SEMI-CLASSICAL DETERMINATION OF EXPONENTIALLY SMALL INTERMODE TRANSITIONS FOR $1+1$ SPACE-TIME SCATTERING SYSTEMS

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ABSTRACT. We consider the semiclassical limit of systems of autonomous PDE's in 1+1 space-time dimensions in a scattering regime. We assume the matrix valued coefficients are analytic in the space variable and we further suppose that the corresponding dispersion relation admits real-valued modes only with one-dimensional polarization subspaces. Hence a BKW-type analysis of the solutions is possible. We typically consider time-dependent solutions to the PDE which are carried asymptotically in the past and as $x \to -\infty$ along one mode only and determine the piece of the solution that is carried for $x \to +\infty$ along some other mode in the future. Because of the assumed non-degeneracy of the modes, such transitions between modes are exponentially small in the semiclassical parameter; this is an expression of the Landau-Zener mechanism. We completely elucidate the space-time properties of the leading term of this exponentially small wave, when the semiclassical parameter is small, for large values of x and t, when some avoided crossing of finite width takes place between the involved modes.

1. INTRODUCTION

Various physical models of wave propagation in space and time are modelled by means of linear systems of autonomous Partial Differential Equations (PDE's), with smooth or analytic coefficients in the space variable $x \in \mathbb{R}^n$. The solutions to such systems are usually difficult to compute in general and one often resorts to asymptotic studies in the limit where the wavelength involved is short with respect to the typical length scale of the problem, on adapted time scales. This regime is often called space-time adiabatic regime or semiclassical regime, due to its relevance in Quantum Mechanics. Typical examples of that situation are the short wavelength approximation of the wave equation, of Maxwell equations and of the Klein-Gordon equation. Similarly, the semiclassical analysis of the Dirac equation, of the Schrödinger equation in solid state physics, or for particles with spin in magnetic fields, and the Born-Oppenheimer approximation in molecular physics belong to the same type of problems. This is true also for certain Quantum systems whose dynamics is constrained in nanotubes or waveguides. Also, the study of shallow water waves in some linearized regime gives rise to the linearized KdV or Boussinesq equations that share similar properties. Plasma physics is another source of physically relevant models entering this category. See e.g. [38], [2], [16], [36], [1]...

From the mathematical point of view, it gives rise to singularly perturbed problems for linear systems of PDE's. These problems are tackled with success by means pseudo-differential operator techniques and/or BKW methods which provide asymptotic solutions up to errors of order $O(\varepsilon^m)$, where ε is the ratio of length scales, and m depends on the peculiarities of the problem. See the monographs [16], [9], [10], [8], [30], [36] for example.

The first step in the study of autonomous linear systems consists is using separation of variables to reduce the problem to a stationary system, parametrized by an energy variable conjugated to the time variable. Superpositions of stationary solutions allow to reconstruct solutions to the full time-dependent problem. Then, one determines the dispersion relations or modes of the corresponding symbol, and the associated polarization subspaces. We will assume that all modes are real valued, i.e. we will consider dispersive waves, according to [38]. In the semiclassical limit, when these real valued modes do not exhibit crossings as the position and energy parameters vary, the dynamics of the waves decouples inside the polarization subspaces in the following sense: to leading order, independent waves driven by the different

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scalar dispersion relations propagate along the corresponding polarization subspaces without interacting. In particular, transitions between isolated modes, or rather between the corresponding polarization subspaces, are forbidden in the semiclassical limit. Moreover, in the scattering limit, these semiclassical transitions are typically of order $O(\varepsilon^{\infty})$, respectively $O(e^{-\Gamma/\varepsilon})$ for some $\Gamma > 0$, in a smooth, respectively analytic context. See e.g. [17], [33], [31], [34], [13], [4], [5], ... This phenomenon goes under the name Landau-Zener mechanism, according to the analysis of the adiabatic approximation of the time dependent Schrödinger equation (in an ODE context) which yields transitions of this order between isolated eigenvalues, [39], [27], [28], [20], [6],... Let us recall here that in case the modes experience crossings at some point, the transitions may be of finite order in ε, indeed of zeroth order in some cases, in the semiclassical limit [16]. Their determination is technically quite different and we do not address these situations.

Although extremely small, the transitions between isolated modes computed in the scattering limit are quite relevant from a physical point of view in the various examples above. It is therefore desirable for an ingoing wave prepared at large negative times along one polarization mode, to determine the asymptotics as $\varepsilon \to 0$ of the part of the waves that propagate for large positive, but finite, times along another mode, be it a transmitted or reflected wave. In a semiclassical context, to achieve such a goal one is lead to further require the initial wave to be well localized in energy.

It is the aim of this paper to determine such exponentially small transmitted waves for quite general autonomous linear systems of PDE's in 1+1 space-time dimensions, when the coefficients are analytic and possess limits they reach sufficiently fast as $|x| \to \infty$.

While the conditions allowing the determination of exponentially small transitions between isolated modes for a variety of physical situations are rather well understood now in a ODE context, or in the language and setting sketched above, for stationary solutions, see [22], [23], [20], [29], [35], [14], [24], [21], [11], [12] [18], [3], [32], ... , it is well known that the description of inter-mode transitions in a time-dependent context requires more work. The only mathematical results we are aware of regarding this issue concern the Born-Oppenheimer approximation in molecular physics [19].

The paper [19] is mainly motivated by molecular physics considerations and the asymptotic descriptions provided there rely heavily on peculiarities of the Born-Oppenheimer approximation considered. However, as will become clear, the general strategy of the analysis is actually model independent and, at the price of sometimes substantial modifications, it can be adapted to fit the various models and situations mentioned above. The importance and frequency of the mechanism of inter-mode transitions in various fields of applied mathematics is the main motivation for the present work. Our aim is to extract practical conditions on a system of PDE's in 1+1 space-time dimensions under which the exponentially small pieces of propagating waves describing inter-mode transitions in a scattering regime can actually be computed, in the semiclassical limit. In that sense, the present paper can be viewed as a generalization of [19].

Let us describe more precisely the autonomous systems we will be dealing with, the type of results we get and the underlying strategy we use to prove these results. Since it requires a fair amount of notations and hypotheses to give a precise statement of our main result, Theorem 6.1, we remain at a rather informal level in this introduction.

Let $\mathcal{R}(x, i\varepsilon\partial_t, i\varepsilon\partial_x)$ be the differential operator:

$$\mathcal{R}(x, i\varepsilon\partial_t, i\varepsilon\partial_x) = \sum_{l\in\{0,\dots,m\}, n\in\{0,\dots,r\}} A_{ln}(x)(i\varepsilon\partial_x)^l(i\varepsilon\partial_t)^n, \tag{1.1}$$

where the $d \times d$ matrix valued coefficients $A_{ln}(x)$ are independent of t and analytic in x a neighborhood of the real axis. Assuming the matrices $A_{ln}(x)$ possess limit as $|x| \to \infty$ which they reach fast enough, we want to describe the small ε behavior of certain solutions $\phi(x, t, \varepsilon)$ to the evolution equation

$$\mathcal{R}(x, i\varepsilon\partial_t, i\varepsilon\partial_x)\phi(x, t, \varepsilon) = 0, \tag{1.2}$$

for $x \in \mathbb{R}$, in the scattering regime t large, in $L^2(\mathbb{R})$.

The $d \times d$ matrix valued symbol, $R(x, E, k)$ corresponding to $\mathcal{R}(x, i\varepsilon\partial_t, i\varepsilon\partial_x)$ writes

$$R(x, E, k) = \sum_{l \in \{0,\dots,m\}, n \in \{0,\dots,r\}} A_{ln}(x) k^l E^n, \tag{1.3}$$

where we call the dual variables E and k the energy and the momentum variables respectively. The energy parameter will be taken in a window $\Delta \subset \mathbb{R}$ specified below. The associated dispersion relations or modes are defined as the set of roots $\{k_j(x, E)\}$ of the polynomial equation in k, of degree md, for $x \in \mathbb{R}$ and $E \in \Delta$,

$$\det R(x, E, k) = 0. \tag{1.4}$$

Our main assumption regarding the type of PDE we consider reads as follows: we suppose there exists an energy window Δ such that for all $E \in \Delta$, and all $x \in \mathbb{R}$, there exist md distinct real valued modes $\{k_j(x, E)\}_{0 \leq j \leq md}$. The associated kernels $R(x, E, k_j(x, E))$, $j = 1, \cdots, md$ are then shown to be one-dimensional and their elements, denoted by $\varphi_j(x, E)$, are the polarization vectors.

For comparison and illustration purposes, the case considered in [19] corresponds to $(i\varepsilon\partial_t + \varepsilon^2\partial_x^2/2 + A_{00}(x))\phi(x, t, \varepsilon) = 0$, where $A_{00}(x) = -V(x)$, is the "electronic hamiltonian", *i.e.* a $d \times d$ self-adjoint matrix. It is assumed that $V(x)$ has non-degenerate eigenvalues $\{e_1(x), \cdots, e_d(x)\}$ with associated eigenvectors $\{\varphi_1(x), \cdots, \varphi_d(x)\}$. For large enough energies E, (1.4) yields $\det\,(E - k^2/2 - V(x)) = 0$, which provides the real valued modes $\{-\sqrt{2(E - e_1(x))}, \cdots, -\sqrt{2(E - e_d(x))}, \sqrt{2(E - e_d(x))}, \cdots, \sqrt{2(E - e_d(x))}\}$ and corresponding polarization vectors $\{\varphi_1(x), \cdots, \varphi_d(x), \varphi_d(x), \cdots, \varphi_1(x)\}$.

Our assumption is very close to the definition of linear dispersive systems in nonuniform autonomous medium given in [38], chapter 11. Such linear systems are characterized there by the fact that the dispersion relation can be solved in the form of real roots

$$E = W(k, x), \quad \text{with} \quad \partial_k^2 W(k, x) \neq 0,$$

for k real and $x \in \mathbb{R}$. This notion is also reminiscent of the strictly hyperbolic equations [37]. In [37], a 1+1 first order partial differential equation is called strictly hyperbolic in x if it can be written as:

$$\partial_x \Phi - A(x, t)\partial_t \Phi - B(x, t)\Phi = 0,$$

where the matrix $A(x_0, t_0)$ has real and distinct eigenvalues. If A and B only depend on x, these equations are of the same type as (1.2) for $r = m = 1$. However, our assumption and this notion are different, in general. The author of [37] gives a characterization for strictly hyperbolic systems of the form

$$\partial_x^m \Phi = \sum_{l < m, l + p \leq m} A_{lp}(x, t)\partial_x^l \partial_t^p \Phi$$

in terms of the principal symbol. By contrast, our assumption concerns the total symbol.

Separation of variables allows to construct solutions to (1.2) by means of the formula

$$\phi(x, t, \varepsilon) := \int_\Delta Q(E, \varepsilon) e^{-itE/\varepsilon} \psi_\varepsilon(x, E)\, dE, \tag{1.5}$$

where $\psi_\varepsilon(x, E)$ is a solution to the energy dependent stationary problem

$$\widehat{R}(x, E, i\varepsilon\partial_x)\psi_\varepsilon(x, E) = 0, \tag{1.6}$$

with

$$\widehat{R}(x, E, i\varepsilon\partial_x) = \sum_{l \in \{0,\dots,m\}, n \in \{0,\dots,r\}} A_{ln}(x) E^n (i\varepsilon\partial_x)^l, \tag{1.7}$$

and the function $Q(\cdot, \varepsilon) : \Delta \mapsto \mathbb{C}$ is an energy density which ensures that E belongs to the prescribed window Δ. The dependence of $Q(\cdot, \varepsilon)$ on the parameter ε will be used to localize in energy the waves we want to describe.

Equation (1.6) is a singularly perturbed system of ODE, to which we apply complex BKW techniques. Making use of suitably normalized polarization vectors $\varphi_j(x,E)$, we show that the solutions of (1.6) can be expanded as

$$\psi_\varepsilon(x,E)=\sum_{j=1}^{md} c_j(x,E,\varepsilon)e^{-i\int_0^x k_j(y,E)dy/\varepsilon}\varphi_j(x,E), \tag{1.8}$$

where the $\mathbb{C}$ valued coefficients $c_j(\cdot,E,\varepsilon)$ satisfy some linear ODE, which we analyze in the semiclassical limit $\varepsilon\to 0$. The assumption $E\in\Delta$ imply that the factors $e^{-i\int_0^x k_j(y,E)dy/\varepsilon}$ are phases for all $x\in\mathbb{R}$ with distinct $k_j(x,E)$, and the coefficients c_j are constant in the semi-classical limit, see e.g. [24], [21],

$$c_j(x,E,\varepsilon)=c_j(0,E,\varepsilon)+O(\varepsilon),\quad j=1,\cdots,md. \tag{1.9}$$

The hypotheses on the matrices A_{ln} at infinity ensure the existence of the limits $\varphi_j(\pm\infty,E)$, $k_j(\pm\infty,E)$, $c_j(\pm\infty,E,\varepsilon)$, and the error term in (1.9) is uniform in x. In particular, the stationary on-shell scattering process characterized by the S-matrix

$$S(E,\varepsilon)c(-\infty,E,\varepsilon)=c(+\infty,E,\varepsilon),\quad \text{where}\quad c(+\infty,E,\varepsilon)=\begin{pmatrix} c_1(+\infty,E,\varepsilon)\\ c_2(+\infty,E,\varepsilon)\\ \vdots\\ c_{md}(+\infty,E,\varepsilon)\end{pmatrix}$$

is well defined. Actually, in our analytic framework, the off-diagonal elements of $S(E,\varepsilon)$ are exponentially small, see below. Thus, for $|x|$ large enough, the solutions (1.5) of the time dependent equation (1.2) behave as

$$\phi(x,t,\varepsilon)\simeq\sum_{j=1}^{md}\int_\Delta Q(E,\varepsilon)c_j(\pm\infty,E,\varepsilon)e^{-i(tE+xk_j(\pm\infty,E))/\varepsilon}\varphi_j(\pm\infty,E)\,dE. \tag{1.10}$$

Assuming the asymptotic dispersion relations $E\mapsto k_j(\pm\infty,E)$ are invertible on Δ, the asymptotic solutions (1.10) are given by linear combinations of wave packets associated with each mode and corresponding polarization. The property (1.9) shows that transitions between modes induced by the evolution are vanishing in the semi-classical limit.

We determine the asymptotics of certain exponentially small transitions between modes for solutions that allow to define a scattering process for $|x|$ large, in a time-dependent set up. *Bona fide* scattering processes require the energy and the modes we are interested to be such that there exists a mode supporting ingoing waves on which we start our solution at time $-\infty$ and that there exists another mode describing outgoing waves at time $+\infty$ to which transitions are possible. There exist systems of PDE's that intertain outgoing solutions or ingoing solutions only. Our results do not provide interesting informations for such systems.

For definiteness, let us assume in that introduction, that the energy of the waves is well localized around $E_0\in\Delta\setminus\partial\Delta$ and that, for all $x\in\mathbb{R}$, $\partial_E k_j(x,E_0)<0$. Our sign conventions imply that the asymptotic group velocities are then positive, see in particular Proposition 7.1. This implies that such waves travel from the left to the right and are polarized along $\varphi_j(-\infty,E_0)$ in the remote past. Let us further assume the mode k_n supports outgoing solutions from the left to the right as well, for $x\simeq+\infty$. The incoming waves are thus characterized for x large and negative by stationary solutions corresponding to $c_k(-\infty,E,\varepsilon)=\delta_{kj}$. Hence, the summand with label n of (1.10) corresponding to the coefficient $c_n(+\infty,E,\varepsilon)$, $n\neq j$, determines the exponentially small piece of the wave for x in a neighborhood of $+\infty$ that has made the transition from mode k_j to mode k_n in the course of the evolution, for times t large and positive.

In order to compute the exponentially small asymptotics of the coefficient $c_n(+\infty,E,\varepsilon)$, one uses BKW techniques. That is one considers the equation satisfied by these coefficients in the complex plane and makes use of their multivaluedness around points of degeneracy of the analytic continuations of certain modes. As is well known, the complex BKW method requires the existence of dissipative or canonical domains, e.g. [9], [10], [14], [22], [21], [11],[12], [32], ... which is not easy to prove. In our setup, we rely on the analysis of [21] which proves that in some avoided crossing regime, dissipative domains exist. The notion of avoided crossing requires the introduction of another parameter but we don't want to be specific about this regime yet. Let us only mention here that dissipative domains exist in particular when the mode $k_j(\cdot, E)$ becomes almost degenerate with $k_l(\cdot, E)$, with either $l = j-1$ or $l = l+1$, at one point only on the real axis. The outcome of the analysis is the asymptotic formula for $\varepsilon \to 0$

$$c_n(+\infty, E, \varepsilon) = \tau(E) e^{iS(E)/\varepsilon}(1 + O(\varepsilon)) \tag{1.11}$$

with $S(E) = \kappa(E) + i\gamma(E)$, $\gamma(E) > 0$ and $\tau(E) \in \mathbb{C}^*$. The exponent $S(E)$ is given by some action integral in the complex plane around the relevant complex degeneracy point of the modes $k_j(\cdot, E)$ and $k_n(\cdot, E)$, see (4.9), and the prefactor $\tau(E)$ possesses some geometric meaning [22]. We localize our wave packets in energy by considering typically Gaussian energy densities of the form

$$Q(E, \varepsilon) = P(E, \varepsilon) e^{-(E-E_0)^2 g/(2\varepsilon)}, \tag{1.12}$$

where P has support in Δ and diverges at worst like a polynomial in $1/\varepsilon$ as $\varepsilon \to 0$.

