13) holds true. We can then use Mourre's arguments (cf. [Mo]), following the h-dependence, to obtain the desired result (see also [W2]). □

As remarked in [Jec], the main problem is then to construct a global escape function for P at energy λ. Let us review some situations where the resolvent estimates of Theorem 2.3 have already been obtained.
In the scalar case, the previous Mourre method was successfully followed by C.Grard and A.Martinez in [GM], and then by X.P. Wang (in a more general setting in [W2]), under the non-trapping condition for the symbol at the considered energy. In this case, there is a natural way, given in [GM], to construct a global escape function a: let $g\in C_0^\infty(T^*\mathbb{R}^n)$ with $0\leq g\leq 1$ and $g=1$ on a large bounded domain $D^*\subset p^{-1}(\lambda)$. To construct a in D^*, we set $\{p,a\}=g$ and compose on both sides with the flow ϕ_p^t. This leads to

$(d/dt)(a\circ\phi_p^t) = g\circ\phi_p^t$ pointwise in $T^*\mathbb{R}^n$. By the non-trapping condition, this can be integrated as

$$a\circ\phi_p^t \;=\; -\int_t^\infty g\circ\phi_p^s\, ds\,, \tag{15}$$

which gives a for $t=0$. To exhibit a global escape function, which agrees with a_∞ for $|x|$ large, we combine appropriatly a and a_∞ (see Proposition 3.1 below).
On a formal level, we can reproduce this in the matricial case, if we replace the classical flow by the propagator of the Liouvillean $\{P,\cdot\}$ of P, but we do not see how to ensure the commutation condition required in Definition 2.2.
In [Jec], the matrix case without crossing was studied and we avoided global escape function for P but our method gave the impression that the conjugate operator should be scalar. This condition is irrelevant and let us extract the real basis of the proof.
The initial idea was to seek a conjugate operator of the form $F=\Pi_+\hat{a}_+\Pi_+ + \Pi_-\hat{a}_-\Pi_-$, where $\Pi_\pm(x)$ are the eigenprojectors of $V(x)$ associated to the eigenvalues $\pm\rho(x)$ and where $a_\pm(x,\xi)$ are scalar symbols, and to reduce the commutator $[\hat{P},F]$ to scalar ones, involving p_+ and p_-, leading to the condition that $a_\pm$ is a global escape function for $p_\pm$ at energy λ. On this way, we met the condition $a_+=a_-$ to cancel some uncontrolled term. Since the energy shells $p_+^{-1}(\lambda)$ and $p_-^{-1}(\lambda)$ are disjoint, we were able to construct such an operator by glueing together different functions a_+ and a_-, which were global escape functions for p_+ and p_-, respectively.
This construction seems artificial. From this, we learn that it may be simplier to work on symbols rather than on operators, that the scalarness of F is irrelevant, and that the basis of the proof is the separation of the energy shells. The latter can be expressed by $\theta(p_+)\theta(p_-)=0$ for a function θ as in Definition 2.2 with small enough support. Indeed we can rewrite the proof along the following lines. Choosing $A=a_0\mathrm{I}_2+a_1V$ for scalar, smooth functions a_1 and a_2 (recall that we have to ensure $[P,A]=0$), we have

$$\theta(P)\{P,A\}\theta(P) \;=\; \theta(p_+)^2\{p_+,a_+\}\Pi_+ \,+\, \theta(p_-)^2\{p_-,a_-\}\Pi_- \,+\, \theta(p_+)\theta(p_-)B\,, \tag{16}$$

where B is some matrix (roughly the previous uncontrolled term), $a_\pm=a_0\pm a_1\rho$. Choosing the support of θ small enough, the last term vanishes. Choosing a_+ (resp. a_-) as a global escape function for p_+ (resp. p_-) at energy λ, with $a_+=a_\infty$ (resp. $a_-=a_\infty$) for $|x|$ large, we get the "classical" Mourre estimate (4). Since ρ does not vanish, we can recover a_0, a_1 from a_+ and a_-. Theorem 2.3 gives now the desired resolvent estimates.
In the present situation ($\mathcal{C}\neq\emptyset$), the intersection of the energy shells $p_+^{-1}(\lambda)$ and $p_-^{-1}(\lambda)$ is not empty and is included in $\mathcal{C}^*$. We thus have to understand the effect of this on the construction of global escape functions.
However, to derive a global escape function from an escape function on some compact region in x, we are able to adapt the idea in [GM]. For $R>0$, we set

$$B_R \;:=\; \{x\in\mathbb{R}^n;\, |x|<R\} \quad\text{and}\quad B_R^* \;:=\; B_R\times\mathbb{R}^n\,. \tag{17}$$

Proposition 3.1. *Assume that we have a smooth function A, which is bounded on $E(\lambda;\epsilon_0)$ (cf. (5)) for $\epsilon_0>0$ small enough, such that, for $R>0$ large enough, it is an escape function for P at energy λ on B_R. Then, we can find a smooth function $\widetilde{A}$, which coincides with A_∞ for $|x|$ large enough, and which is a global escape function for P at energy λ.*

Proof: Let $R_1 > 0$ be large enough to have the assumption for R_1 and large enough so that there exists some $c_0 > 0$ such that $\{P, A_\infty\} \geq c_0 \mathrm{I}_2$ on $E(\lambda;\epsilon_0) \setminus B^*_{R_1}$. Let $\widetilde{A} := A_\infty + d\chi A$ with $\chi \in C_0^\infty(\mathbb{R}^n;\mathbb{R})$, $0 \leq \chi \leq 1$, $\chi = 1$ on B_{R_1}, and with $d > 0$ large enough to ensure

$$\sup_{B^*_{R_1} \cap E(\lambda;\epsilon_0)} \left\| \{P, A_\infty\} \right\| \; < \; d\, c_1 \, ,$$

where c_1 is given by the assumption for R_1 (i.e. $\{P, A\} \geq c_1 \mathrm{I}_2$ on $B^*_{R_1} \cap E(\lambda;\epsilon_0)$). Since $\{P, \chi\}$ is scalar, we have

$$\{P, \widetilde{A}\} \;=\; \{P, A_\infty\} + d\{P,\chi\}A + d\chi\{P, A\} \, . \tag{18}$$

Then, on $E(\lambda;\epsilon_0) \cap B^*_{R_1}$, $\{P, \widetilde{A}\} \geq c_1' \mathrm{I}_2$, for some $c_1' > 0$. Now, we choose the variation of χ such that, on $E(\lambda;\epsilon_0)$, $\|d\{P,\chi\}A\| \leq c_0/2$. Let $R > R_1$ be large enough such that $\mathrm{supp}\, \chi \subset B_R$. On $E(\lambda;\epsilon_0) \cap B^*_R$, for $c > 0$ given by the assumption for R, $d\chi\{P, A\} \geq d\chi c \mathrm{I}_2 \geq 0$, thus $\{P, \widetilde{A}\} \geq \min(c_1', c_0/2)\mathrm{I}_2$. Finally $\{P, \widetilde{A}\} \geq c_0 \mathrm{I}_2$ on $E(\lambda;\epsilon_0) \setminus B^*_R$ and $\widetilde{A}$ coincides with A_∞ for $|x| \geq R$. $\square$

4 Codimension 1 crossings.

This section is devoted to the proof of Theorem 2.4. In other words, we are going to construct a global escape function for P for Codimension 1 crossings.

According to the discussion in Section 3, we should look at the situation at the crossing. In fact, one can make the same geometrical analysis near $\mathcal{C}^*$ or rather $T^*\mathcal{C}$ as for Codimension 2 crossing (see Appendix B). Since, locally on $T^*\mathcal{C}$, the existence of an escape function does not imply the existence of a scalar one, as for Codimension 2 crossings, we do not expect that the geometrical situation at $T^*\mathcal{C}$ produces a local obtruction as in Section 5. However, this situation does produce such an obstruction to the existence of a scalar escape function at $T^*\mathcal{C}$ (as shown in Appendix B). So we really have to exploit the two degrees of freedom given by the commutation condition, namely look for a function $A = a_0 \mathrm{I}_2 + a_1 \widetilde{V} = a_+ \tilde{\Pi}_+ + a_- \tilde{\Pi}_-$ (so that $[A, V] = 0$ everywhere) with eventually non-zero a_1. Furthermore, like in Section 3, we have

$$\begin{aligned} \{P, A\} \;&=\; \{\tilde{p}_+, a_+\}\tilde{\Pi}_+ + \{\tilde{p}_-, a_-\}\tilde{\Pi}_- \\ &\quad + 2\tilde{\rho}\Big(2a_1\xi - \tau(\nabla_\xi a_0)\Big) \cdot \Big(\tilde{\Pi}_+(\nabla_x \tilde{\Pi}_+)\tilde{\Pi}_- + \tilde{\Pi}_-(\nabla_x \tilde{\Pi}_+)\tilde{\Pi}_+\Big) \, , \end{aligned} \tag{19}$$

but this time we cannot eliminate the last term by energy localization. Unless this term is zero (this is the case if $\nabla \tilde{\Pi}_+ = 0$ everywhere, that is for a fixed matricial structure of V, see Remark 4.4 below), we need to control it.

