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Semiclassical Resolvent Estimates for Schrödinger Operators with Coulomb Singularities

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Abstract. Consider the Schrödinger operator with semiclassical parameter h, in the limit where h goes to zero. When the involved long-range potential is smooth, it is well known that the boundary values of the operator's resolvent at a positive energy λ are bounded by $O(h^{-1})$ if and only if the associated Hamilton flow is non-trapping at energy λ. In the present paper, we extend this result to the case where the potential may possess Coulomb singularities. Since the Hamilton flow then is not complete in general, our analysis requires the use of an appropriate regularization.

1. Introduction

In the late eighties and the beginning of the nineties, many semiclassical results were obtained in stationary scattering theory. In this setting, the long time evolution of a system is studied via the resolvent, which appears in representation formulae for the main scattering objects. One can distinguish two complementary domains: on the one hand semiclassical results concerning scattering objects at non-trapping energies (when resonances are negligible), and on the other hand studies of resonances and of their influence on scattering objects. We refer to [15, 20, 29, 39, 47] and also to [46] for an overview of the subject. These results often show a Bohr correspondence principle for the scattering states.

Many studies treat (non-relativistic) molecular systems described by a (many body) Schrödinger operator. From a physical point of view, it is natural to let the potential admit Coulomb singularities in that context. In the spectral analysis of the operator, these singularities do not produce difficulties in dimension ≥ 3, thanks to Hardy's inequality (cf. (2.9)).

In the semiclassical regime however, little is known when Coulomb singularities occur. We point out the propagation results in [13, 27, 32]. In the above mentioned domains of stationary scattering theory, we do not know of any semiclassical result, except that of [29,53]. We think that the main obstacle stems from the difficulty to develop a semiclassical version of Mourre's theory (cf. [14,40,47]) in this situation. This task is performed in [29] when all singularities are repulsive, a situation where the associated classical Hamilton flow is complete. Recently semiclassical resolvent estimates (and further interesting results) were obtained by Wang in [53] but in a non optimal framework (see comments below). When attractive singularities occur, the classical flow is not complete anymore, while it can be regularized (cf. [13,27,32]).

The aim of this article is to contribute to the development of such a semiclassical analysis of molecular scattering. In [22,23], the author faced similar difficulties in the study of a matricial Schrödinger operator. He adapted in [24,25] an alternative approach, previously used in [5]. We here follow the same approach, combined with ideas from [6,13,32,52], in order to extend, in the case of potentials with arbitrary Coulomb singularities, a result established in [29,47].

We now introduce some notation and present the main results of this paper.

1.1. The Schrödinger operators

Let $d \in \mathbb{N} := \{0, 1, 2, \ldots\}$ with $d \geq 2$. For $x \in \mathbb{R}^d$, we denote by $|x|$ the usual norm of x and we set $\langle x \rangle := (1 + |x|^2)^{1/2}$. We denote by Δ_x the Laplacian in $\mathbb{R}^d$. We consider a long-range potential V which is smooth except at N' Coulomb singularities ($N' \in \mathbb{N}^*$) located at the sites s_j where $j \in \{1, 2, \ldots, N'\}$. Let

$$\hat{M} := \mathbb{R}^d \setminus \mathcal{S}\,, \quad \text{with} \quad \mathcal{S} := \{s_j; 1 \leq j \leq N'\}$$

and $R_0 := \max\{|s_j| + 1; 1 \leq j \leq N'\}$. Technically, we take $V \in C^\infty(\hat{M}; \mathbb{R})$ such that

$$\exists \rho > 0\,; \quad \forall \alpha \in \mathbb{N}^d\,, \quad \forall x \in \mathbb{R}^d\,, \quad |x| > R_0\,, \quad |\partial_x^\alpha V(x)| = O_\alpha\big(\langle x \rangle^{-\rho-|\alpha|}\big)\,. \tag{1.1}$$

Furthermore, we assume that for all $j \in \{1, 2, \ldots, N'\}$, we can find smooth functions f_j, W_j in $C_0^\infty(\mathbb{R}^d; \mathbb{R})$ such that $f_j(s_j) \neq 0$ and, near s_j,

$$V(x) = \frac{f_j(x)}{|x - s_j|} + W_j(x)\,. \tag{1.2}$$

If $f_j(s_j) < 0$ (resp. $f_j(s_j) > 0$), we say that s_j is an *attractive* (resp. a *repulsive*) *Coulomb singularity*. Let $N \geq 0$ be the number of attractive singularities. We may assume that they are labelled by $\{1, 2, \ldots, N\}$.

Given some $h_* \in]0; 1[$, we introduce a semiclassical parameter $h \in]0; h_*]$. The semiclassical Schrödinger operator is given by $P(h) := -h^2\Delta_x + V$, acting in $\mathrm{L}^2(\mathbb{R}^d)$.

Under the previous assumptions, it is well known that $P(h)$ is self-adjoint (see [8,26,43]). When $d \geq 3$, this fact follows from Hardy's inequality (cf. (2.9)) and from Kato's theorem on relative boundedness. The domain of $P(h)$ then is the Sobolev space $\mathrm{H}^2(\mathbb{R}^d)$, i.e. the domain of the Laplacian. When $d = 2$, self-adjointness follows when considering the quadratic form associated with $P(h)$ and using Kato's theorem on relative boundedness for forms: the form is seen to be closable and bounded below, and the associated self-adjoint operator is $P(h)$ [7,33]. The situation is rather different for $d = 1$ (see Section I.1 in [43]), which is the reason why we exclude this dimension here.

1.2. The function spaces and main notation

For z belonging to the resolvent set $\rho(P(h))$ of $P(h)$, we set $R(z;h) := (P(h)-z)^{-1}$. We are interested in the size of the resolvent $R(z;h)$ as a bounded operator from some space S into its dual S^*, i.e. as an element of the space $\mathcal{L}(\mathrm{S};\mathrm{S}^*)$. We denote by $\|\cdot\|_{\mathrm{S},\mathrm{S}^*}$ the usual operator norm on $\mathcal{L}(\mathrm{S};\mathrm{S}^*)$. If $\mathrm{S} = \mathrm{L}^2(\mathbb{R}^d)$, we also use the notation $\|\cdot\|$ in place of $\|\cdot\|_{\mathrm{S},\mathrm{S}^*}$. The relevant spaces S are introduced below.

If a is a measurable subset of $\mathbb{R}^d$, we denote by $\|\cdot\|_a$ (resp. $\langle\cdot\,,\cdot\rangle_a$) the usual norm (resp. the right linear scalar product) of $\mathrm{L}^2(a)$ (and we skip the subscript a if $a = \mathbb{R}^d$). For $s \in \mathbb{R}$, we denote by L^2_s the weighted L^2-space of measurable functions f such that $x \mapsto \langle x\rangle^s f(x)$ belongs to $\mathrm{L}^2(\mathbb{R}^d)$. Its dual space is identified with L^2_{-s}. For $j \in \mathbb{Z}$, we set

$$c_j := \{x \in \mathbb{R}^d; 2^{j-1} < |x| \leq 2^j\} \quad \text{and} \quad c = \{x \in \mathbb{R}^d; |x| \leq 1\}\,. \tag{1.3}$$

Let B (resp. its homogeneous version $\dot{\mathrm{B}}$) be the space of functions f locally in $\mathrm{L}^2(\mathbb{R}^d)$ (resp. $\mathrm{L}^2(\mathbb{R}^d \setminus \{0\})$) such that

$$\|f\|_{\mathrm{B}} := \|f\|_c + \sum_{j=1}^{\infty} 2^{j/2}\|f\|_{c_j} \quad \left(\text{resp. } \|f\|_{\dot{\mathrm{B}}} := \sum_{j\in\mathbb{Z}} 2^{j/2}\|f\|_{c_j}\right) \tag{1.4}$$

is finite. Its dual B^* (resp. $\dot{\mathrm{B}}^*$) is equipped with

$$\|f\|_{\mathrm{B}^*} := \max\left(\|f\|_c\,;\, \sup_{j\geq 1} 2^{-j/2}\|f\|_{c_j}\right) \quad \left(\text{resp. } \|f\|_{\dot{\mathrm{B}}^*} := \sup_{j\in\mathbb{Z}} 2^{-j/2}\|f\|_{c_j}\right). \tag{1.5}$$

One can easily check that the embeddings $\mathrm{L}^2_s \subset \mathrm{B} \subset \mathrm{L}^2_{1/2}$, for any $s > 1/2$, and $\mathrm{B} \subset \dot{\mathrm{B}}$, are all continuous. Notice that, for $\mathrm{S} = \mathrm{L}^2_s, \mathrm{B}$, and $\dot{\mathrm{B}}$,

$$\forall f \in \mathrm{S}^*\,, \quad \forall g \in \mathrm{S}\,, \quad \bar{f}g \in \mathrm{L}^1 \quad \text{and} \quad \left|\langle f\,, g\rangle\right| \;\leq\; \|f\|_{\mathrm{S}^*}\cdot\|g\|_{\mathrm{S}}\,. \tag{1.6}$$

For $z \in \rho(P(h))$, $R(z;h)$ can be viewed as a bounded operator from L^2_s to L^2_{-s}, for $s \geq 0$, and from B to B^*, being a bounded operator on $\mathrm{L}^2(\mathbb{R}^d)$. When $d \geq 3$, one can show using Hardy's inequality (2.9) that, for $z \in \rho(P(h))$, $R(z;h)$ can even be viewed as a bounded operator from $\dot{\mathrm{B}}$ to $\dot{\mathrm{B}}^*$ (cf. [54]), a stronger result.

Let I be a compact interval included in $]0;+\infty[$ and $d \geq 3$. By [12], we know that I contains no eigenvalue of $P(h)$. By Mourre's commutator theory (cf. [3,40]), we also know that for fixed h, $\|R(\cdot\,;h)\|_{\mathrm{S},\mathrm{S}^*}$ is bounded on $\{z \in \mathbb{C}; \Re z \in I, \Im z \neq 0\}$ whenever $\mathrm{S} = \mathrm{L}^2_s$ $(s > 1/2)$ or $\mathrm{S} = \mathrm{B}$. Adapting an argument by [54], the above norm is even seen bounded when $\mathrm{S} = \dot{\mathrm{B}}$. Summarizing, for $s > 1/2$ and any given

$h > 0$, the following chain of inequalities holds true

$$\sup_{\substack{\Re z \in I \\ \Im z \neq 0}} \|R(z;h)\|_{\mathrm{L}^2_s, \mathrm{L}^2_{-s}} \leq \sup_{\substack{\Re z \in I \\ \Im z \neq 0}} \|R(z;h)\|_{\mathrm{B},\mathrm{B}^*} \leq \sup_{\substack{\Re z \in I \\ \Im z \neq 0}} \|R(z;h)\|_{\dot{\mathrm{B}},\dot{\mathrm{B}}^*} < \infty\,. \tag{1.7}$$

1.3. The non-trapping condition

We now estimate the terms involved in (1.7) as $h \to 0$. When $V = 0$, it is known that

$$\sup_{\substack{\Re z \in I \\ \Im z \neq 0}} \|R(z;h)\|_{\mathrm{S},\mathrm{S}^*} = O(1/h)\,, \tag{1.8}$$

whenever $\mathrm{S} = \mathrm{L}^2_s$ ($s > 1/2$), or $\mathrm{S} = \mathrm{B}$. Our aim is to characterize those potential V for which (1.8) holds true with $\mathrm{S} = \mathrm{B}$.

If $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ and satisfies (1.1), then a characterization of those V's such that (1.8) holds true is well known, at least in the case $\mathrm{S} = \mathrm{L}^2_s$ ($s > 1/2$) or $\mathrm{S} = \mathrm{B}$, as we now describe. Let $T^*\mathbb{R}^d \ni (x,\xi) \mapsto p(x,\xi) := |\xi|^2 + V(x)$ be the symbol of $P(h)$. Since the potential V is bounded below, the speed $|\xi|$ is bounded above on $p^{-1}(\lambda)$, for all energies λ . Thus the particle cannot escape to infinity in finite time and p defines a complete smooth Hamilton flow $(\phi^t)_{t\in\mathbb{R}}$ on $T^*\mathbb{R}^d$. The symbol p is said *non-trapping* at the energy λ whenever

$$\forall (x,\xi) \in p^{-1}(\lambda)\,, \quad \lim_{t\to-\infty} |\phi^t(x,\xi)| = +\infty \quad \text{and} \quad \lim_{t\to+\infty} |\phi^t(x,\xi)| = +\infty\,. \tag{1.9}$$

In many cases it is easy to show trapping by topological criteria, see [34].

Let $\mathrm{S} = \mathrm{L}^2_s$ with $s > 1/2$, or $\mathrm{S} = \mathrm{B}$. Then (1.8) holds true if and only if any energy $\lambda \in I$ is non-trapping for p (cf. [14, 24, 39, 47, 50, 52]). This statement has been extended to the homogeneous space $\mathrm{S} = \dot{\mathrm{B}}$ ($d \geq 3$) by [6], for V's of class C^2 only.

First note that such a characterization is a Bohr correspondence principle: in the limit $h \to 0$, a qualitative property of the classical flow (the non-trapping condition) is connected to a propagation property of the quantum evolution operator $U(t;h) = \exp(-ih^{-1}tP(h))$. Indeed the propagation estimate (3.11) turns out to be equivalent to the above estimate (1.8).

Second, it is also useful to develop a semiclassical, stationary scattering theory (the case $\mathrm{S} = \mathrm{L}^2_s$ actually suffices). If the non-trapping condition is true, one expects to deduce from (1.8) bounds on several scattering objects (as is done when $V \in C^\infty(\mathbb{R}^d)$, cf. [46, 47]). If trapping occurs, one expects that the resonant phenomena have a leading order influence on the scattering objects (cf. [15, 46]).

Of course, these two motivations are still present if Coulomb singularities are allowed.

When only repulsive Coulomb singularities occur, it was proved in [29] that the non-trapping condition implies that (1.8) is true with $\mathrm{S} = \mathrm{L}^2_s$ ($s > 1/2$). If at least one attractive Coulomb singularity is present, the flow is not complete anymore and the previous non-trapping condition does not even make sense. However, it is known that one can "regularize the flow" (see [32] and references therein), and it turns out the regularization is easier to deal with in dimension $d = 2$ and $d = 3$.

In the present paper, we choose to focus on the case $d = 3$, which is the physically important situation. Our study is devoted to generalizing the previous characterization, in a case where the potential admits arbitrary Coulomb singularities. Note that we do expect our results extend to the case $d = 2$.

Let $d = 3$ and assume that $\mathcal{S}$ contains an attractive singularity. Let $(x, \xi) \in T^*\hat{M} = T^*(\mathbb{R}^3 \setminus \mathcal{S})$. As we shall see in Subsection 2.2, there exists some at most countable subset $\mathrm{coll}(x, \xi) \subset \mathbb{R}$ and a smooth function $\phi(\,\cdot\,; x, \xi) : \mathbb{R} \setminus \mathrm{coll}(x, \xi) \longrightarrow T^*\hat{M}$ such that $\phi(\,\cdot\,; x, \xi)$ solves the Hamilton equations generated by the symbol p of $P(h)$ with initial value (x, ξ) (see (2.15) and (2.14) below). Furthermore, for all $t \in \mathbb{R} \setminus \mathrm{coll}(x, \xi)$, $p(\phi(t; x, \xi)) = p(x, \xi)$. The function ϕ replaces the usual flow. It is thus natural to say that p is non-trapping at energy λ whenever

$$\forall (x, \xi) \in p^{-1}(\lambda)\,, \quad \lim_{t \to -\infty} |\pi_x \phi(t; x, \xi)| = +\infty \quad \text{and} \quad \lim_{t \to +\infty} |\pi_x \phi(t; x, \xi)| = +\infty\,, \tag{1.10}$$

where $\pi_x \phi(t; x, \xi)$ denotes the configuration or base component of $\phi(t; x, \xi) \in T^*\hat{M}$.

1.4. Survey

In view of (1.7) and (1.10), we can now state our main result.

Theorem 1.1. *Let V be a potential satisfying the assumptions* (1.1) *and* (1.2)*. If there are no attractive singularities* ($N = 0$)*, let $d \geq 3$ else let $d = 3$. Let I_0 be an open interval included in* $]0; +\infty[$*. The following properties are equivalent.*

1. *For all $\lambda \in I_0$, p is non-trapping at energy λ.*
2. *For any compact interval $I \subset I_0$, there exists $C > 0$ such that, for $h \in]0; h_*]$,*

$$\sup_{\substack{\Re z \in I \\ \Im z \neq 0}} \|R(z; h)\|_{\mathrm{B}, \mathrm{B}^*} \leq C\, h^{-1}\,. \tag{1.11}$$

In [53], the point 2 of Theorem 1.1 is derived from a virial-like assumption, which is stronger than the non-trapping condition. It is assumed there that only one singularity occurs and that (1.2) holds true for a constant f_j. The statement "1 $\Longrightarrow$ 2" of Theorem 1.1 is proved in [29] when $N = 0$. Theorem 1.1 provides the converse. More importantly, it extends the result to the delicate case $N > 0$.

To complete the picture given by Theorem 1.1, we study in Section 5 the non-trapping condition. In the case of a *single* Coulomb singularity, we show that it is always satisfied when the energy λ is large enough, as in the case of a smooth potential (see Remark 5.5). The classically forbidden region in configuration space then is a point (for attracting Coulomb potential), or it is diffeomorphic to a ball (in the repelling case). Conversely Proposition 5.1 says that – irrespective of the number of singularities and the energy – *only* for the case of a single point or ball trapping does not need to occur. In particular, Corollary 5.2 states that trapping always occurs for two or more singularities at large enough energies.

We point out that our proof of Theorem 1.1 gives some additional insight about the case when the non-trapping condition fails at some energy $\lambda > 0$ (cf.

Proposition 4.9). In such a situation, "semiclassical trapping" occurs, as described by (4.1) and (4.2). Notice that a resonance phenomenon (cf. [20, 35]) is a particular case of the quasi-resonance phenomenon defined in [16], the latter being a particular case of our "semiclassical trapping" criterion. Propositions 4.5 and 4.9 show that the "semiclassical trapping" is microlocalized near "trapped trajectories" (see (4.10) for a precise definition). It would be interesting to check whether a (quasi-)resonance phenomenon is related to our "semiclassical trapping" (cf. Remark 4.6). A traditional study of the resonances "created" by a bounded trajectory (see [16] and references therein) would also be of interest. We do hope that the present paper may help to overcome the difficulties due to the singularities.

While the proof of "$2 \Longrightarrow 1$" in Theorem 1.1 follows the strategy developed by [52] for smooth potentials, we use a rather different argument compared to [14, 29, 47] when showing "$1 \Longrightarrow 2$". In these papers, a semiclassical version of Mourre's commutator theory is used (cf. [3, 40]), and the Besov-like space B is replaced by the weaker L^2_s ($s > 1/2$). An alternative approach is given in [5] for compactly supported perturbations of the Laplacian, using a contradiction argument due to G. Lebeau in [36]. This method was adapted in [24] to include long-range, smooth perturbations, the study still being carried out in the space L^2_s ($s > 1/2$). This technique was further developed in [6] to tackle the estimates in the optimal homogeneous space $\dot{\mathrm{B}}$, by combining and adapting an original estimate derived in [42]. Note that both works [42] and [6] only require C^1 resp. C^2 smoothness on the potential. Note also that the extension of Theorem 1.1 to the homogeneous estimate in $\dot{\mathrm{B}}$ still is open. Now, the contradiction argument of [6, 24] is a key ingredient of the present study. Concerning the treatment of the singularities, we stress that our study uses many results from [13], the propagation results being here crucial. The main features we need on the regularization of the classical flow are provided by [13, 32]. Our main new contributions are given in Proposition 3.6 and in Section 4.3.

Finally, we give some nonrelativistic, physical situations for which our result applies. In both examples below, we may add to the operator a smooth exterior potential satisfying (1.1).

Example 1.2. The behaviour of a particle with charge e_0 in the presence of fixed, pointlike ions, with nonzero charges $z_1, \ldots, z_{N'}$, is governed by the operator (here $d = 3$)

$$P_1(h) := -h^2\Delta_x + \sum_{j=1}^{N'} \frac{e_0 z_j}{|x - s_j|} \,. \tag{1.12}$$

The hydrogen atom corresponds to $N' = 1$, $z_1 > 0$, and $e_0 < 0$. Clearly (1.1) and (1.2) hold true. If charges have different sign, the model has attractive and repulsive singularities.

Example 1.3. Consider a molecule with N' nuclei having positive charges $z_1, \ldots, z_{N'}$, binding $K > 0$ electrons with charge -1. We assume the nuclei are fixed (Born–Oppenheimer idealization) and we neglect electron-electron repulsion.