With these ingredients, we prove in Theorem 6.1 that for $t > 0$ large enough, and in the $L^2(\mathbb{R})$ norm, the piece of the wave function that has made the transition from the mode k_j to k_n, is given in the limit $\varepsilon \to 0$ by

$$\begin{aligned} \phi_{nj}(x, t, \epsilon) \quad &\simeq \quad e^{-\alpha_*/\varepsilon} N_*(\varepsilon) \int_{k_n(+\infty, \Delta)} e^{-\lambda_2 (k-k_*)^2/(2\varepsilon)} e^{-i(tE_n^+(k) + kx + \lambda_1(k-k^*))/\varepsilon} \, dk \\ &\qquad + O(1/|t|^\beta) + o(\varepsilon^{3/4} e^{-\operatorname{Re}\alpha_*/\varepsilon} N_*(\varepsilon)). \end{aligned} \tag{1.13}$$

Here $0 < \beta < 1/2$, $k \mapsto E_n^+(k)$ is the inverse function of the asymptotic dispersion relation $E \mapsto k_n(+\infty, E)$. The exponent α_*, the average momentum k_* and factors λ_1, λ_2 (such that $\operatorname{Re}\lambda_2 > 0$) are determined by the action integral S and the energy density Q, and the prefactor $N_*(\varepsilon)$ is polynomial at worse in $1/\varepsilon$. The leading term in (1.13) is of positive L^2 norm, constant in time, and of order $\varepsilon^{3/4}$, up to the prefactors. Moreover, as $\varepsilon \to 0$ and $|t| \to \infty$ this wave is essentially carried on a ball centered at $x = -\partial_k E_n^+(k_*)t$ of radius $\sqrt{t}$, in the L^2 sense, see Proposition 7.1. Finally, the error terms are uniform in ε and t, respectively.

The function (1.13) corresponds to an exponentially small free wave propagating according to the dispersion relation $E_n^+(k)$ with Gaussian momentum profile (within the momentum window $k_n(+\infty, \Delta)$) centered around k_*. Note that the error terms are negligible only for large enough times, actually exponentially large times $t \simeq e^{c/\varepsilon}$, $c > 0$. Let us emphasize one point revealed by the present analysis and that of [19]. The average momentum k_* does not coincide with the naive guess $k_0 \simeq k_n(+\infty, E_0)$, which corresponds to energy conservation. It is actually dependent on the choice of energy density Q. Similarly, the exponential decay rate α_* is not determined by the function $\gamma = \operatorname{Im} S$ only, but depends explicitly on the density Q as well.

In other words, the piece of the wave function that has made the transition is asymptotically given for small ε and large times by the solution to the linear evolution equation, in (rescaled) Fourier space,

$$i\varepsilon\partial_t f(t, k) = E_n^+(k) f(t, k), \quad f(0, k) = e^{-\alpha_*/\varepsilon} N_*(\varepsilon) e^{-\lambda_2(k-k_*)^2/(2\varepsilon)} e^{-i\lambda_1(k-k_*)/\varepsilon} \chi_{k_n(+\infty, \Delta)}. \tag{1.14}$$

Finally, we mention that in case $E_n^+(k)$ is quadratic in k, we can further compute the leading term explicitly, as in [19], which yields a freely propagating Gaussian, see Lemma 6.1. Also, our analysis applies to the description of exponentially small reflected waves, as will be explained below.

The rest of the paper is organized as follows. The precise hypotheses on the operator $\mathcal{R}(x, i\varepsilon_t, i\varepsilon\partial_x)$, are spelled out in the next Section. Section 3 is devoted to the analysis of the corresponding stationary solutions. The BKW method and the avoided crossing situation are presented in Section 4. The construction of time-dependent solutions to the original problem and their scattering properties are given in Section 5. The precise semiclassical analysis in the scattering regime of the time dependent asymptotic waves describing inter-mode transitions is provided in Section 6. Further properties of the asymptotic waves are given in Section 7. A technical Section closes the paper.

2. Hypotheses for the differential operator

We consider a differential operator defined by (1.1) where a supplementary small parameter δ is included to define the avoided crossing regime in which the gap between certain modes are small:

$$\mathcal{R}(x, i\varepsilon\partial_t, i\varepsilon\partial_x, \delta) = \sum_{l\in\{0,\dots,m\}, n\in\{0,\dots,r\}} A_{ln}(x,\delta)(i\varepsilon\partial_x)^l(i\varepsilon\partial_t)^n. \tag{2.1}$$

We recall that

$$\forall (l,n) \in \{0,\dots,m\}\times\{0,\dots,r\}, \quad \forall x\in\mathbb{R}, \quad \forall \delta\in[0,d_0], \quad A_{ln}(x,\delta)\in\mathcal{M}_d(\mathbb{C})$$

and we define:

$$R(x,E,k,\delta) = \sum_{l\in\{0,\dots,m\}, n\in\{0,\dots,r\}} A_{ln}(x,\delta)k^l E^n.$$

Now, we describe the hypotheses on the differential operator $\mathcal{R}$.

(H1): There exist $Y > 0$ and $d_0 > 0$ such that for any $\delta\in[0,d_0]$ the matrix valued functions $z\mapsto A_{ln}(z,\delta)$ are analytic in a strip $\rho_Y = \{z\in\mathbb{C};\ |\mathrm{Im}\, z| < Y\}$ and $(z,\delta)\mapsto A_{ln}(z,\delta)$ is C^3 for any $(z,\delta)\in\rho_Y\times[0,d_0]$.

(H2): There exist $\nu > 1/2$, $c > 0$ and $2mr$ matrix valued C^2 functions $\{\delta\mapsto A_{ln}(\pm\infty,\delta)\}_{l\in\{0,\dots,m\}}^{n\in\{0,\dots,r\}}$ such that $\forall\delta\in[0,d_0]$,:

$$\sup_{z\in\rho_Y, \mathrm{Re}\, z<0} |\mathrm{Re}\, z|^{2+\nu}\|A_{ln}(z,\delta) - A_{ln}(+\infty,\delta)\| + \sup_{z\in\rho_Y, \mathrm{Re}\, z>0} |\mathrm{Re}\, z|^{2+\nu}\|A_{ln}(z,\delta) - A_{ln}(-\infty,\delta)\| < c.$$

Now, we describe the assumption of avoided crossing. We assume that $\Delta\subset\mathbb{R}$ is a compact interval with non-empty interior such that, for any $E\in\Delta$:

(H3): For any $x\in\mathbb{R}$ and any $\delta\in[0,d_0]$, there are md real values $\{k_1(x,E,\delta), k_2(x,E,\delta),\dots,k_{md}(x,E,\delta)\}$ such that $\det R(x,E,k,\delta) = 0$.

For any $\delta\in[0,d_0]$, the values $k_j(x,E,\delta)$ have md distinct limits as $x\to-\infty$ and as $x\to+\infty$ that we denote by $k_j(\pm\infty,E,\delta)$. The labels are chosen as follows.

When $\delta > 0$, the functions $k_j(x,E,\delta)$ are distinct for $x\in[-\infty,+\infty]$ and are labelled by:

$$k_1(x,E,\delta) < k_2(x,E,\delta) < \cdots < k_{md}(x,E,\delta).$$

When $\delta = 0$, the functions $k_j(x,E,0)$ such that $\det R(x,E,k,\delta) = 0$ are given by md real functions that have $p(E) > 0$ finitely many real crossings at $x_1(E) < \cdots < x_{p(E)}(E)$. Precisely, we assume that for some fixed positive $\tilde{Y}$ and for any fixed $E\in\Delta$ that

- The functions $k_j(x,E,0)$ are labelled according to:

$$k_1(-\infty,E,0) < k_2(-\infty,E,0) < \cdots < k_{md}(-\infty,E,0).$$

- For any $j\in\{1,\dots,md\}$, the function $(z,E)\mapsto k_j(z,E,0)$ is continuous on $\rho_{\tilde{Y}}\times\Delta$.
- For any $j\in\{1,\dots,md\}$, the function $z\mapsto k_j(z,E,0)$ is analytic on $\rho_{\tilde{Y}}$.
- For any $l\in\{1,\dots,p(E)\}$, there exist exactly two integers $(i,j)\in\{1,\dots,md\}^2$ such that:

$$k_i(x_l(E),E,0) = k_j(x_l(E),E,0).$$

Besides, we assume that

$$\partial_x(k_i - k_j)(x_l(E),E,0) \neq 0.$$

For certain results, we also impose the condition that these avoided crossings be generic in the sense of [15, 20, 19].

(H4): Fix $E_0\in\Delta$. Near an avoided crossing $(x_0(E_0),E_0)$ of k_i and k_j, there exist three functions $E\mapsto a(E)$, $E\mapsto b(E)$, $E\mapsto c(E)$ such that, in a neighborhood of E_0,

(1) The difference $k_j - k_i$ satisfies:

$$[k_j(z,E,\delta) - k_i(z,E,\delta)]^2 = a^2(E)(z - x_0(E))^2 + 2c(E)(z - x_0(E))\delta + b^2(E)\delta^2 + R_3(z - x_0(E),\delta),$$

where R_3 is a remainder of order 3.

(2) We have:

$$a(E) > 0, \qquad b(E) > 0, \qquad a^2(E)b^2(E) - c^2(E) > 0.$$

According to [26], we know a priori that the functions k_j are analytic in both variables except at the crossing points. The assumptions (**H1**), (**H2**) and (**H3**) imply analyticity in both variables at the real crossing points:

Lemma 2.1. *Assume that* (**H1**), (**H2**) *and* (**H3**) *are satisfied. Then, for Δ small enough,*

1. *the number $p(E)$ does not depend on $E \in \Delta$.*
2. *there exists $Y > 0$ such that $(z,E) \mapsto k_j(z,E,0)$ is analytic on $\rho_Y \times \Delta$, for any $j \in \{1,\dots,md\}$.*
3. *for $l \in \{1,\cdots,p(E)\}$, the function $E \mapsto x_l(E)$ is analytic on Δ.*

We will prove Lemma 2.1 in Section 8.

Similarly, assumptions (**H1**) to (**H4**) imply the following result:

Lemma 2.2. *Under assumptions* (**H1**) *to* (**H4**)*, the functions a, c and b^2 are analytic in a neighborhood of E_0. Besides, $a(E) = |\partial_z(k_i - k_j)(x_0(E),E)|$.*

Lemma 2.2 is proven in Section 8.

Let us end this Section by noting here that our hypotheses imply that the modes are real, but they do not guarantee that the L^2 norm is conserved under the time evolution. This question is addressed in Section 5.

3. Generalized Eigenvectors

In this Section, we assume that R and Δ satisfy (**H3**), and we investigate the properties of the modes, their corresponding polarization vectors and the stationary solutions. For the time being, the parameter $\delta > 0$ is fixed and we drop it in the notation. The generalized eigenvectors $\psi_\varepsilon(x,E) \in \mathbb{C}^d$ are defined as solutions of the time independent equation:

$$\hat{R}(x,E,i\epsilon\partial_x)\psi_\varepsilon(x,E) = 0. \tag{3.1}$$

For any $E \in \Delta$, the set of such solutions is md-dimensional.

We define:

$$\forall l \in \{1,\dots,m\} \quad N_l(x,E) = \sum_{n=0}^{r} A_{ln}(x)E^n \tag{3.2}$$

so that

$$R(x,E,k) = \sum_{l=0}^{m} N_l(x,E)k^l.$$

We first prove the following result:

Lemma 3.1. *We assume that R and Δ satisfy* (**H1**) *and* (**H3**)*. We have the following properties.*

1. *For any $E \in \Delta$ and any $x \in \mathbb{R}$, $N_m(x,E)$ is invertible.*
2. *For $j \in \{1,\dots,m\}$, $(z,E) \mapsto N_j(z,E)$ is analytic in $\rho_Y \times \Delta$.*
3. *If we define $H(x,E)$ by:*

$$H(x,E) = \begin{bmatrix} 0 & Id & 0 & \dots & 0 \\ 0 & 0 & Id & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & Id \\ -(N_m^{-1}N_0)(x,E) & -(N_m^{-1}N_1)(x,E) & -(N_m^{-1}N_2)(x,E) & \dots & -(N_m^{-1}N_{m-1})(x,E) \end{bmatrix}, \tag{3.3}$$

then $\sigma(H(x,E)) = \{k;\ \det(\sum_{l=0}^{m} N_l(x,E)k^l) = 0\} = \{k;\ \det(R(x,E,k)) = 0\}$.

(4) *The functions* $\{(x,E) \mapsto k_j(x,E)\}_{j\in\{1,\dots,md\}}$ *are analytic in* $\mathbb{R} \times \Delta$.

(5) *Ker* $(R(x,E,k_j(x,E))))$ *is one-dimensional.*

Proof. The singular values of $R(x,E,k) = \sum_{l=0}^{m} N_l(x,E)k^l$ are the roots of the polynomial

$$L(k) = \det\left(\sum_{l=0}^{m} N_l(x,E)k^l\right). \tag{3.4}$$

This polynomial is of degree md and the highest coefficient is $\det N_m(x,E)$. According to (**H3**), since L has md distinct roots, $\det N_m(x,E) \neq 0$, which proves (1).

Assertion (2) is immediate, consider (3). A complex number $k \in \sigma(H(x,E))$ if there exists $\Phi \in \mathbb{C}^{md}\backslash\{0\}$ such that $H\Phi = k\Phi$. Block by block computations show that Φ is of the form:

$$\Phi = \begin{pmatrix} \varphi \\ k\varphi \\ \vdots \\ k^{m-1}\varphi \end{pmatrix}, \quad \varphi \in \mathbb{C}^d, \tag{3.5}$$

with $\det(\sum_{l=0}^{m} N_l(x,E)k^l) = 0$ and $\varphi \in \mathrm{Ker}(\sum_{l=0}^{m} N_l(x,E)k^l)$.

Again by [26], (**H3**) with $\delta > 0$ implies that the functions $k_j(x,E)$ are analytic in a complex neighborhood of $\mathbb{R} \times \Delta$ which proves (4). Point (5) follows from (3.5) and the fact that $\sigma(H(x,E))$ is simple

We introduce some normalized eigenvectors of $R(x,E,k_j(x,E))$.

3.1. **Canonical eigenvectors of** $R(x,E,k_j(x,E))$**.** For a matrix A, we denote its adjoint by $A^* = {}^t\overline{A}$.

Fix $j \in \{1,\dots,md\}$. Under (**H3**) and according to [26], we know that there exist two vector valued functions ξ_j and $\xi_j^\dagger$ with values in $\mathbb{C}^d$ such that:

(1) The functions $(x,E) \mapsto \xi_j(x,E)$ and $(x,E) \mapsto \xi_j^\dagger(x,E)$ are analytic on $\mathbb{R} \times \Delta$.

(2) $\forall (x,E) \in \mathbb{R} \times \Delta, \quad \xi_j(x,E) \in \mathrm{Ker}R(x,E,k_j(x,E)), \quad \xi_j^\dagger(x,E) \in \mathrm{Ker}R^*(x,E,k_j(x,E))$.

Definition 3.1. The vector $\varphi_j = \alpha_j\xi_j$, with

$$\alpha_j(x,E) = e^{-\int_0^x \frac{<\xi_j^\dagger, \partial_k R(u,E,k_j)\partial_x\xi_j> + <\xi_j^\dagger, \frac{\partial_x k_j}{2}\partial_k^2 R(u,E,k_j)\partial_x\xi_j>}{<\xi_j^\dagger, \partial_k R(u,E,k_j)\xi_j>}du} \tag{3.6}$$

is called a canonical eigenvector associated to $R(x,E,k_j(x,E))$.

We notice the following facts:

- The vector φ_j does not depend on the choice of $\xi_j^\dagger \in$ Ker $(R^*(x,E,k_j(x,E))))$. In particular, we can choose $\xi_j^\dagger$ so that
$$<\xi_j^\dagger, \xi_j> = 1.$$
- Condition (3.6) may seem artificial but we shall see in the proof of Lemma 3.2 that it corresponds to the Kato normalization of the eigenvectors of $H(x,E)$.

3.2. **Decomposition Lemma.**

Lemma 3.2. *We assume that R and Δ satisfy* (**H3**). *Let $\psi_\varepsilon(x,E)$ be a solution of* (3.1). *There exist md functions $\{(z,E,\varepsilon) \mapsto c_j(z,E,\varepsilon)\}_{j\in\{1,\dots,md\}}$ such that:*

(1) *The function $\psi_\varepsilon(x,E)$ satisfies:*

$$\forall l \in \{0,\dots,m-1\}, \quad (i\varepsilon\partial_x)^l\psi_\varepsilon(x,E) = \sum_{j=1}^{md} c_j(x,E,\varepsilon)k_j^l(x,E)e^{-\frac{i}{\varepsilon}\int_0^x k_j(y,E)dy}\varphi_j(x,E).$$

(2) *If we define*

$$c(x,E,\varepsilon) = \begin{pmatrix} c_1(x,E,\varepsilon) \\ \vdots \\ c_{md}(x,E,\varepsilon) \end{pmatrix},$$

The vector c satisfies the following differential equation:

$$\partial_x c(x,E,\varepsilon) = M(x,E,\varepsilon)c(x,E,\varepsilon), \tag{3.7}$$

where the matrix M is given by:

$$M_{jl}(x,E) = a_{jl}(x,E)e^{i\frac{\Delta_{jl}(x,E)}{\varepsilon}}, \tag{3.8}$$

$$\text{with} \quad \Delta_{jl}(x,E) = \int_0^x [k_j(u,E) - k_l(u,E)]du,$$

$$\text{and} \quad \forall j \in \{1,\ldots,md\}, \quad a_{jj}(x,E) = 0,$$

$$\forall j \neq l, \qquad a_{jl}(x,E) = \frac{1}{k_j(x,E) - k_l(x,E)} \times \tag{3.9}$$

$$\left[\frac{< \varphi_j^\dagger, R(x,E,k_l)\partial_x\varphi_l > + \partial_x k_l < \varphi_j^\dagger, [\partial_k R(x,E,k_l) - \partial_k R(x,E,k_j)]\varphi_l >}{< \varphi_j^\dagger, \partial_k R(x,E,k_j)\varphi_j >}\right].$$

(3) *For any $j \in \{1,\ldots,md\}$, φ_j is a canonical eigenvector of $R(x,E,k_j(x,E))$ and $\varphi_j^\dagger$ is any eigenvector in $KerR^*(x,E,k_j(x,E))$.*

Remark: The set $\{\varphi_j\}_{j\in\{1,\cdots,md\}}$ is a linearly dependent family of vectors in $\mathbb{C}^d$. The decomposition in point (1) above corresponds to the familiar BKW Ansatz in semiclassical analysis, see e.g. [9].