By energy localization, if we ensure the positivity of $\{\tilde{p}_\pm, a_\pm\}$ on $\tilde{p}_\pm^{-1}(\lambda)$, we need the positivity of (19) on $\tilde{p}_+^{-1}(\lambda) \cap \tilde{p}_-^{-1}(\lambda)$. Recall that τ is small on this region and, since we are looking for a function A that coincides with A_∞ for $|x|$ large, the term containing τ in

(19) should be uniformly a $O(|\tau|)$. So it is reasonable to neglect it. For all $(x, \xi) \in T^*\mathbb{R}^n$, let $f_\pm(x) \in \mathbb{C}^2$ be a normalized vector generating the range of $\tilde{\Pi}_\pm(x)$ and let $\psi(x, \xi) = \langle f_-(x), (2\xi \cdot \nabla_x \tilde{\Pi}_+(x)) f_+(x) \rangle \in \mathbb{C}$ where $\langle \cdot, \cdot \rangle$ denotes the usual scalar product in $\mathbb{C}^2$. The positivity of the matrix

$$\begin{aligned} \{P, A\}' \;&:=\; \{P, A\} \,+\, 2\tilde{\rho}\tau(\nabla_\xi a_0) \cdot \Big(\tilde{\Pi}_+(\nabla_x \tilde{\Pi}_+)\tilde{\Pi}_- \,+\, \tilde{\Pi}_-(\nabla_x \tilde{\Pi}_+)\tilde{\Pi}_+\Big) \\ &=\; \{\tilde{p}_+, a_+\}\tilde{\Pi}_+ \,+\, \{\tilde{p}_-, a_-\}\tilde{\Pi}_- \,+\, 4a_1\tilde{\rho}\xi \cdot \Big(\tilde{\Pi}_+(\nabla_x \tilde{\Pi}_+)\tilde{\Pi}_- \,+\, \tilde{\Pi}_-(\nabla_x \tilde{\Pi}_+)\tilde{\Pi}_+\Big) \end{aligned} \tag{20}$$

on $\tilde{p}_+^{-1}(\lambda) \cap \tilde{p}_-^{-1}(\lambda)$, is garanteed by $\{\tilde{p}_+, a_+\} > 0$ on $\tilde{p}_+^{-1}(\lambda)$ and

$$\{\tilde{p}_+, a_+\}\, \{\tilde{p}_-, a_-\} \;>\; |\psi|^2\, (a_+ - a_-)^2 \tag{21}$$

on $\tilde{p}_+^{-1}(\lambda) \cap \tilde{p}_-^{-1}(\lambda)$, since $a_1\tilde{\rho} = (a_+ - a_-)/2$. So, if we require $\{\tilde{p}_+, a_+\} > 0$ on $\tilde{p}_+^{-1}(\lambda)$ and

$$r_0\, \{\tilde{p}_-, a_-\} \;>\; |\psi|^2\, (a_+ - a_-)^2 \tag{22}$$

on $\tilde{p}_-^{-1}(\lambda)$, for some positive function r_0 which coincides with $\{\tilde{p}_+, a_+\}$ on $\tilde{p}_+^{-1}(\lambda) \cap \tilde{p}_-^{-1}(\lambda)$, we get the "classical" Mourre estimate (4), locally in x, if the neglected term is really small enough.
We see that we have to deal with a nonlinear problem. Given a global escape function a_+ for $\tilde{p}_+$, we try to solve for a_- the following nonlinear p.d.e.

$$r_0\, \{\tilde{p}_-, a_-\} \;=\; |\psi|^2\, (a_+ - a_-)^2 \,+\, r r_0\,, \tag{23}$$

on $\tilde{p}_-^{-1}(\lambda)$ for positive functions r, r_0, with $r_0 = \{\tilde{p}_+, a_+\}$ near the crossing. If we compose with the flow $\phi^t_{\tilde{p}_-}$, we need in fact to solve a family of nonlinear, differential equations of Ricatti's type. In particular, we need to adjust a_+, r, and r_0 in order to avoid explosion in finite time, to ensure the boundness of $a_- - a_\infty$ (needed in Proposition 3.1), and to guarantee a suitable smallness of the neglected term. In fact, we do not solve these Ricatti's equations but just show the global (time-)existence of some solutions that ensure the required properties on a_-. To this end, we need the following (known?, partially known?) result on special Ricatti's differential equations.

Proposition 4.1. *Let a, b be non-negative, integrable functions on $\mathbb{R}^+$ such that $I > 0$ and $4IJ < 1$, where*

$$I \;=\; \int_0^{+\infty} a(t)\, dt \quad \text{and} \quad J \;=\; \int_0^{+\infty} b(t)\, dt\,. \tag{24}$$

Then the solution of the following Cauchy problem

$$z' \;:=\; \frac{dz}{dt} \;=\; z^2 a \,+\, b\,,\;\; z(0) = z_0 < 0 \tag{25}$$

is defined and bounded on $\mathbb{R}^+$, provided $-2Iz_0 \in]1 - \sqrt{1 - 4IJ}; 1 + \sqrt{1 - 4IJ}[$. In this case, the solution satisfies

$$\forall t \in \mathbb{R}^+,\;\; z_0 \leq z(t) < 0\,. \tag{26}$$

Proof: see Appendix C. $\square$

Remark 4.2. *Let us point out that, if there exist constants $a_0, b_0 > 0$ such that $a \geq a_0$ and $b \geq b_0$ on some $[t_0, t_0 + T]$ with $t_0 \geq 0$ and $\pi \leq T\sqrt{a_0 b_0}$, then the solution blows up at some $T^* \leq t_0 + T$. Indeed, it suffices to integrate the inequality $z' \geq a_0 z^2 + b_0$. Therefore, we do need a smallness condition in Proposition 4.1. This explains the requirement that $4IJ < 1$. To ensure this condition in the frame of Theorem 2.4, we cannot simply choose a_+ small enough since $|\psi|^2/r_0$ would be large. So, we use another degree of freedom, which does not depend on the Hamilton flows, namely the variation of $\widetilde{V}/\tilde{\rho}$.*

Proof of Theorem 2.4: Let us choose some $\epsilon_0 > 0$ such that the functions $\tilde{p}_\pm$ are non-trapping on $\tilde{p}_\pm^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$, respectively. Recall that we can find $R_1 > 0$ such that $A_\infty = a_\infty \mathrm{I}_2$ (defined in (6)) is an escape function for P at energy λ outside $B^*_{R_1}$ (defined in (17)). Thus, there exists $c_1 > 0$ such that $\{P, A_\infty\} \geq c_1 \mathrm{I}_2$ on $E(\lambda; \epsilon_0) \setminus B^*_{R_1}$. By (19), this implies that $\{\tilde{p}_\pm, a_\infty\} \geq c_1$ on $\tilde{p}_\pm^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \setminus B^*_{R_1}$.
For some $R > R_1$ large enough, we construct, as in [GM], a global escape function a_+ for $\tilde{p}_+$ at energy λ, which coincides with a_∞ on $T^*\mathbb{R}^n \setminus B^*_R$ and satisfies, for some $c > 0$, $\{\tilde{p}_+, a_+\} \geq c$ on $\tilde{p}_+^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$.
Now, we choose $T > 0$ bigger than the supremum of $|a_\infty|$ on $E(\lambda; \epsilon_0) \cap B^*_R$. Therefore $E(\lambda; \epsilon_0) \cap B^*_R \subset \{\beta \in T^*\mathbb{R}^n; -T \leq a_\infty(\beta) \leq T\} \cap E(\lambda; \epsilon_0)$. Denoting $\phi^t_{\tilde{p}_-}$ by ϕ^t for simplicity, we point out that we have a smooth diffeomorphism Φ from $\mathbb{R} \times [\{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\} \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)]$ onto $\tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$, given by $\Phi(t, \beta) = \phi^t(\beta)$, since $\tilde{p}_-$ is non-trapping on $\tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$ and a_∞ is an escape function for $\tilde{p}_-$ on $\tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \setminus B^*_R$. The compact set $\Phi^{-1}(\tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \cap B^*_R)$ is contained in some $[0; T_0] \times K^*$, where $T_0 > 0$ and where K^* is a compact subset of $\{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\} \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$. This way to isolate the region $\tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \cap B^*_R$ is due to [GS].
Let $\chi_1 \in C_0^\infty(\mathbb{R}; \mathbb{R})$ with $\chi_1(t) \geq \sup(t; 1/2)$, $0 \leq \chi_1' \leq 1$, $\chi_1(t) = t$ on $[1; +\infty[$, and $\chi_1 = 1/2$ on $] - \infty; 0]$. In view of (23), we choose

$$\sup\Big(\{\tilde{p}_+, a_+\}; c/2\Big) \leq r_0 := c\, \chi_1\Big(\{\tilde{p}_+, a_+\}/c\Big)\,, \tag{27}$$

$$\sup\Big(\{\tilde{p}_-, a_+\}; c_1/2\Big) \leq r := c_1\, \chi_1\Big(\{\tilde{p}_-, a_+\}/c_1\Big)\,. \tag{28}$$

For $\alpha \in \{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\} \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$, let $k(t; \alpha) := (|\psi|^2/r_0) \circ \phi^t(\alpha) \geq 0$, $h(t; \alpha) := r \circ \phi^t(\alpha)$, and $g(t; \alpha) = a_+ \circ \phi^t(\alpha)$. Notice that the function $(h - g')(\cdot; \alpha)$ is nonnegative and has compact support included in $\mathbb{R}^+$, since $r \geq \{\tilde{p}_-, a_+\}$ with equality on $\tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \setminus B^*_R$. We define

$$I^\pm(\alpha) := \pm \int_0^{\pm\infty} k(t; \alpha)\, dt \geq 0\,,\ J(\alpha) := \int_0^{+\infty} (h - g')(t; \alpha)\, dt \geq 0\,. \tag{29}$$

Due to the non-trapping assumption (on $\tilde{p}_-$), there exists some finite $T_R > 0$ such that, for all $\alpha \in \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$, the Lebesgue measure of the set $\{t \in \mathbb{R}; \phi^t(\alpha) \in B^*_R\}$ is $\leq T_R$. The properties of χ_1 ensure that

$$J(\alpha) \leq T_R \max\Big(1/2\,; \sup_{B^*_R} |\{\tilde{p}_-, a_+\}|\Big) =: T_1\,, \tag{30}$$

for all $\alpha \in \{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\} \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$, and this bound still holds if we increase T. By (27) and (8), we see that, for all $\alpha \in \{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\} \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$,

$$I^{\pm}(\alpha) \;\leq\; \pm(2/c)\,\kappa\,2\sqrt{\lambda}\int_0^{\pm\infty} \langle q(t;\alpha)\rangle^{-1-\delta}\,dt\,, \tag{31}$$

where we wrote $\phi^t_{\tilde{p}_-}(\alpha) = \phi^t(\alpha) = (q(t;\alpha); p(t;\alpha))$. We need some more information on this flow, given in the following lemma. We set $\phi_0^t(\alpha) = (q_0(t;\alpha); p_0(t;\alpha)) := (x + 2t\xi, \xi)$, for $\alpha = (x, \xi)$.