The behaviour of each electron is then governed by $P_1(h)$ in (1.12). Let $h_0 > 0$ be fixed. Let ψ_k be the normalized wavefunction of $P_1(h_0)$ of electron number k. Let $\rho_k = |\psi_k|^2$ be its charge density. Consider another, much heavier particle with charge e_0. Its scattering by the molecule can be described by $P(h)$ where

$$V(x) := e_0 \left(\sum_{j=1}^{N'} \frac{z_j}{|x - s_j|} + \sum_{k=1}^{K} W_k(x) \right), \quad \text{with} \quad W_k(x) := -\int_{\mathbb{R}^d} \frac{\rho_k(q)}{|q-x|}\, dq\,. \tag{1.13}$$

As we show in Section 6, it turns out that the ψ_k's are "nice enough" to make W_k well defined, smooth away from the singularities $s_1, \dots, s_{N'}$, and to make W_k satisfy (1.1). Though (1.2) does not hold, we show the proof of our result applies in this case.

2. Preliminaries

We shall often use well known facts concerning h-pseudodifferential calculus, functional calculus, and semiclassical measures in the sequel. For sake of completeness, we recall here the main results we need, referring to [9, 17, 18, 21, 27, 37, 38, 41, 45] for further details. Since our Schrödinger operator has Coulomb singularities, it does not define a pseudodifferential operator yet. For this reason, we also explain here how we can use pseudodifferential calculus "away from the singularities": the required results are essentially contained in [13]; notice however that we do not need the results in the appendix of [29], which are, by the way, not known if an attractive Coulomb singularity is present. Last, we also recall basic results on the regularization of the Hamilton flow when an attractive singularity is present, referring to [13, 27, 32] for details.

2.1. Symbolic calculus with singularities

Let $d \in \mathbb{N}^*$. For $(r, m) \in \mathbb{R}^2$, we consider the vector space (space of symbols)

$$\Sigma_{r;m} := \Big\{ a \in C^\infty(T^*\mathbb{R}^d)\ ;\ \forall \gamma = (\gamma_x, \gamma_\xi) \in \mathbb{N}^{2d}\,,\ \exists C_\gamma > 0\,; \sup_{(x,\xi)\in T^*\mathbb{R}^d} \langle x \rangle^{-r+|\gamma_x|} \langle \xi \rangle^{-m+|\gamma_\xi|} \big| (\partial^\gamma a)(x,\xi) \big| \leq C_\gamma \Big\}\,. \tag{2.1}$$

If $r, m \leq 0$, then $\Sigma_{r;m}$ is contained in the vector space of bounded symbols, which are smooth functions $a : T^*\mathbb{R}^d \longrightarrow \mathbb{C}$ such that

$$\forall \gamma \in \mathbb{N}^{2d}\,, \quad \exists C_\gamma > 0\,; \quad \sup_{(x,\xi)\in T^*\mathbb{R}^d} \big| (\partial^\gamma a)(x,\xi) \big| \leq C_\gamma\,. \tag{2.2}$$

For a larger class of symbols a, one can define the *Weyl h-quantization* of a, denoted by a_h^w. It acts on $u \in C_0^\infty(\mathbb{R}^d)$ as follows (cf. [9, 38, 41, 45]).

$$\big(a_h^w u\big)(x) \;=\; (2\pi h)^{-d} \int_{\mathbb{R}^d} e^{i\xi\cdot(x-y)/h} a\big((x+y)/2, \xi\big) u(y)\, dy\, d\xi\,. \tag{2.3}$$

If a is a bounded symbol, then a_h^w extends to a bounded operator on $\mathrm{L}^2(\mathbb{R}^d)$, uniformly with respect to h, by Calderón–Vaillancourt's theorem (cf. [9,38,45]). We shall also use the following functional calculus of Helffer–Sjöstrand, which can be found in [9,38]. Given $\theta \in C_0^\infty(\mathbb{R})$, one can construct an almost analytic extension $\theta^{\mathbb{C}} \in C_0^\infty(\mathbb{C})$ (with $\overline{\partial}\theta^{\mathbb{C}}(z) = \mathcal{O}(\Im(z)^\infty)$). Let H be a self-adjoint operator in some Hilbert space. The bounded operator $\theta(H)$, defined by the functional calculus of self-adjoint operators, can be written as

$$\theta(H) \;=\; \frac{-1}{\pi}\int_{\mathbb{C}} \overline{\partial}\theta^{\mathbb{C}}(z)\cdot(z-H)^{-1}\,d\mathcal{L}_2(z)\,. \tag{2.4}$$

where $\mathcal{L}_2$ denotes the Lebesgue mass on $\mathbb{C}$.

Let us now recall some well known facts about semiclassical measures, which can be found in [17, 18, 27, 37]. Let $(u_n)_n$ be a bounded sequence in $\mathrm{L}^2(\mathbb{R}^d)$. Up to extracting a subsequence, we may assume that it is pure, i.e. it has a unique semiclassical measure μ. By definition μ is a finite, nonnegative Radon measure on the cotangent space $T^*\mathbb{R}^d$. Furthermore, there exists a sequence $h_n \to 0$ such that, for any $a \in C_0^\infty(T^*\mathbb{R}^d)$,

$$\lim_{n\to\infty} \langle u_n\,,\, a_{h_n}^w u_n\rangle = \int_{T^*\mathbb{R}^d} a(x,\xi)\,\mu(dx\,d\xi) =: \mu(a)\,. \tag{2.5}$$

One may relate the total mass of μ to the L^2-norm of the u_n's (see [18], or [27,37]), through the following

Proposition 2.1 ([18]). *Let $(u_n)_n$ be a pure bounded sequence in $\mathrm{L}^2(\mathbb{R}^d)$ such that*

$$\lim_{R\to+\infty}\ \limsup_{n\to\infty} \int_{|x|\geq R} |u_n(x)|^2\,dx = 0\,, \tag{2.6}$$

$$\lim_{R\to+\infty}\ \limsup_{n\to\infty} \int_{|\xi|\geq R/h_n} |\mathcal{F}u_n\,(x)|^2\,d\xi = 0\,, \tag{2.7}$$

where $\mathcal{F}u_n$ denotes the Fourier transform of u_n. Then the sequence $(\|u_n\|^2)_n$ converges to the total mass $\mu(T^*\mathbb{R}^d)$ of its semiclassical measure μ.

Proof. See the proof of Proposition 1.6 in [18]. □

Besides, transformation of the semiclassical measure upon composition of the u_n's with a diffeomorphism is described in the

Proposition 2.2 ([18]). *Let $\Phi : U \longrightarrow V$ be a C^∞ diffeomorphism between two open subsets of $\mathbb{R}^p$ $(p \geq 1)$. Let $\Phi_c : T^*U \longrightarrow T^*V$ be the symplectomorphism*

$$(y,\eta)\ \mapsto\ \Big(\Phi(y)\,;\,\big(\Phi'(y)^T\big)^{-1}\eta\Big)\,. \tag{2.8}$$

Here $\Phi'(y)^T$ denotes the transpose of $\Phi'(y)$. Given $a \in C_0^\infty(T^*V)$, let $b \in C_0^\infty(T^*U)$ be defined by $b = a\circ\Phi_c$. Then, for every compact subset K of V,

$$\lim_{h\to 0}\ \sup_{\substack{\|u\|\leq 1\\ \operatorname{supp} u\subset K}} \big\|(a_h^w u)\circ\Phi - b_h^w(u\circ\Phi)\big\| = 0\,.$$

Let K be a compact subset of V and $(u_n)_n$ be a pure bounded sequence in $\mathrm{L}^2(V)$ such that, for all n, $\operatorname{supp} u_n \subset K$. Denote by μ its semiclassical measure. Then the sequence $(u_n \circ \Phi)_n$ is bounded in $\mathrm{L}^2(U)$, its semiclassical measure $\tilde{\mu}$ is given by $|\mathrm{Det}\Phi'|^{-1}\Phi_c^{-1}(\mu)$, and $\mu(a) = \tilde{\mu}(b)$.

Proof. See the proof of Lemma 1.10 in [18]. □

We now focus on the treatment of Coulomb singularities in dimension $d \geq 3$, in combination with the h-pseudodifferential framework. To begin with, let us recall Hardy's inequality.

$$\forall f \in C_0^\infty(\mathbb{R}^d)\,, \quad \int_{\mathbb{R}^d} \frac{|f(x)|^2}{|x|^2}\,dx \;\leq\; \frac{4}{(d-2)^2}\,\|\nabla_x f\|^2 = \frac{4}{h^2(d-2)^2}\,\|h\nabla_x f\|^2\,, \tag{2.9}$$

where the last bound is relevant in the present, semiclassical regime.

We next discuss how one can use h-pseudodifferential calculus "away from the singularities". Recall that $\hat{M} = \mathbb{R}^d \setminus \mathcal{S}$. Let $\chi \in C_0^\infty(\mathbb{R}^d)$ with $\chi = 1$ near the set $\mathcal{S}$ of all singularities . Define the (truncated) h-pseudodifferential operator

$$P_\chi(h) := -h^2\Delta_x + (1-\chi)V\,. \tag{2.10}$$

Its symbol

$$T^*\mathbb{R}^d \ni (x,\xi) \mapsto p_\chi(x,\xi) = |\xi|^2 + \bigl(1-\chi(x)\bigr)V(x) \tag{2.11}$$

belongs to $\Sigma_{0;2}$ (cf. (2.1)). The following lemma is essentially proved in [13].

Lemma 2.3. *Let $d \geq 3$. Let $\chi \in C_0^\infty(\mathbb{R}^d)$ with $\chi = 1$ near $\mathcal{S}$ and $\theta \in C_0^\infty(\mathbb{R})$. Let $P_\chi(h)$ be given by (2.10). Let $T > 0$, $k, k' \in \mathbb{R}$, $r, m \in \mathbb{R}$, and $[-T;T] \ni t \mapsto a(t) \in \Sigma_{r;m}$ be a continuous function such that, for all $t \in [-T;T]$, $a(t) = 0$ near $\operatorname{supp}\chi$.*

Then, in $C^0([-T;T];\mathcal{L}(\mathrm{L}^2_k;\mathrm{L}^2_{k'}))$,

$$\bigl(P(h) - P_\chi(h)\bigr)\bigl(a(\,\cdot\,)\bigr)_h^w = O(h^2)\,, \tag{2.12}$$

$$\text{and, if} \quad m \leq 2\,, \quad \Bigl(\theta\bigl(P(h)\bigr) - \theta\bigl(P_\chi(h)\bigr)\Bigr)\bigl(a(\,\cdot\,)\bigr)_h^w = O(h^2)\,. \tag{2.13}$$

Proof. Let $r, m, k, k' \in \mathbb{R}$. For $a \in \Sigma_{r;m}$ and $f \in \mathcal{S}(\mathbb{R}^d)$, the Schwartz space on $\mathbb{R}^d$,

$$\langle\,\cdot\,\rangle^{k'}\bigl(P(h) - P_\chi(h)\bigr)a_h^w\langle\,\cdot\,\rangle^k f = V(-h^2\Delta+1)^{-1}\cdot(-h^2\Delta+1)\chi\langle\,\cdot\,\rangle^{k'}a_h^w\langle\,\cdot\,\rangle^k f\,,$$

where $V(-h^2\Delta+1)^{-1} \in \mathcal{L}(\mathrm{L}^2;\mathrm{L}^2)$ has norm $O(1/h^2)$ by (2.9). Now, if a is replaced by a continuous map $t \mapsto a(t)$ with $a(t) = 0$ near $\operatorname{supp}\chi$ for all t, then, for all $N \in \mathbb{N}$,

$$(-h^2\Delta+1)\chi\langle\,\cdot\,\rangle^{k'}a(*)_h^w\langle\,\cdot\,\rangle^k = O\bigl(h^N\bigr)$$

in $C^0([-T;T];\mathcal{L}(\mathrm{L}^2;\mathrm{L}^2))$, by the usual h-pseudodifferential calculus. This yields (2.12). On the other hand it is known that, for all $k \in \mathbb{R}$, the resolvents $(P(h)+i)^{-1}$ and $(P_\chi(h)+i)^{-1}$ are bounded from L^2_k to L^2_k (see [44], Sect. XIII.8), and, by (2.9), there exists some $\alpha(k) \geq 0$ such that

$$\bigl\|\bigl(P(h)+i\bigr)^{-1}\bigr\|_{\mathcal{L}(\mathrm{L}^2_k;\mathrm{L}^2_k)} = O\bigl(h^{-\alpha(k)}\bigr)\,, \quad \bigl\|\bigl(P_\chi(h)+i\bigr)^{-1}\bigr\|_{\mathcal{L}(\mathrm{L}^2_k;\mathrm{L}^2_k)} = O\bigl(h^0\bigr)\,.$$

Besides, there is a $\chi_1 \in C^\infty(\mathbb{R}^d)$ with $\chi\chi_1 = 0$, $\chi_1 = 1$ at infinity, and $\chi_1 a(t) = a(t)$ for all t. Hence, for all $N \in \mathbb{N}$, $(1-\chi_1)a(*)_h^w\langle\,\cdot\,\rangle^k = O(h^N)$ in $C^0([-T;T];\mathcal{L}(\mathrm{L}^2;\mathrm{L}^2))$. We may now adapt the arguments in the proof of Lemma 3.1 in [13] to get (2.13). □

2.2. Extension of the flow

Here we explain how the usual flow can be extended when attractive singularities occur (more details are given in [27, 32]).

Let $d = 3$. We still denote by p the smooth function defined by

$$p:\ \hat{P} \longrightarrow \mathbb{R}\,,\quad (x,\xi) \mapsto |\xi|^2 + V(x) \quad \text{where} \quad \hat{P} := T^*\hat{M}\,. \tag{2.14}$$

Let π_x (resp. π_ξ) be the projection $T^*\mathbb{R}^d \longrightarrow \mathbb{R}^d$ defined by $\pi_x(x,\xi) := x$ (resp. $\pi_\xi(x,\xi) := \xi$). As for any smooth dynamical system, the hamiltonian initial value problem,

$$\begin{aligned} &\frac{dX}{dt}(t) = \nabla_\xi p\big(X(t);\Xi(t)\big)\,, \quad \frac{d\Xi}{dt}(t) = -\nabla_x p\big(X(t);\Xi(t)\big)\,,\\ &\big(X(0);\Xi(0)\big) = \mathrm{x}^* = (x,\xi) \in \hat{P} \end{aligned} \tag{2.15}$$

has a unique maximal solution $\phi : \hat{D} \to \hat{P}$ with

$$\hat{D} = \Big\{(t,\mathrm{x}^*) \in \mathbb{R}\times\hat{P}\,;\ t \in\,]T^-(\mathrm{x}^*), T^+(\mathrm{x}^*)[\ \Big\}\,,$$

where the functions $T^\pm : \hat{P} \to \overline{\mathbb{R}}$ satisfy $T^- < 0 < T^+$ and are lower resp. upper semi-continuous with respect to the natural topology on the extended line $\overline{\mathbb{R}} := \{-\infty\} \cup \mathbb{R} \cup \{+\infty\}$. In particular, the set $\hat{D} \subseteq \mathbb{R}\times\hat{P}$ is open.

If no attractive singularity is present (i.e. $N = 0$ in the notation of Paragraph 1.1), then $\hat{D} = \mathbb{R}\times\hat{P}$. Otherwise a maximal solution can fall on an attractive singularity s at finite time $T^+(\mathrm{x}^*) > 0$. Such a time is called a *collision time*. In that case, it turns out that, setting

$$\mathrm{coll}(\mathrm{x}^*) := \begin{cases} \emptyset & \text{if } T^-(\mathrm{x}^*) = -\infty,\ T^+(\mathrm{x}^*) = \infty\\ \{T^+(\mathrm{x}^*)\} & \text{if } T^-(\mathrm{x}^*) = -\infty,\ T^+(\mathrm{x}^*) < \infty\\ \{T^-(\mathrm{x}^*)\} & \text{if } T^-(\mathrm{x}^*) > -\infty,\ T^+(\mathrm{x}^*) = \infty\\ \{T^+(\mathrm{x}^*)\} + \mathbb{Z}\big(T^+(\mathrm{x}^*) - T^-(\mathrm{x}^*)\big) & \text{if } T^-(\mathrm{x}^*) > -\infty,\ T^+(\mathrm{x}^*) < \infty \end{cases}$$

$$\text{and} \quad D := \Big\{(t,\mathrm{x}^*) \in \mathbb{R}\times\hat{P}\,;\ t \notin\ \mathrm{coll}(\mathrm{x}^*)\Big\}\,,$$

the map ϕ can be uniquely extended to a smooth map $D \to \hat{P}$, still denoted by ϕ. Even more, when $T^+(\mathrm{x}^*) < \infty$, *backscattering* occurs, that is, for $0 < t < T^+(\mathrm{x}^*) - T^-(\mathrm{x}^*)$, we have

$$\begin{aligned} \pi_x\phi\big(T^+(\mathrm{x}^*) + t;\mathrm{x}^*\big) &= \pi_x\phi\big(T^+(\mathrm{x}^*) - t;\mathrm{x}^*\big)\,,\\ \pi_\xi\phi\big(T^+(\mathrm{x}^*) + t;\mathrm{x}^*\big) &= -\pi_\xi\phi\big(T^+(\mathrm{x}^*) - t;\mathrm{x}^*\big)\,, \end{aligned} \tag{2.16}$$

and one may set $\pi_x\phi(T^+(\mathrm{x}^*);\mathrm{x}^*) = s$. We mention that the momentum $\pi_\xi\phi(\,\cdot\,;\mathrm{x}^*)$ however blows up at $T^+(\mathrm{x}^*)$, in the following sense:

$$\lim_{t\to T_+(\mathrm{x}^*)} |\pi_\xi\phi(t;\mathrm{x}^*)| = \infty\,,$$

$$\text{while} \quad v := \lim_{t\nearrow T_+(\mathrm{x}^*)} \frac{\pi_\xi\phi(t;\mathrm{x}^*)}{|\pi_\xi\phi(t;\mathrm{x}^*)|} = -\lim_{t\searrow T_+(\mathrm{x}^*)} \frac{\pi_\xi\phi(t;\mathrm{x}^*)}{|\pi_\xi\phi(t;\mathrm{x}^*)|} \quad \text{exists}\,.$$

For any $\mathrm{x}^* \in \hat{P}$, we obtain in this way a configuration trajectory $(\pi_x\phi(t;\mathrm{x}^*))_{t\in\mathbb{R}}$, which has a countable set $\mathrm{coll}(\mathrm{x}^*)$ of collision times t_0 for which

$$\lim_{t\to t_0} \pi_x\phi(t;\mathrm{x}^*) \in \{s_j, 1 \le j \le N\} \quad \text{and} \quad \lim_{t\to t_0} |\pi_\xi\phi(t;\mathrm{x}^*)| = \infty\,. \tag{2.17}$$

Although ϕ is not a complete flow on $\hat{P}$, the *broken trajectory* $(\phi(t;\mathrm{x}^*))_{t\in\mathbb{R}\setminus\mathrm{coll}(\mathrm{x}^*)}$ is a solution of (2.15) on $\mathbb{R}\setminus\mathrm{coll}(\mathrm{x}^*)$. Its values lie in the energy shell $p^{-1}(p(\mathrm{x}^*))$. Note that no collision with the repulsive singularities can occur.

For $t \in \mathbb{R}$, it is convenient to introduce $\phi^t : D_t \to \hat{P}$ defined by

$$D_t := \Big\{ \mathrm{x}^* \in \hat{P}\,;\, t \notin \ \mathrm{coll}(\mathrm{x}^*) \Big\} \quad \text{and} \quad \phi^t(\mathrm{x}^*) := \phi(t;\mathrm{x}^*)\,. \tag{2.18}$$

Note further that the Hamiltonian system $(\hat{P}, \omega_0, p)$ with canonical symplectic form ω_0 can be uniquely extended to a smooth Hamiltonian system with a complete flow (see Section 5).

An important feature to analyse the pseudo-flow ϕ is the Kustaanheimo–Stiefel transformation (KS-transform for short). We briefly describe it here and refer to [13, 27, 32, 49], for further details. For $z = (z_0, z_1, z_2, z_3)^T \in \mathbb{R}^4$, let

$$\Lambda(z) = \begin{pmatrix} z_0 & -z_1 & -z_2 & z_3 \\ z_1 & z_0 & -z_3 & -z_2 \\ z_2 & z_3 & z_0 & z_1 \end{pmatrix}.$$

Let $\mathcal{K} : \mathbb{R}^4 \longrightarrow \mathbb{R}^3$ be defined by

$$\mathcal{K}(z) := \Lambda(z)\cdot z = \begin{pmatrix} z_0^2 - z_1^2 - z_2^2 + z_3^3 \\ 2z_0z_1 - 2z_2z_3 \\ 2z_0z_2 + 2z_1z_3 \end{pmatrix}. \quad \text{For all } z \in \mathbb{R}^4\,, \quad |\mathcal{K}(z)| = |z|^2\,. \tag{2.19}$$

We call it the *Hopf map*. See the appendix for more information.