Proof. Let $\psi_\varepsilon(x,E)$ be a solution of (3.1). We define:

$$\Psi_\varepsilon(x,E) = \begin{bmatrix} \psi_\varepsilon(x,E) \\ (i\varepsilon\partial_x)\psi_\varepsilon(x,E) \\ \vdots \\ (i\varepsilon\partial_x)^{m-1}\psi_\varepsilon(x,E) \end{bmatrix}. \tag{3.10}$$

Then $\Psi_\varepsilon(x,E)$ satisfies:

$$i\varepsilon\partial_x\Psi_\varepsilon(x,E) = H(x,E)\Psi_\varepsilon(x,E). \tag{3.11}$$

Equation (3.11) has been studied in [24], [21]. We use the results obtained there and write:

$$H(x,E) = \sum_{j=1}^{md} k_j(x,E)P_j(x,E), \tag{3.12}$$

where the matrix valued functions $P_j(x,E)$ are the one-dimensional eigenprojectors of $H(x,E)$ and satisfy:

$$\sum_{j=1}^{md} P_j(x,E) = I_{md}.$$

Hypothesis (**H3**) implies the existence of a basis of eigenvectors of $H(x,E)$: $\{\Phi_j(x,E)\}_{j=1,\ldots,md}$.

We determine these eigenvectors uniquely (up to a constant depending on E) by requiring them to satisfy:

$$H(x,E)\Phi_j(x,E) = k_j(x,E)\Phi_j(x,E), \quad \forall j = 1,\ldots,md, \tag{3.13}$$

$$P_j(x,E)\partial_x\Phi_j(x,E) = 0, \quad \forall j = 1,\ldots,md. \tag{3.14}$$

Indeed, recall that if $W(x,E)$ is the solution of

$$\partial_x W(x,E) = \sum_{j=1}^{md}(\partial_x P_j(x,E))P_j(x,E)W(x,E), \quad W(0,E) = I_{md}, \tag{3.15}$$

it is well known that $W(x,E)$ satisfies the intertwining identity

$$W(x,E)P_j(0,E) = P_j(x,E)W(x,E), \quad \forall j \in \{1,\dots,md\}.$$

The generator of (3.15) being analytic in E, W is analytic in both variables $(x,E) \in \mathbb{R} \times \Delta$, see [7] section XI.5. Hence,

$$\Phi_j(x,E) := W(x,E)\Phi_j(0,E), \quad \forall j \in \{1,\dots,md\}$$

where $\{\Phi_j(0,E)\}_{j\in\{1,\cdots,md\}}$ is basis of analytic eigenvectors of $H(0,E)$, satisfy

$$P_j(x,E)\Phi_j(x,E) = \Phi_j(x,E) \quad \text{and eq. (3.14).}$$

We refer to [26, 24, 21] for the details.

We will rewrite the eigenprojectors as:

$$P_j(x,E) = \frac{1}{< \Phi_j^\dagger(x,E), \Phi_j(x,E) >} |\Phi_j(x,E) >< \Phi_j^\dagger(x,E)|,$$

where $\Phi_j^\dagger(x,E) \in \mathrm{Ker}(H^*(x,E) - k_j(x,E))$, since $k_j(x,E) = \overline{k_j}(x,E)$.

We use the same notation for duality in $\mathbb{C}^m$ and $\mathbb{C}^{md}$ since no confusion should arise.

Let us begin by specifying equation (3.14) in our case. We consider an eigenvector $\Xi_j(x,E)$ of $H(x,E)$. Ξ_j is written as:

$$\Xi_j(x,E) = \begin{bmatrix} \xi_j(x,E) \\ k_j(x,E)\xi_j(x,E) \\ \vdots \\ k_j^{m-1}(x,E)\xi_j(x,E) \end{bmatrix}, \text{ with } \xi_j(x,E) \in \mathrm{Ker}R(x,E,k_j(x,E)).$$

The vector Φ_j must be of the form $\Phi_j = \alpha_j \Xi_j$, where $\alpha_j \in \mathbb{C}$ and we define $\varphi_j = \alpha_j \xi_j$. Then:

$$\Phi_j = \begin{bmatrix} \varphi_j \\ k_j\varphi_j \\ \vdots \\ k_j^{m-1}\varphi_j \end{bmatrix}.$$

Now, if $\Xi_j^\dagger(x,E) \in \mathrm{Ker}\ (H^*(x,E) - k_j(x,E))$ then Φ_j satisfies (3.14) if:

$$\frac{\partial_x \alpha_j}{\alpha_j} = -\frac{< \Xi_j^\dagger, \partial_x \Xi_j >}{< \Xi_j^\dagger, \Xi_j >}.$$

It remains to choose $\Xi_j^\dagger$ and to compute $< \Xi_j^\dagger, \partial_x \Xi_j >$ and $< \Xi_j^\dagger, \Xi_j >$.

We start with the computation of the vector $\Xi_j^\dagger(x,E)$. It is an eigenvector of $H^*(x,E)$ associated with the eigenvalue $\overline{k_j}(x,E) = k_j(x,E)$. Let $\xi_j^\dagger(x,E) \in \mathrm{Ker}(R^*(x,E,k_j(x,E)))$. We check that we can take

$$\Xi_j^\dagger = \begin{bmatrix} \sum_{l=1}^m k_j^{l-1} N_l^* \xi_j^\dagger \\ \sum_{l=2}^m k_j^{l-2} N_l^* \xi_j^\dagger \\ \vdots \\ N_m^* \xi_j^\dagger \end{bmatrix}.$$

Then:

$$< \Xi_j^\dagger, \Xi_j >= \sum_{p=1}^m k_j^{p-1} \sum_{l=p}^m k_j^{l-p} < N_l^* \xi_j^\dagger, \xi_j >= \sum_{l=1}^m k_j^{l-1} \sum_{p=1}^l < N_l^* \xi_j^\dagger, \xi_j >=< \xi_j^\dagger, \sum_{l=1}^m l k_j^{l-1} N_l \xi_j >$$

$$=< \xi_j^\dagger, \partial_k R(x,E,k_j(x,E))\xi_j > .$$

Similarly, we compute:

$$< \Xi_j^\dagger, \partial_x \Xi_j > = < \xi_j^\dagger, \partial_k R(x,E,k_j)\partial_x \xi_j > + < \xi_j^\dagger, \frac{\partial_x k_j}{2}\partial_k^2 R(x,E,k_j)\partial_x \xi_j > .$$

This implies that φ_j is a canonical eigenvector of $R(x,E,k_j)$.

From [24, 21], we know that any solution to (3.11) can be written as:

$$\Psi_\varepsilon(x,E) = \sum_{j=1}^{md} c_j(x,E,\varepsilon) e^{-\frac{i}{\varepsilon}\int_0^x k_j(y,E)dy}\Phi_j(x,E),$$

where the scalar coefficients c_j satisfy the differential equation: $\partial_x c = Mc$, where M is given by (3.8), and

$$a_{jl} = -\frac{< \Phi_j^\dagger, \partial_x \Phi_l >}{< \Phi_j^\dagger, \Phi_j >}.$$

We compute

$$\begin{aligned} < \Phi_j^\dagger, \partial_x \Phi_l > &= \partial_x k_l \sum_{p=2}^{m}\sum_{q=p}^{m}(q-1)k_j^{q-p}k_l^{p-2} < N_q^* \varphi_j^\dagger, \varphi_l > \\ &+ \sum_{p=1}^{m}\sum_{q=p}^{m} k_j^{q-p}k_l^{p-1} < N_q^* \varphi_j^\dagger, \partial_x \varphi_l > . \end{aligned} \tag{3.16}$$

By interchanging the indices p and q and according to the formula

$$\forall a \neq b, \qquad \sum_{p+l=s} a^p b^l = \frac{a^{s+1} - b^{s+1}}{a-b},$$

we obtain formula (3.9). The first statement of the Lemma stems from formula (3.10). This ends the proof of Lemma 3.2.

3.3. **Behavior of the matrix M.** The following Lemma describes the behavior of the coefficients a_{ij} and phases entering the definition of M.

Lemma 3.3. *We assume that (**H1**), (**H2**) and (**H3**) are satisfied. Then,*

- *The eigenvalues k_j satisfy for any $k \in \mathbb{N}$ and any $l \in \mathbb{N}$:*

(3.17)
$$\forall E \in \Delta, \quad \sup_{x\to+\infty} |x|^{2+\nu}|\partial_E^l \partial_x^k (k_j(x,E) - k_j(+\infty,E))| + \sup_{x\to-\infty} |x|^{2+\nu}|\partial_E^l \partial_x^k (k_j(x,E) - k_j(-\infty,E))| < \infty.$$

- *The eigenvectors φ_j satisfy for any $l \in \mathbb{N}$, uniformly in $E \in \Delta$:*

$$\sup_{x\to+\infty} |x|^{1+\nu}\|\partial_E^l(\varphi_j(x,E) - \varphi_j(+\infty,E))\| + \sup_{x\to-\infty} |x|^{1+\nu}\|\partial_E^l(\varphi_j(x,E) - \varphi_j(-\infty,E))\| < \infty. \tag{3.18}$$

- *Moreover, for any $k \in \mathbb{N}^*$ and $l \in \mathbb{N}$, uniformly in $E \in \Delta$:*

$$\sup_{x\to+\infty} |x|^{2+\nu}\|\partial_E^l \partial_x^k(\varphi_j(x,E) - \varphi_j(+\infty,E))\| + \sup_{x\to-\infty} |x|^{2+\nu}\|\partial_E^l \partial_x^k(\varphi_j(x,E) - \varphi_j(-\infty,E))\| < \infty. \tag{3.19}$$

- *For any $k \in \mathbb{N}$ and any $l \in \mathbb{N}$, the coefficients of the matrix M satisfy uniformly in $E \in \Delta$:*

$$\forall x \in \mathbb{R}, \quad \forall (j,p) \in \{1,\ldots,md\}^2, \quad |\partial_E^l \partial_x^k a_{jp}(x,E)||x|^{2+\nu} < \infty. \tag{3.20}$$

- *Let*

$$\omega_j(\pm\infty,E) = \int_0^{\pm\infty} [k_j(y,E) - k_j(\pm\infty,E)]dy, \tag{3.21}$$

and

$$\int_0^x k_j(y,E)dy = xk_j(\pm\infty,E) + \omega_j(\pm\infty,E) + r_j^{\pm}(x,E). \tag{3.22}$$

Then we have, uniformly in $E \in \Delta$, and for any $n \in \mathbb{N}$,

$$\forall j \in \{1,\dots,md\}, \quad \sup_{x>0} |x|^{1+\nu} |\partial_E^n r_j^+(x,E)| + \sup_{x<0} |x|^{1+\nu} |\partial_E^n r_j^-(x,E)| < \infty. \tag{3.23}$$

We prove Lemma 3.3 in section 8.3.

3.4. **The vector c.** In the following lemma, we describe the behavior of the vector c defined by the ODE (3.7).

Lemma 3.4. *We assume that* (**H1**), (**H2**), *and* (**H3**) *are satisfied.*

- *For any $E \in \Delta$ and $\epsilon > 0$, the limits $c_j(\pm\infty, E, \varepsilon)$ exist for all $j = 1, \cdots, md$.*
- *If the initial conditions to (3.7) are chosen so that $c(-\infty, E, \varepsilon)$ is uniformly bounded in $E \in \Delta$ and $\epsilon > 0$, then we have for some constant C uniform in ε and $E \in \Delta$:*

$$|\partial_E c_j(\pm\infty,E,\varepsilon)| + |c_j(\pm\infty,E,\varepsilon)| < C,$$

$$\sup_{x>0} |x|^{\nu} |\partial_E c_j(x,E,\varepsilon) - \partial_E c_j(+\infty,E,\varepsilon)| + \sup_{x<0} |x|^{\nu} |\partial_E c_j(x,E,\varepsilon) - \partial_E c_j(-\infty,E,\varepsilon)| < C,$$

$$\sup_{x>0} |x|^{1+\nu} |c_j(x,E,\varepsilon) - c_j(+\infty,E,\varepsilon)| + \sup_{x<0} |x|^{1+\nu} |c_j(x,E,\varepsilon) - c_j(-\infty,E,\varepsilon)| < C.$$

Remarks:

i) As the proof shows, the condition $\sup\limits_{\substack{E\in\Delta \\ \varepsilon\to 0}} \|c(-\infty,E,\varepsilon)\| < \infty$ can be replaced by

$$\exists x_0 \in \mathbb{R} \ \text{ such that } \ \sup_{\substack{E\in\Delta \\ \varepsilon\to 0}} \|c(x_0,E,\varepsilon)\| < \infty. \tag{3.24}$$

ii) In the construction of solutions to (1.2) by means of an energy density, we can (and will) always assume that the initial conditions, wherever they are chosen, are uniformly bounded in energy:

$$\exists x_0 \in \mathbb{R} \ \text{ such that } \ \sup_{E\in\Delta} \|c(x_0,E,\varepsilon)\| < \infty. \tag{3.25}$$

iii) The equation being linear, we can actually always assume condition (3.24) holds. This is what we do in the rest of the paper.

We shall prove Lemma 3.4 in section 8.4.

According to Lemma 3.4, we can define the stationary scattering matrix $S(E,\varepsilon)$ by:

$$S(E,\varepsilon)c(-\infty,E,\varepsilon) = c(+\infty,E,\varepsilon). \tag{3.26}$$

In order to describe the time-dependent scattering processes we are interested in, we need more detailed informations about the stationary S-matrix.

4. Complex BKW analysis

In this section, the parameter $\delta > 0$ is still kept fixed. All the information about transmissions and transitions among the asymptotic eigenstates is contained in the asymptotic values of the coefficients $c_j(x, E, \pm\infty)$ defined in section 3.4 and hence in the stationary scattering matrix $S(E,\varepsilon)$. We extract this information by mimicking the complex BKW method of [24] and [21], while keeping track of the E-dependence.

In the simplest setting, the complex BKW method requires hypotheses on the behavior of the so-called Stokes-lines for equation (3.11) in order to provide the required asymptotics. These hypotheses are global in nature, and in general are extremely difficult to check. See *e.g.*, [9, 10]. However, in the physically relevant situation of avoided crossings, they can be easily checked, as is proven in [21] and will be recalled in the next Section. We restrict our attention to these avoided crossing situations.

To study the S-matrix, it is enough to consider the coefficients c_j that are uniquely defined by the conditions

$$c_j(-\infty, E, \varepsilon) = 1 \quad c_k(-\infty, E, \varepsilon) = 0, \quad \text{for all} \quad k \neq j. \tag{4.1}$$

The key of the complex BKW method lies in the multivaluedness of the eigenvalues and the eigenvectors of the analytic generator $H(x, E)$ in the complex x plane.

According to (**H3**), the eigenvalues and eigenvectors of $H(x, E)$ are analytic in x on the real axis. They may have branch points in ρ_Y that are located in

$$\Omega(E) = \{z \in \rho_Y \ ; \ \exists\, j \neq l \quad \text{such that} \quad k_j(z, E) = k_l(z, E)\} \tag{4.2}$$

4.1. **The set** $\Omega(E)$**.** By the Schwarz reflection principle, for any $E \in \Delta$, we have $\overline{\Omega}(E) = \Omega(E)$. Besides, the set $\bigcup\limits_{E\in\Delta} \Omega(E)$ is bounded in ρ_Y.

We have the following description of $\Omega(E)$, see [21]:

Lemma 4.1. *Fix $E_0 \in \Delta$. There exists a neighborhood Δ_0 of E_0 and a finite number R of bounded open sets $\{\Omega_i\}_{i\in\{1,\dots,R\}}$ in $\rho_Y \cap \mathbb{C}_+$ such that:*

- *For any $E \in \Delta_0$, $\Omega(E) \subset \bigcup_1^R \Omega_i \bigcup_1^R \overline{\Omega_i}$.*
- *For all $i \in \{1, \dots, R\}$, $\Omega_i \cap \mathbb{R} = \emptyset$.*
- *For any $E \in \Delta_0$, and $i \in \{1, \dots, R\}$, Ω_i contains only one crossing point. This point is a crossing point for finitely many distinct couples of modes.*

We define $\Omega = \bigcup_1^R \Omega_i \bigcup_1^R \overline{\Omega_i}$.

Under our genericity hypotheses, we have the following local behavior at a complex crossing point $z_0 \in \Omega(E_0)$,:

$$k_j(z, E_0) - k_l(z, E_0) \simeq \gamma(E_0)(z - z_0)^{1/2}(1 + O(z - z_0)).$$

The eigenprojectors of $H(x, E)$ also admit multivalued extensions in $\rho_Y \setminus \Omega(E)$, but they diverge at generic eigenvalue crossing points. We only have to deal with generic crossing points. To see what happens to a multivalued function f in $\rho_Y \setminus \Omega$ when we turn around a crossing point, we adopt the following convention: For E fixed, we denote by $f(z, E)$ the analytic continuation of f defined in a neighborhood of the origin along some path from 0 to z. Then we perform the analytic continuation of $f(z, E)$ along a negatively oriented loop that surrounds only one connected component Ω_i of Ω. We denote by $\tilde{f}(z, E)$ the function we get by coming back to the original point z. We define ζ_0 to be a negatively oriented loop, based at the origin, that encircles only Ω_i when $\Omega_i \in \mathbb{C}_+$. When $\Omega_i \in \mathbb{C}_-$, we choose ζ_0 to be positively oriented.

We now fix $\Omega_i \in \mathbb{C}_+$. For any $E \in \Delta_0$, if we analytically continue the set of eigenvalues $\{k_j(z, E)\}_{j=1}^{md}$, along a negatively oriented loop around Ω_i, we get the set $\{\widetilde{k}_j(z, E)\}_{j=1}^{md}$ with

$$\widetilde{k}_j(z, E) = k_{\pi_0(j)}(z, E), \quad \text{for} \quad j = 1, \cdots, md,$$

where

$$\pi_0 : \ \{1, 2, \cdots, m\} \to \{1, 2, \cdots, md\} \tag{4.3}$$

is a permutation that depends on Ω_i. As a consequence, the eigenvectors Φ_j possess multi-valued analytic extensions in $\rho_Y \backslash \Omega$. The analytic continuation $\widetilde{\Phi}_j(z, E)$ of $\Phi_j(z, E)$ along a negatively oriented loop around Ω_i, must be proportional to $\Phi_{\pi_0(j)}(z, E)$. Thus, for $j = 1, 2, \cdots, md$, there exists $\theta_j(\zeta_0) \in \mathbb{C}$, such that

$$\widetilde{\Phi}_j(z, E) \ = \ e^{-i\theta_j(\zeta_0, E)}\Phi_{\pi_0(j)}(z, E). \tag{4.4}$$

The above implies a key identity for the analytic extensions of the coefficients $c_j(z, E, \varepsilon)$, $z \in \rho_Y \backslash \Omega$. Since the solutions to (3.11) are analytic for all $z \in \rho_Y$, the coefficients c_j must also be multi-valued. In our setting, Lemma 3.1 of [21] implies the following lemma.