Lemma 4.3. *There exist some $C > 0$ and $\sigma \in [0; 1[$ such that, for $R' \geq R$ large enough and T bigger than the supremum of $|a_\infty|$ on $E(\lambda;\epsilon_0)\cap B^*_{R'}$, $\langle q(t;\alpha)\rangle \geq C\langle t\rangle$, the derivative with respect to α of $\phi^t(\alpha)$ satisfy $|D_\alpha(\phi^t - \phi_0^t)(\alpha)| \leq 1 - \sigma$ on $\mathbb{R} \times [\{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\} \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \setminus K^*]$, $\mathbb{R}^- \times K^*$, and $\mathbb{R}^+ \times \phi^{T_0}(K^*)$. In particular, there exists some $D > 0$ such that, on these three regions,*

$$|D_\xi q(t;\alpha)| \;\leq\; D\langle t\rangle \qquad \textit{and} \qquad |D_x q(t;\alpha)| + |D_x p(t;\alpha)| + |D_\xi p(t;\alpha)| \;\leq\; D\,.$$

Proof: This lemma follows essentially from results in [DG], Chapters 1 and 2. However, for sake of completeness, we sketch a proof in Appendix C. □

By (the first result in) Lemma 4.3, we derive from (31) the finitness of the integrals $I^{\pm}(\alpha)$. Actually, we even obtain that $I^-(\alpha) \leq D_1(R')^{-\delta/2}$, uniformly for $\alpha \in \{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\}\cap\tilde{p}_-^{-1}(]\lambda-\epsilon_0; \lambda+\epsilon_0[)$. We choose R' large enough such that $D_1(R')^{-\delta/2} \leq 1/(8T_1)$. Let T be bigger than the supremum of $|a_\infty|$ on $E(\lambda;\epsilon_0)\cap B^*_{R'}$. Now, considerind (31) again, we choose κ small enough such that, for all $\alpha \in \{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\}\cap\tilde{p}_-^{-1}(]\lambda-\epsilon_0; \lambda+\epsilon_0[)$, $I^+(\alpha) \leq 1/(8T_1)$. In view of (23), we consider the maximal solution $t \mapsto z(t;\alpha)$ of the Ricatti's differential equation, for $\alpha \in \{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\} \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$,

$$\begin{aligned} z'(t;\alpha) \;&:=\; \frac{dz}{dt}(t;\alpha) \;=\; z^2(t;\alpha)k(t;\alpha) + \; h(t;\alpha) \;-\; g'(t;\alpha)\,, \\ z(0;\alpha) \;&=\; -4T_1\,, \end{aligned} \tag{32}$$

keeping in mind that this solution will be $(a_- - a_+)\circ\phi^t(\alpha)$. Thanks to (30), we can apply Proposition 4.1 (if $I^+(\alpha) = 0$, the corresponding solution is defined on $\mathbb{R}^+$ and bounded above by $J(\alpha)$, for any $z_0 \in \mathbb{R}^-$). Thus, the maximal solution is defined on $\mathbb{R}^+$ and satisfies $z_0 \leq z \leq T_1$. On $\mathbb{R}^-$, (32) reduces to $z' = z^2k$. Since $I^-(\alpha) \leq 1/(8T_1)$, the solution is defined on $\mathbb{R}^-$ and satisfies $-4T_1/(1 - 4T_1I^-) \leq z \leq -4T_1$.
Now, we define a_- to be a smooth function on $T^*\mathbb{R}^n$ such that, $a_-\circ\phi^t(\alpha) = a_+\circ\phi^t(\alpha) + z(t;\alpha)$, for all $t \in \mathbb{R}$ and $\alpha \in \{\beta \in T^*\mathbb{R}^n; a_\infty(\beta) = -T\}\cap\tilde{p}_-^{-1}(]\lambda-\epsilon_0; \lambda+\epsilon_0[)$. We can choose this function such that $a_- - a_\infty$ is bounded on $E(\lambda;\epsilon_0)$. Since it satisfies (23) thus (22) on $\tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$, we obtain (21) on $\tilde{p}_+^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$, yielding the positivity of (20) on $\tilde{p}_+^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$. More precisely, we have, for the matrix (20), the lower bound $(cc_1/4)\mathrm{I}_2$ on $\tilde{p}_+^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[) \cap \tilde{p}_-^{-1}(]\lambda - \epsilon_0; \lambda + \epsilon_0[)$. Assume, for a while, that the function $(\nabla_\xi(a_- + a_+))\cdot\nabla_x\tilde{\Pi}_+$ is bounded on $E(\lambda;\epsilon_0)$, then we

choose $\epsilon_0' \in]0;\epsilon_0]$ small enough to ensure that the term containing τ in (20) is $\leq (cc_1/5)\mathrm{I}_2$ on $\tilde{p}_+^{-1}(]\lambda-\epsilon_0';\lambda+\epsilon_0'[)\cap\tilde{p}_-^{-1}(]\lambda-\epsilon_0';\lambda+\epsilon_0'[)$. On $E(\lambda;\epsilon_0')\setminus[\tilde{p}_+^{-1}(]\lambda-\epsilon_0';\lambda+\epsilon_0'[)\cap\tilde{p}_-^{-1}(]\lambda-\epsilon_0';\lambda+\epsilon_0'[)]$, the "classical" Mourre estimate (4) holds true since we ensured $\{\tilde{p}_\pm, a_\pm\} \geq c' > 0$ on $\tilde{p}_\pm^{-1}(]\lambda-\epsilon_0';\lambda+\epsilon_0'[)$. But a_- does not coincide with a_∞ for $|x|$ large. Let $\chi \in C_0^\infty(\mathbb{R}^n;\mathbb{R})$ with $0 \leq \chi \leq 1$ and $\chi = 1$ on B_R. Since $a_- - a_\infty$ is bounded on $E(\lambda;\epsilon_0')$, we can choose the variation of χ small enough such that $a_+\tilde{\Pi}_+ + (\chi a_- + (1-\chi)a_\infty)\tilde{\Pi}_-$ is a global escape function for P at energy λ.
So, to end the proof, we show that $(\nabla_\xi(a_- + a_+))\cdot\nabla_x\tilde{\Pi}_+$ is bounded on $E(\lambda;\epsilon_0)$. By (8), the function $(\nabla_\xi a_\infty)\cdot\nabla_x\tilde{\Pi}_+$ is bounded there, so it suffices to show that $(\nabla_\xi(a_- - a_+))$ is bounded, since $a_+ = a_\infty$ for $|x|$ large enough. We just have to show the boundness of $\nabla_\xi(a_- - a_+)$ on $\tilde{p}_-^{-1}(]\lambda-\epsilon_0;\lambda+\epsilon_0[)\setminus\Phi([0;T_0]\times K^*)$, since we remove a compact set. By (the second result in) Lemma 4.3, it suffices to bound $D_\alpha[(a_- - a_+)\circ\phi^t(\alpha)]$ on the three regions given in Lemma 4.3. In the two first regions, the function $(a_- - a_+)\circ\phi^t(\alpha)$ coincides with the function z, while, on the third region, it equals the function $\tilde{z}(t;\alpha) := z(t+T_0;\phi^{-T_0}(\alpha))$, which is the solution of the equation (32) with initial condition $\tilde{z}(0;\alpha) = z(T_0;\phi^{-T_0}(\alpha)) < 0$. But, on the relevant regions, we have the following explicit formula

$$z(t;\alpha) \;=\; \frac{-(1+\epsilon)T_1}{-(1+\epsilon)T_1 + \int_0^t k(s;\alpha)\,ds} \tag{33}$$

for z and the same for $\tilde{z}$ with $-(1+\epsilon)T_1$ replaced by $z(T_0;\phi^{-T_0}(\alpha))$, since the function $(h-g')(t;\alpha)$ vanishes. Notice that $D_\alpha[z(T_0;\phi^{-T_0}(\alpha))]$ is bounded on $\phi^{T_0}(K^*)$. By Lemma 4.3,

$$\begin{aligned}\left|D_\xi\int_0^t k(s;\alpha)\,ds\right| \;&\leq\; \int_0^{+\infty}\Big\{\left|D_x[|\psi|^2/r_0)]\circ\phi^t(\alpha)\right|\cdot\left|D_\xi q(t;\alpha)\right| \\ &\qquad + \left|D_\xi[|\psi|^2/r_0]\circ\phi^t(\alpha)\right|\cdot\left|D_\xi p(t;\alpha)\right|\Big\}\,dt \\ &\leq\; C'\int_0^{+\infty}\Big\{\langle q(t;\alpha)\rangle^{-3-2\delta}\langle t\rangle \;+\; \langle q(t;\alpha)\rangle^{-2-2\delta}\Big\}\,dt \;\leq\; C''\,,\end{aligned}$$

uniformly on the regions given in Lemma 4.3. On the same regions, we find in the same way a bound for $|D_x\int_0^t k(s;\alpha)\,ds|$. This yields the boundness of $D_\alpha z(t;\alpha)$ and $D_\alpha\tilde{z}(t;\alpha)$ on the relevant regions. □