Let $\mathbb{R}^3_\pm := \{(x_1, x_2, x_3) \in \mathbb{R}^3; \pm x_1 > 0\}$ and $z \in \mathbb{R}^4$. It turns out (see [13]) that, if $x := \mathcal{K}(z) \in \mathbb{R}^3_+$, $\mathcal{A}_+(z) := \sqrt{2}(x_1 + |z|)^{-1/2}(z_0 + iz_3) \in S^1$ and, if $x := \mathcal{K}(z) \in \mathbb{R}^3_-$, $\mathcal{A}_-(z) := \sqrt{2}(-x_1 + |z|)^{-1/2}(z_1 + iz_2) \in S^1$. Furthermore, one can explicitly construct smooth maps $\mathcal{J}_\pm : \mathbb{R}^3_\pm \times S^1 \longrightarrow \mathbb{R}^4$ such that, locally,

$$(\mathcal{K}, \mathcal{A}_\pm) \circ \mathcal{J}_\pm = \mathrm{Id} \quad \text{in} \quad \mathbb{R}^3_\pm \times S^1 \quad \text{and}$$
$$\mathcal{J}_\pm \circ (\mathcal{K}, \mathcal{A}_\pm) = \mathrm{Id} \quad \text{in} \quad \mathcal{J}_\pm(\mathbb{R}^3_\pm \times S^1)\,. \tag{2.20}$$

For $z = \mathcal{J}_\pm(x;\theta)$, for $x \in \mathbb{R}^3_\pm$ and $\theta \in S^1$, we have $dz = C|x|^{-1}dx\,d\theta$ for some constant $C > 0$. In particular, there exists $C' > 0$ such that, for all $f, g : \mathbb{R}^3 \longrightarrow \mathbb{C}$ measurable,

$$\int_{\mathbb{R}^3} |x|^{-1} \cdot |f(x)g(x)|\,dx = C' \int_{\mathbb{R}^4} |f \circ \mathcal{K}(z)\, g \circ \mathcal{K}(z)|\,dz\,. \tag{2.21}$$

It is useful to consider the following extension to phase space. For $\mathrm{z}^* = (z;\zeta) \in T^*\mathbb{R}^4$, we set as usual $\pi_z \mathrm{z}^* = z$ and $\pi_\zeta \mathrm{z}^* = \zeta$. If $(x;\xi) \in T^*(\mathbb{R}^3 \setminus \{0\})$, let $z \in \mathbb{R}^4$ such that $x = \mathcal{K}(z) = \Lambda(z) \cdot z$ (z is not unique). Then, we define

$$\zeta := 2\Lambda(z)^T \xi = 2 \begin{pmatrix} z_0 & z_1 & z_2 \\ -z_1 & z_0 & z_3 \\ -z_2 & -z_3 & z_0 \\ z_3 & -z_2 & z_1 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}, \tag{2.22}$$

which is a solution of the equation $2|x|\xi = \Lambda(z)\zeta$. The *KS-transform* is defined by

$$\mathcal{K}^* : T^*\big(\mathbb{R}^4 \setminus \{0\}\big) \longrightarrow T^*\big(\mathbb{R}^3 \setminus \{0\}\big)\,, \quad \mathcal{K}^*(z;\zeta) = \left(\Lambda(z) \cdot z\,;\, \frac{1}{2|z|^2}\Lambda(z) \cdot \zeta\right). \tag{2.23}$$

Assume that an attractive singularity sits at 0. Recall that, by (1.2), $V(x) = f(x)/|x| + W(x)$ on $\Omega \setminus \{0\}$, where $\Omega := \{x \in \mathbb{R}^3; |x| < r\}$ for some $r > 0$, with $f, W \in C_0^\infty(\mathbb{R}^d;\mathbb{R})$. Let $\tilde{\Omega} := \mathcal{K}^{-1}(\Omega)$. Let $\mathrm{x}_0^* = (x_0;\xi_0) \in \hat{P}$ be such that the first collision of $(\pi_x \phi(t;\mathrm{x}_0^*))_{t\in\mathbb{R}}$ takes place at 0 at time $t_+(\mathrm{x}_0^*) > 0$. Let $\mathcal{T}_0$ be the connected component of $\big\{t \in \mathbb{R};\ \pi_x\phi(t;\mathrm{x}_0^*) \in \Omega\big\}$ containing $t_+(\mathrm{x}_0^*)$. Let $z_0 \in \mathbb{R}^4$ be such that $x_0 = \mathcal{K}(z_0)$ and let ζ_0 be the ζ given by (2.22) with $(z;\xi) = (z_0;\xi_0)$. For $\mathrm{t}^* = (t;\tau) \in T^*\mathbb{R}$, $\mathrm{z}^* = (z;\zeta) \in T^*\mathbb{R}^4$, let $\tilde{p}(\mathrm{t}^*;\mathrm{z}^*) := |\zeta|^2 + f \circ \mathcal{K}(z) + |z|^2(W \circ \mathcal{K}(z) - \tau)$. Since $\tilde{p}$ is smooth on $T^*\mathbb{R} \times T^*\mathbb{R}^4 = T^*(\mathbb{R}_t \times \mathbb{R}^4_z)$, independent of t, and since its Hamilton vector field at point $(t,\tau;z,\zeta)$ is given by $(-|z|^2, 0; 2\zeta, 2\tau z)$ outside a compact region in (z,ζ), there exists a unique maximal solution $\mathbb{R} \ni s \mapsto \big(t(s);\tau(s);z(s);\zeta(s)\big) = (\mathrm{t}^*(s);\mathrm{z}^*(s))$ to the Hamilton equations associated with $\tilde{p}$

$$\begin{pmatrix} (dz/ds)(s) &=& \nabla_\zeta \tilde{p}\,(\mathrm{t}^*(s);\mathrm{z}^*(s)) & \quad (d\zeta/ds)(s) &=& -\nabla_z \tilde{p}\,(\mathrm{t}^*(s);\mathrm{z}^*(s)) \\ (dt/ds)(s) &=& \nabla_\tau \tilde{p}\,(\mathrm{t}^*(s);\mathrm{z}^*(s)) & \quad (d\tau/ds)(s) &=& -\nabla_t \tilde{p}\,(\mathrm{t}^*(s);\mathrm{z}^*(s)) \end{pmatrix}, \tag{2.24}$$

with initial condition $(\mathrm{t}^*(0);\mathrm{z}^*(0)) = (\mathrm{t}_1^*;\mathrm{z}_1^*)$. We denote it by

$$\begin{aligned} \tilde{\phi}(s;\mathrm{t}_1^*;\mathrm{z}_1^*) &:= \big(\mathrm{t}^*(s;\mathrm{t}_1^*;\mathrm{z}_1^*);\mathrm{z}^*(s;\mathrm{t}_1^*;\mathrm{z}_1^*)\big) \\ &= \big(t(s;\mathrm{t}_1^*;\mathrm{z}_1^*);\tau(s;\mathrm{t}_1^*;\mathrm{z}_1^*);z(s;\mathrm{t}_1^*;\mathrm{z}_1^*);\zeta(s;\mathrm{t}_1^*;\mathrm{z}_1^*)\big)\,. \end{aligned}$$

Let $(\mathrm{t}_0^*;\mathrm{z}_0^*) = (0;p(\mathrm{x}_0^*);z_0;\zeta_0)$. It turns out that, for all $t_1 \in \mathcal{T}_0$, there exists a unique $s \in \mathbb{R}$ such that $t_1 = t(s;\mathrm{t}_0^*;\mathrm{z}_0^*)$. Furthermore, if $t_1 \neq t_+(\mathrm{x}_0^*)$, $z(s;\mathrm{t}_0^*;\mathrm{z}_0^*) \neq 0$ and

$$\phi(t_1;\mathrm{x}_0^*) = \phi\big(t(s;\mathrm{t}_0^*;\mathrm{z}_0^*);\mathrm{x}_0^*\big) = \mathcal{K}^*\big(\mathrm{z}^*(s;\mathrm{t}_0^*;\mathrm{z}_0^*)\big)\,. \tag{2.25}$$

3. Towards the non-trapping condition

The aim of this section is to prove the implication "2 $\Longrightarrow$ 1" of Theorem 1.1. We thus assume that 2 holds true and we want to show that p is non-trapping at energy λ, for all $\lambda \in I_0$. Let λ_0 be such an energy. We can find a compact interval $I \subset I_0$ such that λ_0 belongs to the interior of I. By assumption, (1.11) holds true for I. This implies, by (1.7), that (1.8) holds true for $\mathrm{S} = \mathrm{L}^2_s$, for any $s > 1/2$. As in [25], we follow the strategy in [52]. We translate the bound on the resolvent into a bound on a time integral of the associated propagator

$$U(t;h) := \exp\big(-ih^{-1}tP(h)\big)\,. \tag{3.1}$$

If an attractive singularity is present (and $d = 3$), we need some information on the time-dependent microlocalization of $U(t;h)u_h$, for some family $(u_h)_h$ of $\mathrm{L}^2(\mathbb{R}^3)$ functions. Most of it is already available in [13]. We also need some well-known facts on the classical flow, which we borrow from [32]. In Subsection 3.1, we shall recall results from [13, 32] and extend them a little bit. Then we proceed with the announced proof in Subsection 3.2. In the repulsive case ($N = 0$ and $d \geq 3$), we show in Subsection 3.3 that Wang's proof may be carried over with minor changes.

3.1. Coherent states evolution

In this subsection we are interested in the case where an attractive singularity occurs (i.e. $N > 0$) but the results hold true for $N = 0$. Better results in the latter case are given in Subsection 3.3. Proposition 3.6 is the main result of the subsection.

Before considering the time evolution of coherent states, we recall some basic facts on the classical dynamics, in particular on the dilation function

$$a_0 : T^*\mathbb{R}^d \longrightarrow \mathbb{R}\,, \quad a_0(x,\xi) := x\cdot\xi\,.$$

Lemma 3.1. *Consider a dimension $d \geq 2$ and energies $\lambda > 0$.*

1. *Then for some $R_1 = R_1(\lambda) \geq R_0$ and all $\mathrm{x}_0^* := (x_0,\xi_0) \in p^{-1}(]\lambda/2;\infty[)$*

$$|x_0| \geq R_1 \implies \{p, a_0\}(\mathrm{x}_0^*) \geq \lambda/2\ , \quad \textit{and} \tag{3.2}$$

$$\liminf_{t\to\pm\infty} |\pi_x\phi(t;\mathrm{x}_0^*)| > R_1 \implies \lim_{t\to\pm\infty} |\pi_x\phi(t;\mathrm{x}_0^*)| = +\infty\,. \tag{3.3}$$

2. *For any $T, R > 0$, there is some $R_2 > R_1$ such that, for all $\mathrm{x}_0^* = (x_0,\xi_0) \in p^{-1}(]\lambda/2;2\lambda[)$*

$$\big(|x_0| > R_2\big) \implies \big(|\pi_x\phi(t;\mathrm{x}_0^*)| > R \textit{ for all } t \in [-T;T]\big)\,. \tag{3.4}$$

Proof. We shortly recall the standard arguments. Thanks to the decay properties (1.1) of V,

$$\{p, a_0\}(\mathrm{x}_0^*) = 2\big(p(\mathrm{x}_0^*) - V(x_0)\big) - \big\langle x_0, \nabla V(x_0)\big\rangle \geq \lambda/2$$

for large $|x_0|$, implying (3.2). As the dilation function a_0 is the time derivative of the phase space function $|x|^2/2$, composed with ϕ, the second time derivative of the latter function is eventually bounded below by $\lambda/2 > 0$, if the l.h.s. of (3.3) is satisfied. Thus $t \mapsto |\pi_x \phi(t; \mathrm{x}_0^*)|^2$ goes to infinity, showing (3.3). Let $V_0 = \inf_{|x|\geq R_0} V(x)$. Relation (3.4) follows, since the speed is bounded by $|\xi_0| \leq (4\lambda - 2V_0)^{1/2} < \infty$. □

For $h \in]0; h_*]$ the *dilation operator* E_h on $\mathrm{L}^2(\mathbb{R}^d)$, given by $E_h(f)(x) := h^{-d/4} f(h^{-1/2}x)$, is unitary, as are the *Weyl operators*

$$w(\mathrm{x}_0^*; h) := \exp\bigl(ih^{-1/2}(x_0 \cdot x - \xi_0 \cdot D_x)\bigr) \quad \text{for} \quad \mathrm{x}_0^* := (x_0, \xi_0) \in T^*\mathbb{R}^d\,,$$

(cf. [21], p. 151, [11]). The *coherent states operators*, microlocalized at x_0^*, are

$$c(\mathrm{x}_0^*; h) := E_h \cdot w(\mathrm{x}_0^*; h)\,. \tag{3.5}$$

A direct computation gives that

$$E_h^* a_h^w E_h = \bigl(a(h^{1/2}\star; h^{-1/2}\star)\bigr)_1^w\,,$$
$$c(\mathrm{x}_0^*; h)^* a_h^w c(\mathrm{x}_0^*; h) = \bigl(a(x_0 + h^{1/2}\star; \xi_0 + h^{-1/2}\star)\bigr)_1^w\,,$$

where $b(\star;\star)$ denotes the symbol $(x;\xi) \mapsto b(x;\xi)$. It is known (cf. [51]) that

$$\forall a \in \Sigma_{0,0}\,, \quad \forall f \in \mathcal{S}(\mathbb{R}^d)\,, \quad c(\mathrm{x}_0^*; h)^* a_h^w c(\mathrm{x}_0^*; h) f = a(\mathrm{x}_0^*) f + O(h)\,, \tag{3.6}$$

where $\mathcal{S}(\mathbb{R}^d)$ denotes the Schwartz space on $\mathbb{R}^d$. Let u_h be the function given by

$$u_h := c(\mathrm{x}_0^*; h)\, \pi^{-d/4} \exp\bigl(-|\cdot|^2/2\bigr)\,. \tag{3.7}$$

Then $(u_h)_h$ is a family of $\mathrm{L}^2(\mathbb{R}^d)$-normalized coherent states microlocalized at x_0^*. We collect properties of the family $(U(\,\cdot\,; h)u_h)_h$ of the propagated states.

In the remainder part of Subsection 3.1 we consider initial conditions in phase space

$$\mathrm{x}_0^* := (x_0, \xi_0) \in \hat{P} \quad \text{with energy} \quad \lambda := p(\mathrm{x}_0^*) > 0$$

and the associated coherent states $(u_h)_h$ microlocalized at x_0^*.

In [13] the following *energy localization* of $(u_h)_h$ is obtained. We give a short proof using Lemma 2.3.

Lemma 3.2 ([13]). *Let $d \geq 3$ and $\theta \in C_0^\infty(\mathbb{R})$ such that $\theta = 1$ near λ. Then, in $\mathrm{L}^2(\mathbb{R}^d)$, $(1 - \theta(P(h)))u_h = O(h)$.*

Proof. Let $\chi, \tilde{\chi} \in C_0^\infty(\mathbb{R}^d)$ with $\chi, \tilde{\chi} = 1$ near $\mathcal{S}$, $\chi, \tilde{\chi} = 0$ near $x_0 = \pi_x \mathrm{x}_0^*$, and $\chi\tilde{\chi} = \chi$. From (3.7), we see that $\tilde{\chi} u_h = O(h)$ in $\mathrm{L}^2(\mathbb{R}^d)$. By Lemma 2.3,

$$\Bigl(1-\theta\bigl(P(h)\bigr)\Bigr)u_h = \Bigl(1-\theta\bigl(P(h)\bigr)\Bigr)(1-\tilde{\chi})u_h + O(h) = \Bigl(1-\theta\bigl(P_\chi(h)\bigr)\Bigr)(1-\tilde{\chi})u_h + O(h)\,,$$

in $\mathrm{L}^2(\mathbb{R}^d)$, where $P_\chi(h)$ is as in (2.10). Besides, thanks to (3.6) and using (2.11),

$$\begin{aligned}\Bigl(1-\theta\bigl(P(h)\bigr)\Bigr)u_h &= \Bigl(1-\theta\bigl(P_\chi(h)\bigr)\Bigr)u_h + O(h) = \Bigl(1-\theta\bigl(p_\chi(\mathrm{x}_0^*)\bigr)\Bigr)u_h + O(h)\\ &= 0 + O(h)\,.\end{aligned}$$

□

From [13] we pick the following *localization away from singularities*.

Lemma 3.3 ([13]). *Let $d = 3$. Let K be a compact subset of $\mathbb{R}$ such that $K \cap \mathrm{coll}(\mathrm{x}_0^*) = \emptyset$ (cf. (2.17)). If $\sigma \in C_0^\infty(\mathbb{R}^3)$ has small enough a support near the set $\mathcal{S}$ of singularities, then $K \ni t \mapsto \sigma U(t;h)u_h$ is of order $O(h)$ in $C^0(K;\mathrm{L}^2(\mathbb{R}^3))$.*

Proof. See the proof of Theorem 1, p. 25 in [13]. □

A careful inspection of the result in [13] on the frequency set shows that even after a collision, we have the following *localization along our broken trajectories*.

Lemma 3.4. *Let $d = 3$. Let K be a compact subset of $\mathbb{R}$ such that $K \cap \mathrm{coll}(\mathrm{x}_0^*) = \emptyset$ (cf. (2.17)). Let $\epsilon > 0$ and $K \ni t \mapsto a(t;*) \in C_0^\infty(\hat{P})$ be continuous functions such that $a(t;x,\xi) = 0$ if $|x - \pi_x\phi(t;\mathrm{x}_0^*)| \le \epsilon$. Then $(a(\,\cdot\,;*))_h^w U(\,\cdot\,;h)u_h = O(h)$ in $C^0(K;\mathrm{L}^2(\mathbb{R}^3))$.*

Proof. See the proof of Theorem 1, p. 25 in [13]. □

We also need to complete Lemma 3.4 with a *bound* on $(U(\,\cdot\,;h)u_h)_h$ *near infinity in position space* and, since the singularities are far away, we can assume $d \ge 3$. This is the purpose of the following

Lemma 3.5. *Let $d \ge 3$. Let $T > 0$ and $R := \max(R_0; 1 + |x_0|\}$. Let $R_2 > R_1$ large enough such that (3.4) holds true. Let $R_3 > R_2 + 1$ and $\kappa \in C^\infty(\mathbb{R}^d;\mathbb{R})$ such that $\mathrm{supp}\,\kappa \subset \{y \in \mathbb{R}^d;\ |y| > R_2 + 1\}$ and $\kappa = 1$ on $\{y \in \mathbb{R}^d;\ |y| > R_3\}$. Then*

$$\kappa U(\,\cdot\,;h)u_h = O(h) \quad in \quad C^0\big([-T;T];\mathrm{L}^2(\mathbb{R}^3)\big)\,.$$

Proof. The proof is based on an Egorov type estimate which is valid although $P(h)$ is not a pseudodifferential operator.

• Let $\tau \in C_0^\infty(\mathbb{R}^d)$ such that $\tau = 1$ on $\{y \in \mathbb{R}^d; |y| \le R_0\}$ and $\tau = 0$ near the set

$$\pi_x \bigcup_{t\in[-T;T]} \Big(p^{-1}\big(]\lambda/2;2\lambda[\big) \cap \phi^t\Big(\big\{(x,\xi);\ |x| > R_2\big\}\Big)\Big)\,.$$

This is well-defined by (2.18), (3.4), and the choice of R. Let p_τ be defined as in (2.11). Let $\theta \in C_0^\infty(\mathbb{R})$ with $\mathrm{supp}\,\theta \subset]\lambda/2;2\lambda[$ such that $\theta = 1$ near λ. Set

$$a : T^*\mathbb{R}^d \longrightarrow \mathbb{C}\,, \quad a(x,\xi) = \kappa(x)\,\theta\big(p_\tau(x,\xi)\big)\,. \tag{3.8}$$

Thanks to (3.4), $[-T;T] \ni t \mapsto a \circ \phi^t$ is a $\Sigma_{0;0}$-valued, C^1-function. Therefore, by Calderón–Vaillancourt $(a \circ \phi^t)_h^w$ is h-uniformly bounded, and for $t \in [-T;T]$, strongly in $\mathrm{H}^2(\mathbb{R}^d)$,

$$\begin{aligned}
&U(t;h)^* a_h^w U(t;h) - \big(a \circ \phi^t\big)_h^w \qquad (3.9)\\
&\quad = \int_0^t \frac{d}{ds}\big(U(s;h)^*(a\circ\phi^{t-s})_h^w U(s;h)\big)\,ds\\
&\quad = \int_0^t U(s;h)^* \ \left(\frac{i}{h}\big[P(h),(a\circ\phi^{t-s})_h^w\big] + \big((d/ds)a\circ\phi^{t-s}\big)_h^w\right)\ U(s;h)\,ds\,.
\end{aligned}$$

The support properties of a and the choice of τ ensure that, for all $r \in [-T;T]$, $(d/dr)a \circ \phi^r = \{p, a \circ \phi^r\} = \{p_\tau, a \circ \phi^r\}$. Thus, (3.9) equals

$$\int_0^t U(s;h)^* \left(\frac{i}{h}\big[P(h), (a\circ\phi^{t-s})_h^w\big] - \big(\{p_\tau, a\circ\phi^{t-s}\}\big)_h^w \right) U(s;h)\, ds\,.$$

By Lemma 2.3, (3.9) equals

$$\int_0^t U(s;h)^* \left(\frac{i}{h}\big[P_\tau(h), (a\circ\phi^{t-s})_h^w\big] - \big(\{p_\tau, a\circ\phi^{t-s}\}\big)_h^w \right) U(s;h)\, ds + hB_h(t)$$

where $[-T;T] \ni t \mapsto B_h(t) \in \mathcal{L}(\mathrm{L}^2(\mathbb{R}^d))$ is bounded, uniformly with respect to h. By the usual pseudodifferential calculus,

$$[-T;T] \ni r \;\mapsto\; \frac{i}{h}\big[P_\tau(h), (a\circ\phi^r)_h^w\big] - \big(\{p_\tau, a\circ\phi^r\}\big)_h^w \in \mathcal{L}\big(\mathrm{L}^2(\mathbb{R}^d)\big)$$

is $O(h)$ in $C^0\big([-T;T]; \mathcal{L}(\mathrm{L}^2(\mathbb{R}^d))\big)$. Thus, so is (3.9).

