A nonlinear Landau-Zener formula

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A NONLINEAR LANDAU-ZENER FORMULA

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Abstract. We consider a system of two coupled ordinary differential equations which appears as an envelope equation in Bose–Einstein Condensation. This system can be viewed as a nonlinear extension of the celebrated model introduced by Landau and Zener. We show how the nonlinear system may appear from different physical models. We focus our attention on the large time behavior of the solution. We show the existence of a nonlinear scattering operator, which is reminiscent of long range scattering for the nonlinear Schrödinger equation, and which can be compared with its linear counterpart.
Keywords: Nonlinear scattering, Landau-Zener formula, eigenvalue crossing.

1. Introduction

1.1. **Physical motivation.** In the 30's, questions about adiabaticity have begun to be studied and major contributions have been brought by Landau and Zener, independently (see [23] and [28]). The system studied by Zener reads

$$-i\partial_s u = V(s,z)u; \quad u(0) = u_0, \tag{1.1}$$

where $u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \in \mathbb{C}^2$, and the potential V is given by

$$V(s,z) = \begin{pmatrix} s & z \\ z & -s \end{pmatrix}.$$

This system presents an eigenvalue crossing: the eigenvalues of the matrix $V(s,z)$ are $\sqrt{s^2+z^2}$ and $-\sqrt{s^2+z^2}$, and they cross when $s=0$ and $z=0$. One can easily check that the eigenspace associated with $\sqrt{s^2+z^2}$ is asymptotic to $\mathbb{R}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ when $s \to +\infty$, and to $\mathbb{R}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ when $s \to -\infty$. Therefore, a solution $u(s,z)$ asymptotic to $\begin{pmatrix} 0 \\ \alpha(s,z) \end{pmatrix}$ when $s \to -\infty$ is polarized along the $+$ mode. The adiabatic issue consists in asking whether such a solution is still polarized along the $+$ mode when $s \to +\infty$. The adiabatic character of this solution is characterized by the ratio $|u_1(s,z)|^2/|\alpha(s,z)|^2$. It has been proved in the 30's that for (1.1), this ratio is described by the Landau-Zener transition coefficient $e^{-\pi z^2}$ which characterizes the transfer between modes (see Section 1.3 below for details). More generally, for an eigenvalue gap of the form $\sqrt{a^2s^2+b^2z^2} + \mathcal{O}(s^2)$ near $s=0$, the transition coefficient was expected to be $e^{-\pi z^2 b^2/a}$.

This work was supported by the French ANR projects R.A.S. (ANR-08-JCJC-0124-01) and SchEq (ANR-12-JS01-0005-01).

Mathematical proofs of the Landau-Zener formula have been given in the 90's by Hagedorn in [16] for small gaps and, then by Joye in [20]. Later, in [6], [7], Colin de Verdière has performed a classification of pseudodifferential operators with symbols presenting crossings of two eigenvalues. Under some genericity assumptions that we will not detail here, he derives simple model systems thanks to a change of coordinates in the phase space (a canonical transform) and the conjugation by a Fourier Integral Operator (including a Gauge transform). In the case of a system of evolution equations, the reduced systems are closely related with (1.1) (see (1.4) below); for this reason, the system (1.1) appears as a toy-model for understanding eigenvalue crossings.

Recently, a nonlinear version of this system has been introduced in [3], of the form

$$i\frac{\partial}{\partial t}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = H(\gamma)\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \tag{1.2}$$

with the Hamiltonian given by

$$H(\gamma) = \begin{pmatrix} \gamma(t) + \delta\left(|u_2|^2 - |u_1|^2\right) & z \\ z & -\gamma(t) - \delta\left(|u_2|^2 - |u_1|^2\right) \end{pmatrix}, \tag{1.3}$$

where, according to the terminology in [3], $\gamma(t) = \gamma_1 t$ denotes the level separation, z is the coupling constant between the two levels, and δ is a parameter describing the nonlinear interaction. This nonlinear two-level model can be used to understand Landau-Zener tunneling of a Bose-Einstein condensate between Bloch bands in an optical lattice: this has been observed in e.g. [8]. In Section 2, we present a derivation of this model from the nonlinear Schrödinger equation in a rotating frame and a periodic potential. Physical properties of the above system have been investigated in e.g. [19, 22, 21, 24]. We also show how this model can arise under the influence of a double-well potential, as in [21] (see Section 2 for a rapid presentation, and the appendix for a rigorous proof). The goal of this paper is to recast this model in a mathematical framework, and to study some of its properties, in particular as far as the large time regime is concerned.