Remark 4.4. *In some particular case, we do not need to consider a nonlinear problem and can directly derive Theorem 2.4. Assume indeed that $V = \tau\tilde{V}$ everywhere and that $\tilde{V}$ is a constant matrix near $\mathcal{C}$. Then, in (19), the last term equals zero. Therefore, it suffices to use the non-trapping condition on $\tilde{p}_\pm$ to construct independent escape functions $a_\pm$ for $\tilde{p}_\pm$, which equal a_∞ for large $|x|$, as in [GM]. Then the function $A = a_+\tilde{\Pi}_+ + a_-\tilde{\Pi}_-$ is a global escape function for P, which equals A_∞ for large $|x|$.*

5 Codimension 2 crossings.

In this section, we still consider the problem of the existence of global escape function for P, but in the case of Codimension 2 crossings. First of all, we exhibit the obstruction announced in Section 2 and prove Theorem 2.6. Then, we show Proposition 2.8 and its refinement in Remark 2.9.

As already pointed out, if there is some escape function for P near $T^*\mathcal{C}$, then there is a scalar one, for instance its half-trace (see Appendix D). Therefore, we restrict the question to scalar functions. So, we are looking for a smooth function $a : T^*\mathbb{R}^n \longrightarrow \mathbb{R}$ such that, for some $\epsilon_0 > 0$,

$$\{p, a\} \ > \ \sqrt{\{v_1, a\}^2 + \{v_2, a\}^2} \tag{34}$$

on $T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$, where the energy localization $E(\lambda, \epsilon_0)$ is defined in (5). If we denote by σ the second fundamental form on $T^*\mathbb{R}^n$, we can rewrite this condition as

$$\sigma(H_p, H_a) \ > \ \sqrt{\sigma(H_{v_1}, H_a)^2 + \sigma(H_{v_2}, H_a)^2} \tag{35}$$

on $T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$. Since $T^*\mathcal{C}$ is symplectic, we have, for all $\alpha \in T^*\mathcal{C}$,

$$T_\alpha T^*\mathbb{R}^n \ = \ T_\alpha T^*\mathcal{C} \oplus \Big(T_\alpha T^*\mathcal{C}\Big)^\sigma \tag{36}$$

where the second term is the orthogonal space of $T_\alpha T^*\mathcal{C}$ with respect to σ evaluated at α. If we define p' (resp. a') as the restriction of p (resp. a) to $T^*\mathcal{C}$, then, according to the decomposition (36), we have $H_p = H_{p'} + (H_p - H_{p'})$ (resp. $H_a = H_{a'} + (H_a - H_{a'})$), as shown in Appendix B. Therefore, $\sigma(H_p, H_a) = \sigma(H_{p'}, H_{a'}) + \sigma(H_p - H_{p'}, H_a - H_{a'})$. Since $T^*\mathcal{C} \subset \mathcal{C}^*$ and $(T_\alpha\mathcal{C}^*)^\sigma = \mathrm{Vect}(H_{v_1}, H_{v_2})$ (see Appendix B), $\mathrm{Vect}(H_{v_1}, H_{v_2}) \subset (T_\alpha T^*\mathcal{C})^\sigma$ and $\sigma(H_{v_j}, H_a)$ reduces to $\sigma(H_{v_j}, H_a - H_{a'})$, for $j = 1, 2$. So, (35) may be equivalently rewritten as

$$\sigma(H_{p'}, H_{a'}) + \sigma(H_p - H_{p'}, H_a - H_{a'}) \ > \ \sqrt{\sigma(H_{v_1}, H_a - H_{a'})^2 + \sigma(H_{v_2}, H_a - H_{a'})^2} \tag{37}$$

on $T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$. Furthermore, since H_p belongs to $T_\alpha\mathcal{C}^*$, $H_p - H_{p'}$ is in fact in $\mathrm{Vect}(H_{v_1}, H_{v_2})$, as expressed in (11) and shown in Appendix B. Now, we can guess what kind of obstruction may appear. Since $T^*\mathcal{C}$ is symplectic, $\sigma(H_{p'}, H_{a'})$ can be viewed as a Poisson bracket of functions on $T^*\mathcal{C}$ and if $\mathcal{C}$ is compact, for instance, then so is $T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$ and p' cannot have a global escape function. Therefore, the term $\sigma(H_{p'}, H_{a'})$ cannot be positive everywhere on $T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$. Thus, at some point $\alpha \in T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$,

$$\sigma(H_p - H_{p'}, H_a - H_{a'}) \ > \ \sqrt{\sigma(H_{v_1}, H_a - H_{a'})^2 + \sigma(H_{v_2}, H_a - H_{a'})^2}\,, \tag{38}$$

which implies (see Appendix D) that α is not confining for P at the considered energy, according to Definition 2.5. Here, we have introduced the main ingredients of the proofs of Theorem 2.6 and Proposition 2.8.

Proof of Theorem 2.6: Assume that there is an escape function for P on $T^*\mathcal{C}$. Then, by Appendix D, there is a scalar one: a. By the previous discussion, there is some $\epsilon_0 > 0$ such that (37) holds true on $T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$. By assumption, there is a trapped trajectory for p', contained in the confining region for P. On this trajectory, there is a point $\alpha \in T^*\mathcal{C} \cap E(\lambda, \epsilon_0)$ where $\sigma(H_{p'}, H_{a'})$ vanishes. So, (38) holds true at α, which is a contradiction, since the crossing is confining at α. $\square$

Now, we want to prove Proposition 2.8, constructing first an escape function near $T^*\mathcal{C}$ and then near $\mathcal{C}^*$. To this end, we need some notation and notions. Let us define

$$\mathcal{U} \ := \ \Big\{x \in \mathbb{R}^n;\ |\nabla v_1(x)|\,|\nabla v_2(x)| \ > \ |\nabla v_1(x)\cdot \nabla v_2(x)|\Big\} \quad \text{and} \quad \mathcal{U}^* \ := \ \mathcal{U}\times \mathbb{R}^n\,. \quad (39)$$

By assumption, the open set $\mathcal{U}$ contains $\mathcal{C}$. We recall (17), since the escape function should coincide with A_∞ outside some B_R^*. We have already described $T^*\mathcal{C}$, namely in (9). For $x\in\mathcal{C}$, we have the direct sum

$$T_x^*\mathbb{R}^n \ = \ T_x^*\mathcal{C} \oplus N_x^*\mathcal{C}\,, \quad (40)$$

where the conormal space $N_x^*\mathcal{C}$ to $\mathcal{C}$ over x is defined by

$$N_x^*\mathcal{C} \ := \ \Big\{\xi \in T_x^*\mathbb{R}^n;\ \xi \in (T_x\mathcal{C})^\perp\Big\}\,. \quad (41)$$

We denote by P_x^N (resp. P_x^T) the projection onto $N_x^*\mathcal{C}$ (resp. $T_x^*\mathcal{C}$) associated to the decomposition (40).

The assumptions 1 and 2 in Proposition 2.8 are independent, as the previous discussion shows. Thus, we consider them separately to prove this proposition. Some more work will give the refinement given in Remark 2.9.

Assume that assumption 1 of Proposition 2.8 holds true. In view of (37), we look for a function a such that $H_a - H_{a'} = 0$ and such that a' is an escape function for p'. So, we construct such an escape function, which is defined on $T^*\mathcal{C}$ only, and extend it to some neighborhood of $T^*\mathcal{C}$. To this end, avoiding local coordinates, we use a vector field that is conormal to $\mathcal{C}^*$. Precisely, we consider, the differential equation

$$\frac{dy_t}{dt} \ = \ -\nabla\rho^2(y_t)\,,\ y_0 \ = \ x\,. \quad (42)$$

There exists some open set $\mathcal{U}_1$ with $\mathcal{C}\subset\mathcal{U}_1\subset\mathcal{U}$ such that, for $x\in\mathcal{U}_1$, the maximal solution of (42) is well defined for all $t\geq 0$, the limit $y(x)$ of $y(t;x)$, as $t\to+\infty$, exists and defines a smooth function of x on $\mathcal{U}_1$ with values in $\mathcal{C}$, which coincides with the identity on $\mathcal{C}$. Furthermore, for $(x,\xi)\in T^*\mathcal{U}_1$, we can construct $\eta(x,\xi)\in T^*_{y(x)}\mathcal{U}_1$ such that η is smooth on $T^*\mathcal{U}_1$ with values in $T^*\mathcal{C}$, and such that $\eta(x,\xi)=\xi$ and $\nabla v_j\cdot\nabla_\xi\eta(x,\xi)=0$ on $T^*\mathcal{C}$, for $j=1,2$. All these properties are proved in Appendix D.