• Since $a \circ \phi^t$ vanishes near x_0, for $t \in [-T;T]$, $t \mapsto (a\circ\phi^t)_h^w u_h$ is $O(h)$ in $C^0\big([-T;T]; L^2\big)$, by (3.6). Thus so is $U(\,\cdot\,;h)\,(a\circ\phi^t)_h^w\, u_h$.

• Using the previous points, the Lemmata 3.2 and 2.3, the fact that $\theta(P(h))$ and $U(t,h)$ commute, and the usual pseudodifferential calculus,

$$\begin{aligned}\kappa U(t;h)u_h &= \kappa U(t;h)\theta\big(P(h)\big)u_h + O(h) = \kappa\theta\big(P(h)\big)U(t;h)u_h + O(h)\\ &= \kappa\theta\big(P_\tau(h)\big)U(t;h)u_h + O(h) = \big(\kappa\theta(p_\tau)\big)_h^w U(t;h)u_h + O(h)\\ &= U(t;h)\,\big(\kappa\theta(p_\tau)\circ\phi^t\big)_h^w u_h + O(h) = O(h)\,. \end{aligned} \tag{3.10}$$

□

From these lemmata, we can deduce the following information on the time evolution of the coherent states u_h.

Proposition 3.6. *Let $N > 0$ and $d = 3$. Let K be a compact subset of $\mathbb{R}$ such that $K \cap \mathrm{coll}(\mathrm{x}_0^*) = \emptyset$ (cf. (2.17)). Let $\tau \in C_0^\infty(\mathbb{R}^3)$ with $\tau = 1$ near 0. For $t \in \mathbb{R}$ and $x \in \mathbb{R}^3$, set $\tau_t(x) := \tau(x - \pi_x\phi(t;\mathrm{x}_0^*))$. Take the support of τ small enough such that, for all $t \in K$, $\mathrm{supp}\,(\tau_t) \cap \mathcal{S} = \emptyset$. Then, for any $a \in \Sigma_{0;0}$ and any $t \in K$,*

$$a_h^w\, U(t;h)u_h = (\tau_t a)_h^w\, U(t;h)u_h + e(t)\,,$$

where $K \ni t \mapsto e(t)$ is $O(h)$ in $C^0(K; \mathrm{L}^2(\mathbb{R}^d))$.

Proof. Let $T > 0$ such that $K \subset [-T;T]$. Let $\kappa_0, \kappa_1 \in C^\infty(\mathbb{R}^3;\mathbb{R})$ such that $\kappa_0 + \kappa_1 = 1$ and $\kappa := \kappa_1$ satisfies the assumptions of Lemma 3.5. Then, by Lemma 3.5,

$$a_h^w\, U(t;h)u_h = a_h^w\, \kappa_0\, U(t;h)u_h + O(h)\,,$$

in $C^0(K) := C^0(K; \mathrm{L}^2(\mathbb{R}^d))$. Now let $\sigma_0 \in C_0^\infty(\mathbb{R}^3;\mathbb{R})$ such that $\sigma_0 = 1$ near s_j for any $1 \le j \le N'$, and, for all $t \in K$, $\mathrm{supp}\,\sigma_0 \cap \mathrm{supp}\,\tau_t = \emptyset$. Upon possibly decreasing the support of σ_0, we may apply Lemma 3.3. This yields

$$a_h^w\, U(t;h)u_h = a_h^w\, \kappa_0\,(1-\sigma_0)\, U(t;h)u_h + O(h)\,,$$

in $C^0(K)$. Let $\sigma \in C_0^\infty(\mathbb{R}^3;\mathbb{R})$ such that $\sigma = 1$ near each singularity s_j and $\sigma\sigma_0 = \sigma$. For an energy cutoff θ as in Lemma 3.2, we obtain, as in the proof of Lemma 3.5 (see (3.10)),

$$a_h^w\,\kappa_0\,(1-\sigma_0)\,U(t;h)u_h = a_h^w\,\kappa_0\,(1-\sigma_0)\,\theta\big(P_\sigma(h)\big)\,U(t;h)u_h + O(h)\,,$$

in $C^0(K)$, since $1-\sigma_0$ is localized away from the singularities. By pseudodifferential calculus,

$$a_h^w\,U(t;h)u_h = b_h^w\,U(t;h)u_h + O(h)\,,$$

in $C^0(K)$, where $b := \theta(p_\sigma)\,(1-\sigma_0)\,\kappa_0\,a \in C_0^\infty(\hat{P})$. Applying Lemma 3.4 to $a(t) = (1-\tau_t)b$,

$$a_h^w\,U(t;h)u_h = (\tau_t b)_h^w U(t;h)u_h + O(h) = \big((1-\sigma_0)\,\kappa_0\,\tau_t a\big)_h^w U(t;h)u_h + O(h)\,,$$

in $C^0(K)$. Since $\tau_t\,(1-\sigma_0)\,\kappa_0 = \tau_t$, for all $t \in K$, we obtain the desired result. □

3.2. Necessity of the non-trapping condition

Assuming $N > 0$ and $d = 3$, we want to show that (1.11) implies the non-trapping condition, yielding the proof of "$2 \Longrightarrow 1$". The proof below actually works if $N = 0$, but a more straightforward and easier proof is provided in Subsection 3.3.

In view of (1.7), we assume (1.8) for $\mathrm{S} = \mathrm{L}_s^2$ with $s > 1/2$. This means that, for any $\theta \in C_0^\infty(I_0;\mathbb{R})$, $\langle\cdot\rangle^{-s}\theta(P(h))$ is Kato smooth with respect to $P(h)$ (by Theorem XIII.30 in [44]). This can be formulated in the following way (cf. Theorem XIII.25 in [44]). There exists $C_s > 0$ such that for any $\theta \in C_0^\infty(I_0;\mathbb{R})$,

$$\forall u \in \mathrm{L}^2(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}} \big\|\langle\cdot\rangle^{-s}\,U(t;h)\,\theta\big(P(h)\big)u\big\|^2\,dt \le C_s \cdot \|u\|^2\,. \tag{3.11}$$

uniformly in $h \in]0;h_*]$. Take $\lambda \in I_0$ and a function $\theta \in C_0^\infty(I_0;\mathbb{R})$ such that $\theta = 1$ near λ. Let $\mathrm{x}_0^* := (x_0,\xi_0) \in p^{-1}(\lambda)$ and consider the coherent states u_h given by (3.7). Let $(t_j)_{j\in J}$, with $J \subset \mathbb{N}^*$, be the set of collision times of the broken trajectory $(\phi(t;\mathrm{x}_0^*))_{t\in\mathbb{R}}$ (cf. (2.17)). Eq. (3.11) implies that, for all $T > 0$ and all $h \in]0;h_*]$,

$$\int_{[-T;T]} \big\|\langle\cdot\rangle^{-s}\,U(t;h)\,\theta\big(P(h)\big)u_h\big\|^2\,dt \le C_s\,.$$

We know from Subsection 2.2 that the collision times in $\mathrm{coll}(\mathrm{x}_0^*)$ have positive minimal distance $T^+(\mathrm{x}_0^*) - T^-(\mathrm{x}_0^*)$. Thus we can choose $\epsilon > 0$ smaller than one fourth of that distance, and define for $T > 0$ the compact sets

$$K(T) := \Big\{t \in [-T,T];\, \mathrm{dist}\big(t,\mathrm{coll}(\mathrm{x}_0^*)\big) \ge \epsilon\Big\}\,.$$

Notice that the length of $K(T)$ goes to infinity when $T \to \infty$, while

$$\int_{K(T)} \big\|\langle\cdot\rangle^{-s}\,U(t;h)\,\theta\big(P(h)\big)u_h\big\|^2\,dt \le C_s\,.$$

By energy localization of the coherent state (Lemma 3.2) and Pythagoras' theorem,

$$\int_{K(T)} \|\langle\cdot\rangle^{-s}\,U(t;h)\,u_h\|^2\,dt + O_T(h) \le 2C_s\,, \tag{3.12}$$

where $O_T(h)$ is a T-dependent $O(h)$. We apply Proposition 3.6 for the bounded symbol $(x,\xi) \mapsto a(x,\xi) = \langle x\rangle^{-s}$ and the compact $K(T)$ introduced above. This yields

$$\int_{K(T)} \|\tau_t \langle\,\cdot\,\rangle^{-s}\, U(t;h)\, u_h\|^2\, dt + O_T(h) \le 2C_s\,.$$

We can require that the support of the function τ is so small that, for all $t \in K(T)$, $\operatorname{supp}(\tau_t) \cap \mathcal{S} = \emptyset$ and $\tau_t^2 \langle\,\cdot\,\rangle^{-2s} \ge (1/2)\tau_t^2 \langle \pi_x\phi(t;\mathrm{x}_0^*)\rangle^{-2s}$. Therefore,

$$\int_{K(T)} \big\langle \pi_x\phi(t;\mathrm{x}_0^*)\big\rangle^{-2s} \big\langle U(t;h)u_h\,,\, \tau_t^2 U(t;h)u_h\big\rangle\, dt + O_T(h) \le 4C_s\,.$$

Now, we apply Proposition 3.6 again for the bounded symbol $(x,\xi) \mapsto a(x,\xi) = 1$, yielding

$$\int_{K(T)} \big\langle \pi_x\phi(t;\mathrm{x}_0^*)\big\rangle^{-2s} dt + O_T(h) \le 4C_s\,, \tag{3.13}$$

since the u_h are normalized. Letting h tend to 0, we obtain, for all $T > 0$,

$$\int_{K(T)} \big\langle \pi_x\phi(t;\mathrm{x}_0^*)\big\rangle^{-2s} dt \le 4C_s\,. \tag{3.14}$$

Assume semi-boundedness of the trajectory, that is, for some $t_0 \in \mathbb{R}$,

$$\big\{\pi_x\phi(t;\mathrm{x}_0^*)\,,\, \pm t \ge t_0\big\} \;\subset\; \{y \in \mathbb{R}^3; |y| \le R_1\}\,, \tag{3.15}$$

then, by (3.14), $4C_s$ is larger than R_1^{-2s} times the length of

$$K(T) \setminus \{t \in \mathbb{R}; \pm t < t_0\} = [-T;T] \setminus \Big\{t \in \mathbb{R}; \pm t < t_0 \text{ and } \operatorname{dist}\big(t, \operatorname{coll}(\mathrm{x}_0^*)\big) < \epsilon\Big\}\,.$$

This is a contradiction since the latter tends to ∞ as $T \to \infty$. Thus (3.15) is false and we can apply (3.3), yielding the non-trapping condition (1.10).

3.3. The repulsive case

Here we consider the case where any singularity is repulsive (i.e. $N = 0$) and $d \ge 3$. We want to show that (1.11) implies the non-trapping condition. Thanks to Proposition 3.7 below, we show that Wang's proof can be followed in the present case, yielding a much simpler proof than the one in Subsection 3.2.

First of all, we show that an important ingredient in Wang's proof is available, namely the following weak version of Egorov's theorem.

Proposition 3.7. *Let $N = 0$ and $d \ge 3$. Let $T > 0$ and $a \in \Sigma_{0;0}$. Let $\theta, \gamma \in C_0^\infty(\mathbb{R})$ such that $\gamma\theta = \theta$. Then $[-T;T] \ni t \mapsto \gamma(p)(a \circ \phi^t)$ is a $\Sigma_{0;0}$-valued, C^1-function. Furthermore, there exists $C > 0$, depending on θ and a, such that, for any $\epsilon > 0$, for any $t \in [-T;T]$,*

$$U(t;h)^* a_h^w U(t;h)\theta\big(P(h)\big) = \Big(\big(\gamma(p)(a \circ \phi^t)\big)_h^w + r(t)\Big)\theta\big(P(h)\big)\,,$$

where $[-T;T] \ni t \mapsto r(t)$ is bounded by $C\epsilon + O_{\epsilon,T}(h)$ in $C^0\big([-T;T]; \mathcal{L}(\mathrm{L}^2(\mathbb{R}^d))\big)$.

Proof. Let $\epsilon > 0$. Since the singularities are repulsive, there exists some $\sigma_0 \in C_0^\infty(\mathbb{R}^d, [0,1])$ which equals 1 near each singularity, such that, $\epsilon^2 V \geq 1$ on the support of σ_0 and $(\sigma_0 \circ \pi_x)(\gamma \circ p) = 0$. Thus, for $g \in \mathrm{L}^2(\mathbb{R}^d)$ and $f = \theta(P(h))U(t;h)g$,

$$\begin{aligned}\|\sigma_0 f\|^2 &\leq \langle f\,,\, \sigma_0^2 \epsilon^2 V f\rangle + \epsilon^2 \langle \sigma_0 f\,,\, -h^2\Delta\, \sigma_0 f\rangle \\ &\leq \epsilon^2 \big\langle \sigma_0^2 f\,,\, P(h) f\big\rangle + \epsilon^2 \big\langle \sigma_0 f\,,\, [-h^2\Delta, \sigma_0] f\big\rangle \\ &\leq C_\theta^2 \epsilon^2 \|f\|^2 + \epsilon^2 \big\langle \sigma_0 f\,,\, [-h^2\Delta, \sigma_0] f\big\rangle\,,\end{aligned}$$

where C_θ depends only on θ. Since $[-h^2\Delta, \sigma_0]\theta(P(h)) = O_\epsilon(h)$ in $\mathcal{L}(\mathrm{L}^2(\mathbb{R}^d))$,

$$\big\|\sigma_0 \theta\big(P(h)\big) U(t;h)\big\| \leq C_\theta \epsilon + O_\epsilon(h) \tag{3.16}$$

in $C^0\big([-T;T]; \mathcal{L}(\mathrm{L}^2(\mathbb{R}^d))\big)$. Let $\sigma \in C_0^\infty(\mathbb{R}^d)$ with $\sigma = 1$ near each singularity such that $\sigma\sigma_0 = \sigma$. Using (3.16), Lemma 2.3, and pseudodifferential calculus,

$$\begin{aligned}U(t;h)^* a_h^w U(t;h)\theta\big(P(h)\big) &= U(t;h)^* \big(a(1-\sigma_0)\big)_h^w \gamma\big(P_\sigma(h)\big)\; U(t;h)\theta\big(P(h)\big) + r_1(t) \\ &= U(t;h)^* \big(a(1-\sigma_0)\gamma(p)\big)_h^w\, U(t;h)\theta\big(P(h)\big) + r_2(t)\,,\end{aligned}$$

where the r_j are bounded by $C\epsilon + O_\epsilon(h)$ in $C^0\big([-T;T]; \mathcal{L}(\mathrm{L}^2(\mathbb{R}^d))\big)$. By the choice of σ_0, $a(1-\sigma_0)\gamma(p) = a\gamma(p) =: a_\gamma$. Furthermore, for all $t \in [-T;T]$, $a_\gamma \circ \phi^t = \gamma(p)(a \circ \phi^t)$ and $(d/dt) a_\gamma \circ \phi^t = \{p, a_\gamma \circ \phi^t\} = \{p_\sigma, a_\gamma \circ \phi^t\}$. This allows us to follow the arguments in the proof of Lemma 3.5 showing that (3.9) with $a = a_\gamma$ is $O_{\epsilon,T}(h)$ in $C^0\big([-T;T]; \mathcal{L}(\mathrm{L}^2(\mathbb{R}^d))\big)$. □

Let $\lambda \in I_0$. As in Subsection 3.2, (1.11) implies the existence of some constant $C_s > 0$ such that (3.11) holds true, for $\theta \in C_0^\infty(I_0;\mathbb{R})$ with $\theta(\lambda) = 1$. Since no collision occurs, we choose $K(T) = [-T;T]$, take $a : (x,\xi) \mapsto \langle x\rangle^{-2s}$, and write (3.12) as

$$\int_{[-T;T]} \big\langle U(t;h)u_h\,,\, a_h^w U(t;h)u_h\big\rangle\, dt + O_T(h) \leq 2C_s\,. \tag{3.17}$$

By Lemma 3.2, Proposition 3.7 with $\epsilon = C_s$, and (3.6),

$$\big\langle U(t;h)u_h, a_h^w U(t;h)u_h\big\rangle = \Big\langle u_h, \big(\gamma(p)(a\circ\phi^t)\big)_h^w u_h\Big\rangle + b_1(t) = \big\langle \pi_x \phi(t;\mathrm{x}_0^*)\big\rangle^{-2s} + b_2(t)$$

where the b_j are bounded by $CC_s + O(h)$ in $C^0([-T,T])$. This yields (3.13), with bound $4C_s$ replaced by $(2+C)C_s$, and the non-trapping condition as in Subsection 3.2.

4. Semiclassical trapping

This section is devoted to the proof of the implication "1 $\Longrightarrow$ 2" of Theorem 1.1. We assume the non-trapping condition true on I_0 and we want to prove the bound (1.11), for any compact interval $I \subset I_0$. Here we follow the strategy in [5,24]. We assume that the bound (1.11) is false, for some I. This means precisely that the following situation occurs, which we call "semiclassical trapping". There exist a sequence $(f_n)_n$ of nonzero functions of $\mathrm{H}^2(\mathbb{R}^d)$, a sequence $(h_n)_n \in]0;h_0]^{\mathbb{N}}$ tending to zero, and a sequence $(z_n)_n \in \mathbb{C}^{\mathbb{N}}$ with $\Re(z_n) \to \lambda \in I$ and $\Im(z_n)/h_n \to r \geq 0$, such that

$$\|f_n\|_{\mathrm{B}^*} = 1 \quad \text{and} \quad \big\|\big(P(h_n) - z_n\big) f_n\big\|_{\mathrm{B}} = o(h_n)\,. \tag{4.1}$$

As in [6], we shall see that "the $(f_n)_n$ has no B^*-mass at infinity" (see Proposition 4.2 below). This yields the existence of some large $R_1' > 0$, of a sequence $(g_n)_n$ of nonzero functions of $\mathrm{H}^2(\mathbb{R}^d)$, of a sequence $(h_n)_n \in]0; h_0]^{\mathbb{N}}$ tending to zero, and of a sequence $(\lambda_n)_n \in \mathbb{R}^{\mathbb{N}}$ with $\lambda_n \to \lambda \in I$, such that

$$\operatorname{supp} g_n \subset \{x \in \mathbb{R}^3; |x| \leq R_1'\}\,, \quad \|g_n\| = 1\,, \quad \text{and}$$
$$\big\|\big(P(h_n) - \lambda_n\big) g_n\big\| = o(h_n)\,. \tag{4.2}$$

Possibly after extraction of a subsequence, we may assume that the sequence $(g_n)_n$ has a unique semi-classical measure μ, satisfying (2.5) with u_n replaced by g_n (see Lemma 4.3).

Now, we look for a contradiction with the non-trapping condition. While, in the regular case, it is quite easy to show the invariance of μ under the flow generated by p, this is not clear in the present situation. We shall show the invariance for repulsive singularities in Subsection 4.2. In Subsection 4.3 however, we only show a weaker form of invariance, if there is an attractive singularity. This Subsection 4.3 contains the main novelty of the paper.

The other steps of the strategy are essentially the same as in [24], as explained in Subsection 4.1. If the reader is only interested in the bound (1.11) with B replaced by some L^2_s ($s > 1/2$), we propose a simpler proof in Subsection 4.4.

4.1. Main lines of the proof

In this subsection, we give the main steps leading to the contradiction between the "semiclassical trapping" and the non-trapping condition. Here we focus on the steps which are essentially proved as in [24].

Lemma 4.1. *The sequence* $\big(\|f_n\|^2 \Im(z_n)/h_n\big)_n$ *goes to* 0 *and* $\lim_{n\to\infty} \Im(z_n)/h_n = 0$.

Proof. We write $\|f_n\|^2 \Im(z_n) = \Im\,\langle f_n\,,\,(P(h_n) - z_n) f_n\rangle$, which is $o(h_n)$ by (1.6) and (4.1). This gives the first result. Now, assume that $r > 0$. Since $\|f_n\|^2(\Im(z_n)/h_n)$ goes to 0, $\|f_n\|$ must go to 0, while $\|f_n\| \geq \|f_n\|_{\mathrm{B}^*} = 1$. This is a contradiction. □

Using (1.1), we show as in [6] the following localization in position space.