Lemma 4.2. *For any $j = 1, \ldots, md$, we have*

$$\widetilde{c}_j(z, E, \varepsilon)\ e^{-i\int_{\zeta_0} k_j(u,E)\,du/\varepsilon}\ e^{-i\,\theta_j(\zeta_0,E)} \ = \ c_{\pi_0(j)}(z, E, \varepsilon) \tag{4.5}$$

where ζ_0 and $\pi_0(j)$ are defined as above and are independent of $E \in \Delta_0$.

Remark: Since Ω has a finite number of connected components, it is straightforward to generalize the study of the analytic continuations around one crossing point to analytic continuations around several crossing points. The loop ζ_0 can be rewritten as a concatenation of finitely many individual loops, each encircling only one connected component of Ω. The permutation π_0 is given by the composition of associated permutations. The factors $e^{-i\theta_j(\zeta_0,E)}$ in (4.4) are given by the product of the factors associated with the individual loops. The same is true for the factors $\exp\Big(-i\int_{\zeta_0} k_j(z,E)\,dz/\varepsilon\Big)$ in Lemma 4.2.

4.2. **Dissipative domains.** We now describe how to use the above properties in order to control the limit $\varepsilon \to 0$. The details may be found in [21].

The idea is to integrate the integral equation corresponding to (3.7) along paths that go above (or below) one or several crossing points, and then to compare the result with the integration performed along the real axis. As $z \to -\infty$ in ρ_Y these paths become parallel to the real axis so that the coefficients take the same asymptotic value $c_m(-\infty, E, \varepsilon)$ along the real axis and the integration paths. Since the solutions to (3.11) are analytic, the results of these integrations must agree as $\mathrm{Re}\, z \to \infty$. Therefore, (4.5) taken at $z = \infty$ yields the asymptotics of $c_{\pi_0(j)}(\infty, E, \varepsilon)$, provided we can control $\widetilde{c}_j(z, E, \varepsilon)$ in the complex plane. We argue below that this can be done in the so-called dissipative domains of the complex plane. We do not go into the details of these notions because a result of [21] will enable us to get sufficient control on $\widetilde{c}_j(z, E, \varepsilon)$ in the avoided crossing situation, to which we restrict our attention.

We recall that Δ_{jl} is defined in (3.8). We rewrite (3.7) as an integral equation:

$$c_j(x, E, \varepsilon) = c_j(x_0, E, \varepsilon) + \int_{x_0}^{x} \sum_l a_{jl}(x', E) e^{\frac{i\Delta_{jl}(x',E)}{\varepsilon}} c_l(x', E, \varepsilon) dx'. \tag{4.6}$$

By explicit computation, we check that (4.6) can be extended to $\rho_Y \setminus \Omega$. We integrate by parts in (4.6) to see that (4.6) with $x_0 = -\infty$ can be rewritten as:

$$\begin{aligned} \widetilde{c}_m(z, E, \varepsilon) \ &= \ \delta_{jm} - i\varepsilon \sum_l \frac{\widetilde{a}_{ml}(z, E)}{\widetilde{k}_m(z, E) - \widetilde{k}_l(z, E)}\, e^{i\widetilde{\Delta}_{ml}(z,E)/\varepsilon}\, \widetilde{c}_l(z, E, \varepsilon) \\ &\quad + i\varepsilon^2 \sum_l \int_{-\infty}^{z} \left(\frac{\partial}{\partial z'} \frac{\widetilde{a}_{ml}(z', E)}{\widetilde{k}_m(z', E) - \widetilde{k}_l(z', E)} \right) e^{i\widetilde{\Delta}_{ml}(z',E)/\varepsilon}\, \widetilde{c}_l(z', E, \varepsilon)\, dz' \\ &\quad + i\varepsilon \sum_{l,p} \int_{-\infty}^{z} \frac{\widetilde{a}_{ml}(z', E)\, \widetilde{a}_{lp}(z', E)}{\widetilde{k}_m(z', E) - \widetilde{k}_l(z', E)}\, e^{i\widetilde{\Delta}_{mp}(z',E)/\varepsilon}\, \widetilde{c}_p(z', E, \varepsilon)\, dz', \end{aligned} \tag{4.7}$$

as long as the chosen path of integration does not meet Ω. Here, $\widetilde{\ }$ denotes the analytic continuation along the chosen path of integration of the corresponding function defined originally on the real axis. This distinguishes $\widetilde{c}_m(\infty, E, \varepsilon)$ from $c_m(\infty, E, \varepsilon)$ computed along the real axis as $x \to \infty$. These quantities may differ since the integration path may pass above (or below) points of Ω. If the exponential factors in (4.7) are all uniformly bounded when $\varepsilon \to 0$, as it is the case when the integration path coincides with the real axis, it is straightforward to get bounds of the type

$$c_m(z, E, \varepsilon) \ = \ \delta_{jm} \ + \ O_E(\varepsilon). \tag{4.8}$$

However, when dealing with $\tilde{c}_m$ in the complex plane, these exponential factors are usually not uniformly bounded and one needs to restrict integration paths to certain domains in which useful estimates can be obtained:

One defines a *Dissipative domain* for index j, $D_j \subset \rho_Y \setminus \Omega$ associated with the initial condition (4.1), by the conditions:

- $D_j \subset \rho_Y \setminus \Omega$ and $\sup_{z\in D_j} \operatorname{Re} z = \infty, \inf_{z\in D_j} \operatorname{Re} z = -\infty$,
- For any $z \in D_j$ and any index $k \in \{1, \dots, md\}$, there exists a path $\gamma^k \subset D_j$, parametrized by $u \in (-\infty, t]$ which the regularity properties

$$\lim_{u\to-\infty} \operatorname{Re}\gamma^k(u) = -\infty \ , \ \gamma^k(t) = z \ \text{ and } \ \sup_{z\in D_j} \sup_{u\in(-\infty,t]} |\partial_u \gamma^k(u)| < \infty$$

- γ^k satisfies the monotonicity properties

$$u \mapsto \operatorname{Im} \widetilde{\Delta}_{jk}(\gamma^k(u)) \ \text{ is non-decreasing on } \ (-\infty, t].$$

Again, as it is well known, the existence of paths from $-\infty$ to $+\infty$ passing above (or below) points in Ω and along which the exponentials can be controlled is difficult to check in general. We can overcome these complications by restricting attention to avoided crossing situations where the existence of dissipative domains for all indices has been proven in [21], see hypothesis **(AC)** below. The interest of the definition above lies in the following property.

When a dissipative domains exists for the index j, (4.5) and (4.8) imply

$$c_{\pi_0(j)}(\infty, E, \varepsilon) \ = \ e^{-i\int_{\zeta_0} k_j(u,E)\,du/\varepsilon} \ e^{-i\,\theta_j(\zeta_0,E)} \ (1 + O_E(\varepsilon)), \tag{4.9}$$

where the $O_E(\varepsilon)$ estimate is uniform for $E \in \Delta_0$. This is the main result of Proposition 4.1 in [21] for our purpose, under the assumption that a dissipative domain D_j exists.

In our context, all quantities depend on $E \in \Delta_0$. However, by carefully following the proof of Proposition 4.1 of [21], it is not difficult to check that the estimate (4.8) is uniform for $E \in \Delta_0$. For later purposes, we also note here that under the same hypotheses on the exponential factors, $\frac{\partial}{\partial E}\widetilde{c}_m(z, E, \varepsilon)$ is uniformly bounded for $0 < \varepsilon < \varepsilon_0$ and $E \in \Delta_0$ for some fixed ε_0, by differentiation of (4.7). See the proof of Lemma 3.4 for this property on the real axis.

4.3. **Avoided crossings.** We now make use of the avoided crossing situation, that allows us to prove the existence of dissipative domains. We thus restore the parameter δ in the notation. We therefore work under **(H3)** and under the following assumption on the patterns of crossings for the modes $\{k_j(x, E, 0)\}$:

(AC):

- For all $x < x_1(E)$,

$$k_1(x, E, 0) < k_2(x, E, 0) < \cdots < k_{md}(x, E, 0).$$

- For all $j < l \in \{1, 2, \cdots, md\}$, there exists at most one $x_r(E)$ with

$$k_j(x_r(E), E, 0) \ - \ k_l(x_r(E), E, 0) \ = \ 0,$$

and if such an $x_r(E)$ exists, we have

$$\frac{\partial}{\partial x}\left(k_j(x_r(E), E, 0) - k_l(x_r(E), E, 0)\right) \ > \ 0. \tag{4.10}$$

- For all $j \in \{1, 2, \cdots, md\}$, the mode $k_j(x, E, 0)$ crosses modes whose indices are all superior to j or all inferior to j.

To any given pattern of real crossings for the group $\{k_j(x, E, 0)\}$, with $E \in \Delta_0$, we associate a permutation π as follows. The modes $\{k_j(x, E, 0)\}$ are labelled in ascending order at $x \simeq -\infty$, by (**H3**). Since there are no real crossings for $E \in \Delta$ and as $x \to +\infty$, the values $\{k_j(x, E, 0)\}$ are ordered uniformly in $E \in \Delta$ at $x = +\infty$. If $k_j(+\infty, E, 0)$ is the k^{th} eigenvalue in ascending order at $x = +\infty$, the permutation π is defined by

$$\pi(j) = k. \tag{4.11}$$

Let E be in a sufficiently small interval Δ_0. For a loop ζ_0 that surrounds all the complex crossing points and π_0 the associated permutation (see (4.5)), π_0 corresponds to the permutation π.

We can now restate the main result of [21] that describes the asymptotics of the coefficients defined in (4.7). We only have to check that, for small $\delta > 0$, dissipative domains exist and do not depend on $E \in \Delta_0$. We refer to [21] for the details. The construction of these dissipative domains is based on a perturbation of the case $\delta = 0$. By mimicking the arguments of [21], as in [19] we obtain that estimates of the type (4.9) are true for certain indices j and n, determined by the permutation (4.11):

Theorem 4.1. *Assume that* (**H1**) *to* (**H3**) *are satisfied and that* (**AC**) *holds. If $\delta > 0$ and Δ_0 are small enough, the $\pi(j), j$ elements of the matrix $S(E,\varepsilon)$, with $\pi(j)$ defined in* (4.11) *have small ε asymptotics for all $j = 1, \cdots, md$ given by*

$$S_{\pi(j),j}(E,\varepsilon) \;=\; \prod_{l=j}^{\pi(j)\mp 1} e^{-i\theta_l(\zeta_l,E,\delta)}\, e^{i\int_{\zeta_l} k_l(z,E,\delta)\,dz/\varepsilon}\,(1+O_{E,\delta}(\varepsilon)), \qquad \pi(j)\, \begin{cases} > j \\ < j \end{cases}$$

where, for $\pi(j) > j$ (resp. $\pi(j) < j$), ζ_l, $l = j, \cdots, \pi(j)-1$ (resp. $l = j, \cdots, \pi(j)+1$), denotes a negatively (resp. positively) oriented loop based at the origin which encircles the complex domain Ω_r (resp. $\overline{\Omega_r}$) corresponding to the avoided crossing between $k_l(x,E,\delta)$ and $k_{l+1}(x,E,\delta)$ (resp. $k_{l-1}(x,E,\delta)$). The $\int_{\zeta_l} k_l(z,E,\delta)\,dz$ denotes the integral along ζ_l of the analytic continuation of $k_l(0,E,\delta)$, and $\theta_l(\zeta_l,E,\delta)$ is the corresponding factor defined by (4.4).

Remark: Under our regularity hypotheses in δ, it is easy to get the following properties, see [20],

$$\lim_{\delta\to 0} \int_{\zeta_l} k_l(z,E,\delta)\,dz = 0.$$

Let us emphasize here that we do not have access to all off-diagonal elements of the S-matrix; those we can asymptotically compute are determined by the pattern of avoided crossings. Moreover, there are cases in which one can compute all elements of the S-matrix, due to supplementary symmetries in the problem, see [25]. Sometimes, the coefficients to which we have access are not even the largest ones in the avoided crossing situation, as shown in [25].

On the basis of steepest descent arguments, transitions between modes that do not display avoided crossings, *i.e.*, that are separated by a gap of order 1 as $\delta \to 0$, are expected to be exponentially smaller than the transitions we control by means of Theorem 4.1, as δ shrinks to zero. Since the coefficients in the exponential decay rates given by the theorem vanish in the limit $\delta \to 0$, it is enough to show that the decay rates of the exponentially small transitions between well separated levels are independent of δ.

That is the meaning of the following proposition, which is proven in [19]:

Proposition 4.1. *We assume that* (**H3**) *is satisfied. Further assume that the eigenvalues of $H(x,E,\delta)$ can be separated into two distinct groups $\sigma_1(x,E,\delta)$ and $\sigma_2(x,E,\delta)$ that display no avoided crossing for $E \in \Delta$, i.e., such that*

$$\inf_{\substack{\delta\geq 0, E\in\Delta \\ x\in\rho_Y\cup\{\pm\infty\}}} \operatorname{dist}(\sigma_1(x,E,\delta),\, \sigma_2(x,E,\delta)) \;\geq\; g \;>\; 0.$$

Let $P(x,E,\delta)$ and $Q(x,E,\delta) = \mathbb{I} - P(x,E,\delta)$ be the projectors onto the spectral subspaces corresponding to $\sigma_1(x,E,\delta)$ and $\sigma_2(x,E,\delta)$ respectively, and let $U_\varepsilon(x,x_0,E,\delta)$ be the (space-) evolution operator corresponding to the equation

$$i\,\varepsilon\,\frac{d}{dx}\,U_\varepsilon(x,x_0,E,\delta) \;=\; H(x,E,\delta)\; U_\varepsilon(x,x_0,E,\delta), \qquad \text{with} \qquad U_\varepsilon(x_0,x_0,E,\delta) = \mathbb{I}. \tag{4.12}$$

Then, for any $\delta > 0$, there exists $\varepsilon_0(\delta)$, $C(\delta) > 0$ depending on δ, and $\Gamma > 0$ independent of δ, such that for all $\varepsilon \leq \varepsilon_0(\delta)$,

$$\lim_{\substack{x\to\infty \\ x_0\to-\infty}} \;\|\, P(x,E,\delta)\, U_\varepsilon(x,x_0,E,\delta)\, Q(x_0,E,\delta)\,\| \;\leq\; C(\delta)\; e^{-\Gamma/\varepsilon}.$$

This Proposition implies that the stationary transitions between modes without an avoided crossing are exponentially smaller than transitions between modes displaying an avoided crossings. It also shows that in any case, these transitions are all exponentially small.

Let us end this section by remarking that we have always specified initial conditions at $x = -\infty$. Obviously, the BKW analysis can be equally performed for coefficients whose initial conditions are specified at $x = +\infty$, *mutatis mutandis.*

5. Exact solutions to the time-dependent equation

In this Section, we construct solutions to

$$\mathcal{R}(x, i\varepsilon\partial_t, i\varepsilon\partial_x)\phi(x,t,\varepsilon) = 0, \quad x \in \mathbb{R} \tag{5.1}$$

by taking time-dependent superpositions of the generalized eigenvectors $\psi_\varepsilon(x, E)$, for $E \in \Delta$, studied in Section 3. We investigate particularly these exact solutions in the scattering regime of large but finite times t, and for any fixed $\varepsilon > 0$, not necessarily small.

The superpositions of generalized eigenvectors depend on an energy density $Q(E,\varepsilon)$ that might be complex valued. We assume that the following regularity conditions holds:

(C0): The density $E \mapsto Q(E,\varepsilon)$ is supported on Δ and is C^1 on Δ, for any fixed ε.
Moreover, (3.25) is true.

In this Section, the parameter δ is fixed and we omit it in the notations. We work under the hypotheses (**H1**), (**H2**), and (**H3**) and we define:

$$\phi(x,t,\varepsilon) = \int_\Delta \psi_\varepsilon(x,E)e^{\frac{-itE}{\varepsilon}}Q(E,\varepsilon)dE = \sum_{j=1}^{md}\phi_j(x,t,\varepsilon), \tag{5.2}$$

where

$$\phi_j(x,t,\varepsilon) = \int_\Delta c_j(x,E,\varepsilon)e^{\frac{-i\int_0^x k_j(y,E)dy}{\varepsilon}}\varphi_j(x,E)e^{\frac{-itE}{\varepsilon}}Q(E,\varepsilon)dE. \tag{5.3}$$

Since the integrand is smooth and Δ is compact, $\phi(x,t,\varepsilon)$ is an exact solution of (1.2).

We also get from the decomposition (3.10) for all $l = 0, \cdots, m-1$,

$$\begin{aligned}(i\varepsilon\partial_x)^l\phi(x,t,\varepsilon) &= \sum_{j=1}^{md}\int_\Delta c_j(x,E,\varepsilon)e^{\frac{-i\int_0^x k_j(y,E)dy}{\varepsilon}}k_j^l(x,E)\varphi_j(x,E)e^{\frac{-itE}{\varepsilon}}Q(E,\varepsilon)dE \\ &\equiv \sum_{j=1}^{md}\phi_j^{[l]}(x,t,\varepsilon),\end{aligned} \tag{5.4}$$

with the convention $\phi_j^{[0]}(x,t,\varepsilon) = \phi_j(x,t,\varepsilon)$. Note, however, that in general $(i\varepsilon\partial_x)^l\phi_j(x,t,\varepsilon) \neq \phi_j^{[l]}(x,t,\varepsilon)$.

The behavior of $\phi_j(x,t,\varepsilon)$ for large x can be understood under the following supplementary assumption **(GV):**

$$\forall j \in \{1,\dots,md\}, \quad \forall E \in \Delta, \quad \partial_E k_j(\pm\infty, E) \neq 0. \tag{5.5}$$

Let us note that condition (**GV**) is quite natural. Indeed, with our sign conventions, $-1/\partial_E k_j$ is the group velocity of the asymptotic waves (5.9). Our condition says that we want to describe waves with non-zero asymptotic velocity. Moreover, **(GV)** also imposes the presence of at least one time derivative in the definition of the differential operator $\mathcal{R}(x, i\varepsilon\partial_t, i\varepsilon\partial_x, \delta)$.