Proposition 5.1. *Under the assumptions of Proposition 2.8, with condition 1, there exist a smooth, scalar function $A=a\mathrm{I}_2$, which equals A_∞ for $|x|$ large enough, and some $R>0$ large enough such that A is an escape function for P at energy λ on $[T^*\mathcal{C}\cap B_R^*]\cup T^*\mathbb{R}^n\setminus B_R^*$.*

Proof: Let $R_1>0$ be large enough such that, for some $c_1>0$, $\{P,A_\infty\}\geq c_1\mathrm{I}_2$ on $E(\lambda,\epsilon_0)\setminus B_{R_1}^*$. Let $g'\in C_0^\infty(T^*\mathcal{C};\mathbb{R})$ with $0\leq g'\leq 1$ and $g'=1$ on $T^*\mathcal{C}\cap B_{R_1}^*$. Since p' is non-trapping at energy λ, we can find a smooth, bounded function a' on $T^*\mathcal{C}$ which satisfies (15) (where g' and p' replace g and p, respectively) on $(p')^{-1}(]\lambda-\epsilon_0;\lambda+\epsilon_0[)=T^*\mathcal{C}\cap E(\lambda,\epsilon_0)$ (decreasing eventually ϵ_0). Now, we choose a smooth function a_1 on $T^*\mathbb{R}^n$ such that $a_1(x,\xi)=a'(y(x),\eta(x,\xi))$ on $\mathcal{U}_1^*$ and it is also bounded, and we set $A_1=a_1\mathrm{I}_2$. By the choice of η, its restriction to $T^*\mathcal{C}$ is a' and $H_{a_1} - H_{a'_1}$ vanishes on $T^*\mathcal{C}$. This implies, by (37), that $\{P, A_1\} \geq \mathrm{I}_2$ (resp. $\{P, A_1\} \geq 0$) on $E(\lambda, \epsilon_0) \cap T^*\mathcal{C} \cap B^*_{R_1}$ (resp. $E(\lambda, \epsilon_0) \cap T^*\mathcal{C}$). We set $A = A_\infty + d\chi A_1$ for some constant $d > 0$ and some cut-off χ, as in Propostion 3.1. Following the arguments of the proof of Propostion 3.1, we can choose d and χ such that A is a scalar escape function for P at energy λ on $[B^*_R \cap T^*\mathcal{C}] \cup T^*\mathbb{R}^n \setminus B^*_R$, for $R \geq R_1$ large enough. Moreover, A equals A_∞ for $|x|$ large. □

Next, we consider the other condition in Proposition 2.8, condition 2. Under this condition, we want to obtain (37) through (38). Therefore, it is natural to seek a function a_1 of the form $a_1(x, \xi) := \beta_1(x, \xi)\xi \cdot \nabla v_1(x) + \beta_2(x, \xi)\xi \cdot \nabla v_2(x)$, which satisfies $a_1 = 0$ and $\nabla_\xi a_1 = \beta_1 \nabla v_1(x) + \beta_2 \nabla v_2$ on $T^*\mathcal{C}$. In view of (38) and its meaning (see Appendix D), in view of (11) rewritten near $T^*\mathcal{C}$ with smooth functions μ_1 and μ_2 (see Appendix B), we choose the bounded, smooth functions on $\mathcal{U}^*$

$$\beta_1 = \Big(\mu_1 |\nabla v_2|^2 - \mu_2 (\nabla v_1 \cdot \nabla v_2)\Big)/\mu^2 , \tag{43}$$

$$\beta_2 = \Big(\mu_2 |\nabla v_1|^2 - \mu_1 (\nabla v_1 \cdot \nabla v_2)\Big)/\mu^2 , \tag{44}$$

where $\mu = (1 + \mu_1^2 + \mu_2^2)^{1/2} \geq 1$. This defines a bounded, smooth function a_1 on $\mathcal{U}^*$.

Proposition 5.2. *Under the assumptions of Proposition 2.8, with condition 2, there exist a smooth, scalar function $A = a\mathrm{I}_2$, which equals A_∞ for $|x|$ large enough, and $R > 0$ large enough such that A is an escape function for P at energy λ on $[T^*\mathcal{C} \cap B^*_R] \cup T^*\mathbb{R}^n \setminus B^*_R$.*

Proof: Let $A_1 = a_1 \mathrm{I}_2$, for $a_1 := \beta_1(\xi \cdot \nabla v_1) + \beta_2(\xi \cdot \nabla v_2)$, where the functions β_1, β_2 are defined in (43) and (44). Since $a_1 = 0$ on $T^*\mathcal{C}$, (34) reduces to (38). Notice that (38) only depends on $\nabla_\xi a_1 = \beta_1 \nabla v_1 + \beta_2 \nabla v_2$. Thus (38) holds true on $T^*\mathcal{C}$, by the choice of β_1, β_2 (see Appendix B). We set $A = A_\infty + d\chi A_1$ for some constant $d > 0$ and some cut-off χ, as in Propostion 3.1. As in the proof of Propostion 3.1, we can find such A satisfying the requirement of Proposition 5.2. □

Now, we try to construct an escape function near $\mathcal{C}^*$. Our idea is to add to the previous escape function on $T^*\mathcal{C}$ a scalar function $\xi \cdot \nabla w^2(x)$, where $w(x)$ is small near $\mathcal{C}$, in order to get rid of the matricial structure of P. Indeed, the off-diagonal terms of $\{P, \xi \cdot \nabla w^2\}$ are small, while the diagonal, up to a small term, is $4|\xi \cdot \nabla w|^2 \mathrm{I}_2$. It is quite natural to choose $w = \rho$, since, for $x \in \mathcal{C}$ and $\xi \notin T^*_x\mathcal{C}$, if $|\xi|^2$ is positive so is also $|P^N_x \xi|^2$, yielding the positivity we want to use. We define the smooth, scalar function $A_N = a_N \mathrm{I}_2$ with

$$\forall (x, \xi) \in T^*\mathbb{R}^n , \qquad a_N(x, \xi) = \xi \cdot \nabla \rho^2(x) . \tag{45}$$

Notice that it is bounded on $E(\lambda, \epsilon_0)$. Furthermore, for any $R > 0$, there exists some $c_R > 0$ such that, on $E(\lambda, \epsilon_0) \cap B^*_R$,

$$\{P, A_N\}(x, \xi) \geq c_R |P^N_x \xi|^2 \mathrm{I}_2 + O_R(|\rho(x)|) . \tag{46}$$

Proposition 5.3. *Assume that we have a smooth function A, which coincides with A_∞ for $|x|$ large enough and is an escape function for P at energy λ on $[T^*\mathcal{C}\cap B^*_{R'}]\cup T^*\mathbb{R}^n\setminus B^*_{R'}$, for some $R'>0$. Then, we can find a smooth, scalar function $\widetilde{A}$, which coincides with A_∞ for $|x|$ large enough, and $R>0$ large enough, such that $\widetilde{A}$ is an escape function for P at energy λ on $[\mathcal{C}\cap B_R]\cup\mathbb{R}^n\setminus B_R$.*

Proof: Let $R_1\geq R'$ be large enough such that $A=A_\infty$ outside $B^*_{R_1}$ and such that there exists $c_1>0$ for which $|\xi|^2\geq c_1$ and $\{P,A_\infty\}\geq c_1/2$ on $E(\lambda;\epsilon_0)\cap T^*\mathbb{R}^n\setminus B^*_{R_1}$. There exists some $c_1'>0$ such that $\{P,A\}\geq c_1'\mathrm{I}_2$ on $E(\lambda;\epsilon_0)\cap T^*\mathcal{C}\cap B^*_{R_1}$. By a continuity argument, we can find $\sigma>0$ such that $(x,\xi)\in E(\lambda;\epsilon_0)\cap\mathcal{C}^*\cap B^*_{R_1}$ and $|P^N_x\xi|<\sigma|\xi|$ imply that $\{P,A\}(x,\xi)\geq c_1'/2\mathrm{I}_2$. Now, by (46), $(x,\xi)\in E(\lambda;\epsilon_0)\cap\mathcal{C}^*\cap B^*_{R_1}$ and $|P^N_x\xi|\geq\sigma|\xi|$ imply that $\{P,A_N\}(x,\xi)\geq c_{R_1}\sigma^2c_1\mathrm{I}_2$, where $c_{R_1}>0$ is given by (46) for $R=R_1$. Let $d>0$ be a constant large enough such that

$$\sup_{B^*_{R_1}\cap E(\lambda;\epsilon_0)}\left\|\{P,A\}\right\| \;<\; d\,c_{R_1}\,\sigma^2c_1\,.$$

As in the proof of Proposition 3.1, we set $\widetilde{A}=A+d\chi A_N$ where $\chi\in C_0^\infty(\mathbb{R}^n;\mathbb{R})$, $0\leq\chi\leq1$, $\chi=1$ on B_{R_1}, and write (18). On $E(\lambda;\epsilon_0)\cap\mathcal{C}^*\cap B^*_{R_1}$, we have $\{P,\widetilde{A}\}\geq c'\mathrm{I}_2$, for some $c'>0$, since $\chi=1$ on B_{R_1}. Now we can follow the arguments in the proof of Proposition 3.1 to ensure the desired result. $\square$