Proposition 4.2. *There exists* $R_0' > R_0$ *such that* $\lim_{n\to\infty} \|\mathbb{1}_{\{|\cdot|>R_0'\}} f_n\|_{\mathrm{B}^*} = 0$.

Proof. Let $a \in \Sigma_{0;0}$. It is known that $(a_h^w)_{h \in]0;h_*]}$ is uniformly bounded in $\mathcal{L}(L^2_s; L^2_s)$ for any $s \in \mathbb{R}$. Even more, using a partition of unity adapted to the decomposition $\mathbb{R}^d = c \cup (\cup_{j\geq 1} c_j)$ from (1.3), say $1 = \tau(x) + \sum_{j\geq 1} \tau_j(x)$, and writing, for any $u \in B^*$, the identity $u = \tau\, u + \sum_{j\geq 1} \tau_j\, u$, standard pseudodifferential calculus and almost orthogonality properties allow to easily establish that $(a_h^w)_{h\in]0;h_*]}$ is uniformly bounded in $\mathcal{L}(B^*; B^*)$ (see [6] for a complete proof). Now, let $\alpha_n := \langle f_n, i h_n^{-1} [P(h_n), a_{h_n}^w] f_n\rangle$. Expanding the commutator, using (1.6), (4.1) and Lemma 4.1, we observe that $\alpha_n \to 0$. For any $s > 1/2$, $(f_n)_n$ is bounded in

L^2_{-s}, since $\mathrm{L}^2_s \subset B$. Now, we assume that a vanishes near the set $\mathcal{S}$ of all singularities. We can find $\chi \in C_0^\infty(\mathbb{R}^d;\mathbb{R})$ such that $a\chi = 0$ and $\chi = 1$ near the singularities. By Lemma 2.3 with $k = k' = -s$,

$$\alpha_n = \Big\langle f_n\,,\, ih_n^{-1}\big[P_\chi(h_n), a^w_{h_n}\big] f_n\Big\rangle + O(h_n)\,.$$

Let $\theta \in C_0^\infty(\mathbb{R};\mathbb{R})$ with $\theta = 1$ near I and $\tilde{\theta} := 1 - \theta$. Since $z_n \to \lambda \in I$, $(\|\tilde{\theta}(P(h_n))(P(h_n) - z_n)^{-1}\|)_n$ is uniformly bounded. Thus there exists $C > 0$ such that

$$\begin{aligned}\big\|\tilde{\theta}\big(P(h_n)\big)f_n\big\|_{B^*} &\le \max\Big(\big\|\tilde{\theta}\big(P(h_n)\big)f_n\big\|_c\,;\, \sup_{j\ge 1} 2^{-j/2}\big\|\tilde{\theta}\big(P(h_n)\big)f_n\big\|_{c_j}\Big)\\ &\le C\big\|\big(P(h_n) - z_n\big)f_n\big\| = o(h_n)\,, \end{aligned}\qquad (4.3)$$

since (4.1) implies that $\|(P(h_n) - z_n)f_n\| = o(h_n)$. Using further that, for $s \in]1/2;1]$, $\langle\,\cdot\,\rangle^s ih_n^{-1}[P_\chi(h_n), a^w_{h_n}]$ is uniformly bounded,

$$\alpha_n = \Big\langle f_n\,,\, ih_n^{-1}\big[P_\chi(h_n), a^w_{h_n}\big]\theta\big(P(h_n)\big) f_n\Big\rangle + O(h_n)\,.$$

Since $ih_n^{-1}[P_\chi(h_n), a^w_{h_n}]$ is a h-pseudodifferential operator, we may apply Lemma 2.3 with $k = k' = -s$, yielding

$$\alpha_n = \Big\langle f_n\,,\, ih_n^{-1}\big[P_\chi(h_n), a^w_{h_n}\big]\theta\big(P_\chi(h_n)\big) f_n\Big\rangle + O(h_n)\,.$$

Using similar arguments again, we arrive at

$$\alpha_n = \Big\langle \theta\big(P_\chi(h_n)\big)f_n\,,\, ih_n^{-1}\big[P_\chi(h_n), a^w_{h_n}\big]\theta\big(P_\chi(h_n)\big) f_n\Big\rangle + O(h_n)\,. \qquad (4.4)$$

Now we specify the symbol a more carefully. By [6] (see Proposition 8 and the second step of the proof of Proposition 7 therein), we can find $c > 0$ and a function $\chi_1 \in C_0^\infty(\mathbb{R}^d)$ such that, for all $\beta = (\beta_j) \in \ell^1$ with $|\beta|_{\ell^1} = 1$, there exists a symbol $a \in \Sigma_{0;0}$ satisfying the following properties. The function $\chi_1 = 1$ on a large enough neighbourhood of 0 and of the support of χ. The semi-norms of a in $\Sigma_{0;0}$ are bounded independently of β and, uniformly with respect to β,

$$\alpha_n \;\ge\; c\cdot \left|\sum_j \beta_j 2^{-j}\big\|(1-\chi_1)\theta\big(P_\chi(h_n)\big)f_n\big\|^2_{c_j}\right| + o(1)\,.$$

By the above arguments, $\alpha_n \to 0$, uniformly in β. This implies that

$$\sup_j 2^{-j}\big\|(1-\chi_1)\theta\big(P_\chi(h_n)\big)f_n\big\|^2_{c_j} \quad \text{and therefore} \quad \sup_j 2^{-j/2}\big\|(1-\chi_1)\theta\big(P_\chi(h_n)\big)f_n\big\|_{c_j}$$

tend to 0. In other words, $\|(1-\chi_1)\theta(P_\chi(h_n))f_n\|_{B^*} \to 0$. Since $B \subset \mathrm{L}^2_{1/2-\epsilon}$ continuously, for any $\epsilon > 0$, we derive from Lemma 2.3 that

$$\Big\|(1-\chi_1)\Big(\theta\big(P_\chi(h_n)\big) - \theta\big(P(h_n)\big)\Big)f_n\Big\|_{B^*} \;\to\; 0\,,$$

yielding $\|(1-\chi_1)f_n\|_{B^*} \to 0$, thanks to (4.3). Now the desired result follows for R_0' large enough such that $|x| \geq R_0' \Longrightarrow \chi_1(x) = 0$. □

Lemma 4.3. *Let $R_1' > R_0'$. There exist a sequence $(g_n)_n$ of nonzero functions of $\mathrm{H}^2(\mathbb{R}^d)$, bounded in $\mathrm{L}^2(\mathbb{R}^d)$ and having a unique semiclassical measure μ, a sequence $(h_n)_n \in]0; h_*]^{\mathbb{N}}$ tending to zero, and a sequence $(\lambda_n)_n \in \mathbb{R}^{\mathbb{N}}$ with $\lambda_n \to \lambda \in I$, such that (4.2) holds true.*

Proof. Let $\tau, \kappa \in C_0^\infty(\mathbb{R}^d; \mathbb{R})$ be such that $\operatorname{supp}\tau, \operatorname{supp}\kappa \subset \{x \in \mathbb{R}^d; |x| \leq R_1'\}$, $\kappa = 1$ on $\{x \in \mathbb{R}^d; |x| \leq R_0'\}$, and $\tau\kappa = \kappa$. The sequence $(\tau f_n)_n$ is bounded in $\mathrm{L}^2(\mathbb{R}^d)$. Possibly after extraction of a subsequence, we may assume that it has a unique semiclassical measure μ. We shall show that

$$\operatorname{supp}\mu \subset \left\{(x,\xi) \in T^*\mathbb{R}^d; |x| \leq R_0'\right\}, \tag{4.5}$$

$$\operatorname{supp}\mu \cap T^*(\mathbb{R}^d \setminus \mathcal{S}) \subset p^{-1}(\lambda)\,. \tag{4.6}$$

By Proposition 4.2, $\|\mathbb{1}_{\{|\cdot|>R_0'\}}\tau f_n\|$ goes to 0. Using (2.5), this implies (4.5). Now let $a \in C_0^\infty(T^*\mathbb{R}^d)$ be such that $a = 0$ near $p^{-1}(\lambda) \cup \mathcal{S}$. Since $(\|\langle\cdot\rangle^{-1} f_n\|)_n$ is bounded by (4.1),

$$\begin{aligned}\langle \tau f_n\,,\, a_{h_n}^w \tau f_n\rangle &= \left\langle \tau f_n\,,\, (\tau a)_{h_n}^w f_n\right\rangle + O(h_n)\\ &= \left\langle \tau f_n\,,\, (\tau a)_{h_n}^w \theta\big(P(h_n)\big) f_n\right\rangle + O(h_n)\\ &\quad + \left\langle \tau f_n\,,\, (\tau a)_{h_n}^w \tilde\theta\big(P(h_n)\big)\big(P(h_n)-z_n\big)^{-1}\left(P(h_n)-z_n\right) f_n\right\rangle,\end{aligned} \tag{4.7}$$

where $\theta \in C_0^\infty(\mathbb{R}; \mathbb{R})$ with $\theta = 1$ near λ, such that $\theta(p)a = 0$, and $\tilde\theta = 1-\theta$. By (4.1), $\|(P(h_n)-z_n)f_n\| = o(h_n)$ and the last term in (4.7) is a $o(h_n)$. We can find $\chi \in C_0^\infty(\mathbb{R}^d; \mathbb{R})$ such that $a\chi = 0$ and $\chi = 1$ near the singularities. By Lemma 2.3, we recover

$$\langle \tau f_n\,,\, a_{h_n}^w \tau f_n\rangle = \left\langle \tau f_n\,,\, (\tau a)_{h_n}^w \theta\big(P_\chi(h_n)\big) f_n\right\rangle + O(h_n) = O(h_n)$$

since $a\theta(p_\chi) = 0$. By (2.5), this yields (4.6).

The symbol of $[-h_n^2\Delta, \kappa]$ belongs to $\Sigma_{-\infty,1}$ and is supported in $\{(x,\xi) \in T^*\mathbb{R}^d; R_0' < |x| < R_1'\}$. Let $\tilde\tau \in C_0^\infty(\mathbb{R}^d)$ such that $\tilde\tau = 1$ on $\operatorname{supp}\nabla\kappa$ and $\operatorname{supp}\tilde\tau \subset \{x \in \mathbb{R}^d; R_0' < |x| < R_1'\}$. Then

$$\begin{aligned}[-h_n^2\Delta, \kappa] f_n &= [-h_n^2\Delta, \kappa]\tilde\tau f_n = [-h_n^2\Delta, \kappa]\left(P_\chi(h_n)+i\right)^{-1}\left(P_\chi(h_n)+i\right)\tilde\tau f_n\\ &= [-h_n^2\Delta, \kappa]\left(P_\chi(h_n)+i\right)^{-1}[-h_n^2\Delta, \tilde\tau] f_n\\ &\quad + [-h_n^2\Delta, \kappa]\left(P_\chi(h_n)+i\right)^{-1}\tilde\tau\left(P(h_n)-z_n\right) f_n\\ &\quad + [-h_n^2\Delta, \kappa]\big(P_\chi(h_n)+i\big)^{-1}(i+z_n)\tilde\tau f_n =: r_1 + r_2 + r_3\,.\end{aligned}$$

Standard pseudodifferential calculus together with Proposition 4.2 provide $r_1 = o(h_n^2)$, $r_2 = o(h_n^2)$, and $r_3 = o(h_n)$ in $\mathrm{L}^2(\mathbb{R}^d)$. Thus, setting $g_n := \kappa f_n$,

$$\big(P(h_n)-z_n\big) g_n = \kappa\big(P(h_n)-z_n\big) f_n + o(h_n) = o(h_n)$$

in $\mathrm{L}^2(\mathbb{R}^d)$. By Proposition 4.2 and (4.1), $\|g_n\| \to c$, with $c > 0$, and $\Im(z_n)g_n = o(h_n)$ in $\mathrm{L}^2(\mathbb{R}^d)$, by Lemma 4.1. Setting $\lambda_n := \Re(z_n)$, we obtain $\|(P(h_n) - \lambda_n)g_n\| = o(h_n)$. Using (2.5) and the previous arguments, μ is the unique semiclassical measure of $(g_n)_n$. □

We now collect properties of the g_n and their semiclassical measure μ, defined in Lemma 4.3.

Lemma 4.4. *Let $a \in C_0^\infty(T^*\mathbb{R}^d)$ such that $a = 0$ near the set $\mathcal{S}$ of all singularities.*

1. *Then $\mu(\{p, a\}) = 0$ ("μ is invariant under the flow").*
2. *If $a = 0$ near $p^{-1}(\lambda)$ or near $\{(x, \xi) \in T^*\mathbb{R}^d; |x| \leq R_0'\}$ then $\mu(a) = 0$.*
3. *Let $\tau \in C^\infty(\mathbb{R}^d)$ such that $\tau = 0$ near $\mathcal{S}$. Then the sequence $(\|\tau i h_n \nabla g_n\|)_n$ is bounded.*

Proof. 1) Let $\chi \in C_0^\infty(\mathbb{R}^d; \mathbb{R})$ such that $a\chi = 0$ and $\chi = 1$ near the set $\mathcal{S}$ of all singularities. In particular, $\{p, a\} = \{p_\chi, a\}$. By Lemma 2.3,

$$a_n := \Big\langle g_n \,,\, i h_n^{-1}\big[P(h_n), a_{h_n}^w\big] g_n \Big\rangle = \Big\langle g_n, i h_n^{-1}\big[P_\chi(h_n), a_{h_n}^w\big] g_n \Big\rangle + O(h_n) \qquad (4.8)$$

$$= \big\langle g_n, (\{p_\chi, a\})_{h_n}^w g_n \big\rangle + O(h_n)\,. \qquad (4.9)$$

By (2.5), the r.h.s. of (4.9) goes to $\mu(\{p_\chi, a\})$, as $n \to \infty$. As in [24], we replace $P(h_n)$ by $P(h_n) - \lambda_n$ in the commutator on the l.h.s. of (4.8) and expand the commutator. Using (4.2), we show that $a_n = o(1)$, as $n \to \infty$, yielding $\mu(\{p, a\}) = 0$.

2) The second assertion was established in the proof of Lemma 4.3.

3) Let $\tau \in C^\infty(\mathbb{R}^d)$ with support in $\hat{M}$. Since $\operatorname{supp} g_n \subset \{|x| \leq R_1'\}$,

$$\big|\big\langle \tau^2 g_n \,,\, h_n^2 \Delta_x g_n \big\rangle\big| \leq \Big|\Big\langle \tau^2 g_n \,,\, \big(P(h_n) - \lambda\big) g_n \Big\rangle\Big| + O(n^0)\,,$$

where $O(n^0)$ means $O(1)$ as $n \to \infty$. Thus

$$\big\langle i h_n \nabla_x g_n \,,\, \tau^2 i h_n \nabla_x g_n \big\rangle \leq 2h_n \big|\big\langle (\nabla_x \tau) g_n \,,\, \tau i h_n \nabla_x g_n \big\rangle\big| + O(n^0)$$

$$\|\tau i h_n \nabla_x g_n\|^2 \leq O(h_n) \cdot \|\tau i h_n \nabla_x g_n\| + O(n^0)\,,$$

yielding the boundedness of $(\|\tau i h_n \nabla g_n\|)_n$. □

We introduce

$$B_\pm(\lambda) := \big\{\mathrm{x}^* \in p^{-1}(\lambda);\ 0 \leq \pm t \ \mapsto\ \pi_x \phi(t; \mathrm{x}^*) \quad \text{is bounded}\big\} \qquad (4.10)$$

and $B(\lambda) := B_+(\lambda) \cap B_-(\lambda)$. By (3.3), the non-trapping condition (1.10) exactly means that $B_+(\lambda)$ and $B_-(\lambda)$ are empty.

Proposition 4.5. *Let $d \geq 3$ if $N = 0$ else let $d = 3$. The measure μ is nonzero.*

If $N = 0$, μ vanishes near the (repulsive) singularities, is invariant under the complete flow $t \mapsto \phi^t$, and $\operatorname{supp} \mu \subset B(\lambda)$.

If $N > 0$, then, outside the attractive singularities, μ is supported in $B(\lambda)$ that is

$$\operatorname{supp} \mu \cap T^*(\mathbb{R}^3 \setminus \mathcal{S}) \subset B(\lambda)\,. \qquad (4.11)$$

Proof. For the case of purely repulsive singularities (i.e. $N = 0$) the proof is given in Subsection 4.2. The other case appears in Subsection 4.3. □

Remark 4.6. If (1.11) is really false, one expects that the f_n are "close to some resonant state". Proposition 4.5 and Proposition 4.9 below roughly say that this resonant state should be microlocalized on trajectories in $B(\lambda)$. However, it does not give any information above the attractive singularities. If the potential V is smooth (i.e. $N = N' = 0$), the arguments used in [24] actually prove Proposition 4.5 in this case.

Lemma 4.7. *Let $d \geq 3$ if $N = 0$ else let $d = 3$. If p is non-trapping at energy λ (cf. (1.10)) then $\mu = 0$.*

Proof. Let $N = 0$. By Proposition 4.5, $\operatorname{supp} \mu \subset B(\lambda)$, which is empty by the non-trapping condition. Thus $\mu = 0$. The other case is treated in Subsection 4.3. □

Now Proposition 4.5 and Lemma 4.7 produce the desired contradiction.

4.2. Repulsive singularities

We show Proposition 4.5 for the case $N = 0$, $d \geq 3$, by first showing a decay estimate for the Fourier transform of the g_n's.

Since we only have repulsive singularities, there exists some positive c such that

$$\big\langle g_n\,,\,(-h_n^2\Delta_x)\,g_n\big\rangle + \sum_{j=1}^{N'}\big\langle g_n\,,\,(1/|\cdot - s_j|)\,g_n\big\rangle \leq c\Big\langle g_n\,,\,\big(P(h_n)-\lambda\big)g_n\Big\rangle + O(n^0)\,. \quad (4.12)$$

By Lemma 4.3, $\|(P(h_n)-\lambda)g_n\| \to 0$ and the r.h.s of (4.12) is bounded. Now, we show that $\mu \neq 0$. Let $\chi \in C_0^\infty(\mathbb{R}^d;\mathbb{R})$ such that $0 \leq \chi \leq 1$ and $\chi = 1$ near 0. Let us denote by $\mathcal{F}g$ the Fourier transform of g. Setting $\chi_R(\xi) = \chi(\xi/R)$, for $R > 0$ and $\xi \in \mathbb{R}^d$, we observe that

$$\Big\langle \mathcal{F}g_n\,,\,\frac{(1-\chi_R)(h_n\,\cdot)}{|h_n\,\cdot|^2}\,|h_n\,\cdot|^2\mathcal{F}g_n\Big\rangle \leq \frac{O(n^0)}{R^2}\,\big\langle g_n\,,\,(-h_n^2\Delta)g_n\big\rangle\,.$$

The bracket on the r.h.s is bounded uniformly w.r.t. R. Thus

$$\lim_R \limsup_n \big\langle \mathcal{F}g_n\,,\,(1-\chi_R)(h_n\,\cdot)\mathcal{F}g_n\big\rangle = 0\,. \quad (4.13)$$

Recall that, for all n, $\operatorname{supp} g_n \subset \{|x| \leq R_1'\}$ (cf. Lemma 4.3). By Proposition 2.1, this implies that $\|g_n\|^2 \to \mu(\mathbb{1})$, yielding $\mu \neq 0$. Now let $\tau \in C_0^\infty(\mathbb{R};\mathbb{R}^+)$ be supported on a neighborhood of the singularities such that $\tau = 1$ near them. Since $V - \lambda$ is large and positive near the singularities, we can choose the support of τ such that,

$$\|\tau g_n\|^2 \leq \big\langle \tau g_n\,,\,(V-\lambda)\tau g_n\big\rangle\,. \quad (4.14)$$

Thus

$$\left\langle \tau g_n \, , \, (-h_n^2 \Delta_x) \, \tau g_n \right\rangle + \|\tau g_n\|^2 \leq 2 \left\langle \tau g_n \, , \, (P - \lambda) \tau g_n \right\rangle = o(1) \, , \qquad (4.15)$$

using Lemma 4.4. In particular, $\|\tau g_n\|^2 \to \mu(\tau^2)$ (cf. Proposition 2.1) and $\|\tau g_n\| \to 0$. Thus μ is supported away from the (repulsive) singularities. By Lemma 4.4, we conclude that μ is invariant under the flow $(\phi^t)_{t\in\mathbb{R}}$. If the trajectory $t \mapsto \pi_x \phi^t(x,\xi)$ goes to infinity when $\pm t \to +\infty$, then the invariance of μ under the flow implies that μ vanishes on this trajectory. This shows that $\operatorname{supp} \mu \subset B(\lambda)$ and finishes the proof of Proposition 4.5 in the case $N = 0$ and $d \geq 3$.