We have

Lemma 5.1. *Assume that* (**H1**)*,* (**H2**)*,* (**H3**)*,* (**C0**) *and* (**GV**) *are satisfied. Let*

$$K_+ = \sup_{E\in\Delta,\ j\in\{1,\dots,md\}} \frac{1}{|\partial_E k_j(\pm\infty, E)|} > 0$$

and

$$K_- = \inf_{E\in\Delta,\ j\in\{1,\dots,md\}} \frac{1}{|\partial_E k_j(\pm\infty,E)|} > 0.$$

Fix $\alpha \in (0,1)$. Then, there exists $C_\varepsilon > 0$ such that, for x large enough and for either $t = 0$ or any $t \neq 0$ and x satisfying:

$$|x/t| > \frac{K_+}{1-\alpha} \quad \textit{or} \quad |x/t| < \frac{K_-}{1+\alpha},$$

we have for all $j = 1, \cdots, md$:

$$\|\phi_j(x,t,\varepsilon)\| < \frac{C_\varepsilon}{|x|} \quad \textit{and} \quad \|\phi_j^{[l]}(x,t,\varepsilon)\| < \frac{C_\varepsilon}{|x|},$$

where $l \in [0,\cdots,m-1]$ and $\|\cdot\|$ is the norm in $\mathbb{C}^m$.

Specializing to the j'th mode, there exist $x_0^\pm(j) \in \mathbb{R}^\pm$ and $C_\varepsilon(j)$, independent of time, such that for any $\beta \in (0,1)$ and any $l \in [0,\cdots,m-1]$, if $|t| > 1$ with $\mathrm{sign}\,(t) = \pm\mathrm{sign}\,(\partial_E k_j(\pm\infty,E))$ and $\pm x \geq \pm x_0^\pm(j)$ then

$$\|\phi_j^{[l]}(x,t,\varepsilon)\| < \frac{C_\varepsilon(j)}{|t|^\beta |x|^{(1-\beta)}}. \tag{5.6}$$

Remarks:
i) As direct corollaries, we get that $\phi_j^{[l]}(\cdot,t,\varepsilon)$, and thus $(\varepsilon\partial_x)^l\phi(\cdot,t,\varepsilon)$ belong to $L^2(\mathbb{R})$, for any $t\in\mathbb{R}$, and any $l = 0,\cdots,m-1$. Moreover,

$$\sup_{|t|\leq 1} \|(\varepsilon\partial_x)^l\phi(\cdot,t,\varepsilon)\|_{L^2(\mathbb{R})} = O(C_\varepsilon). \tag{5.7}$$

ii) The behavior in ε of C_ε and $C_\varepsilon(j)$ cannot be estimated under hypothesis **(C0)** only. However, anticipating on our eventual choice of $Q(E,\varepsilon)$, see (6.1) below, if the energy density satisfies

$$\sup_{\substack{E\in\Delta\\ \varepsilon>0}} (|Q(E,\varepsilon)| + |\varepsilon\partial_E Q(E,\varepsilon)|) < \infty, \tag{5.8}$$

and assuming (3.24), then the constants C_ε and $C_\varepsilon(j)$ are actually uniform in $\varepsilon \to 0$, as easily checked from the proof and Lemma 3.4.
iii) The complicated looking second statement simply says the following, for $0 < \beta < 1/2$. In the asymptotic regions where $\phi_j^{[l]}$ is driven by the asymptotic group velocity $-1/\partial_E k_j(\pm\infty,E)$, if time flows in the wrong direction, in the sense that the wave is driven out of these regions, then the L^2 norm over those regions decreases.
iv) We prove this Lemma in section 8.5.

In a scattering regime, we expect our solutions to behave as freely propagating waves along independent modes. Let us introduce such asymptotic waves $\phi(x,t,\varepsilon,\pm\infty)$:

$$\phi(x,t,\varepsilon,\pm\infty) = \sum_{j=1}^{md} \phi_j(x,t,\varepsilon,\pm\infty),$$

with

$$\phi_j(x,t,\varepsilon,\pm\infty) = \int_\Delta c_j(\pm\infty,E,\varepsilon) e^{\frac{-i(k_j(\pm\infty,E)x+\omega_j(\pm\infty,E))}{\varepsilon}} \varphi_j(\pm\infty,E) e^{\frac{-itE}{\varepsilon}} Q(E,\varepsilon)dE. \tag{5.9}$$

With respect to (5.3), the only dependence left in the space variable in the integrand is in the exponent. The index $\pm\infty$ refers to the choice of asymptotic mode $k_j(\pm\infty,E)$ and polarization $\varphi_j(\pm\infty,E)$ taken in the definition. Note the relation

$$(5.10)\qquad (i\varepsilon\partial_x)^l\phi_j(x,t,\varepsilon,\pm\infty) = \int_\Delta c_j(\pm\infty,E,\varepsilon)e^{-i(k_j(\pm\infty,E)x+\omega_j(\pm\infty,E))/\varepsilon}k_j^l(\pm\infty,E)\varphi_j(\pm\infty,E)e^{-itE/\varepsilon}Q(E,\varepsilon)dE \equiv \phi_j^{[l]}(x,t,\varepsilon,\pm\infty).$$

We also remark that since $\phi_j^{[l]}(x,t,\varepsilon,\pm\infty)$ are constructed as integrals in the same way as $\phi_j^{[l]}(x,t,\varepsilon)$ are, only with simpler integrands, then they also satisfy the estimates based on this structure. In particular, (5.6) holds without restriction on the boundary of the x-region:
For any $x_0\in\mathbb{R}$, there exists a constant $C_\varepsilon^\pm(j,x_0)$ such that for any $\beta\in(0,1)$ and any $l\in[0,\cdots,m-1]$, if $|t|>1$ with $\text{sign}\,(t)=\pm\text{sign}\,(\partial_E k_j(\pm\infty,E))$ and $\pm x\geq\pm x_0^\pm(j)$, then

$$(5.11)\qquad \|\phi_j^{[l]}(x,t,\varepsilon,\pm\infty)\| < \frac{C_\varepsilon^\pm(j,x_0)}{|t|^\beta|x|^{(1-\beta)}}.$$

Again, assuming (3.24) and (5.8), $C_\varepsilon^\pm(j,x_0)$ can be chosen uniformly as $\varepsilon\to 0$.

Finally, $\phi_j^{[l]}(x,0,\varepsilon,-\infty)$ determines $\phi_j^{[l]}(x,0,\varepsilon,+\infty)$ by means of (3.7).

While the waves $\phi_j(x,t,\varepsilon,\pm\infty)$ are not localized in space, we expect them to be approximations of solutions to (5.1) in neighborhoods of $x=\pm\infty$ only. Hence the following construction:

Let $x\mapsto\omega(x)\in[0,1]$ be a function such that $\omega(x)=1$ if $x\geq 1$ and $\omega(x)=0$ if $x\leq 0$. We define asymptotic waves corresponding to $\phi_j(x,t,\varepsilon,+\infty)$ for $x>1$ and to $\phi_j(x,t,\varepsilon,-\infty)$ for $x<-1$ as follows:

$$\begin{aligned}\phi_j^{[l]}(x,t,\varepsilon,a) &= \omega(x)\phi_j^{[l]}(x,t,\varepsilon,+\infty)+(1-\omega(x))\phi_j^{[l]}(x,t,\varepsilon,-\infty).\\ (5.12)\qquad \phi^{[l]}(x,t,\varepsilon,a) &= \sum_{j=1}^{md}\phi_j^{[l]}(x,t,\varepsilon,a).\end{aligned}$$

Under our hypotheses, it is easy to compute the L^2 norm of these different asymptotic states by means of the rescaled Fourier transform $\mathcal{F}_\varepsilon$ defined as:

$$(5.13)\qquad (\mathcal{F}_\varepsilon\, g(\cdot))(x) \;=\; \frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}} g(k)\,e^{-ikx/\varepsilon}\,dk.$$

Lemma 5.2. *Assume* (**H1**)*,* (**H2**)*,* (**H3**)*,* (**C0**) *and* (**GV**)*. Then there exists D_ε such that for all $j=1,\cdots,md$, all $l=0,\cdots,m-1$ and all $t\in\mathbb{R}$*

$$\|(i\varepsilon\partial_x)^l\phi_j(\cdot,t,\varepsilon,\pm\infty)\|_{L^2(\mathbb{R})}\leq D_\varepsilon.$$

Remarks:
i) As a direct corollary, $\|(i\varepsilon\partial_x)^l\phi(\cdot,t,\varepsilon,\pm\infty)\|=O(D_\varepsilon)$. Moreover, $\|\phi_j^{[l]}(\cdot,t,\varepsilon,a)\|_{L^2(\mathbb{R})}=O(D_\varepsilon)$ and therefore $\|\phi^{[l]}(\cdot,t,\varepsilon,a)\|_{L^2(\mathbb{R})}=O(D_\varepsilon)$.
ii) Again, further assuming (5.8) and (3.24), we get $D_\varepsilon=\sqrt{\varepsilon}D$, with D uniform in ε.

Proof. Under (**GV**), the reciprocal functions of $E\mapsto k_j(\pm\infty,E)$ all exist on Δ and we denote them by $k\mapsto E_j^\pm(k)$, $j=1,\cdots,md$. Hence, using (5.10) and a change of variables, we can write

$$(i\varepsilon\partial_x)^l\phi_j(x,t,\varepsilon,\pm\infty)=\phi_j^{[l]}(x,t,\varepsilon,\pm\infty)=\sqrt{2\pi\varepsilon}(\mathcal{F}_\varepsilon\,\widehat{\phi}_j^{[l]}(\cdot,t,\varepsilon,\pm\infty))(x),$$

where

$$\widehat{\phi}_j^{[l]}(k,t,\varepsilon,\pm\infty)=c_j(\pm\infty,E_j^\pm(k),\varepsilon)e^{-i\omega_j(\pm\infty,E_j^\pm(k))/\varepsilon}k^l\varphi_j(\pm\infty,E_j^\pm(k))e^{-itE_j^\pm(k)/\varepsilon}Q(E_j^\pm(k),\varepsilon)\partial_k E_j^\pm(k).$$

By Plancherel formula,

$$\|(i\varepsilon\partial_x)^l\phi_j(\cdot,t,\varepsilon,\pm\infty)\|_{L^2(\mathbb{R})}=\sqrt{2\pi\varepsilon}\|\widehat{\phi}_j^{[l]}(\cdot,t,\varepsilon,\pm\infty)\|_{L^2(\mathbb{R})}\equiv D_\varepsilon,$$

where D_ε is uniform in $t \in \mathbb{R}$.

Finally, as expected, we show that the exact solutions (5.2) behave more and more like the corresponding free asymptotic waves (5.12), in L^2 norm, as time gets large. Furthermore, we show that (5.2) cannot get trapped on a compact set of $\mathbb{R}$ as time goes to infinity, since its L^2 norm vanishes for $|t| \to \infty$ on such sets:

Proposition 5.1. *Assume that* (**H1**), (**H2**), (**H3**), (**GV**) *and* (**C0**) *are satisfied. Then, there exists $C_\varepsilon > 0$ such that we have for any $|t| > 0$, $\forall j \in \{1, \dots, md\}$ and $\forall l \in \{0, \dots, m-1\}$:*

$$\|\phi_j^{[l]}(\cdot, t, \varepsilon) - \phi_j^{[l]}(\cdot, t, \varepsilon, a)\|_{L^2(\mathbb{R})} < \frac{C_\varepsilon}{|t|}.$$

Moreover, for any bounded interval $I \in \mathbb{R}$,

$$\|\phi_j^{[l]}(\cdot, t, \varepsilon)\|_{L^2(I)} < \frac{\tilde{C}_\varepsilon}{|t|},$$

for some $\tilde{C}_\varepsilon$ depending on I.

Remarks:
i) As a direct corollary,

$$\|(i\varepsilon\partial_x)^l \phi(\cdot, t, \varepsilon) - \phi^{[l]}(\cdot, t, \varepsilon, a)\|_{L^2(\mathbb{R})} < \frac{C_\varepsilon}{|t|}.$$

ii) Further assuming (5.8) and (3.24), we can take $C_\varepsilon = C$, and $\tilde{C}_\varepsilon = \tilde{C}$ uniformly as $\varepsilon \to 0$, see the proof.
iii) The estimate is independent of the signs of t and of the asymptotic group velocities, because the definition of $\phi^{[l]}(\cdot, t, \varepsilon, a)$ takes into account the asymptotic waves travelling in both asymptotic regions. See the example below for an illustration.
iv) We prove this Proposition in 8.6.

In order to have a better understanding of the localization properties for large times of the asymptotic approximation $\phi_j^{[l]}(\cdot, t, \varepsilon, a)$, we need to look at the signs of the group velocities $-/\partial_E k_j(\pm\infty, E)$ of its components (5.9). Different cases occur that we list below.

Corollary 5.1. *Assume* (**H1**), (**H2**), (**H3**), (**GV**) *and* (**C0**) *are satisfied. Then there exists a constant H_ε such that and for any $0 < \beta < 1/2$ and $|t| \geq 1$,*

$$\begin{aligned}
&\{\ \partial_E k_j(-\infty, E)\partial_E k_j(+\infty, E) < 0 \ \ \textit{and} \ \ t\partial_E k_j(+\infty, E) < 0\ \} \\
&\qquad \Rightarrow \|\phi_j^{[l]}(\cdot, t, \varepsilon, a) - (\phi_j^{[l]}(\cdot, t, \varepsilon, -\infty) + \phi_j^{[l]}(\cdot, t, \varepsilon, +\infty))\|_{L^2(\mathbb{R})} \leq \frac{H_\varepsilon}{|t|^\beta}, \\
&\{\ \partial_E k_j(-\infty, E)\partial_E k_j(+\infty, E) > 0 \ \ \textit{and} \ \ t\partial_E k_j(+\infty, E) > 0\ \} \\
&\qquad \Rightarrow \|\phi_j^{[l]}(\cdot, t, \varepsilon, a) - \phi_j^{[l]}(\cdot, t, \varepsilon, -\infty)\|_{L^2(\mathbb{R})} \leq \frac{H_\varepsilon}{|t|^\beta}, \\
&\{\ \partial_E k_j(-\infty, E)\partial_E k_j(+\infty, E) > 0 \ \ \textit{and} \ \ t\partial_E k_j(+\infty, E) < 0\ \} \\
&\qquad \Rightarrow \|\phi_j^{[l]}(\cdot, t, \varepsilon, a) - \phi_j^{[l]}(\cdot, t, \varepsilon, +\infty)\|_{L^2(\mathbb{R})} \leq \frac{H_\varepsilon}{|t|^\beta}, \\
&\{\ \partial_E k_j(-\infty, E)\partial_E k_j(+\infty, E) < 0 \ \ \textit{and} \ \ t\partial_E k_j(+\infty, E) > 0\ \} \\
&\qquad \Rightarrow \|\phi_j^{[l]}(\cdot, t, \varepsilon, a)\|_{L^2(\mathbb{R})} \leq \frac{H_\varepsilon}{|t|^\beta},
\end{aligned}$$

Proof. Just make use of the definition (5.12), of (5.11) and of the support properties of ω.

Remark: Again, if (5.8) and (3.24) are true, the constant H_ε is uniform in ε.

Another consequence of Lemmas 5.1 and 5.2, equation (5.7) and Proposition 5.1 is the following estimate

Corollary 5.2. *Assume* (**H1**), (**H2**), (**H3**) *and* (**C0**) *are satisfied. Then, there exists* $F_\varepsilon > 0$ *such that for all* $l = 0, \cdots, m-1$,

$$\sup_{t\in\mathbb{R}} \|(\varepsilon\partial_x)^l \phi(x,t,\varepsilon)\|_{L^2(\mathbb{R})} \le F_\varepsilon.$$

If, furthermore, (5.8) and (3.24) are true, F_ε *can be chosen as* F*, uniform in* $\varepsilon \to 0$.

Hence, if the L^2 norm is not conserved under the time evolution (1.2), it remains uniformly bounded in time. Moreover, it is also uniformly bounded in ε, for the type of energy densities that we will use below, see (6.1), with (5.8) and (3.24). Hence, in that case, the L^2 norm of our solutions at any time is proportional to that they had at any initial time t_0:

$$\|\phi(\cdot,t,\varepsilon)\|_{L^2(\mathbb{R})} \le F\|\phi(\cdot,t_0,\varepsilon)\|_{L^2(\mathbb{R})}. \tag{5.14}$$

Let us illustrate some of the notions of this Section by means of an explicitly solvable example. Consider the following scalar linear PDE:

$$(\tanh(x) i\epsilon\partial_t - i\epsilon\partial_x)\phi(x,t,\epsilon) = 0. \tag{5.15}$$

The corresponding dispersion relation yields $k(x,E) = E\tanh(x)$ as unique mode, which satisfies **(GV)**. As the equation is ε-independent, we take $\varepsilon = 1$. The general solution reads $\phi(x,t,1) = f(t + \ln(\cosh(x)))$, where f is any regular function. To have a solution obtained by means of a superposition of generalized eigenvectors $e^{-iE\int_0^x \tanh(y)dy}$ according to some compactly supported energy density, we must have

$$f(t+\ln(\cosh(x))) = \int_\Delta e^{-iE\int_0^x \tanh(y)dy} e^{-iEt} Q(E,1)dE = \int_\Delta e^{-iE(t+\ln(\cosh(x)))} Q(E,1)dE.$$

Hence, $f = \sqrt{2\pi}(\mathcal{F}_1 Q(\cdot,1))$ and is therefore L^2, analytic and goes to zero at infinity.

That the L^2 norm is not conserved in general under our hypotheses is now easily seen: Since $0 \le \ln(\cosh(x))$ is even and behave as $|x|$ for x large, one checks that we have $\lim_{t\to-\infty} \|\phi(\cdot,t,1)\|_{L^2(\mathbb{R})} = O(\|f(\cdot)\|_{L^2(\mathbb{R})}) > 0$, whereas, $\lim_{t\to+\infty} \|\phi(\cdot,t,1)\|_{L^2(\mathbb{R})} = 0$.