Justification of Remark 2.9: Under the assumptions of this remark, it suffices to construct an escape function on $T^*\mathcal{C}$, since the expected result will then follow from Proposition 5.3.
Let $\mathcal{B}\subset(p')^{-1}(\lambda)$ be the closure of the trapping region of p'. We assume that there are open sets U_1^*,U_2^* of $T^*\mathbb{R}^n$ such that $\mathcal{B}\subset(p')^{-1}(\lambda)\cap U_1^*\subset(p')^{-1}(\lambda)\cap\overline{U_1^*}\subset(p')^{-1}(\lambda)\cap U_2^*$, and that the last region is not confining for P at energy λ. Notice that $(p')^{-1}(\lambda)=E(\lambda)\cap T^*\mathcal{C}$.
Let $R_1>0$ be large enough such that, for some $c_1>0$, $\{P,A_\infty\}\geq c_1\mathrm{I}_2$ on $E(\lambda)\setminus B^*_{R_1}$. Let $g'\in C_0^\infty(T^*\mathcal{C};\mathbb{R})$ with $0\leq g'\leq1$, $g'=1$ on $B^*_{R_1}\cap T^*\mathcal{C}\cap(T^*\mathbb{R}^n\setminus U_2^*)$ and $\operatorname{supp}g'\subset T^*\mathbb{R}^n\setminus U_1^*$. As in [GM] (see (15)), we can construct a smooth, bounded function a' on $T^*\mathcal{C}$ such that $\{p',a'\}'=g'\geq0$ on $(p')^{-1}(\lambda)$, where $\{\cdot,\cdot\}'$ denotes the Poisson bracket on $T^*\mathcal{C}$. Let $\chi'\in C_0^\infty(T^*\mathcal{C};\mathbb{R})$ with $0\leq\chi'\leq1$, $\chi'=1$ on $B^*_{R_1}\cap T^*\mathcal{C}\cap U_1^*$, $\operatorname{supp}\chi'\subset T^*\mathcal{C}\cap U_2^*$, and $\chi'+g'\geq1/2$ on $B^*_{R_1}\cap T^*\mathcal{C}$. Now we construct a smooth, bounded function a_1 as in the proof of Proposition 5.1. Similarly, we extend χ' on $\mathcal{U}_1^*$ to χ. Let $a_2=\beta_1(x,\xi)\xi\cdot\nabla v_1(x)+\beta_2(x,\xi)\xi\cdot\nabla v_2(x)$ on $\mathcal{U}^*$, where the functions β_1 and β_2 are given in (43) and (44). In particular, there exists $c_2>0$ such that, on $E(\lambda)\cap B^*_{R_1}\cap T^*\mathcal{C}$, $\{P,\chi a_2\mathrm{I}_2\}=\chi'\{P,a_2\mathrm{I}_2\}\geq c_2\chi'\mathrm{I}_2$, since $a_2=0$ on $T^*\mathcal{C}$. Let $a=a_1+a_2$ and $A=a\mathrm{I}_2$.
On $E(\lambda)\cap B^*_{R_1}\cap T^*\mathcal{C}$, we thus have $\{P,A\}\geq c\mathrm{I}_2$, for some $c>0$. Notice that $\{P,A\}\geq0$ on $E(\lambda)\cap T^*\mathcal{C}$. Now, we define $\widetilde{A}=a_\infty+d\chi_0A$ like in the proof of Proposition 3.1, that we can follow to get Remark 2.9. $\square$

Appendix.

A Sharp Gårding inequality.

Here we sketch a proof of the sharp Gårding inequality for matricial symbols. We just adapt a known proof for scalar symbols to matricial ones.

For bounded symbols A, valued in the non-negative, real symetric matrices, we want to show that there exists a constant C such that, in the sense of bounded self-adjoint operators on L^2, $\hat{A} \geq C\,h$, where $\hat{A}$ is the Weyl h-quantization of A :

$$C_0^\infty(\mathbb{R}^n;\mathbb{C}^2) \ni u \;\mapsto\; (\hat{A}u)(x) \;=\; (2\pi h)^{-n} \int_{\mathbb{R}^n} e^{i\xi\cdot(x-y)/h} A\Big((x+y)/2,\xi\Big)u(y)\,dyd\xi\,.$$

For any bounded, matrix-valued symbol A, we define A_1 by

$$A_1(x,\xi) \;:=\; (\pi h)^{-n} \int_{T^*\mathbb{R}^n} e^{-[(x-y)^2+(\xi-\eta)^2]/h} A(y,\eta)\,dyd\eta\,.$$

We observe that A_1 is also a bounded symbol and that the difference $A - A_1$ is $O(h)$ in this class of symbols. Let $\tilde{A}$ be the Anti-Wick h-quantization of A, that is $\hat{A}_1$, the Weyl h-quantization of A_1. By the Calderon-Vaillancourt theorem (which works for matricial pseudodifferential operators), the bounded operator $\hat{A} - \tilde{A}$ on L^2 is $O(h)$ in the corresponding norm. So it suffices to prove $\tilde{A} \geq 0$, provided $A \geq 0$, to get the result. To this end, we can write, for all $u \in C_0^\infty$,

$$\langle u, \tilde{A}u\rangle \;=\; \int_{T^*\mathbb{R}^n} e^{-y^2/h}\,|U(y,\eta)|^2\,A(y,\eta)\,dyd\eta\,,$$

where U may be expressed in terms of u. Thus, if A is nonnegative so is $\tilde{A}$.

B Geometrical properties.

In this part, we collect some geometrical facts for both types of crossings. We use the notation introduced in Section 5. Since we want to consider functions defined near $\mathcal{C}^*$, we need to extend the geometrical objects of Section 5 to some neighborhood of $\mathcal{C}^*$.
We set, for $\epsilon = (\epsilon_1,\epsilon_2) \in \mathbb{R}^2 \setminus \{(0,0)\}$, $\mathcal{C}(\epsilon) := v_1^{-1}(\epsilon_1) \cap v_2^{-1}(\epsilon_2)$, the intersection of the ϵ_1-level set of v_1 and the ϵ_2-level set of v_2. The set $\mathcal{C}(\epsilon)\cap\mathcal{U}$ is a codimension 2 submanifold of $\mathcal{U}$. We define the sets $\mathcal{C}^*(\epsilon) := \mathcal{C}(\epsilon)\times\mathbb{R}^n$. For $x \in \mathcal{C}(\epsilon)\cap\mathcal{U}$, we have, as in (40), $T_x^*\mathbb{R}^n = T_x^*\mathcal{C}(\epsilon) \oplus N_x^*\mathcal{C}(\epsilon)$ where the cotangent space $T_x^*\mathcal{C}(\epsilon)$ (resp. the conormal space $N_x^*\mathcal{C}(\epsilon)$) of $\mathcal{C}(\epsilon)$ at x is defined as in (9) (resp. (41)). We still denote by P_x^T (resp. P_x^N) the natural projection onto $T_x^*\mathcal{C}(\epsilon)$ (resp. $N_x^*\mathcal{C}(\epsilon)$) associated to this direct sum. Notice that, for $\epsilon = (0,0)$, we find objects, defined in Section 5. So, in this case, we simply pull out the symbol "$(0,0)$" at the end keeping this way a coherent notation.
Recall first that the Hamilton field $H_a(\beta)$ of some smooth function a on $T^*\mathbb{R}^n$ at $\beta \in T^*\mathbb{R}^n$ is the unique vector $w \in T_\beta T^*\mathbb{R}^n$ such that the differential $da(\beta)$ of a at β is given by $\sigma_\beta(w,\cdot)$, where σ_β is the value of the fundamental 2-form at β. Furthermore, if $\mathcal{D}^*$ is some level set of a, then, for any $\beta \in \mathcal{D}^*$, the orthogonal set to $T_\beta\mathcal{D}^*$ w.r.t. the form σ_β

is $(T_\beta \mathcal{D}^*)^\sigma = \mathrm{Vect}(H_a(\beta))$.
For $\alpha \in T^*\mathcal{C}(\epsilon) \cap \mathcal{U}^*$, the space $T_\alpha T^*\mathcal{C}(\epsilon)$ is symplectic and we have

$$T_\alpha T^*\mathbb{R}^n \;=\; T_\alpha T^*\mathcal{C}(\epsilon) \oplus \Big(T_\alpha T^*\mathcal{C}(\epsilon)\Big)^\sigma . \tag{47}$$

For any smooth function a defined on $\mathcal{U}^*$, we denote by a' its restriction to $T^*\mathcal{C}(\epsilon) \cap \mathcal{U}^*$. Since the restriction of da of a to $T_\alpha T^*\mathcal{C}(\epsilon)$ equals da', we have, by definition of the Hamilton fields, $H_a(\alpha) - H_{a'}(\alpha) \in (T_\alpha T^*\mathcal{C}(\epsilon))^\sigma$. Therefore, according to (47), $H_a(\alpha)$ splits into $H_{a'}(\alpha) + (H_a(\alpha) - H_{a'}(\alpha))$. For Codimension 2 crossings, we have, since $H_{v_1}(\alpha)$ and $H_{v_2}(\alpha)$ are independent, $(T_\alpha \mathcal{C}^*(\epsilon))^\sigma = \mathrm{Vect}(H_{v_1}(\alpha), H_{v_2}(\alpha))$. Furthermore, since v_1 and v_2 only depend on x, $\sigma(H_{v_1}, H_{v_2})$ is zero at α. Thus $(T_\alpha \mathcal{C}^*(\epsilon))^\sigma \subset T_\alpha \mathcal{C}^*(\epsilon)$. Obviously, $T_\alpha T^*\mathcal{C}(\epsilon) \subset T_\alpha \mathcal{C}^*(\epsilon)$, so $\mathrm{Vect}(H_{v_1}(\alpha), H_{v_2}(\alpha)) \subset (T_\alpha T^*\mathcal{C}(\epsilon))^\sigma$. By an argument of dimension, we even have $T_\alpha \mathcal{C}^*(\epsilon) = \mathrm{Vect}(H_{v_1}(\alpha), H_{v_2}(\alpha)) \oplus T_\alpha T^*\mathcal{C}(\epsilon)$. Since $p = |\xi|^2 + u(x)$, we see, thanks to (9), that $\sigma_\alpha(H_{v_1}(\alpha), H_p(\alpha)) = \sigma_\alpha(H_{v_2}(\alpha), H_p(\alpha)) = 0$, that is $H_p(\alpha) \in T_\alpha \mathcal{C}^*(\epsilon)$. Therefore, according to the previous decomposition,