4.3. The general case in dimension 3

In this subsection, we assume that $N > 0$ and $d = 3$ and we give successively the proofs of Proposition 4.5 and Lemma 4.7 (at the end of the subsection). In view of (4.13) and of Proposition 2.1, we want to show that $\langle g_n, (-h_n^2 \Delta_x) g_n \rangle$ is bounded to get $\mu \neq 0$. We also need a kind of invariance of μ under the pseudo-flow ϕ^t (cf. (2.18)). To realize this programme, we want to use the KS-transform (2.23) to lift the property (4.2) in $\mathbb{R}^4$, locally near each attractive singularity.

Let $(\tau_j)_{0\leq j\leq N} \in (C_0^\infty(\mathbb{R}^d;\mathbb{R}^+))^{N+1}$ be such that

- $\sum_{j=0}^N \tau_j^2 = 1$ near $\{x \in \mathbb{R}^d; |x| \leq R_1'\}$,
- for $1 \leq j \leq N$, $\tau_j = 1$ near s_j and is supported away from the other singularities,
- $\tau_0 = 1$ near the set of repulsive singularities and is supported away from the other singularities.

There exists $c > 0$ such that

$$\sum_{j=N+1}^{N'} \left\langle \tau_0 g_n \, , \, (1/|x - s_j|) \, \tau_0 g_n \right\rangle \ \leq c \left\langle \tau_0 g_n \, , \, (V - \lambda) \tau_0 g_n \right\rangle . \qquad (4.16)$$

Thus

$$\begin{aligned} &\left\langle \tau_0 g_n \, , \, (-h_n^2 \Delta_x) \, \tau_0 g_n \right\rangle + \sum_{j=N+1}^{N'} \left\langle \tau_0 g_n \, , \, (1/|x - s_j|) \, \tau_0 g_n \right\rangle \\ &\qquad \leq (1 + c) \left\langle \tau_0 g_n \, , \, (P - \lambda) \tau_0 g_n \right\rangle + O(n^0) = O(n^0) \, . \qquad (4.17) \end{aligned}$$

Here we used the fact that $\langle \tau_0 g_n, (P - \lambda) \tau_0 g_n \rangle \to 0$, by Lemma 4.3 and Lemma 4.4. Let $1 \leq j \leq N$. For the same reason, $\langle \tau_j g_n, (P - \lambda) \tau_j g_n \rangle \to 0$. Thus, since $(V - f_j/|\cdot - s_j|)\tau_j$ is bounded,

$$\left| \left\langle \tau_j g_n \, , \, (-h_n^2 \Delta_x) \, \tau_j g_n \right\rangle + \left\langle \tau_j g_n \, , \, (f_j/|\cdot - s_j|) \, \tau_j g_n \right\rangle \right| = O(n^0) \, . \qquad (4.18)$$

We introduce the KS-transformation (cf. (2.23)) which is adapted to the singularity at s_j: $x = \mathcal{K}_j(z_j) := s_j + \mathcal{K}(z_j)$ (cf. (2.19)) and, for $x \neq s_j$,

$$(x, \xi) = \mathcal{K}_j^*(z; \zeta) := (s_j, 0) + \mathcal{K}^*(z; \zeta) \, . \qquad (4.19)$$

For all n, let $\tilde{g}_{n,j} := g_n \circ \mathcal{K}_j$. Let $\chi_j \in C_0^\infty(\mathbb{R}^3)$ such that $\chi_j \tau_j = \chi_j$, $\chi_j = 1$ near s_j, and $\chi_j \tau_k = 0$, for $k \neq j$. Denote by $\tilde{\chi}_j$ the function $\chi_j \circ \mathcal{K}_j$. For $\lambda' \in \mathbb{R}$, we introduce the differential operator in $\mathbb{R}^4_{z_j}$

$$\tilde{P}_j(h; \lambda') := -h^2 \Delta_{z_j} + \big((\tau_j V) \circ \mathcal{K}_j - \lambda'\big) \, |\cdot|^2 \,, \tag{4.20}$$

which can be seen as the Weyl h-quantization of the symbol

$$T^*\mathbb{R}^4 \ni (z_j, \zeta_j) \;\mapsto\; \tilde{p}_{j,\lambda'}(z_j, \zeta_j) \;:=\; |\zeta_j|^2 + \Big((\tau_j V)\big(\mathcal{K}(z_j)\big) - \lambda'\Big) \cdot |z_j|^2 \,. \tag{4.21}$$

Notice that $\tilde{p}_{j,\lambda'} \in \Sigma_{2;2}$. We can write, for $z_j \in \operatorname{supp} \tilde{\chi}_j$,

$$\begin{aligned} |z_j|^2 &\Big((\tau_j V)\big(\mathcal{K}_j(z_j)\big) - \lambda'\Big) \\ &= f_j(s_j) + \Big(f_j\big(\mathcal{K}_j(z_j)\big) - f_j\big(\mathcal{K}_j(0)\big)\Big) + |z_j|^2 \Big(W_j\big(\mathcal{K}_j(z_j)\big) - \lambda'\Big) \\ &=: f_j(s_j) + \tilde{W}_{j,\lambda'}(z_j) \,. \end{aligned} \tag{4.22}$$

So $\tilde{W}_{j,\lambda'}$ is a quadratic perturbation of the constant $f_j(s_j)$, vanishing at s_j, and

$$\tilde{P}_j(h; \lambda') = -h^2 \Delta_{z_j} + f_j(s_j) \,+\, \tilde{W}_{j,\lambda'} \,. \tag{4.23}$$

Lemma 4.8. *Let $1 \leq j \leq N$. The sequence $(\tilde{g}_{n,j})_n = (g_n \circ \mathcal{K}_j)_n$ is bounded in $\mathrm{L}^2(\mathbb{R}^4)$. Up to subsequence, we may assume that it has a unique semiclassical measure $\tilde{\mu}_j$. Besides,*

$$\forall n \in \mathbb{N}, \quad \operatorname{supp} \tilde{g}_{n,j} \subset \big\{z_j ; |z_j| \leq (R_0 + R_1')^{1/2}\big\} \,, \tag{4.24}$$

$$\text{and} \quad \tilde{\chi}_j \tilde{P}_j(h_n; \lambda_n) \tilde{g}_{n,j} = o(h_n) \quad \text{in} \quad \mathrm{L}^2(\mathbb{R}^4) \,. \tag{4.25}$$

Let $\tilde{\phi}_j^s := \tilde{\phi}_j(s; \cdot)$ be the Hamiltonian flow associated to $(t, \lambda', z, \zeta) \mapsto \tilde{p}_{j,\lambda'}(z, \zeta)$ by (2.24). Let $\tilde{b} \in C_0^\infty(T^*\mathbb{R}^4)$ and $T_b := \{s > 0; \forall t \in [0; s] \,, (\tilde{b} \circ \tilde{\phi}_j^t)(1 - \tilde{\chi}_j) = 0\}$. Then, for $s \in T_b$,

$$\tilde{\mu}_j(\tilde{b}) = \tilde{\mu}_j\big(\tilde{b} \circ \tilde{\phi}_j^s\big) \,. \tag{4.26}$$

Proof. • Eq. (4.24) follows from the scaling $|\mathcal{K}(z)| = |z|^2$ of the Hopf map (see (2.19)) and the estimate (4.2) for the support of g_n .

• Since $(-h_n^2 \Delta_x + V - \lambda_n) g_n = o(h_n)$ and $g_n = O(n^0)$ in $\mathrm{L}^2(\mathbb{R}^3)$, we use (2.19), (2.21), and the arguments of Proposition 2.1 in [13] to get

$$|\cdot|^{-1} \tilde{\chi}_j \tilde{P}_j(h_n; \lambda_n) \tilde{g}_{n,j} = o(h_n) \quad \text{and} \quad |\cdot| \tilde{g}_{n,j} = O(n^0) \quad \text{in} \quad \mathrm{L}^2(\mathbb{R}^4) \,. \tag{4.27}$$

This yields (4.25).

• Now, we show that $\tilde{\chi}_j \tilde{g}_{n,j} = O(n^0)$ in $\mathrm{L}^2(\mathbb{R}^4)$. Together with (4.27), this then will imply the desired boundedness of $(\tilde{g}_{n,j})_n$ in $\mathrm{L}^2(\mathbb{R}^4)$.

Thanks to (2.19), (2.21), and to Part 3 of Lemma 4.4,

$$\|\mathbb{1}_{\operatorname{supp} \nabla \tilde{\chi}_j} h_n \nabla_{z_j} \tilde{g}_{n,j}\| = O\big(\|\mathbb{1}_{\operatorname{supp} \nabla \chi_j} h_n \nabla_x g_n\|\big) = O(n^0) \,, \tag{4.28}$$

$$\|\mathbb{1}_{\operatorname{supp} \nabla \tilde{\chi}_j} \tilde{g}_{n,j}\| = O\big(\|\mathbb{1}_{\operatorname{supp} \nabla \chi_j} g_n\|\big) = O(n^0) \,. \tag{4.29}$$

Let $A_{n,j} := (z_j \cdot h_n \nabla_{z_j} + h_n \nabla_{z_j} \cdot z_j)/(2i)$ and

$$a_{n,j} := \Big\langle \tilde{g}_{n,j}\,,\, h_n^{-1}\big[\tilde{P}_j(h_n;\lambda_n), i\tilde{\chi}_j A_{n,j}\tilde{\chi}_j\big]\,\tilde{g}_{n,j}\Big\rangle\,.$$

Expanding the commutator and using (4.27), we see, on one hand, that

$$\begin{aligned} |a_{n,j}| &\le o(n^0)\cdot\big(h_n\|\mathbb{1}_{\operatorname{supp}\nabla\tilde{\chi}_j}\tilde{g}_{n,j}\| + \|\tilde{\chi}_j i h_n \nabla_{z_j}\tilde{g}_{n,j}\| + O(n^0)\big) \\ &\le o(n^0)\cdot\|\tilde{\chi}_j i h_n \nabla_{z_j}\tilde{g}_{n,j}\| + o(n^0)\,, \end{aligned} \tag{4.30}$$

thanks to (4.29). On the other hand, writing $2iA_{n,j} = 2z_j\cdot h_n\nabla_{z_j} + 4h_n$,

$$\begin{aligned} a_{n,j} = \Big\langle \tilde{g}_{n,j}, 2\big[-h_n^2\Delta_{z_j}, \tilde{\chi}_j^2\big]\tilde{g}_{n,j}\Big\rangle - 2\Re\Big\langle (z_j\cdot h_n\nabla_{z_j})\tilde{\chi}_j\tilde{g}_{n,j}, h_n^{-1}\big[-h_n^2\Delta_{z_j},\tilde{\chi}_j\big]\tilde{g}_{n,j}\Big\rangle \\ + \Big\langle \tilde{\chi}_j\tilde{g}_{n,j}, h_n^{-1}\big[\tilde{P}_j(h_n;\lambda_n), z_j\cdot h_n\nabla_{z_j}\big]\,\tilde{\chi}_j\tilde{g}_{n,j}\Big\rangle\,. \end{aligned}$$

By (4.28) and (4.29),

$$\Big| a_{n,j} - \Big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, h_n^{-1}\big[\tilde{P}_j(h_n;\lambda_n), iA_{n,j}\big]\,\tilde{\chi}_j\tilde{g}_{n,j}\Big\rangle\Big| = O(n^0)\,.$$

As a differential operator, $h_n^{-1}[\tilde{P}_j(h_n;\lambda_n), iA_{n,j}] = 2(-h_n^2\Delta_{z_j}) - z_j\cdot\nabla_{z_j}\tilde{W}_{j,\lambda_n}(z_j)$ (cf. (4.23)) and, by (4.24), there exists some $c_j > 0$ such that, for all n and for all $z_j \in \operatorname{supp}\tilde{g}_{n,j}$, $|z_j\cdot\nabla_{z_j}\tilde{W}_{j,\lambda_n}(z_j)| \le c_j|z_j|^2$. By (4.27),

$$\big| a_{n,j} - \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, -2h_n^2\Delta_{z_j}\,\tilde{\chi}_j\tilde{g}_{n,j}\big\rangle\big| = O(n^0)\,.$$

This, together with (4.30), implies that

$$0 \le \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, -2h_n^2\Delta_{z_j}\,\tilde{\chi}_j\tilde{g}_{n,j}\big\rangle \le o(n^0)\cdot\|\tilde{\chi}_j i h_n\nabla_{z_j}\tilde{g}_{n,j}\| + O(n^0)\,. \tag{4.31}$$

Writing

$$\begin{aligned} \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, -h_n^2\Delta_{z_j}\,\tilde{\chi}_j\tilde{g}_{n,j}\big\rangle = \|\tilde{\chi}_j i h_n\nabla_{z_j}\tilde{g}_{n,j}\|^2 + h_n^2\|(\nabla_{z_j}\tilde{\chi}_j)\tilde{g}_{n,j}\|^2 \\ + 2h_n\Re\big\langle (\nabla_{z_j}\tilde{\chi}_j)\tilde{g}_{n,j}\,,\, \tilde{\chi}_j i h_n\nabla_{z_j}\tilde{g}_{n,j}\big\rangle \end{aligned}$$

and using again (4.28) and (4.29), we arrive at

$$\|\tilde{\chi}_j i h_n\nabla_{z_j}\tilde{g}_{n,j}\|^2 \le o(n^0)\cdot\|\tilde{\chi}_j i h_n\nabla_{z_j}\tilde{g}_{n,j}\| + O(n^0)\,.$$

This yields

$$\|\tilde{\chi}_j i h_n\nabla_{z_j}\tilde{g}_{n,j}\| = O(n^0) \quad\text{and}\quad \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, -h_n^2\Delta_{z_j}\,\tilde{\chi}_j\tilde{g}_{n,j}\big\rangle = O(n^0)\,. \tag{4.32}$$

Now

$$\begin{aligned} \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, \tilde{P}_j(h_n;\lambda_n)\tilde{\chi}_j\tilde{g}_{n,j}\big\rangle = \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, \tilde{\chi}_j\tilde{P}_j(h_n;\lambda_n)\tilde{g}_{n,j}\big\rangle \\ + \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, [-h_n^2\Delta_{z_j},\tilde{\chi}_j]\tilde{g}_{n,j}\big\rangle \end{aligned}$$

and is bounded by (4.27), (4.28), and (4.29). Thus

$$\begin{aligned} \big\langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, -h_n^2\Delta_{z_j}\,\tilde{\chi}_j\tilde{g}_{n,j}\big\rangle + f(s_j)\|\tilde{\chi}_j\tilde{g}_{n,j}\|^2 + \langle \tilde{\chi}_j\tilde{g}_{n,j}\,,\, \tilde{W}_{j,\lambda_n}\tilde{\chi}_j\tilde{g}_{n,j}\rangle \\ = O(n^0)\,. \end{aligned} \tag{4.33}$$

In (4.33), the first and third terms are $O(n^0)$, by (4.32) and by (4.27) respectively. Since $f_j(s_j) \neq 0$, we conclude that $(\tilde{\chi}_j\tilde{g}_{n,j})_n$ is bounded in $\mathrm{L}^2(\mathbb{R}^4)$.

• We now show the invariance (4.26). It suffices to show that, for all $\lambda \in \mathbb{R}$ and all $\tilde{b} \in C_0^\infty(T^*\mathbb{R}^4)$ such that $\tilde{b}(1-\tilde{\chi}_j) = 0$, $\tilde{\mu}_j(\{\tilde{p}_{j,\lambda}, \tilde{b}\}) = 0$. Take such a $\tilde{b}$ and $\lambda \in \mathbb{R}$. Since $\tilde{b}_{h_n}^w$ is uniformly bounded,

$$\Big\langle \tilde{g}_{n,j}, ih_n^{-1}\big[\tilde{\chi}_j \tilde{P}_j(h_n;\lambda_n), \tilde{b}_{h_n}^w\big]\tilde{g}_{n,j}\Big\rangle = o(n^0)\,,$$

by expanding the commutator, using (4.25), and using the boundedness in $\mathrm{L}^2(\mathbb{R}^4)$ of $(\tilde{g}_{n,j})_n$. Now we compute the leading term of the commutator and arrive at

$$\begin{aligned} o(n^0) &= \big\langle \tilde{g}_{n,j}, \{\tilde{\chi}_j\tilde{p}_{j,\lambda_n}, \tilde{b}\}_{h_n}^w \tilde{g}_{n,j}\big\rangle + O(h_n) = \big\langle \tilde{g}_{n,j}, \{\tilde{\chi}_j\tilde{p}_{j,\lambda}, \tilde{b}\}_{h_n}^w \tilde{g}_{n,j}\big\rangle + o(n^0) \\ &= \big\langle \tilde{g}_{n,j}, \{\tilde{p}_{j,\lambda}, \tilde{b}\}_{h_n}^w \tilde{g}_{n,j}\big\rangle + o(n^0)\,, \end{aligned}$$

since $\tilde{\chi}_j = 1$ on the support of $\tilde{b}$. Thus $\tilde{\mu}_j(\{\tilde{p}_{j,\lambda}, \tilde{b}\}) = 0$. As in the proof of (4.6), we see that $\operatorname{supp}\tilde{\mu}_j \subset (\tilde{p}_{j,\lambda})^{-1}(0)$. Since the last two components of $\tilde{\phi}_j^s(\,\cdot\,,\lambda,\,\cdot\,,\,\cdot\,)$ actually form the flow generated by $\tilde{p}_{j,\lambda}$, we obtain (4.26). □

Proof of Proposition 4.5. Let $1 \le j \le N$. The boundedness of the sequence $(\tilde{\chi}_j\tilde{g}_{n,j})_n$ in $\mathrm{L}^2(\mathbb{R}^4)$ precisely means that $(\langle \chi_j g_n\,,\,(1/|\cdot - s_j|)\chi_j g_n\rangle)_n$ is bounded (cf. (2.21)) and so is also $(\langle \tau_j g_n\,,\,(1/|\cdot - s_j|)\tau_j g_n\rangle)_n$. By (4.18), this implies that $(\langle \tau_j g_n\,,\,-h_n^2\Delta_x\tau_j g_n\rangle)_n$ is bounded. By the IMS localization formula (cf. Chapter 3.1 of [8]),

$$\langle g_n\,,\,-h_n^2\Delta_x g_n\rangle = \sum_{j=0}^{N}\langle \tau_j g_n\,,\,-h_n^2\Delta_x\tau_j g_n\rangle - h_n^2\sum_{j=0}^{N}\|(\nabla_x\tau_j)g_n\|^2 = O(n^0)\,, \quad (4.34)$$

thanks to (4.17). As in Subsection 4.2, we can derive (4.13) and prove that $\mu \neq 0$.

Consider a trajectory $(\phi(t;\mathrm{x}_0^*))_{t\notin\mathrm{coll}(\mathrm{x}_0^*))}$ such that $\pi_x\phi(t;\mathrm{x}_0^*)$ goes to infinity as $t \to \pm\infty$. If it does hit a singularity then $\pi_x\phi(t;\mathrm{x}_0^*)$ must come from infinity, hit the singularity and then go back to infinity ($\mathrm{coll}(\mathrm{x}_0^*)$ contains one point). Since μ vanishes on some $\{\mathrm{x}^* \in T^*\mathbb{R}^3; |x| \ge C\}$, μ vanishes near the tail(s) of $(\phi(t;\mathrm{x}_0^*))_{t\notin\mathrm{coll}(\mathrm{x}_0^*))}$ which is (are) inside this set. By invariance (cf. Lemma 4.4), μ vanishes near each $\phi(t;\mathrm{x}_0^*)$, for $t \notin \mathrm{coll}(\mathrm{x}_0^*)$. This proves (4.11). □

Proof of Lemma 4.7. Let $1 \le j \le N$ and $\tilde{\tau} \in C_0^\infty(\mathbb{R}^4)$ with $\tilde{\tau}(1-\tilde{\chi}_j) = 0$ and $\tilde{\tau} = 0$ near $z_j = 0$. Then $|\tilde{\tau}|^2\tilde{\mu}_j$ is the semiclassical measure of $(\tilde{\tau}\tilde{g}_{n,j})_n$ (see [18]). We may assume that $\tau = \tilde{\tau}\circ J_{j,+}$ is well defined. By (2.21), $\|\tau g_n|\cdot|^{-1/2}\|^2 = \|\tilde{\tau}\tilde{g}_{n,j}\|^2$. By (2.19), $\tau_1 := \tau|\cdot|^{-1/2}$ is smooth. Thus $\langle \tau_1 g_n, (P-\lambda)\tau_1 g_n\rangle \to 0$, by Lemma 4.3 and Lemma 4.4. This yields the bound (4.34) and Eq. (4.13) with g_n replaced by $\tau_1 g_n$. By Proposition 2.1, $\|\tau_1 g_n\|^2 \to |\tau_1|^2\mu(\mathbb{1})$. But the latter is zero since, by Proposition 4.5 and the non-trapping assumption, μ may only have mass above the attractive singularities. Thus $\lim\|\tilde{\tau}\tilde{g}_{n,j}\| = 0$. This implies that $\tilde{\chi}_j\tilde{\mu}_j$ may only have mass above $z_j = 0$.