Let us investigate the asymptotic waves corresponding to (5.15). Using $k(\pm\infty, E) = \pm E$, we find

$$\phi(x,t,1,\pm\infty) = \int_\Delta e^{\mp ixE} e^{-iEt} Q(E,1)dE = \sqrt{2\pi}(\mathcal{F}_1 Q(\cdot,1))(t\pm x).$$

Hence,

$$\phi(x,t,1,a) = \omega(x)\sqrt{2\pi}(\mathcal{F}_1 Q(\cdot,1))(t+x) + (1-\omega(x))\sqrt{2\pi}(\mathcal{F}_1 Q(\cdot,1))(t-x),$$

which, as $t \to -\infty$, is significant at both large and positive values of x and large and negative values of x. Accordingly, for $t \simeq -\infty$, $f(t+\ln(\cosh(x)))$ is significant at values of $\ln(\cosh(x)) \simeq |x| \simeq |t|$, i.e. for $x \simeq \pm|t|$. The picture is that of two bumps at plus and minus infinity in space that travel towards one another with unit velocity and disappear as they collide. This is correctly captured by the approximation $\phi(x,t,1,a)$, for large times.

6. Semi-classical transitions asymptotics

6.1. **The transition integral.** We assume here we are in an avoided crossing situation, and we do not explicit the dependence in the variable $\delta > 0$ in the notation. We have obtained the asymptotics of the scattering matrix $S(E,\varepsilon)$ in Section 4. We now compute the small ε-asymptotics of the integrals that describe the asymptotic states $\phi_j(x,t,\varepsilon,\pm\infty)$ given by (5.9) as $|t| \to \infty$, for the different channels.

We assume that j is such that (4.1) holds and let $n = \pi(j)$ be given by (4.11).

We choose our energy density $Q(E,\varepsilon)$ to be more and more sharply peaked near a specific value $E_0 \in \Delta\setminus\partial\Delta$ as $\varepsilon \to 0$. As a result, we obtain semiclassical wavepackets that are well localized in phase space. This is a physically reasonable choice that allows for a complete semiclassical treatment.

More precisely we consider,

$$Q(E,\varepsilon) \;=\; e^{-G(E)/\varepsilon}\, e^{-i\,J(E)/\varepsilon}\, P(E,\varepsilon), \tag{6.1}$$

where

(C1): The real-valued function $G \geq 0$ is in $C^3(\Delta)$, is independent of δ and has a unique non-degenerate absolute minimum value of 0 at E_0 in the interior of Δ. This implies that

$$G(E) \;=\; g\,(E-E_0)^2/2 \;+\; O(E-E_0)^3, \qquad \text{where} \qquad g>0.$$

(C2): The real-valued function J is in $C^3(\Delta)$.

(C3): The complex-valued function $P(E,\varepsilon)$ is in $C^1(\Delta)$ and satisfies

$$\sup_{\substack{E\in\Delta\\ \varepsilon\geq 0}} \left|\frac{\partial^n}{\partial E^n}\, P(E,\varepsilon)\right| \;\leq\; C_n, \qquad \text{for} \qquad n=0,\,1. \tag{6.2}$$

Remarks:
i) Typical interesting choices of Q are $G \,=\, g\,(E-E_0)^2$, $J=0$, and P an ε-dependent multiple (the equation (1.2) is linear) of a smooth function with at most polynomial growth in $(E-E_0)/\varepsilon$.
ii) We want to emphasize the fact that a Gaussian energy density does not give rise in general to a Gaussian solution. See the discussion in the Introduction and Section 6 of [19].

The leading inter-modes transitions are described by the asymptotics of those coefficients $c_l(\pm\infty,E,\varepsilon)$ that satisfy

$$c_k(-\infty,E,\varepsilon) \;=\; \delta_{j,k} \tag{6.3}$$

$$c_n(+\infty,E,\varepsilon) \;=\; e^{-i\theta_j(\zeta,E)}\; e^{i\int_\zeta k_j(z,E)dz/\varepsilon}\;(1+O_E(\varepsilon)), \tag{6.4}$$

where $n=\pi(j)=j\pm 1$. We recall that the error term $O_E(\varepsilon)$ depends analytically on the energy E in a neighborhood of the compact set Δ. We have already noted in the comments after Theorem 4.1 that the term $O_E(\varepsilon)$ satisfies (6.2).

Theorem 6.1. *Assume* **(H1)** *to* **(H3)**, **(AC)** *and* **(GV)**. *Let $Q(\cdot,\epsilon)$ be the energy density supported on the interval Δ defined in (6.1) which satisfies* **(C1)**, **(C2)**, *and* **(C3)**. *Let $\phi(x,t,\varepsilon)$ be a solution of equation (5.1) of the form (5.2). Assume $\partial_E k_j(-\infty,E)<0$ on Δ, for some j and suppose that the solution is characterized in the past by*

$$\lim_{t\to-\infty}\|\phi(\cdot,t,\varepsilon)-\phi(\cdot,t,\varepsilon,a)\|_{L^2(\mathbb{R})}=0,$$

where, as $t\to-\infty$,

$$\omega(x)\phi(x,t,\varepsilon,a)=\int_\Delta Q(E,\varepsilon)e^{-itE/\varepsilon}e^{-i(xk_j(-\infty,E)+\omega_j(-\infty,E))/\varepsilon}\varphi_j(-\infty,E)dE+O(1/|t|^\beta).$$

Let $n=\pi(j)$ be given by (4.11), and let

$$\alpha(E) \;=\; G(E)\,+\,\mathrm{Im}\,(\int_\zeta k_j(z,E)\,dz), \tag{6.5}$$

$$\kappa(E) \;=\; J(E)\,-\,\mathrm{Re}\,(\int_\zeta k_j(z,E)\,dz)\,+\,\omega_n(+\infty,E). \tag{6.6}$$

Assume E^* is the unique absolute minimum of $\alpha(\cdot)$ in $\mathrm{Int}\,\Delta$ and define $k^*=k_n(+\infty,E^*)$. Let $k\mapsto E_n^\pm(k)$ be the inverse function of $E\mapsto k_n(\pm\infty,E)$ on Δ.

Then, there exist $\delta_0>0$, $p>0$ arbitrarily close to $5/4$, and a function $\varepsilon_0:(0,\delta_0)\to\mathbb{R}^+$, such that for all $0<\beta<1/2$, $\delta<\delta_0$, and $\varepsilon<\varepsilon_0(\delta)$, the following asymptotics hold as $t\to-\mathrm{sign}\,(\partial_k E_n^+(k^*))\infty$, in $L^2(\mathbb{R})$ norm:

$$\begin{aligned}\phi_n(x,t,\varepsilon)=&\sqrt{2\pi\varepsilon}P(E^*,\varepsilon)e^{-\alpha(E^*)/\varepsilon}e^{-i\kappa(E^*)/\varepsilon}\varphi_n(+\infty,E^*)e^{-i\,\theta_j(\zeta,E^*)}\partial_k E_n^+(k^*)\times\\ &\times\mathcal{F}_\varepsilon(e^{-itE_n^+(\cdot)/\varepsilon}e^{-\Lambda(\cdot)/\varepsilon}\chi_{k_n(+\infty,\Delta)})+O(e^{-\alpha(E^*)/\varepsilon}\varepsilon^p)+O\left(1/|t|^\beta\right),\end{aligned} \tag{6.7}$$

where

$$\Lambda(k) = \frac{\lambda_2}{2}(k-k^*)^2 + i\lambda_1(k-k^*), \ \textit{with } \lambda_1 = \partial_k E_n^+(k^*)\kappa'(E^*),$$

$$\lambda_2 = [\partial_k E_n^+(k^*)]^2\alpha\text{"}(E^*) + i\left[\kappa\text{"}(E^*)[\partial_k E_n^+(k^*)]^2 + \kappa'(E^*)\partial_k^2 E_n^+(k^*)\right],$$

and $\chi_{k_n(+\infty,\Delta)}$ *is the characteristic function of the set* $k_n(+\infty,\Delta)$.
Moreover, if $t \to \operatorname{sign}(\partial_k E_n^+(k^*))\infty$, *then* $\|\phi_n(x,t,\varepsilon)\|_{L^2(\mathbb{R})} = O\left(1/|t|^\beta\right)$.

Remarks:
0) The first error term is uniform in t whereas the second error term is uniform in ε.
i) The same result holds for ϕ, and $\phi_n(+\infty)$, replaced by $(i\varepsilon\partial)^l\phi$, and $(i\varepsilon\partial)^l\phi_n(+\infty)$ respectively, with $\{l = 0,\cdots,m-1\}$, at the expense of a multiplication of the prefactor by $k_n(+\infty,E^*)^l$.
ii) As will be made explicit in Section 7 below, the L^2 norm of the leading term expressed as a Fourier transform is positive, of order $\varepsilon^{1/4}$, and independent of time. The leading term hence becomes meaningful for times t that are of order $|t| \simeq e^{c/\varepsilon}$, for some $c > 0$ at least. We get control over this time scale far beyond the Ehrenfest or Heisenberg times of Quantum semiclassical analysis thanks to our scattering setup.
iii) The leading term clearly satisfies the asymptotic PDE (1.14).
iv) The energy E^* depends explicitly on the properties of the involved modes and on the energy density $Q(E,\varepsilon)$ as well.
v) The space-time localization properties of the leading term are further discussed in Section 7.
vi) Also, as mentioned earlier, we can specify the coefficients c_l at $x = +\infty$ instead.
vii) The proof of the Theorem is given in the last Section of the paper.

Let us finally discuss our hypotheses and interpret our result. The condition on the sign of $\partial_E(k_j(-\infty,E))$ says that the group velocity of $\phi_j(x,t,\varepsilon,-\infty)$ is positive, so that $\phi(x,t,\varepsilon,a)$ is non trivial as $t\to-\infty$ for negative x's and describes an ingoing wave. If the asymptotic group velocity of the mode $k_n(x,E)$ is positive as $x\to+\infty$, our results describes an outgoing *transmitted wave* for large positive times, as discussed in the introduction. If the asymptotic group velocity $-\partial_k E_n^+(k)$ is negative, we describe another ingoing wave along mode n, for large negative times and large positive x's, arising during the evolution, which, as time goes to $+\infty$, goes to zero. Note also that if the asymptotic group velocity of mode $k_j(x,E)$ at $x=+\infty$ is positive, then an order one wave, in the sense that $c_j(+\infty,E,\varepsilon) = 1+O(\varepsilon)$, propagates along positive x's for positive times. If the asymptotic group velocity of mode $k_j(x,E)$ at $x=+\infty$ is negative, there is no wave propagating along positive x's to the right, for large positive times, but another ingoing wave from large positive x's and large negative times.

Therefore, in case $-\partial_k E_n^+(k)$ is negative and both $-\partial_k E_j^-(k)$ and $-\partial_k E_j^+(k)$ are positive, running the evolution *backwards in time*, we have an ingoing wave (of order one in the sense above) on mode j, for $x\to+\infty$ and $t\to+\infty$, and, as $t\to-\infty$, we have an outgoing wave on mode j, for $x\to-\infty$, and another exponentially small outgoing wave on mode n, for $x\to+\infty$, whose asymptotics is determined by our Theorem. Hence, we describe the asymptotics of a *reflected wave* in mode n. Note that reflected waves on other modes may be present as well. In any case, they are exponentially small.

Finally, in case $-\partial_k E_n^+(k)$ and $-\partial_k E_j^+(k)$ are both negative, we describe a scattering process in which we have ingoing solutions on the modes j and n, that all disappear as time goes to $+\infty$, in a similar way as what happens in the illustration ending the previous Section.

6.2. **Perturbative results in δ.** We assume that (**H4**) is also satisfied and restore back δ in the notation. We have the following sharper result concerning the behavior as $\delta\to0$ of the quantities involved in the description of the asymptotic wave:

Proposition 6.1. *Further assuming* (**H4**), *we have the following as* $\delta\to0$, *for* $E\in\Delta$:

$$\operatorname{Im}\int_\zeta (k_i - k_j)(z,E,\delta)\ dz = D(E)\delta^2 + O(\delta^3),$$

with $D(E) = \frac{\pi}{4}\frac{a^2(E)b^2(E)-c^2(E)}{a^3(E)}$.

This implies that $(E,\delta)\mapsto \mathrm{Im}\int_\zeta (k_i-k_j)(z,E,\delta)dz$ *is a positive function.*

Let $\alpha(E,\delta)=G(E)+\mathrm{Im}\int_\zeta (k_i-k_j)(E,\delta)$. *There exists* $E^*(\delta)$ *such that*

$$\partial_E\alpha(E^*(\delta),\delta)=0.$$

It satisfies:

$$E^*(\delta)=E_0-\frac{D'(E_0)}{g}\delta^2+O(\delta^3).$$

The results above hold provided one knows $E^*(\delta)$ is the unique absolute minimum of α in the set Δ, which is generically true. Again, if there are several minima, one simply adds the corresponding contributions. Note also that if the constant g characteristic of the energy density is of order δ^2, the difference E_0-E^* is of order one as δ shrinks to zero. This corresponds to a "wide" energy density of width ε/δ^2 around E_0. This result is a straightforward consequence of the Implicit Function Theorem, the proof of which we omit.

6.3. **Explicit computation in case $E_n^+(k)$ is quadratic.** In this paragraph, we assume that $k\mapsto E_n^+(k)$ is quadratic:

$$\forall k\in k_n(\Delta,+\infty),\quad \partial_k^3E_n^+(k)=0. \tag{6.8}$$

This is true for all modes in the study of the Born-Oppenheimer approximation, see [19]. This situation allows for an explicit determination of the leading term in the asymptotic wave. We also assume that the function α has a unique absolute minimum $E^*(\delta)$. For sufficiently small δ, this minimum is non degenerate and satisfies $E^*(\delta)\in\mathrm{Int}\Delta$.

The following result is proven in Section 8:

Lemma 6.1. *Assume that* $k\mapsto E_n^+(k)$ *is quadratic and that* α *has a unique absolute minimum* $E^*(\delta)\in Int\Delta$. *There exists* $p\in]3/4,5/4[$ *such that, as* $\varepsilon\to 0$*:*

$$\begin{aligned}\phi_n(x,t,\varepsilon,+\infty)&=e^{-\alpha(E^*)/\varepsilon}e^{-i\kappa(E^*)/\varepsilon}\varphi_n(+\infty,E^*)e^{-i\,\theta_j(\zeta,E^*)}P(E^*,\varepsilon)\partial_kE_n^+(k^*)\times\\&\times\frac{\sqrt{2\pi\varepsilon}e^{-i(k^*x+tE^*)/\varepsilon}}{[\lambda_2+i\partial_k^2E_n^+(k^*)t]^{1/2}}e^{-\frac{(\lambda_1+\partial_kE_n^+(k^*)t+x)^2}{2\varepsilon(\lambda_2+i\partial_k^2E_n^+(k^*)t)}}+O(e^{-\alpha(E^*)/\varepsilon}\varepsilon^p),\end{aligned} \tag{6.9}$$

Remarks:
i) The leading term in that case is a freely propagating Gaussian, i.e. an exact solution to

$$i\varepsilon\partial_tg(x,t,\varepsilon)=\left(E^*+\partial_kE_n^+(k^*)(i\varepsilon\partial_x-k^*)+\frac{\partial_k^2E_n^+(k^*)}{2}(i\varepsilon\partial_x-k^*)^2\right)g(x,t,\varepsilon),$$

centered at $x_c(t)=-\partial_kE_n^+(k^*)t-\lambda_1$, of width $\sqrt{\varepsilon t}$ and of L^2 norm of order $\varepsilon^{3/4}$.
ii) In the general case, the error terms involved in the course of the computation are not uniform in time, which prevents us to get such an explicit form for the asymptotic wave. Nevertheless, we show in the next Section that we can get a fairly accurate description of such asymptotic waves, for large times and small ε.

7. Space-time properties of the asymptotic waves

As seen above, the interpretation of our results makes use of the space-time properties the different asymptotic waves $\phi_j(x,t,\varepsilon,\pm\infty)$ in terms of which the time-dependent scattering processes are expressed. The present Section is devoted to a thorough description of the space-time properties of the leading term of these waves as $\varepsilon\to 0$ and $|t|\to\infty$.

We first note that Theorem 6.1 also holds for the wave $\phi_j(x,t,\varepsilon,\pm\infty)$, which characterized by the asymptotics $c_j(\pm\infty,E,\varepsilon)=1+O_E(\varepsilon)$. It suffices to replace the index n by j, the values E^* and k^* by E_0 and k_0, and to set $\alpha(E)=G(E)$ and $\theta_j(\zeta,E)\equiv 0$. Note in particular, that $\alpha(E_0)=0$, as it should be.

Therefore, the space-time properties of the asymptotic waves along modes j and $\pi(j) = n$ are encoded in the Fourier transform

$$\mathcal{F}_\varepsilon\,(e^{-itE_l^\sigma(\cdot)/\varepsilon}e^{-\Lambda(\cdot)/\varepsilon}\chi_{k_l(+\infty,\Delta)})(x) \;=\; \frac{1}{\sqrt{2\pi\varepsilon}}\int_{k_l(\sigma,\Delta)} e^{-i(kx+tE_l^\sigma(k))/\varepsilon}e^{-\Lambda(k)/\varepsilon}\,dk, \tag{7.1}$$

where the index l stands for j or n, and σ for $+$ or $-$. We will also denote k^* or k_0, respectively E^* or E_0, depending on the context, by $\tilde{k}$, respectively $\tilde{E}$. We can make use of the positivity of the real part of the function $\Lambda(k)$ and of Parseval's formula to regularize and localize the integrand as follows. Let $\eta \in C_0^\infty(\mathbb{R})$ with support in $[-1,1]$ and $\eta(k) \equiv 1$ in a neighborhood of $k = 0$. Set $\eta_\varepsilon(k) := \eta((k-\tilde{k})/\varepsilon^\tau)$, with $0 < \tau < 1/2$. Then, if $k \notin \operatorname{supp}(\eta_\varepsilon)$, $|e^{-\Lambda(k)/\varepsilon}| = O(\varepsilon^\infty)$. Therefore, we have in L^2 norm,

$$\begin{aligned}\mathcal{F}_\varepsilon\,(e^{-itE_l^\sigma(\cdot)/\varepsilon}e^{-\Lambda(\cdot)/\varepsilon}\chi_{k_l(+\infty,\Delta)})(x) &= \frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}} e^{-i(kx+tE_l^\sigma(k))/\varepsilon}e^{-\Lambda(k)/\varepsilon}\eta_\varepsilon(k)\,dk + O(\varepsilon^\infty)\\ &= \mathcal{F}_\varepsilon\,(e^{-itE_l^\sigma(\cdot)/\varepsilon}e^{-\Lambda(\cdot)/\varepsilon}\eta_\varepsilon(\cdot))(x) + O(\varepsilon^\infty),\end{aligned} \tag{7.2}$$

where the error term is uniform in t. Note also that by Parseval again,

$$\begin{aligned}\left\|\mathcal{F}_\varepsilon\,(e^{-itE_l^\sigma(\cdot)/\varepsilon}e^{-\Lambda(\cdot)/\varepsilon}\eta_\varepsilon(\cdot))\right\|^2_{L^2(\mathbb{R}_x)} &= \sqrt{\varepsilon}\int_{\mathbb{R}} e^{-\operatorname{Re}\lambda_2 z^2}\,dz + O(\varepsilon^\infty)\\ &= \sqrt{\frac{\varepsilon 2\pi}{[\partial_k E_l^\sigma(\tilde{k})]^2\alpha"(\tilde{E})}} + O(\varepsilon^\infty),\end{aligned} \tag{7.3}$$

uniform in t. Hence, the L^2 norm of the asymptotic state in Theorem 6.1 is positive, independent of time and of order $\varepsilon^{3/4}$.