$$\forall \alpha \in T^*\mathcal{C}(\epsilon) \cap \mathcal{U}^*, \qquad H_p(\alpha) \;=\; \Big(\mu_1(\alpha) H_{v_1}(\alpha) + \mu_2(\alpha) H_{v_2}(\alpha)\Big) \;+\; H_{p'}(\alpha)\,, \tag{48}$$

for some smooth, real functions μ_1, μ_2. Here, p' is the restriction of p to $T^*\mathcal{C}(\epsilon)$. Of course, we have the same situation for Codimension 1 crossings, that is, for $\mathcal{U} = \{x \in \mathbb{R}^n; \nabla\tau(x) \neq 0\}$ and $\alpha \in \mathcal{C}^*(\epsilon) \cap \mathcal{U}^*$, $T_\alpha \mathcal{C}^*(\epsilon) = \mathrm{Vect}(H_\tau(\alpha)) \oplus T_\alpha T^*\mathcal{C}(\epsilon)$, $H_p(\alpha) \in T_\alpha \mathcal{C}^*(\epsilon)$, and the corresponding decomposition

$$\forall \alpha \in T^*\mathcal{C}(\epsilon) \cap \mathcal{U}^*,\; H_p(\alpha) \;=\; \mu(\alpha) H_\tau(\alpha) \;+\; H_{p'}(\alpha)\,, \tag{49}$$

for some smooth, real function μ. The phenomenon described in Section 5 appears also here. If we consider a <u>scalar</u> function a, then the positivity of $\{P, a\mathrm{I}_2\}$ on $E(\lambda)$ implies the inequality

$$\sigma(H_{p'}, H_{a'}) \;+\; \sigma(H_p - H_{p'}, H_a - H_{a'}) \;>\; \tilde{\rho}|\sigma(H_\tau, H_a - H_{a'})|$$

on $T^*\mathcal{C} \cap E(\lambda)$. If $\sigma(H_{p'}, H_{a'})$ is not everywhere positive on $T^*\mathcal{C} \cap E(\lambda)$ (if $\mathcal{C}$ is compact, for instance), then we must have $\mu > \tilde{\rho}$ everywhere on $T^*\mathcal{C} \cap E(\lambda)$.

C Codimension 1.

For the construction of escape functions, we need some result on a special case of Ricatti's differential equations, which might be not completely included in the litterature, and some properties of Hamilton flows, essentially contained in [DG], that we sketch here.

Proof of Proposition 4.1 : By the Cauchy-Lipschitz theorem, we have local existence and uniqueness of solution. We consider the maximal solution, defined on $[0; T^*[$, for some $T^* > 0$. Assume that there exists some $t_1 \in [0; T^*[$ such that $z(t_1) = 0$. Then, since $|z(t)| \leq |z_0|$ on $[0; t_1]$, $z' \leq a z_0 z + b$ on $[0; t_1]$. Therefore, we obtain on $[0; t_1]$,

$$\begin{aligned} z(t) \;&\leq\; z_0 \exp\Big(z_0 \int_0^t a(s)\,ds\Big) \;+\; \int_0^t b(s) \exp\Big(z_0 \int_s^t a(v)\,dv\Big)\,ds \\ &\leq\; z_0 \exp\Big(z_0 \int_0^t a(s)\,ds\Big) \;+\; \int_0^t b(s)\,ds\,, \end{aligned}$$

since $z_0 < 0$ and $a \geq 0$. Using the convexity of the exponential function, we see that

$$0 \;=\; z(t_1) \;\leq\; z_0 \,+\, z_0^2 \int_0^t a(s)\,ds \,+\, \int_0^t b(s)\,ds \;\leq\; z_0 \,+\, z_0^2 I \,+\, J\,.$$

Since $1-4IJ > 0$, we arrive at a contradiction for $2Iz_0 \in]-1-\sqrt{1-4IJ}; -1+\sqrt{1-4IJ}[\subset]-\infty; 0]$. Thus, for such z_0, the solution is defined on R^+ and negative. Since z is non-decreasing, it satisfies (26). □

Proof of Lemma 4.3 : Let a be a global escape function for $\tilde{p}_-$ at energy λ, such that $a = a_\infty$ outside $B^*_{R'}$. Thus, there exists $c_1 > 0$ such that $\{\tilde{p}_-, a\} \geq c_1$ on $\tilde{p}_-^{-1}(]\lambda-\epsilon_0; \lambda+\epsilon_0[)$, for small enough $\epsilon_0 > 0$. On this region, if we take β with $a(\beta) = 0$ then, for all t, $c_2\langle q(t;\beta)\rangle \geq |a \circ \phi^t(\beta)| \geq c_1|t|$, for $c_2 > 0$ independent of t and β (see Theorem 2.4.3 in [DG]). Thus, there exists $c > 0$ such that, uniformly, $\langle q(t;\beta)\rangle \geq c\langle t\rangle$, yielding the first result of Lemma 4.3 in the last two regions. For the first one, $\langle q(t;\alpha)\rangle = \langle q(t-t_1;\beta)\rangle$, for some β satisfying $a(\beta) = 0$ and some $t_1 \geq 0$. Using the previous estimate for $q(t;\beta)$ and the fact that $t_1 \leq T/c_1$, we get the first result for the first region.
In the spirit of [DG], we introduce a time-dependent effective force. Let $\chi \in C^\infty(\mathbb{R};\mathbb{R})$ such that $0 \leq \chi \leq 1$, $\chi = 0$ on $]-\infty; 1/2]$, and $\chi = 1$ on $[1; +\infty[$. We set, for $t \in \mathbb{R}$ and $x \in \mathbb{R}^n$, $F(t;x) = \chi(\langle x\rangle/(C\langle t\rangle))\chi(x/R')(-\nabla_x(u - \tau\tilde{p}))(x)$. For the three regions we consider, $(q(t;\alpha); p(t;\alpha))$ is the solution of the Hamilton system

$$\frac{dq}{dt}(t;\alpha) \;=\; 2p(t;\alpha)\,, \qquad \frac{dp}{dt}(t;\alpha) \;=\; F\Big(t, q(t;\alpha)\Big)\,,$$

starting at $\alpha = (x,\xi)$ at $t = 0$. As usual, this is equivalent to

$$\frac{dq}{dt}(t;\alpha) \;=\; 2p(t;\alpha)\,, \qquad q(t;\alpha) \;=\; q_0(t;\alpha) \,+\, 2\int_0^t (t-s)F\Big(s, q(s;\alpha)\Big)\,ds\,.$$

The function $t \mapsto z(t;\alpha) := q(t;\alpha) - q_0(t;\alpha)$ is solution of $\mathcal{P}(z) = z$ where

$$\mathcal{P}(v)(t) \;:=\; 2\int_0^t (t-s)F\Big(s, v(s) + q_0(t;\alpha)\Big)\,ds\,. \tag{50}$$

Let $\mathcal{B}$ be the Banach space of the functions $t \mapsto v(t)$, such that $\|v\|_{\mathcal{B}} := \sup_{t\in\mathbb{R}} |v(t)/t| < \infty$, equiped with the norm $\|\cdot\|_{\mathcal{B}}$. As in Theorem 1.5.1 in [DG], we want to use the fixed point Theorem. By definition of F, we see that $\mathcal{P}(v)$ belongs to $\mathcal{B}$. Derivating w.r.t. v, we see that $\|D_v\mathcal{P}(v)\|_{\mathcal{B}} \leq c(R')^{-\delta/2}$ by (2), showing that $\mathcal{P}$ is a contraction on $\mathcal{B}$, for R' large enough. Similarly we get $\|D_\xi\mathcal{P}(v)\| \leq c(R')^{-\delta/2}$, since $|D_\xi q_0(s;\alpha)| \leq C\langle s\rangle$. Since z is a fixed point of $\mathcal{P}$, $D_\xi\mathcal{P}(z) = (1 - D_v\mathcal{P}(z))D_\xi z$. Therefore $D_\xi z$ belongs to $\mathcal{B}$ and $\|D_\xi z\|_{\mathcal{B}} \leq c(R')^{-\delta/2}$. Along the same lines, we show that $D_x z$ belongs to $\mathcal{B}$ and that $\|D_x z\|_{\mathcal{B}} \leq c(R')^{-\delta/2}$. Choosing R' large enough, we can ensure the second result of Lemma 4.3. □

D Codimension 2.

In this part, we prove that the existence of an escape function for P near $T^*\mathcal{C}$, for a Codimension 2 crossing, implies the existence of a scalar one, we relate the confining condition to some positivity, and we consider some tools used in Proposition 5.1.