Now let $\tau \in C_0^\infty(\mathbb{R}^3)$ supported near s_j and inside the set $\chi_j^{-1}(1)$, and set $\tilde{\tau} = \tau\circ\mathcal{K}_j$. Let $\tilde{\varphi} \in C_0^\infty(T^*\mathbb{R}^4)$ such that $\tilde{\varphi} = 1$ on a neighborhood of $(\tilde{p}_{j,\lambda})^{-1}(0)\cap(\operatorname{supp}\tilde{\chi}_j \times \mathbb{R}^4)$. Let $r \in \mathbb{R}$. For n large enough, the well defined symbols $\tilde{\tau}(1-$

$\tilde{\varphi})(\tilde{p}_{j,\lambda_n})^{-1}$ belong to $\Sigma_{r,-2}$ and form a bounded sequence in this set. Writing $\tilde{\tau}(1-\tilde{\varphi}) = \tilde{\tau}(1-\tilde{\varphi})(\tilde{p}_{j,\lambda_n})^{-1}\cdot\tilde{\chi}_j\tilde{p}_{j,\lambda_n}$ and using pseudodifferential calculus and (4.25),

$$\big(\tilde{\tau}(1-\tilde{\varphi})\big)^w_{h_n}\tilde{g}_{n,j} = \big(\tilde{\tau}(1-\tilde{\varphi})(\tilde{p}_{j,\lambda_n})^{-1}\big)^w_{h_n}\tilde{\chi}_j\tilde{P}_j(h_n;\lambda_n)\tilde{g}_{n,j}+O(h_n) = O(h_n) \quad (4.35)$$

in $\mathrm{L}^2(\mathbb{R}^4)$. Notice that if $(0,\zeta)\in(\tilde{p}_{j,\lambda})^{-1}(0)$ then $|\zeta|^2 = -f(s_j)\neq 0$ and $\zeta\neq 0$. Now, using (2.19), we can choose the support of τ small enough around $z=0$ such that, for some $s_0'>0$, $\operatorname{supp}(\tilde{\tau}\tilde{\varphi})\circ\tilde{\phi}(s';\,\cdot\,)\subset\tilde{\chi}_j^{-1}(1)$, for $0\le s'\le s_0'$, and $(\tilde{\tau}\tilde{\varphi})\circ\tilde{\phi}(s';\,\cdot\,)=0$ near $\{0\}\times\mathbb{R}^4\subset T^*\mathbb{R}^4$. Using (2.21), (4.35), and (2.5) applied to $\tilde{g}_{n,j}$ and $\tilde{\mu}_j$,

$$\|\tau g_n\|^2 = \|\tilde{\tau}\tilde{g}_{n,j}|\cdot|\,\|^2 = \|\tilde{\tau}\tilde{\varphi}\tilde{g}_{n,j}|\cdot|\,\|^2 + O(h_n) = \tilde{\mu}_j(\tilde{\tau}^2\tilde{\varphi}^2|\cdot|^2) + o(n^0)\,.$$

By (4.26), $\tilde{\mu}_j(\tilde{\tau}^2\tilde{\varphi}^2|\cdot|^2) = \tilde{\mu}_j((\tilde{\tau}^2\tilde{\varphi}^2|\cdot|^2)\circ\tilde{\phi}(s_0';\,\cdot\,)) = 0$, by the choice of s_0'. Therefore $\lim\|\tau g_n\|^2 = 0$, yielding $\mu=0$ near s_j. Thus $\mu=0$. □

Actually, if trapping occurs, we have the following stronger result on the measure μ.

Proposition 4.9. *Let $N>0$ and $d=3$. If $\mathrm{x}^*\in\operatorname{supp}\mu\cap T^*(\mathbb{R}^3\setminus\mathcal{S})$ and $t\notin\operatorname{coll}(\mathrm{x}^*)$ then $\phi(t;\mathrm{x}^*)\in\operatorname{supp}\mu$.*

Proof. Let $1\le j\le N$. Let $\mathrm{x}_0^* := (x_0,\xi_0)\in p^{-1}(\lambda)$ such that $\chi_j=1$ near x_0. By the properties of the KS-transform (4.19) (cf. (2.22)), there exists $\mathrm{z}_0^* = (z_0,\zeta_0)\in T^*\mathbb{R}^4$ such that $\mathrm{x}_0^* = \mathcal{K}_j^*(\mathrm{z}_0^*)$. Let $\mathrm{t}_0^* = (0,p(\mathrm{x}_0^*)) = (0,\lambda)$. We consider the trajectory $\{\pi_x\phi^t(\mathrm{x}_0^*), t\in\mathbb{R}\}$ and assume that it hits the singularity s_j at time t_0. Let $t'>t_0$ such that $\chi_j(\pi_x\phi(t';\mathrm{x}_0^*))=1$. There exists some $s'\in\mathbb{R}$ such that $t' = t_j(s';\mathrm{t}_0^*,\mathrm{z}_0^*)$ (cf. (2.25)). Here $t_j(s;\mathrm{t}^*,\mathrm{z}^*)$ is the first component of the flow $\tilde{\phi}_j(s;\mathrm{t}^*,\mathrm{z}^*)$ given by (2.25) with $\tilde{p}$ replaced by (4.21). Let $\tau_0\in C_0^\infty(\mathbb{R}^3)$ such that $\chi_j=1$ near $\operatorname{supp}\tau_0$, $\tau_0=1$ near x_0, and $\tau_0=0$ near s_j. The semiclassical measure μ_1 of the sequence $(\tau_0 g_n)_n$, viewed as a bounded sequence in $\mathrm{L}^2(\mathbb{R}^3\times S^1)$, is $\mu\otimes 1\otimes\delta_0$ on $T^*\mathbb{R}^3\times T^*S^1$. Let $\psi\in C_0^\infty(\mathbb{R})$ such that $\psi=1$ near 0 and $K_0\subset\subset\mathbb{R}^3$ be a vicinity of ξ_0. Let $a\in C_0^\infty(T^*\mathbb{R}^3)$ such that $\tau_0=1$ near $\pi_x\operatorname{supp}a$ and $\pi_\xi\operatorname{supp}a\subset K_0$. For $(\mathrm{x}^*;\theta^*) := (x;\xi;\theta;\sigma)\in T^*\mathbb{R}^3\times T^*S^1$, set $a_1(\mathrm{x}^*;\theta^*) = \psi(\sigma)a(\mathrm{x}^*)$. Let $\psi_1+\psi_2=1$ be a smooth partition of unity on S^1. Notice that

$$\mu(a) = \tau_0\mu(a) = \tau_0\mu_1(a_1) = \sum_{k=1}^{2}\tau_0\mu_1(a_1\psi_k)\,. \quad (4.36)$$

For each $k\in\{1;2\}$, we may apply Proposition 2.2 with $u_n = \tau_0 g_n\psi_k\in\mathrm{L}^2(\mathbb{R}^3\times S^1)$ and $\Phi = (\mathcal{K}_j,\mathcal{A}_{j,+})$, since $(\mathcal{K}_j,\mathcal{A}_{j,+})$ is a local diffeomorphism near $\operatorname{supp}\tau_0\times\operatorname{supp}\psi_k$ by (2.20). Thus $((\tau_0\psi_k)\circ(\mathcal{K}_j,\mathcal{A}_{j,+}))\tilde{\mu}_j(\tilde{b}_k) = \tau_0\mu_1(a_1\psi_k)$, where $\tilde{b}_k = (a_1\psi_k)\circ(\mathcal{K}_j,\mathcal{A}_{j,+})_c$, since $((\tau_0\psi_k)\circ(\mathcal{K}_j,\mathcal{A}_{j,+}))\tilde{\mu}_j$ is the semiclassical measure of $((\tau_0 g_n\psi_k)\circ(\mathcal{K}_j,\mathcal{A}_{j,+}))_n$. Now we can choose K_0 and $\operatorname{supp}\tau_0$ small enough such that, for all $k\in\{1;2\}$, $\tilde{b}_k\circ\tilde{\phi}_j^{s'}=0$ near $\{0\}\times\mathbb{R}^4$ and $(1-\tilde{\chi}_j)\tilde{b}_k\circ\tilde{\phi}_j^t=0$, for $0\le t\le s'$. Thus (4.26) holds true with $s=s'$ and $\tilde{b}=\tilde{b}_k$. Let $\tilde{\tau}_k\in C_0^\infty(\mathbb{R}^4)$ such that $\tilde{\chi}_j=1$ near $\operatorname{supp}\tilde{\tau}_k$, $\tilde{\tau}_k=1$ near $\pi_z\operatorname{supp}\tilde{b}_k\circ\tilde{\phi}_j^{s'}$, and $\tilde{\tau}_k=0$ near

$z_j = 0$. We may assume that $\mathcal{J}_{j,+}$ is a local diffeomorphism with local inverse $(\mathcal{K}_j, \mathcal{A}_{j,+})$ near $\pi_z \mathrm{supp}\, \tilde{b}_k \circ \tilde{\phi}_j^{s'}$ (cf. (2.20)). Thus we can apply Proposition 2.2 with $u_n = \tilde{\tau}_k \tilde{g}_{n,j} \in \mathrm{L}^2(\mathbb{R}^4)$ and $\Phi = \mathcal{J}_{j,+}$. This yields $\tilde{\tau}_k \tilde{\mu}_j (\tilde{b}_k \circ \tilde{\phi}_j^{s'}) = \tau_k \mu_1(a_{s',k})$, where $\tau_k = \tilde{\tau}_k \circ \mathcal{J}_{j,+}$ and $a_{s',k} = \tilde{b}_k \circ \tilde{\phi}_j^{s'} \circ (\mathcal{J}_{j,+})_c$. Now we see that, if μ is zero near $\phi(t'; \mathrm{x}_0^*)$, then we can choose K_0 and $\mathrm{supp}\, \tau_0$ small enough such that $\tau_k \mu_1(a_{s',k}) = 0$, for $k \in \{1; 2\}$. By (4.36), this implies that $\mu(a) = 0$, for a with small enough support near x_0^*. Since we can reverse the time direction, we get the desired result. □

4.4. A simpler proof for weighted L^2 estimates

In Subsections 4.1, 4.2, and 4.3, we proved that the non-trapping condition implies the Besov estimate (1.11). By (1.7), the latter implies the existence of some $C > 0$ such that, for all $s > 1/2$,

$$\sup_{\substack{\Re z \in I \\ \Im z \neq 0}} \|R(z; h)\|_{\mathrm{L}^2_s, \mathrm{L}^2_{-s}} \leq C \cdot h^{-1}, \tag{4.37}$$

a weighted L^2 estimate. This derivation of (4.37) from the non-trapping condition uses Proposition 4.2, the proof of which is based on arguments borrowed from [6]. The latter are rather involved since, in [6], the potential is assumed to be C^2 only. In particular, a special pseudodifferential calculus, adapted to this low regularity, is used there. Since our potential here is C^∞ outside the singularities, we want to give a simpler proof of the following, slightly weaker result.

Proposition 4.10. *Under the assumptions of Theorem* 1.1*, we assume that p is non-trapping at each energy $\lambda \in I_0$. Then, for any compact interval $I \subset I_0$ and any $s > 1/2$, there exists $C_s > 0$ such that* (4.37) *holds true with $C = C_s$.*

Proof. Let $d \geq 3$. We can follow the arguments in Subsections 4.1, 4.2, and 4.3, if Proposition 4.2 is replaced by

$$\exists R_0' > R_0 ; \quad \lim_{n \to \infty} \left\| \mathbb{1}_{\{|\cdot| > R_0'\}} f_n \right\|_{\mathrm{L}^2_{-s}} = 0 . \tag{4.38}$$

Indeed, for functions localized in $\{x \in \mathbb{R}^d; |x| \leq R_0'\}$, the norms $\|\cdot\|_B$ and $\|\cdot\|_{\mathrm{L}^2_s}$ are equivalent and so are the norms $\|\cdot\|_{B^*}$ and $\|\cdot\|_{\mathrm{L}^2_{-s}}$. So we are left with the proof of (4.38). We follow the proof of Proposition 4.2 and arrive at (4.4). Now, by [24], we can find $c > 0$, a function $\chi_1 \in C_0^\infty(\mathbb{R}^d)$, and a symbol $a \in \Sigma_{0;0}$ satisfying the following properties. The function $\chi_1 = 1$ on a large enough neighbourhood of 0 and of the support of χ and

$$\alpha_n \ \geq \ c \cdot \left\| (1 - \chi_1) \theta\big(P_\chi(h_n)\big) f_n \right\|^2_{\mathrm{L}^2_{-s}} + o(1) .$$

Following again the proof of Proposition 4.2, we get (4.38). □

5. On the validity of the non-trapping condition

The aim of this section is to provide examples both of validity and of invalidity of the non-trapping condition (1.10). As we shall see in Corollary 5.2 below, the non-trapping property is seldom fulfilled if there is some singularity ($N' > 0$), even at positive energies. This is in strong contrast to the smooth case, for which p is always non-trapping at large enough positive energies.

To study the non-trapping condition (1.10) when an attractive singularity is present (and $d = 3$), we need to review the regularization of the Hamilton flow of p, described in Section 2, in a more sophisticated way. Recall that $\hat{M} = \mathbb{R}^3 \setminus \mathcal{S}$. Let ω_0 be the natural symplectic two-form on $T^*\mathbb{R}^3$ given by $\sum_{j=1}^3 dx_i \wedge d\xi_i$ and also its restriction to $\hat{P}$. It is well known (see [32], Thm. 5.1) that there exists an extension (M, ω, m) of the Hamiltonian system $(\hat{P}, \omega_0, p)$, where as a set the six-dimensional smooth manifold M equals

$$M := \hat{P} \cup \bigcup_{i=1}^{N} (\mathbb{R} \times S^2)\,.$$

Here the ith copy $\mathbb{R} \times S^2$ parameterizes energy and direction of the particle colliding with the attractive singularity s_i. Using the symplectic form ω on M, the Hamiltonian function $m \in C^\infty(M)$ generates a smooth complete flow

$$\Phi : \mathbb{R} \times M \longrightarrow M\,, \quad (t; \mathrm{x}^*) \mapsto \Phi(t; \mathrm{x}^*) =: \Phi^t(\mathrm{x}^*)\,. \tag{5.1}$$

A collision time for $\mathrm{x}^* \in M$ is a time t_0 such that $\Phi(t_0; \mathrm{x}^*) \notin \hat{P}$. If t is not a collision time for $\mathrm{x}^* \in \hat{P}$ then $\Phi(t; \mathrm{x}^*) = \phi(t; \mathrm{x}^*)$, defined just before (2.17).

Proposition 5.1. *Consider for $d = 2$ or 3 a regular value $\lambda > 0$ of V. If the set*

$$\mathcal{H}_\lambda := \left\{x \in \mathbb{R}^d;\, V(x) \geq \lambda \text{ or } x \in \mathcal{S}\right\}$$

is not homeomorphic to a d-dimensional ball or a point, then p is trapping at energy λ, i.e. (1.10) *is false.*

Proof. We write $\mathcal{H}_\lambda$ as the disjoint union $\tilde{\mathcal{H}}_\lambda \dot{\cup} \{s_1, \ldots, s_N\}$ with

$$\tilde{\mathcal{H}}_\lambda := \left\{x \in \mathbb{R}^d;\, V(x) \geq \lambda \text{ or } x \in \{s_{N+1}, \ldots, s_{N'}\}\right\}.$$

Then $\tilde{\mathcal{H}}_\lambda$ is a d-dimensional manifold with boundary, since by assumption λ is a regular value of V. It is compact since by assumption $\lim_{|x|\to\infty} V(x) = 0$ but $\lambda > 0$. Notice that $\tilde{\mathcal{H}}_\lambda$ is a neighbourhood of the repulsive singularities $s_{N+1}, \ldots, s_{N'}$, but there exist neighbourhoods of the attractive singularities $s_1, \ldots, s_N$ that are disjoint from $\tilde{\mathcal{H}}_\lambda$. In the presence of repulsive singularities $\tilde{\mathcal{H}}_\lambda$ is nonempty. In any case, $\mathcal{H}_\lambda$ is a nonempty compact set. We denote by $\mathrm{Int}(\mathcal{H}_\lambda)$ the interior of $\mathcal{H}_\lambda$. Now we assume that $\mathcal{H}_\lambda$ is not homeomorphic to a d-dimensional ball nor to a point, and we construct a periodic orbit, thus proving trapping. We discern two cases.

First case: $\mathcal{H}_\lambda$ has two or more connected components.

Here the idea is to construct a periodic orbit (using curve shortening), whose projection on configuration space is a curve connecting two components of $\mathcal{H}_\lambda$. Let $g_{\rm Euclid}$ denotes the euclidean metric on $\mathbb{R}^d$. We now use the Jacobi metric $\hat{g}_\lambda$, defined on $\mathbb{R}^d \setminus \mathcal{H}_\lambda$ by

$$\hat{g}_\lambda(q) := \big(\lambda - V(q)\big) g_{\rm Euclid} \,. \tag{5.2}$$

It is known (see e.g. [28] and [4]) that for regular curves $c : [0,1] \to \mathbb{R}^d \setminus \mathrm{Int}(\mathcal{H}_\lambda)$ with $c(1) = s_i$ $(i \le N)$ the length

$$\mathcal{L}(c) := \lim_{t \nearrow 1} \int_0^t \sqrt{\hat{g}_\lambda\big(c(s)\big)\big(\dot{c}(s), \dot{c}(s)\big)}\, ds$$

is finite. By compactness of $\mathcal{H}_\lambda$ the number ℓ of connected components of $\mathcal{H}_\lambda$ is finite. Denoting them by $\mathcal{H}_{\lambda;1}, \dots, \mathcal{H}_{\lambda;\ell}$, for $1 \le i < j \le \ell$

$$D_\lambda(i,j) := \inf_{c : c(0) \in \mathcal{H}_{\lambda;i}\,,\, c(1) \in \mathcal{H}_{\lambda;j}} \mathcal{L}(c) > 0\,,$$

that is, the different components have positive geodesic distances.

Taking R large enough, we can ensure that these mutual distances are smaller than the corresponding geodesic distance of the $\mathcal{H}_{\lambda;i}$ to the region $\{x \in \mathbb{R}^d; |x| \ge R\}$.

The (standard) approach is to consider the negative gradient flow of the *energy functional*

$$\mathcal{E}(c) := \int_0^1 \hat{g}_\lambda\big(c(s)\big)\big(\dot{c}(s), \dot{c}(s)\big)\, ds\,, \quad \text{with} \quad c(0) \in \mathcal{H}_{\lambda;i_0} \quad \text{and} \quad c(1) \in \mathcal{H}_{\lambda;i_1}$$

in order to approximate geodesic segments, which are then critical points of $\mathcal{E}$ with respect to these boundary conditions.

Due to the degeneracy of the Jacobi metric (5.2) at $\partial(\mathbb{R}^d \setminus \mathcal{H}_\lambda)$ still no Palais–Smale condition is satisfied for $\mathcal{E}$, that is, a vanishing gradient of $\mathcal{E}$ at c does not ensure that c is a geodesic (see Klingenberg [30], Chapter 2.4 for a discussion of the Palais–Smale condition).

However, as λ is assumed to be a regular value of V, the regularization technique devised by Seifert in [48] and later by Gluck and Ziller in [19] can be applied to yield a geodesic segment of length equal to $D_\lambda(i_0, i_1) = \min_{i<j} D_\lambda(i,j) > 0$, with $c(0) \in \mathcal{H}_{\lambda;i_0}$ and $c(1) \in \mathcal{H}_{\lambda;i_1}$.

We denote the restriction of the flow Φ^t to $m^{-1}(\lambda)$ by Φ^t_λ. Away from the end points, and up to time parameterization, the geodesic segment in the Jacobi metric corresponds to a segment of a Φ^t_λ-solution curve. See [1], Thm. 3.7.7 for a proof.

This segment is part of a periodic orbit, whose period is twice the time needed to parametrize the segment:

- If $V(c(i_k)) = \lambda$, then (by our regularity assumption for the value λ) $\nabla V(c(i_k)) \neq 0$. Furthermore the geodesic segment at this point has a normalized tangent

$$\lim_{s \nearrow i_k} \|c(s) - c(i_k)\|^{-1}\big(c(s) - c(i_k)\big)$$

which is parallel to $\nabla V(c(i_k))$ (see [19], Sect. 6). Thus the solution curve can be continued by *time reversal* (cf. (2.16))

$$c(i_k + s) := c(i_k - s) \quad (s > 0)\,. \tag{5.3}$$

- Similarly, if instead $c(i_k) \in \{s_1, \dots, s_N\}$, that is, $c(t)$ converges to an attracting singularity, then, time reversal (5.3) again continues the geodesic segment c and thus the Φ_λ^t-solution curve as well.

In both cases we thus constructed a periodic Φ_λ-orbit.

Second case: $\mathcal{H}_\lambda$ has only one component, which however is not homeomorphic to a d-dimensional ball nor a point. Thus it is a connected compact d-dimensional submanifold of $\mathbb{R}^d$ with boundary not homeomorphic to $\mathbb{S}^{d-1}$.