Now, as $k_l(\sigma\infty,\cdot)$ is analytic in $E \in \Delta$, the same is true for the inverse function $E_l^\sigma(\cdot)$ in $k \in k_l(+\infty,\Delta)$. Moreover, $e^{-\Lambda(\cdot)/\varepsilon}\eta_\varepsilon(\cdot)$ is in C_0^∞, so that we can apply stationary phase methods to describe the large t and x behavior of (7.2).

Proposition 7.1. *Let η_ε be as above and $1 > \alpha > 1/2$ and assume $\partial_k E_l^\sigma(\tilde{k}) \neq 0$. Define for all $|t| \geq 1$,*

$$C_t(\varepsilon) = \cup_{|k-\tilde{k}|\leq\varepsilon^\tau}\,\{x \in \mathbb{R}\,|\,|x + \partial_k E_l^\sigma(k)t| \leq |t|^\alpha\}$$

Then, there exist $\varepsilon_0 > 0$ and $c(n) > 0$, such that for all $\varepsilon < \varepsilon_0$, all $n \in \mathbb{N}$ and all $|t| \geq 1/\varepsilon^{1/(1-\alpha)}$,

$$\begin{aligned}\left\|\frac{1}{\sqrt{2\pi\varepsilon}}\int_{\mathbb{R}} e^{-i(kx+tE_l^\sigma(k))/\varepsilon}e^{-\Lambda(k)/\varepsilon}\eta_\varepsilon(k)\,dk\right\|_{L^2(\mathbb{R}\setminus C_t(\varepsilon))} &\leq c(n)\frac{\varepsilon^{1/2+\tau}}{|t|^{3\alpha/2-1}}\left(\frac{\varepsilon}{|t|^{2\alpha-1}}\right)^n\\ &= O\left(\left(\frac{\varepsilon}{|t|^{2\alpha-1}}\right)^\infty\right).\end{aligned} \tag{7.4}$$

Remarks:
i) The Proposition says, essentially, that the whole L^2 mass of the asymptotic wave in Theorem 6.1 is located at time t in (a slightly larger) neighborhood of size $\sqrt{|t|}$ of the point propagating with the group velocity $-\partial_k E_l^\sigma(\tilde{k})$, up to arbitrarily small corrections as $\varepsilon/|t|^{2\alpha-1} \to 0$.
ii) The Proposition actually also holds if $\varepsilon = 1$, if one is not interested in the small ε behavior.
iii) The condition $|t| \geq 1/\varepsilon^{1/(1-\alpha)}$ actually represents no restriction in our case, since we need to work with exponentially large times in ε, in order to have a meaningful leading order term in Theorem 6.1.
iv) The proof is given in the last Section.

While we don't need to assume anything on the direction of propagation of the involved waves for Theorem 6.1 to hold, it's usefulness in describing time-dependent scattering processes is revealed by the above interpretation based on these directions of propagation.

8. Technicalities

8.1. **Proof of Lemma 2.1.** We first prove that if Δ is small enough, p is independent of E. Fix $E_0 \in \Delta$ and x_0 such that $(k_i - k_j)(x_0, E_0) = 0$. By hypothesis $k_i - k_j$ is continuous, then, by Cauchy formula, $\partial_x(k_i - k_j)$ is continuous and $\partial_x(k_i - k_j) \neq 0$ in a neighborhood of (x_0, E_0). By local inversion, the set $\{E \in \Delta \; ; \; p(E) = p(E_0)\}$ is open. Thus, for any $E \in \Delta$, $p(E)$ is constant.

By linear perturbation theory, there exists $Y > 0$ such that there are no non real crossings in ρ_Y, for any $E \in \Delta$.

We have the following result:

Lemma 8.1. *Fix $i \neq j$. The functions k_i and k_j have the following properties*
1. *The function $(z, E) \mapsto k_i(z, E, 0) + k_j(z, E, 0)$ is analytic on $\rho_Y \times \Delta$.*
2. *The function $(z, E) \mapsto (k_i(z, E, 0) - k_j(z, E, 0))^2$ is analytic on $\rho_Y \times \Delta$.*

Proof. According to [26], we know that we only have to check the analyticity of $k_i + k_j$ and $(k_i - k_j)^2$ in a neighborhood of a crossing, actually a branch point (x_0, E_0). Let $P(z, E)$ be the 2-dimensional projector on the λ-group corresponding to the eigenvalues $k_i(z, E, 0)$ and $k_j(z, E, 0)$. Let Γ be a small a closed path in $\mathbb{C}$ surrounding $k_i(x_0, E_0)$. For (z, E) in a neighborhood of (x_0, E_0), we can write :

$$P(z, E) = \frac{1}{2i\pi} \int_\Gamma (H(z, E, 0) - \lambda)^{-1} d\lambda.$$

As H and thus its resolvent on Γ are analytic in (z, E), this implies that $(z, E) \mapsto P(z, E)$ is analytic in a neighborhood of (x_0, E_0). We consider $\{\varphi_1(x_0, E_0), \varphi_2(x_0, E_0)\}$ a basis of $P(x_0, E_0)\mathbb{C}^{md}$ and we define:

$$\varphi_1(z, E) = P(z, E)\varphi_1(x_0, E_0) \quad ; \quad \varphi_2(z, E) = P(z, E)\varphi_2(x_0, E_0).$$

Then, in a neighborhood of (x_0, E_0), $\{\varphi_1(z, E), \varphi_2(z, E)\}$ is an analytic basis of $P(z, E)\mathbb{C}^{md}$. The matrix $M(z, E)$ of $P(z, E)H(z, E, 0)_{|P(z,E)\mathbb{C}^{md}}$ on the basis $\{\varphi_1(z, E), \varphi_2(z, E)\}$ has analytic coefficients. Besides, $\sigma(P(z, E)H(z, E, 0)_{|P(z,E)\mathbb{C}^{md}}) = \{k_i(z, E, 0), k_j(z, E, 0)\}$. This implies that $\det M(z, E) = k_i(z, E, 0)k_j(z, E, 0)$ and $\operatorname{tr} M(z, E) = k_i(z, E, 0) + k_j(z, E, 0)$. We finish the proof with the identity $(k_i - k_j)^2 = (k_i + k_j)^2 - 4k_ik_j$. This ends the proof of Lemma 8.1.

We define:

$$\Lambda = \{(z, E)/\exists i \neq j/ \quad (k_i - k_j)(z, E, 0) = 0\} \subset \mathbb{R} \times \Delta.$$

According to [26], it suffices to prove that the functions $\{k_j\}_{j=1,\dots,md}$ are analytic in a neighborhood of any $(x_0, E_0) \in \Lambda$. Fix $(x_0, E_0) \in \Lambda$. There exist i and j such that $k_i(x_0, E_0, 0) = k_j(x_0, E_0, 0)$. For $l \neq j$ and $l \neq i$, k_l is analytic in a neighborhood of (x_0, E_0). By using Lemma 8.1, it suffices to prove that $(z, E) \mapsto (k_i(z, E, 0) - k_j(z, E, 0))$ is analytic at (x_0, E_0). The function $g(z, E) = (k_i - k_j)^2(z, E, 0)$ is analytic in a neighborhood V of (x_0, E_0). Besides, since $k_i - k_j$ is real for any (x, E) in $V \cap \mathbb{R}^2$, we have:

$$g(x, E) \geq 0, \quad \forall (x, E) \in V \cap \mathbb{R}^2.$$

We write the Taylor expansion of $(z, E) \mapsto g(z, E)$. There exist $(\alpha,\ \beta,\ \gamma) \in \mathbb{R}^3$ such that:

$$g(z, E) = [\alpha(z - x_0)]^2 + [\beta(z - x_0) + \gamma(E - E_0)]^2 + o((z - x_0)^2 + (E - E_0)^2).$$

We start with proving that there exist $(\tilde{\beta},\ \tilde{\gamma}) \in \mathbb{R}^2$ such that

$$g(z, E) = [\tilde{\beta}(z - x_0) + \tilde{\gamma}(E - E_0)]^2 + o((z - x_0)^2 + (E - E_0)^2).$$

We know that, for any $E \in \Delta$, the function $z \mapsto \sqrt{g(z, E)}$ is analytic. For $|E - E_0|$ and $|z - x_0|$ small enough, we have that:

$$\sqrt{g(z, E)} = \sqrt{(\alpha^2 + \beta^2)\left(z - x_0 + \frac{\gamma\beta(E - E_0)}{\alpha^2 + \beta^2}\right)^2 + \frac{\gamma^2\alpha^2(E - E_0)^2}{\alpha^2 + \beta^2} + o((z - x_0)^2 + (E - E_0)^2)}.$$

The function $z \mapsto \sqrt{g(z, E)}$ can be analytically continued in a neighborhood of x_0 only if $\gamma\alpha = 0$. This proves the announced result, with $(\tilde{\beta},\ \tilde{\gamma}) = (\beta,\ \gamma)$ or $(\tilde{\beta},\ \tilde{\gamma}) = (\sqrt{\alpha^2 + \beta^2}, 0)$.

We notice that we have the following relations:

$$|\partial_x(k_i - k_j)(x_0, E_0)| = |\tilde\beta| \neq 0.$$

$$|\partial_E(k_i - k_j)(x_0, E_0)| = |\tilde\gamma|.$$

To end the proof, it remains to show that:

$$g(z, E) = [\tilde\beta(z - x_0) + \tilde\gamma(E - E_0)]^2 + O(|\tilde\beta(z - x_0) + \tilde\gamma(E - E_0)|^3 + |E - E_0|[\tilde\beta(z - x_0) + \tilde\gamma(E - E_0)]^2).$$

We change variables for $u = \tilde\beta(z - x_0) + \tilde\gamma(E - E_0)$ and $e = (E - E_0)$.

Since $\tilde\beta \neq 0$, this map is bijective and we consider the function $\tilde g$:

$$\tilde g(u, e) = g\left(\frac{u - \tilde\gamma e}{\tilde\beta} + x_0, e + E_0\right).$$

We write the Taylor expansion of $\tilde g$ near $(0, 0)$:

$$\tilde g(u, e) = u^2 + \sum_{l+q\geq 3} a_{lq} u^l e^q.$$

Since $\tilde g$ is real positive on a neighborhood of $(0, 0)$, we obtain that $a_{1q} = 0$, for any $q \geq 2$. This implies:

$$\tilde g(u, e) = u^2\left(1 + \sum_{l\geq 2, q\geq 1} a_{lq} u^{l-2} e^q\right) = u^2\left(1 + O(|e| + |ue|)\right).$$

Point (3) is an immediate consequence of (2) and of Rouché's Theorem. It ends the proof of Lemma 2.1.

8.2. **Proof of Lemma 2.2.** A proof similar to the proof of Lemma 8.1 shows that the function $(z, E) \mapsto (k_i - k_j)^2(z, E, \delta)$ is analytic for δ small enough and that $(z, E, \delta) \mapsto (k_i - k_j)^2(z, E, \delta)$ is C^3.

For $\delta = 0$, Lemma 2.1 implies that $a(E) = |\partial_z(k_i - k_j)(x_0(E), E, 0)|$ is analytic in $E \in \Delta$. For $\delta > 0$, we define:

$$r_1(z, E, \delta) = \frac{(k_i - k_j)^2(z, E, \delta) - a^2(E)(z - x_0(E))^2}{2\delta}.$$

The function $E \mapsto \partial_z r_1(x_0(E), E, \delta) = c(E) + O(\delta)$ is analytic and $O(\delta)$ is uniform in E. Thus we can apply Weierstrass's Theorem to get that the function c satisfies $c(E) = \lim_{\delta\to 0} \partial_z r_1(x_0(E), E, \delta)$ and is analytic in $E \in \Delta$. We also define:

$$r_2(z, E, \delta) = \frac{(k_i - k_j)^2(z, E, \delta) - a^2(E)(z - x_0(E))^2 - 2c(E)(z - x_0(E))\delta}{\delta^2}.$$

Similarly, the function b^2 such that $b^2(E) = \lim_{\delta\to 0} r_2(x_0(E), E, \delta)$ is analytic.

8.3. **Proof of Lemma 3.3.** We fix $\delta > 0$ and drop it from the notation. For $\rho > 0$, we denote by $V_\rho(\Delta) = \{\mathcal{E} \in \mathbb{C}\ ;\ \mathrm{dist}(\mathcal{E}, \Delta) < \rho\}$.

By perturbation theory, there exists $Y > 0$ and $\rho > 0$, depending on δ, such that $(z, E) \mapsto k_j(z, E)$ is analytic on $\rho_Y \times V_\rho(\Delta)$ and:

$$\inf_{i\neq j, (z,E)\in\rho_Y\times V_\rho(\Delta)} (k_i(z, E) - k_j(z, E)) > 0.$$

Hence, for $a > 0$ small enough, we can write the eigenprojector $P_j(z, E)$ as:

$$P_j(z, E) = \frac{1}{2i\pi}\int_{|\lambda - k_j(z,E)|=a} [H(z, E) - \lambda]^{-1} d\lambda.$$

We recall the identity

$$[H(z, E) - \lambda]^{-1} - [H(\infty, E) - \lambda]^{-1} = [H(z, E) - \lambda]^{-1}[H(\infty, E) - H(z, E)][H(\infty, E) - \lambda]^{-1}$$

and the fact that $H(\cdot, E)$ and its derivatives with respect to E satisfy the analog of **H2** uniformly in $E \in V_\rho(\Delta)$. This implies that for any $j \in \{1, \dots, md\}$, for any $l \in \mathbb{N}$, and uniformly in $E \in V_\rho(\Delta)$:

$$
\sup_{\mathrm{Re}\, z>0} |\mathrm{Re}\, z|^{2+\nu} \|\partial_E^l (P_j(z,E) - P_j(+\infty, E))\| + \sup_{\mathrm{Re}\, z<0} |\mathrm{Re}\, z|^{2+\nu} \|\partial_E^l (P_j(z,E) - P_j(-\infty, E))\| < \infty. \tag{8.1}
$$

We consider the vector $\Phi_j(0, E)$ satisfying (3.14) for $z = 0$ and which is analytic in E. Consider the identities

$$
k_j(z,E) = \mathrm{tr}\,(P_j(z,E)H(z,E)), \quad \Phi_j(z,E) = W(z,E)\Phi_j(0,E),
$$

and Cauchy formula:

$$
\partial_E^l \partial_x^p [k_j(x,E) - k_j(\pm\infty, E)] = \frac{p!l!}{(2i\pi)^2} \oint_{|\mathcal{E}-E|=r} \oint_{|z-x|=r'} \frac{[k_j(z,\mathcal{E}) - k_j(\pm\infty, \mathcal{E})]}{(\mathcal{E}-E)^{l+1}(z-x)^{p+1}} dz d\mathcal{E},
$$

for r and r' small enough. Then, (3.17) follows. To get (3.19), one also makes use of the differential equation satisfied by $W(\cdot, E)$, of the estimate (8.1) and one considers the first d components of $\Phi_j(z,E)$ only.

The explicit formula (3.9) and the decay of $\partial_x k_j$ and of $\partial_x \varphi_j$ yields formula (3.20).
Finally, estimate (3.23) is a direct consequence of the definitions (3.21) and (3.22) and of (3.17).

8.4. **Proof of Lemma 3.4.** The proof of Lemma 3.4 is virtually identical to the one of Lemma 3.1 in [19], once the properties of the matrix $M(x, E, \varepsilon)$ have been established. Therefore, we just give here the main steps of the first part of the argument for the reader's convenience.

Because of (3.20), we know that there exists C such that, uniformly in E and ε,

$$
\int_0^\infty \|M(y,E,\varepsilon)\| dy < C.
$$

Expressing the solutions of equation (3.7) as Dyson series:

$$
\begin{aligned}
c(x,E,\varepsilon) \;&=\; \sum_{n=0}^{\infty} \int_0^x \int_0^{x_1} \cdots \int_0^{x_{n-1}} \\
&\times\; M(x_1,E,\varepsilon) M(x_2,E,\varepsilon) \cdots M(x_n,E,\varepsilon) dx_1 dx_2 \cdots dx_n \; c(0,E,\varepsilon),
\end{aligned} \tag{8.2}
$$

we obtain the usual bound:

$$
\| c(x,E,\varepsilon) \| \;\leq\; e^{\int_0^\infty \|M(y,E,\varepsilon)\|\, dy} \; \| c(0,E,\varepsilon) \|.
$$

Thus, we get from (8.2) that $c(x,E,\varepsilon)$ is bounded as $x \to \pm\infty$. Next we show that $\|c(x,E,\varepsilon) - c(y,E,\varepsilon)\|$ is arbitrarily small for large x and y, so that $\lim_{x\to\infty} c(x,E,\varepsilon) = c(\infty,E,\varepsilon)$ exists. It is enough to consider

$$
c(x,E,\varepsilon) \;-\; c(y,E,\varepsilon) \;=\; -\int_x^y M(z,E,\varepsilon)\, c(z,E,\varepsilon)\, dz.
$$

The expression above with $y = \pm\infty$, and the properties of M, c, just proven yield the bound

$$
c(x,E,\varepsilon) - c(\pm\infty,E,\varepsilon) = O(< x >^{-(1+\nu)}).
$$

Finally, if $\|c(\pm\infty,E,\varepsilon)\|$ is further assumed to be uniformly bounded in $E \in \Delta$ and $\varepsilon \to 0$, it is enough to consider the initial conditions (4.1), by linearity. Then, by integration by parts, see (4.7) and (4.8), we get,

$$
c(x,E,\varepsilon) \;=\; O(1),
$$

uniformly in $E \in \Delta$, $\varepsilon \to 0$ and $x \in \mathbb{R}$. Hence, all bounds above are uniform in $E \in \Delta$ and $\varepsilon \to 0$.