Scalar escape function for Codimension 2 crossings: We want to show that the existence of an escape function A for P at energy λ on $T^*\mathcal{C}$ implies the existence of a scalar one, namely its half-trace a_0.
Notice that a_0 is a smooth function on $T^*\mathbb{R}^n$. Since $[P, A] = 0$, we can write $A = a_0 \mathrm{I}_2 + a_1 V$ outside $\mathcal{C}^*$, for a smooth function a_1 on $T^*\mathbb{R}^n \setminus \mathcal{C}^*$. Since A is smooth everywhere, so is the function $a_1 V$ and so are the functions $v_1 a_1$ and $v_2 a_1$. Since v_1 and v_2 are independent coordinates near $\mathcal{C}$, we see, using Taylor expansion with rest integral for the functions $v_1 a_1$ and $v_2 a_1$, that a_1 extends to a smooth function on $T^*\mathbb{R}^n$. Next we compute $\{P, A\}$, defined in (14), and obtain

$$\{P, A\} \; = \; \Big(\{p, a_0\} - (1/2)\nabla_\xi a_1 \cdot \nabla \rho^2\Big)\, \mathrm{I}_2 \; + \; \{p, a_1\}\, V \; + \; \{V, a_0\} \; + \; 2a_1 \xi \cdot \nabla V \, .$$

For $x \in \mathcal{C}$, $(\nabla \rho^2)(x) = 0$ and $V(x) = 0$, and for $(x, \xi) \in T^*\mathcal{C}$, $\xi \cdot \nabla V(x) = 0$. Therefore, on $T^*\mathcal{C}$, $\{P, A\} = \{P, a_0\}$. This proves the expected result. $\square$

Confining condition: In the main text, we use the following result for the independent vectors $\nabla v_1(x)$ and $\nabla v_2(x)$ when x belongs to $\mathcal{C}$.
Let e_1, e_2 be two independent vectors in $\mathbb{R}^m$ $(m \geq 2)$. We shall prove that, given $\mu_1, \mu_2 \in \mathbb{R}$, there exist $\lambda_1, \lambda_2 \in \mathbb{R}$ such that

$$(\lambda_1 e_1 + \lambda_2 e_2) \, \cdot \, (\mu_1 e_1 + \mu_2 e_2) \; > \; \sqrt{(\lambda_1 |e_1|^2 + \lambda_2 e_1 \cdot e_2)^2 + (\lambda_1 e_1 \cdot e_2 + \lambda_2 |e_2|^2)^2} \, , \qquad (51)$$

if and only if $\mu_1^2 + \mu_2^2 > 1$. And, in this case, we can exhibit λ_1, λ_2 satisfying (51).
To this end, we set $x = \lambda_1 |e_1|^2 + \lambda_2 e_1 \cdot e_2$ and $y = \lambda_1 e_1 \cdot e_2 + \lambda_2 |e_2|^2$. Notice that $(\lambda_1 e_1 + \lambda_2 e_2) \cdot (\mu_1 e_1 + \mu_2 e_2) = \mu_1 x + \mu_2 y$. So, the condition (51) means that the scalar product of the vectors (μ_1, μ_2) and (x, y) in $\mathbb{R}^2$ must be greater than the norm of (x, y). This is only possible if the norm of (μ_1, μ_2) is greater than 1. In this case, we have the solution $(x, y) = (\mu_1, \mu_2)$. Since e_1 and e_2 are independent, $\Delta := |e_1|^2 |e_2|^2 - (e_1 \cdot e_2)^2 > 0$ so we can recover (λ_1, λ_2) from (x, y). In particular, (51) is satisfied for $\lambda_1 = (\mu_1 |e_2|^2 - \mu_2 (e_1 \cdot e_2))/\Delta$ and $\lambda_2 = (\mu_2 |e_1|^2 - \mu_1 (e_1 \cdot e_2))/\Delta$. $\square$

Properties of the differential equation (42): Let $z \in \mathcal{C}$. Since $z \in \mathcal{U}$, we can find a bounded open set $\mathcal{U}_z$, with $z \in \mathcal{U}_z \subset \mathcal{U}$, and a smooth diffeomorphism

$$\begin{array}{rcl} \phi_z : \mathcal{U}_z & \longrightarrow & \mathcal{W}_z \\ x & \mapsto & \Big(v_1(x), v_2(x), v_3(x), \cdots, v_n(x)\Big) \, , \end{array}$$

onto some open set $\mathcal{W}_z$ in $\mathbb{R}^n$, such that $x \in \mathcal{U}_z$ and $a_1^2 + a_2^2 \leq \rho^2(x)$ imply $(a_1, a_2, v_3(x), \cdots, v_n(x)) \in \mathcal{W}_z$. For the maximal solution of (42), defined on $[0; T^*[$, starting at $x \in \mathcal{U}_z$,

$(d/dt)\rho^2(y_t) = -|\nabla\rho^2|^2(y_t)$, so the function $t \mapsto \rho^2(y_t)$ is nonincreasing. Thus, y_t stays in $\mathcal{U}_z$, for all $t \in [0; T^*[$. Therefore $T^* = \infty$. Furthermore, we can find some $c > 0$ such that $|\nabla\rho^2|^2 \geq c\rho^2$ on $\mathcal{U}_z$. This implies that $(d/dt)\rho^2(y_t) \leq -c\rho^2(y_t)$ and further that $\rho^2(y_t) \leq \exp(-ct)\rho^2(x)$. Since $\phi_z(y_t) = (v_1(y_t), v_2(y_t), v_3(x), \cdots, v_n(x))$, we conclude that $y(x) := \lim_{t\to+\infty} y_t$ exists, belongs to $\mathcal{C}$, and that y equals the smooth function $x \mapsto \phi_z^{-1}(0, 0, v_3(x), \cdots, v_n(x))$ on $\mathcal{U}_z$. So it is well defined and smooth on $\mathcal{U}_1 := \cup_{z\in\mathcal{C}}\mathcal{U}_z$. Since $\phi_z \circ y \circ \phi_z^{-1}$ is the restriction to $\mathcal{W}_z$ of a projection, we see that $y'(x)$ is bijective from $T_x\mathcal{C}(\epsilon)$, for $\epsilon = (v_1(x), v_2(x))$, onto $T_{y(x)}\mathcal{C}$ and equals the identity for $x \in \mathcal{C}$. Thus, so is its transposed map ${}^t(y'(x))$ from $T^*_{y(x)}\mathcal{C}$ onto $T^*_x\mathcal{C}(\epsilon)$. For any $\xi \in T^*_x\mathbb{R}^n$, there exists an unique $\eta(x,\xi) \in T^*_{y(x)}\mathcal{C}$ such that ${}^t(y'(x))\eta(x,\xi) = P_x^T\xi$. This defines a smooth function η, which satisfies, on $T^*\mathcal{C}$, $\eta(x,\xi) = \xi$ and $\nabla v_j \cdot \nabla_\xi \eta(x,\xi) = 0$ for $j = 1, 2$.

References

[DG] J. Dereziński, C. Grard : *Scattering theory of classical and quantum N-particle systems.* Springer-Verlag 1997.

[FG] C.Fermanian, P.Grard : *Mesures semi-classiques et croisement de modes.* Sminaire EDP, 1999-2000, Exp. No. XVIII, École Polytechnique. To appear in Bulletin de la SMF.

[FH] R.Froese, I.Herbst : *Realizing holonomic constraints in classical and quantum mechanics.* Comm. Math. Phys. 220, 489-535 (2001).

[GM] C.Gérard, A.Martinez : *Principe d'absorption limite pour des opérateurs de Schrödinger à longue portée.* C.R. Acad. Sci. 306, 121-123, 1988.

[GS] C.Gérard, J.Sjöstrand : *Semiclassical resonances generated by a closed Trajectory of hyperbolic type.* Comm. Math. Phys. 108, 391-421 (1987).

[Ha] G.A.Hagedorn : *Molecular propagation through electron energy level crossings.* Memoirs AMS 536, vol. 111, 1994.

[HS] B.Helffer, J.Sjöstrand : *Opérateurs de Schrödinger avec champs magnétiques faibles et constants.* Exposé No. XII, Séminaire EDP, février 1989, Ecole Polytechnique.

[H] L.Hörmander : *The analysis of linear partial differential operators III.* Springer-Verlag Berlin Heidelberg 1983.

[Jec] Th.Jecko : *Estimations de la résolvante pour une molécule diatomique dans l'approximation de Born-Oppenheimer.* Comm. Math. Phys. 195, 3, 585-612, 1998.

[K] T. Kato : *Pertubation theory for linear operators.* Springer-Verlag 1995.

[Kl] M.Klein : *On the absence of resonances for Schrödinger operators with non-trapping potentials in the classical limit.* Comm. Math. Phys. 106, 485-494 (1986).

[Mo] E.Mourre : *Absence of singular continuous spectrum for certain self-adjoint operators.* Commun. in Math. Phys. 78, 391-408, 1981.

[Ne1] L.Nédélec : *Résonances pour l'opérateur de Schrödinger matriciel.* Ann.IHP vol 65, 2, 1996, 129-162.

[Ne2] L.Nédélec : *Resonances for matrix Schrödinger operators.* Duke Math. J., vol. 106, n^o 2, 2001, 209-236.

[RS2] M.Reed, B.Simon : *Methods of Modern Mathematical Physics, Tome II : Fourier Analysis, Self-adjointness.* Academic Press 1979.

[Ro] D.Robert : *Autour de l'approximation semi-classique.* Birkhäuser 1987.

[RT] D.Robert, H.Tamura : *Semiclassical estimates for resolvents and asymptotics for total cross-section.* Ann. IHP Vol. 46, 1987, p. 415-442.

[W1] X.P.Wang : *Time-delay operators in semiclassical limit II. Short-range potentials* Trans. AMS Vol. 322, 1, 1990, p. 395-415.

[W2] X.P.Wang : *Semiclassical resolvent estimates for N-body Schrödinger operators.* J. Funct. Anal. 97, 466-483 (1991).