- If $\mathbb{R}^d \setminus \mathrm{Int}(\mathcal{H}_\lambda)$ contains a compact connected component, then this arises as the projection on configuration space of a connected component of the regularized energy surface $m^{-1}(\lambda)$. This flow-invariant component is compact too, and thus consists of trapped orbits.
- If, however $\mathbb{R}^d \setminus \mathrm{Int}(\mathcal{H}_\lambda)$ does not contain a compact component, it necessarily is connected since $d \geq 2$ and $\mathcal{H}_\lambda$ is compact. In this situation, the boundary $\partial\mathcal{H}_\lambda$ consists of one component, which is not homeomorphic to $\mathbb{S}^{d-1}$. In this situation Corollary 3.3 of [31] ensures the existence of a periodic so–called brake orbit, that is a trapped orbit in the terminology of our paper (although [31] treats smooth potentials, in the case at hand all singularities of our potential are repelling. Thus the dynamics at energy λ is unaffected by the singularities.). □

A converse of Proposition 5.1 does not hold true in general. That is, there are potentials like Yukawa's potential $V(x) = -e^{-|x|}/|x|$ for which $\mathcal{H}_\lambda$ consists only of one point but still there are trapped orbits for small $\lambda > 0$, see [28]. Yet Proposition 5.1 gives us the

Corollary 5.2. *Consider for $d = 2$ or 3 a regular value $\lambda > 0$ of V.*

If $N > 1$ or if $N = 1$ and $N' > N$, then p is trapping at energy λ.

If $N' \geq 2$ then p is trapping at energy λ, for λ large enough.

Proof. In all cases, $\mathcal{H}_\lambda$ has several connected components. Thus Proposition 5.1 gives the result. □

However one can find non-trapping situations as in Examples 5.3 and 5.4 below.

Example 5.3. Let $N' \in \mathbb{N}^*$. Let V be defined on $\mathbb{R}^d \setminus \mathcal{S}$ by $V(x) = \sum_{j=1}^{N'} f_j/|x - s_j|$ with $f_j > 0$, for any $1 \leq j \leq N'$. It satisfies (1.2) with $N = 0$. For $0 < \lambda < (\sum_{j=1}^{N'} |s_j|/f_j)^{-1}$, p is non-trapping at energy λ.

Proof. Recall that $a_0(x,\xi) = x \cdot \xi$. For $(x,\xi) \in p^{-1}(\lambda)$,

$$\{p, a_0\}(x,\xi) = 2|\xi|^2 + \sum_{j=1}^{N'} f_j x \cdot \frac{x - s_j}{|x - s_j|^3} = |\xi|^2 + \lambda + \sum_{j=1}^{N'} f_j s_j \cdot \frac{x - s_j}{|x - s_j|^3}$$
$$\geq \lambda - \sum_{j=1}^{N'} \frac{|s_j|\lambda^2}{f_j} = \lambda \left(1 - \lambda \sum_{j=1}^{N'} \frac{|s_j|}{f_j}\right) > 0 \,.$$

Here we used that $0 < f_j/|x - s_j| \leq \lambda$, for $(x,\xi) \in p^{-1}(\lambda)$. Now standard arguments yields the result (see the proof of Lemma 3.1, for instance). □

Example 5.4. Let $\lambda, c, \rho > 0$ and $W \in C^\infty(\mathbb{R}^d; \mathbb{R})$ such that

$$\forall \alpha \in \mathbb{N}^d \,, \quad \exists C_\alpha > 0 \,; \quad \forall x \in \mathbb{R}^d \,, \quad |\partial_x^\alpha W(x)| \leq C_\alpha \langle x \rangle^{-\rho - |\alpha|} \,.$$

Let $V \in C^\infty(\mathbb{R}^d \setminus \{0\}; \mathbb{R})$ defined by $V(x) = -c/|x| + W(x)$. Depending on c and λ, one can find small enough $(C_\alpha)_{|\alpha| \leq 1}$'s such that p is non-trapping at energy λ.

Proof. The function $\tilde{p}$ defined just before (2.24) takes the following form: $\tilde{p}(\mathrm{t}^*; \mathrm{z}^*) = \tilde{p}(t, \tau; z, \zeta) = |\zeta|^2 - c + |z|^2 (W \circ \mathcal{K}(z) - \tau)$. Let $b_0 : T^*\mathbb{R} \times T^*\mathbb{R}^d \longrightarrow \mathbb{R}$ be defined by $b_0(\mathrm{t}^*; \mathrm{z}^*) = \zeta \cdot z$. Then

$$\{\tilde{p}\,,\, b_0\}(\mathrm{t}^*; \mathrm{z}^*) = 2\tilde{p}(\mathrm{t}^*; \mathrm{z}^*) + 2c + |z|^2 \big(4\tau - 4W \circ \mathcal{K}(z) - z \cdot \nabla_z (W \circ \mathcal{K})(z)\big) \,. \quad (5.4)$$

Thanks to (2.19), we can choose the $(C_\alpha)_{|\alpha| \leq 1}$'s small enough such that, for $\tau = \lambda > 0$, the last term in (5.4) is everywhere non-negative. Thus, on $\tilde{p}^{-1}(]-c/2; c/2[)$, $\{\tilde{p}\,,\, b_0\} \geq c$. This implies that, for any solution $s \mapsto (t(s), \lambda; z(s), \zeta(s))$ of (2.24) leaving in $\tilde{p}^{-1}(0)$, the function $s \mapsto |z(s)|^2$ is strictly convex. It must go to infinity in both time s directions. By (2.25), this implies that any broken trajectory $(\phi(t; \mathrm{x}^*))_{t \in \mathbb{R} \setminus \mathrm{coll}(\mathrm{x}^*)}$ with $p(\mathrm{x}^*) = \lambda$ goes to infinity in both time t directions. □

Remark 5.5. By inspection of (5.4) we see that, for a potential of the form $V(x) = \frac{f(x)}{|x|} + W(x)$ with $f(0) < 0$ and meeting (1.1), no trapping occurs for high enough energies.

6. Scattering by a molecular potential

We now show that our analysis can be applied to Example 1.3.

The potential $x \mapsto \sum_j e_0 z_j |x - s_j|^{-1}$ of $P_1(h_0)$ is smooth on $\hat{M} = \mathbb{R}^3 \setminus \{s_1, \ldots, s_{N'}\}$ and satisfies (1.1). By local elliptic regularity (see [43], Thm. IX.26), the electronic eigenfunctions $\psi_k \in \mathrm{L}^2(\mathbb{R}^3)$ of $P_1(h_0)$ are smooth on $\hat{M}$. Furthermore, they are continuous on $\mathbb{R}^3$ (see [8], Thm. 2.4) and the corresponding eigenvalues E_k are negative by [12] (see also [8], Thm. 4.19). Using [2] outside the ball $B := \{x \in \mathbb{R}^3; |x| \leq R_0\}$ (cf. (1.1)), one can show that the ψ_k's decay exponentially. This means, for any k, that there exists $c_k, C_k > 0$ such that

$$x \notin B \implies |\psi_k(x)| \leq C_k e^{-c_k |x|} \,. \quad (6.1)$$

By (1.1), the result in [2] can be applied to the derivatives of the ψ_k outside B. Thus (6.1) holds true for these derivatives with possibly different constants c_k, C_k. For any $j \in \{1, \dots, N'\}$, it turns out that $\psi_{kj} : \mathbb{R}^4 \ni z \mapsto \psi_k(s_j + \mathcal{K}(z))$, with $\mathcal{K}(z)$ defined in (2.19), is smooth near $z = 0$. Indeed, we can show as in [13] (see also the proof of (4.25) in Lemma 4.8) that the equation $P_1(h_0)\psi_k = E_k\psi_k$ can be lifted to a Schrödinger equation in $\mathbb{R}^4$ with smooth potential solved by the function ψ_{kj}. Again, the elliptic regularity gives the desired result. Therefore the charge densities $\rho_k := |\psi_k|^2$ are smooth on $\hat{M}$ and continuous on $\mathbb{R}^d$. The ρ_k and their derivatives satisfy (6.1). For any $j \in \{1, \dots, N'\}$, $\rho_{kj} : \mathbb{R}^4 \ni z \mapsto \rho_k(s_j + \mathcal{K}(z))$ is smooth near $z = 0$. This allows us to obtain the following properties for the W_k.

Proposition 6.1. *Let $k \in \{1, \dots, K\}$. The potential W_k is smooth on $\hat{M}$, continuous on $\mathbb{R}^3$, and satisfies* (1.1). *For any $j \in \{1, \dots, N'\}$, the function $W_{kj} : \mathbb{R}^4 \ni z \mapsto W_k(s_j + \mathcal{K}(z))$, with $\mathcal{K}(z)$ defined in* (2.19), *is smooth near $z = 0$.*

Proof. Since $|\cdot|^{-1} \in \mathrm{L}^1(\mathbb{R}^3) + \mathrm{L}^\infty(\mathbb{R}^3)$, $\rho_k \in \mathrm{L}^1(\mathbb{R}^3)$, and ρ_k is continuous, W_k is well defined and continuous on $\mathbb{R}^3$. Let $j \in \{1, \dots, N'\}$, $y \in \hat{M}$, and consider a partition of unity in $\mathbb{R}^3$ of the form $\sum_{j=0}^{N'} \chi_j = 1$ with $\chi_j \in C_0^\infty$ and $\chi_j = 1$ near s_j, for $j \geq 1$, and $\chi_0 = 1$ near y. Denoting by $*$ the convolution product, we can write near y, for any k and any multiindex $\alpha \in \mathbb{N}^d$,

$$D_x^\alpha W_k = D_x^\alpha(\rho_k * |\cdot|^{-1}) = \sum_{j=1}^{N'} (\rho_k \chi_j) * D_x^\alpha |\cdot|^{-1} + \big(D_x^\alpha(\rho_k \chi_0)\big) * |\cdot|^{-1} \tag{6.2}$$

(as distributions). This defines a continuous function near y. Using the exponential decay of the functions ρ_k, we can show that W_k satisfies (1.1).

Let $j \in \{1, \dots, N'\}$. We want to show that the function $\mathbb{R}^4 \ni z \mapsto (\rho_k * |\cdot|^{-1})(s_j + \mathcal{K}(z))$ is a constant times the function $\mathbb{R}^4 \ni z \mapsto (\rho_{kj} * |\cdot|^{-2})(z)$. Notice that, for an $f \in C(\mathbb{R}^4) \cap \mathrm{L}^1(\mathbb{R}^4)$, $f * |\cdot|^{-2}$ is a well defined continuous function since $|\cdot|^{-2} \in \mathrm{L}^1(\mathbb{R}^4) + \mathrm{L}^\infty(\mathbb{R}^4)$. Now, it is convenient to view $\mathbb{R}^4$ as the quaternion space $\mathbb{H}$ and to use the representation of $\mathcal{K}$ on this space (see the appendix). In particular, one can use formula (3) from [13], saying that for $x := \mathcal{K}(Y)$, $Y \in \mathbb{H}$, $|Y|^2\, dY = c \cdot dx\, d\theta$ for some constant $c > 0$ ($d\theta$ is uniquely defined by (2.20), compare also with the group action (A.4)). Then, using Lemma 6.2 below, we get

$$\begin{aligned}
(\rho_{kj} * |\cdot|^{-2})(Z) &= \int_{\mathbb{R}^4} \frac{\rho_k(s_j + \mathcal{K}(Y))}{|Y - Z|^2} |Y|^2 dY \\
&= c \cdot \int_{\mathbb{R}^3 \times S^1} \frac{\rho_k(s_j + x)}{|Y(x,\theta) - Z|^2} dx\, d\theta \\
&= c' \cdot \int_{\mathbb{R}^3} \frac{\rho_k(s_j + x)}{|x - \mathcal{K}(Z)|} dx \\
&= c' \cdot \int_{\mathbb{R}^3} \frac{\rho_k(s_j + x)}{|s_j + x - s_j - \mathcal{K}(Z)|} dx \\
&= c'(\rho_k * |\cdot|^{-1})\big(s_j + \mathcal{K}(Z)\big)\,,
\end{aligned}$$

for $Z \in \mathbb{H}$, and $c' > 0$. Now, since ρ_{kj} is smooth near 0 and $|\cdot|^{-1}$ is smooth away from 0, we can use a formula similar to (6.2) to show that $\rho_{kj} * |\cdot|^{-2}$ is smooth near 0. □

Lemma 6.2. *For $X, Z \in \mathbb{H}$ with $\mathcal{K}(Z) \neq \mathcal{K}(X)$*

$$\int_0^{2\pi} |\exp(I_1\theta)Z - X|^{-2}\, d\theta = 2\pi \cdot |\mathcal{K}(Z) - \mathcal{K}(X)|^{-1}\,.$$

Proof. Assuming the condition, both sides are well-defined. Then, using the definition of the real part of a quaternion (see appendix)

$$\begin{aligned}
&\int_0^{2\pi} |\exp(I_1\theta)Z - X|^{-2}\, d\theta \\
&= \int_0^{2\pi} \Big(|Z|^2 + |X|^2 - 2\mathrm{Re}\Big(\big(\cos(\theta) + I_1\sin(\theta)\big)ZX^*\Big)\Big)^{-1} d\theta \\
&= \int_0^{2\pi} \Big(|Z|^2 + |X|^2 - 2\big(\mathrm{Re}(ZX^*)\cos(\theta) + \mathrm{Re}(I_1ZX^*)\sin(\theta)\big)\Big)^{-1} d\theta \\
&= \int_0^{2\pi} \Big(|Z|^2 + |X|^2 - 2\sqrt{\big(\mathrm{Re}(ZX^*)\big)^2 + \big(\mathrm{Re}(I_1ZX^*)\big)^2}\cos(\psi)\Big)^{-1} d\psi \\
&= 2\pi \cdot \Big((|Z|^2 + |X|^2)^2 - 4\big(\mathrm{Re}(ZX^*)\big)^2 - 4\big(\mathrm{Re}(I_1ZX^*)\big)^2\Big)^{-1/2} \\
&= 2\pi \cdot |Z^*I_1Z - X^*I_1X|^{-1} = 2\pi \cdot |\mathcal{K}(Z) - \mathcal{K}(X)|^{-1}\,,
\end{aligned}$$

the last two equations being due to (A.5) and (A.3). □

Now we are able to explain why the proof of our results can be adapted to treat the potential V defined in (1.13). In the proof of the necessity of the non-trapping condition in Section 3, the results away from the singularities work since V satisfies (1.1). Since the W_{kj} are smooth near 0, the results in [13] (see Lemmata 3.3 and 3.4) are still valid. Since each W_k is bounded, it is small compared to a repulsive potential $+|\cdot - s_j|^{-1}$ near the corresponding repulsive singularity s_j. So Section 3.3 is also valid. In the proof of the converse in Section 4, the results away from the singularities hold true since (1.1) is still valid. The fact that the W_k is small compared to the size of a singular potential $\pm|\cdot - s_j|^{-1}$ near the corresponding singularity s_j explains why Section 4.2 works and also the validity of (4.18). The fact that the W_{kj} are smooth near 0, ensures that Lemma 4.8 still works.

Appendix A. The Hopf map

We use the following notation for the quaternion algebra over $\mathbb{R}$:

$$\mathbb{H} := \left\{ \begin{pmatrix} w_1 & -w_2 \\ \bar{w}_2 & \bar{w}_1 \end{pmatrix} \middle| \, w_1, w_2 \in \mathbb{C} \right\} \cong \mathbb{R}^4$$

with matrix multiplication, and basis

$$(I_0, I_1, I_2, I_3) := \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} \right).$$

The direct sum decomposition $\mathbb{H} = \mathbb{R} \cdot \mathbb{1} \oplus \mathrm{Im}\mathbb{H}$ with

$$\mathrm{Im}\mathbb{H} := \{Z \in \mathbb{H} \mid Z^2 = \lambda \cdot \mathbb{1} \text{ with } \lambda \leq 0\} = \mathrm{Span}_{\mathbb{R}}(I_1, I_2, I_3)$$

into real and imaginary space is orthogonal w.r.t. the inner product

$$\mathbb{H} \times \mathbb{H} \to \mathbb{R}, \quad \langle X, Y \rangle := \frac{1}{2} \mathrm{tr}(XY^*),$$

$X \mapsto X^* := \bar{X}^t$ being the conjugation. The norm $|X| := \langle X, X \rangle^{\frac{1}{2}}$ is multiplicative:

$$|XY| = |X|\,|Y| \quad (X, Y \in \mathbb{H}).$$

The *real part* of a quaternion equals $\mathrm{Re}(X) := \frac{1}{2}\mathrm{tr}(X)$.

See, e.g., [10] for more information on $\mathbb{H}$. The *Hopf map* equals

$$\mathcal{K} : \mathbb{H} \to \mathrm{Im}\mathbb{H}, \quad \mathcal{K}(Z) := Z^* I_1 Z = i \begin{pmatrix} w_1\bar{w}_1 - w_2\bar{w}_2 & -2\bar{w}_1 w_2 \\ -2w_1\bar{w}_2 & w_2\bar{w}_2 - w_1\bar{w}_1 \end{pmatrix} \tag{A.3}$$

which is a surjection $\mathbb{R}^4 \to \mathbb{R}^3$ whose preimages are the orbits of the isometric group action

$$\alpha_0 : S^1 \to \mathrm{Aut}(\mathbb{H}), \quad \alpha_0(\theta)(Z) := \exp(\theta I_1) Z. \tag{A.4}$$

This action is free on $\mathbb{H} \setminus \{0\}$. We call $\mathcal{K}$ the Hopf map, since its restriction to S^3 is the Hopf fibration $S^3 \longrightarrow S^2$ with fibre S^1.

Writing $w_1 := z_0 + iz_3$, $w_2 := z_2 + iz_1$ we get formula (2.19) in the basis (I_1, I_2, I_3) of $\mathrm{Im}\mathbb{H}$. Finally we prove the formula

$$|Z^* I_1 Z - X^* I_1 X| = \sqrt{(|Z|^2 + |X|^2)^2 - 4\Big(\big(\mathrm{Re}(ZX^*)\big)^2 + \big(\mathrm{Re}(I_1 Z X^*)\big)^2\Big)} \tag{A.5}$$

used in Section 6.

Notice that, for all $A, B \in \mathbb{H}$, $\mathrm{Re}(I_k A^*) = -\mathrm{Re}(I_k A)$, $\mathrm{Re}(A^*) = \mathrm{Re}(A)$, $\mathrm{Re}(A^* A) = |A|^2$, and

$$\mathrm{Re}(AB) = \mathrm{Re}(A)\mathrm{Re}(B) - \sum_{k=1}^{3} \mathrm{Re}(I_k A)\mathrm{Re}(I_k B). \tag{A.6}$$

Setting $A := I_1 Z X^*$ and $B := I_1 X Z^*$ in (A.6), we get

$$\begin{aligned} \mathrm{Re}\big((I_1 Z X^*)(I_1 X Z^*)\big) = &-\big(\mathrm{Re}(XZ^*)\big)^2 - \big(\mathrm{Re}(I_1 X Z^*)\big)^2 \\ &+ \big(\mathrm{Re}(I_2 X Z^*)\big)^2 + \big(\mathrm{Re}(I_3 X Z^*)\big)^2. \end{aligned}$$

Similarly it follows from (A.6) that $|A|^2 = \sum_{k=0}^{3} (\mathrm{Re}(I_k A))^2$, so that for $A := ZX^*$,

$$|Z|^2\,|X|^2 = |A|^2 = \big(\mathrm{Re}(ZX^*)\big)^2 + \big(\mathrm{Re}(I_1 Z X^*)\big)^2 + \big(\mathrm{Re}(I_2 X Z^*)\big)^2 + \big(\mathrm{Re}(I_3 X Z^*)\big)^2.$$

So

$$\begin{aligned}
|Z^*I_1Z - X^*I_1X|^2 &= (Z^*I_1Z - X^*I_1X)(-Z^*I_1Z + X^*I_1X) \\
&= Z^*I_1(-|Z|^2)I_1Z + X^*I_1(-|X|^2)I_1X \\
&\quad + (Z^*I_1ZX^*I_1X) + (Z^*I_1ZX^*I_1X)^* \\
&= |Z|^4 + |X|^4 + 2\mathrm{Re}\big((I_1ZX^*)(I_1XZ^*)\big) \\
&= |Z|^4 + |X|^4 + 2\Big(- \big(\mathrm{Re}(XZ^*)\big)^2 - \big(\mathrm{Re}(I_1XZ^*)\big)^2 \\
&\quad + \big(\mathrm{Re}(I_2XZ^*)\big)^2 + \big(\mathrm{Re}(I_3XZ^*)\big)^2\Big) \\
&= (|Z|^2 + |X|^2)^2 - 4\Big(\big(\mathrm{Re}(ZX^*)\big)^2 + \big(\mathrm{Re}(I_1ZX^*)\big)^2\Big)\,.
\end{aligned}$$

This proves the claim.

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