Getting similar bounds on the derivatives of c with respect to E which are uniform in ε and $E \in \Delta$ requires a little more work. The argument is identical to that used in [19]. We resort again to integration by parts in (4.6) with $x_0 = -\infty$, differentiate with respect to E, and make use of Gronwall Lemma to get bounds. We do not give the details and refer to Section 7 of [19].

8.5. **Proof of Lemma 5.1.** Again, we mimic the proof of Lemma 4.1 in [19]. It suffices to rewrite:

$$e^{-i(\int_0^x k_j(y,E)dy+tE)/\epsilon} \;=\; i\epsilon\,\frac{\frac{\partial}{\partial E}e^{-i(\int_0^x k_j(y,E)dy+tE)/\epsilon}}{\left(t+\int_0^x \frac{\partial}{\partial E}k_j(y,E)dy\right)}.$$

We compute:

$$\begin{aligned}
\phi_j(x,t,\varepsilon) &= i\varepsilon\left[\frac{c_j(x,E,\varepsilon)Q(E,\varepsilon)\varphi_j(x,E,\varepsilon)}{t+\int_0^x \partial_E k_j(y,E)dy}e^{-i(\int_0^x k_j(y,E)dy+tE)/\varepsilon}\right]_{\partial\Delta}\\
&- i\varepsilon\int_\Delta \frac{\partial_E[c_j(x,E,\varepsilon)Q(E,\varepsilon)\varphi_j(x,E,\varepsilon)]}{t+\int_0^x \partial_E k_j(y,E)dy}e^{-i(\int_0^x k_j(y,E)dy+tE)/\varepsilon}dE\\
&+ i\varepsilon\int_\Delta \frac{c_j(x,E,\varepsilon)Q(E,\varepsilon)\varphi_j(x,E,\varepsilon)e^{-i(\int_0^x k_j(y,E)dy+tE)/\varepsilon}}{[t+\int_0^x \partial_E k_j(y,E)dy]^2}\int_0^x \partial_E^2 k_j(y,E)dydE.
\end{aligned}\tag{8.3}$$

By Lemma 3.3 we have for x large enough:

$$t+\int_0^x \partial_E k_j(y,E)dy = x\left[\partial_E k_j(\pm\infty,E)+\frac{t}{x}+O\left(\frac{1}{x}\right)\right].$$

Under the restrictions put on x/t, we obtain that for a constant C_ε independent of t:

$$\|\phi_j(x,t,\varepsilon)\| \le \frac{C_\varepsilon}{|x|}.$$

Now, for any $l\in\{0,\cdots,m-1\}$, we have:

$$\phi_j^{[l]}(x,t,\varepsilon) = \int_\Delta c_j(x,E,\varepsilon)k_j^l(x,E)\varphi_j(x,E)e^{\frac{-i(\int_0^x k_j(y,E)dy+Et)}{\varepsilon}}Q(E,\varepsilon)\;dE,$$

so that a similar computation gives the result.

The last estimate makes use of the fact that under the given conditions stated on the signs of x and t, and for $|x|$ large enough, uniformly in time and energy,

$$|t+\int_0^x \partial_E k_j(y,E)dy| \ge |t+x\partial_E k_j(\pm\infty,E)|/2 \ge (|t|+|x|)c,\tag{8.4}$$

for some $c>0$. The result follows from the elementary inequality $(x+y)\ge x^\beta y^{1-\beta}$, for any $x,y\ge 0$ and any $\beta\in(0,1)$, and the arguments used above.

8.6. **Proof of Proposition 5.1.** We adapt the proof of Proposition 4.1 in [19] and we only give the main steps.

i) We rewrite:

$$\begin{aligned}
&\phi_j^{[l]}(x,t,\varepsilon)-\phi_j^{[l]}(x,t,\varepsilon,\pm\infty) =\\
&\int_\Delta [k_j^l(x,E)\varphi_j(x,E)-k_j^l(\pm\infty,E)\varphi_j(\pm\infty,E)]e^{\frac{-i\int_0^x k_j(y,E)dy}{\varepsilon}}c_j(x,E,\varepsilon)Q(E,\varepsilon)e^{-itE/\varepsilon}\;dE+\\
&\int_\Delta k_j^l(\pm\infty,E)\varphi_j(\pm\infty,E)e^{\frac{-i(k_j(\pm\infty,E)x+\omega_j(\pm\infty,E))}{\varepsilon}}[e^{-ir_j^\pm(x,E)/\varepsilon}-1]c_j(x,E,\varepsilon)Q(E,\varepsilon)e^{-itE/\varepsilon}\;dE+\\
&\int_\Delta k_j^l(\pm\infty,E)\varphi_j(\pm\infty,E)e^{\frac{-i(k_j(\pm\infty,E)x+\omega_j(\pm\infty,E))}{\varepsilon}}[c_j(x,E,\varepsilon)-c_j(\pm\infty,E,\varepsilon)]Q(E,\varepsilon)e^{-itE/\varepsilon}\;dE.
\end{aligned}\tag{8.5}$$

ii) To obtain a factor $1/t$, we integrate by parts. For any regular function f, we have:

$$\int_\Delta f(x,E,\varepsilon)e^{-itE/\varepsilon}dE = \left[\frac{i\varepsilon}{t}\;f(x,E,\varepsilon)\;e^{-itE/\varepsilon}\right]_{\partial\Delta} - \frac{i\varepsilon}{t}\int_\Delta \partial_E f(x,E,\varepsilon)\;e^{-itE/\varepsilon}dE.\tag{8.6}$$

iii) We apply equation (8.6) for the three terms in (8.5).

iv) The estimates of Lemma 3.3 and Lemma 3.4 prove that there exists $C_\varepsilon > 0$ such that:

$$\sup_{x\to\pm\infty} |x|^\nu \|[\phi_j^{[l]}(x,t,\varepsilon) - \phi_j^{[l]}(x,t,\varepsilon,\pm\infty)]\| < \frac{C_\varepsilon}{|t|}.$$

v) The identity $\phi_j^{[l]}(x,t,\varepsilon) = \omega(x)\phi_j^{[l]}(x,t,\varepsilon) + (1-\omega(x))\phi_j^{[l]}(x,t,\varepsilon)$ and support considerations on the definition of $\phi_j^{[l]}(x,t,\varepsilon,a)$ yield the first result.

vi) The second estimate follows from (8.6) applied to the definition of $\phi_j^{[l]}(x,t,\varepsilon)$.

8.7. **Proof of Theorem 6.1.** Taking into account the results of Section 5, we are left with the computation of the following integral:

$$T(\varepsilon,x,t) = \int_\Delta \tilde{P}(E,\varepsilon)e^{-\alpha(E)/\varepsilon}e^{-i\kappa(E)/\varepsilon}e^{-itE/\varepsilon}e^{-ixk_n(+\infty,E)/\varepsilon}\varphi_n(+\infty,E)dE,$$

with $\tilde{P}(E,\varepsilon) = P(E,\varepsilon)e^{-i\theta_j(\zeta,E)}(1+O_E(\varepsilon))$, where $O_E(\varepsilon)$ is defined in (6.4). We already remarked that $\tilde{P}(E,\varepsilon)$ satisfies **C3** as well. Again, wa adapt the arguments of [19].

In terms of the variable $k = k_n(+\infty, E)$, we rewrite T as:

$$\int_{k_n(\Delta,+\infty)} \tilde{P}(E_n^+(k),\varepsilon)e^{-\alpha(E_n^+(k))/\varepsilon}e^{-i\kappa(E_n^+(k))/\varepsilon}e^{-itE_n^+(k)/\varepsilon}e^{-ixk/\varepsilon}\varphi_n(+\infty,E_n^+(k))(\partial_k E_n^+)(k)dk.$$

We can see T as the rescaled Fourier transform (see (5.13)) of the function:

$$S(\varepsilon,k,t) = \sqrt{2\pi\varepsilon}\tilde{P}(E_n^+(k),\varepsilon)e^{-\alpha(E_n(+\infty,k))/\varepsilon}e^{-i\kappa(E_n^+(k))/\varepsilon}e^{-itE_n^+(k)/\varepsilon}\varphi_n(+\infty,E_n^+(k))(\partial_k E_n^+)(k).$$

We follow the analysis done in [19] and expand S around k^*

$$\alpha(E_n^+(k)) = \alpha(E^*) + [\partial_k E_n^+(k^*)]^2\alpha\text{"}(E^*)\frac{(k-k^*)^2}{2} + O((k-k^*)^3),$$

where $\alpha\text{"}(E^*) > 0$. We define:

$$\tilde{\kappa}(k) = \kappa(E_n^+(k)),$$
$$\tilde{\kappa}(k) = \tilde{\kappa}(k^*) + \tilde{\kappa}'(k^*)(k-k^*) + \tilde{\kappa}\text{"}(k^*)\frac{(k-k^*)^2}{2} + O((k-k^*)^3).$$

We also have:

$$\tilde{P}(E_n^+(k),\varepsilon) = P(E_n^+(k^*),\varepsilon)e^{-i\theta_j(\zeta,E_n^+(k^*))} + O((k-k^*)) + O(\varepsilon).$$
$$(\partial_k E_n^+)(k)\varphi_n(+\infty,E_n^+(k)) = (\partial_k E_n^+)(k^*)\varphi_n(+\infty,E_n^+(k^*)) + O((k-k^*)).$$

We can then follow the computations of [19]. We set $\mu(\varepsilon) = \varepsilon^s$, with $1/3 < s < 1/2$, so that $\mu(\varepsilon)^3/\varepsilon << 1 << \mu(\varepsilon)/\sqrt{\varepsilon}$, as $\varepsilon \to 0$. Using Parseval formula and thanks to the properties of α, the restriction of the integration set to the interval $[k^*-\mu(\varepsilon), k^*+\mu(\varepsilon)]$ causes an error, in the L^2 sense, of order $e^{-\alpha(E^*)/\varepsilon}\varepsilon^\infty$. On that set, the overall error $\mathrm{err}(\varepsilon)$ stemming from the expansion around k^* is $\mathrm{err}(\varepsilon) = O(\varepsilon + \varepsilon^s + \varepsilon^{3s-1}) = O(\varepsilon^{3s-1})$, with our values of s. The L^2 norm of the error term can thus be estimated by Parseval formula to yield

$$\left\| \int_{[k^*-\mu(\varepsilon),k^*+\mu(\varepsilon)]} \mathrm{err}(\varepsilon)e^{-\alpha(E^*)/\varepsilon}e^{-\Lambda(k)/\varepsilon}e^{-itE_n^+(k)/\varepsilon}e^{-ixk/\varepsilon}\, dk \right\| = O\left(\mathrm{err}(\varepsilon)e^{-\alpha(E^*)/\varepsilon}\varepsilon^{3/4}\right),$$

uniformly in t. The interval of integration can then be restored to its initial value $k_n(+\infty,\Delta)$ at the expense of another error of order $e^{-\alpha(E^*)/\varepsilon}\varepsilon^\infty$. Therefore, we obtain that there exists $3/4 < p < 5/4$ so that in L^2-norm and with an error term that is uniform in t:

$$\begin{aligned} T(\varepsilon,x,t) &= e^{-\alpha(E^*)/\varepsilon}P(E^*,\varepsilon)e^{-i\theta_j(\zeta,E^*)}e^{-i\tilde{\kappa}(E^*)/\varepsilon}\varphi_n(+\infty,E^*)\partial_k E_n^+(k^*)\times \\ &\times \int_{k_n(+\infty,\Delta)} e^{-\Lambda(k)/\varepsilon}e^{-itE_n^+(k)/\varepsilon}e^{-ikx/\varepsilon}dk + O(e^{-\alpha(E^*)/\varepsilon}\varepsilon^p). \end{aligned} \tag{8.7}$$

8.8. **Proof of Lemma 6.1.** To prove Lemma 6.1, it suffices to compute:

$$\int_{k_n(+\infty,\Delta)} e^{-\Lambda(k)/\varepsilon} e^{-itE_n^+(k)/\varepsilon} e^{-ikx/\varepsilon} dk.$$

According to (6.8), we have:

$$E_n^+(k) = E_n^+(k^*) + \partial_k E_n^+(k^*)(k-k^*) + \frac{\partial_k^2 E_n^+(k^*)}{2}(k-k^*)^2.$$

With the same arguments as in [19], we can expand the interval of integration to the whole line at the expense of an error that is uniform in t, and in the L^2 sense:

$$\int_{k_n(+\infty,\Delta)} e^{-\Lambda(k)/\varepsilon} e^{-itE_n^+(k)/\varepsilon} e^{-ikx/\varepsilon} dk = \int_{-\infty}^{+\infty} e^{-\Lambda(k)/\varepsilon} e^{-itE_n^+(k)/\varepsilon} e^{-ikx/\varepsilon} dk + O(\varepsilon^\infty).$$

The rest of the proof follows from the formula:

$$\int_{-\infty}^{\infty} e^{-(M(k-k^*)^2/2+iN(k-k^*))/\varepsilon}\, dk \;=\; \sqrt{\frac{\varepsilon 2\pi}{M}}\; e^{-\frac{N^2}{2\varepsilon M}},$$

with

$$M = \lambda_2 + i\partial_k^2 E_n^+(k^*)t,$$
$$N = \lambda_1 + \partial_k E_n^+(k^*)t + x.$$

8.9. **Proof of Proposition 7.1.** We will make use of the following Lemma whose proof we omit.

Lemma 8.2. *Let f and u_ε be $C_0^\infty(\mathbb{R},\mathbb{R})$. Provided $f'(k) \neq 0$ on* supp u_ε*, we have for any $n \in \mathbb{N}$*

$$\int_{\mathbb{R}} e^{-if(k)/\varepsilon} u_\varepsilon(k)\, dk = (-i\varepsilon)^n \int_{\mathbb{R}} e^{-if(k)/\varepsilon} \left(\left(\cdots \left(\left(\frac{u_\varepsilon(k)}{f'(k)} \right)' \frac{1}{f'(k)} \right)' \cdots \right)' \frac{1}{f'(k)} \right)' dk\ ,$$

where there are n factors $1/f'(k)$. Moreover, setting $g = 1/f'$, there exist constants $c(j, r_1, \cdots, r_n) \in \mathbb{R}$ such that

$$\left(\left(\cdots \left((u_\varepsilon g)' g \right)' \cdots \right)' g \right)' = \sum_{j=0}^{n} \sum_{\substack{r_1,\cdots,r_n \\ \sum_{i=1}^n r_i = j}} c(j, r_1, \cdots, r_n) u_\varepsilon^{(n-j)} g^{(r_1)} g^{(r_2)} \cdots g^{(r_n)},$$

where $h^{(k)}$ denotes the k^{th} derivative of h.

In our case, $f'(k) = x + \partial_k E_l^\sigma(k)t$, so that explicit computations show the existence of smooth functions on S_ε, the support of $u_\varepsilon = e^{-\Lambda(k)/\varepsilon}\eta_\varepsilon$, $k \mapsto c_{j,n}(k)$ which are independent of x and t and such that

$$\left(\frac{1}{f'(k)} \right)^{(n)} = \sum_{j=0}^{n} c_{j,n}(k) \frac{t^j}{(x + \partial_k E_l^\sigma(k)t)^{j+1}}. \tag{8.8}$$

Then, we get from the above

Lemma 8.3. *Assume $\partial_k E_l^\sigma(\tilde{k}) \neq 0$ and consider (x,t) such that $\inf_{k\in S_\varepsilon} |x + \partial_k E_l^\sigma(k)t| > 0$. For any $n \in \mathbb{N}$, there exists a positive constant $C(n)$, uniform in (x,t) and ε such that*

$$\left| \int_{\mathbb{R}} e^{-i(kx+tE_l^\sigma(k))/\varepsilon} e^{-\Lambda(k)/\varepsilon} \eta_\varepsilon(k)\, dk \right| \leq C(n)\varepsilon^\tau \sum_{r=0}^{n} \frac{(\varepsilon|t|)^r}{\left(\inf_{k\in S_\varepsilon} |x + \partial_k E_l^\sigma(k)t|\right)^{r+n}}, \tag{8.9}$$

for all $\varepsilon < \varepsilon_0$, where ε_0 is uniform in n and (x,t).

Remark: The Lemma actually holds for any value of ε if one is not interested in the behavior in that parameter.

Proof. One first notes that by scaling and by our choice of τ the successive derivatives of $u_\varepsilon = e^{-\Lambda(k)/\varepsilon}\eta_\varepsilon$ satisfy $\sup_{k\in\mathbb{R}} u_\varepsilon^{(j)}(k) = O(1/\varepsilon^j)$, if ε is small enough. Then, formula (8.8) and the restriction $\sum_{i=1}^n r_i = j$ in the second point of Lemma 8.2 give the possible numbers of factors $\frac{t^j}{(x+\partial_k E_l^\sigma(k)t)^{j+1}}$ in the integrand. Finally, the fact that all functions of k involved are smooth, together with $|S_\varepsilon| = \varepsilon^\tau$ yield the result.

To end the proof of the Proposition, we note that on the complement of $C_t(\varepsilon)$, the right hand side of (8.9) is bounded above by

$$\frac{C(n)\varepsilon^\tau \varepsilon |t|^{1-\alpha}}{(\inf_{k\in S_\varepsilon}|x+\partial_k E_l^\sigma(k)t|)}\left(\frac{\varepsilon}{|t|^{2\alpha-1}}\right)^{n-1},$$

using the fact that $\varepsilon|t|^{1-\alpha} > 1$. Explicit computation of the L^2 norm of $(\inf_{k\in S_\varepsilon}|x+\partial_k E_l^\sigma(k)t|)$ on the complement of $C_t(\varepsilon)$ yields the result.

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