1.2. **Mathematical setting.** The classification of crossings performed in [6] and [7] in the one hand, and in [12] on the other hand, produces model problems of the form

$$-i\partial_s u = \begin{pmatrix} s & G \\ G^* & -s \end{pmatrix} u; \quad u(0) = u_0 \in \mathcal{H}^2, \tag{1.4}$$

where $\mathcal{H}$ is a Hilbert space and G an operator on $\mathcal{H}$. Equation (1.1) corresponds to $\mathcal{H} = \mathbb{C}$ and $G = z \in \mathbb{R}$, as in [23] and [28] (see also [12] and [6]). Other choices of the pair $(\mathcal{H}, G)$ are relevant:

(1) In [7] and [17], $G = z_1 + iz_2$ and $\mathcal{H} = \mathbb{C}$.
(2) In [7] and [10], $G = \partial_z - z$ and $\mathcal{H} = L^2(\mathbb{R})$.
(3) In [17], [14] and [9], $G = q(z)$ is a quaternion, $z \in \mathbb{R}^4$ and $\mathcal{H} = \mathbb{C}^2$.
(4) In [9] and [12], G is a semiclassical pseudodifferential operator on the space $\mathcal{H} = L^2(\mathbb{R}^k)$, $k = 1, 2, 3\dots$

For this reason, we will focus on the following abstract problem

$$-i\partial_s u = \begin{pmatrix} s & G \\ G^* & -s \end{pmatrix} u + \delta F(u)u; \quad u(0) = u_0 \in \mathcal{H}^2, \tag{1.5}$$

which is the nonlinear counterpart of (1.4) and contains the systems coming from physics such as (1.2)–(1.3). The nonlinearity $F : \mathcal{H}^2 \to \mathcal{L}(\mathcal{H}^2)$ is of the form

$$F(u) = \mathrm{diag}(F_1(u), F_2(u)),$$

where for $(A, B) \in \mathbb{R}^2$, the operator $\mathrm{diag}(A, B)$ acts on $\mathcal{H}^2$ as

$$\mathrm{diag}(A, B)(u_1, u_2) = (Au_1, Bu_2),$$

and where the functions $F_j : \mathbb{C}^2 \to \mathbb{R}$ satisfy

$$F_j(u) = f_j(\|u_1\|^2_{\mathcal{H}}, \|u_2\|^2_{\mathcal{H}}), \tag{1.6}$$

with $f_j \in \mathcal{C}^2(\mathbb{R}^2; \mathbb{R})$ and $\nabla^2 f_j$ bounded. By the change of variable $s = t\sqrt{\gamma_1}$, we are left with (1.5) with $G = z/\sqrt{\gamma_1}$ and $F_j(u) = (-1)^j \delta \gamma_1^{-1/2}(|u_2|^2 - |u_1|^2)$ for $j \in \{1, 2\}$.

We make the following assumption on the operator G: for any $\chi \in \mathcal{C}^0(\mathbb{R})$,

$$\chi(GG^*)G = G\chi(G^*G) \ \text{ and } \ \chi(G^*G)G^* = G^*\chi(GG^*), \tag{1.7}$$

where the operators $\chi(GG^*)$ and $\chi(G^*G)$ are defined by functional calculus. This assumption is satisfied in the first three examples above. The situation is more complicated in the fourth one where it only holds at leading order in the semiclassical parameter.

We also assume that the domains $\mathcal{D}(GG^*)$ and $\mathcal{D}(G^*G)$ are dense subsets of $\mathcal{H}$.

Lemma 1.1. *Let $u_0 \in \mathcal{H}^2$. Under the above assumptions,* (1.5) *has a unique, global solution $u \in C(\mathbb{R}; \mathcal{H}^2)$. It satisfies the following conservation law*

$$\frac{d}{ds}\left(\|u_1(s)\|^2_{\mathcal{H}} + \|u_2(s)\|^2_{\mathcal{H}}\right) = 0.$$

Proof. Denote by $U(s_2, s_1)$ the linear operator which maps $u^{\mathrm{lin}}(s_1)$ to $u^{\mathrm{lin}}(s_2)$, where u^{lin} solves the linear equation

$$-i\partial_s u^{\mathrm{lin}} = \begin{pmatrix} s & G \\ G^* & -s \end{pmatrix} u^{\mathrm{lin}}.$$

It satisfies $U(s, s) = \mathrm{Id}$, $U(s, \tau)U(\tau, \sigma) = U(s, \sigma)$, and is unitary on $\mathcal{H}^2$. By Duhamel's principle, (1.5) becomes

$$u(s) = U(s, 0)u_0 + i\delta \int_0^s U(s, \sigma) \left(F(u)u\right)(\sigma) d\sigma.$$

Local existence follows by a standard fixed point argument (Cauchy-Lipschitz), with a local existence time which depends only on $\|u_0\|_{\mathcal{H}^2}$. We then note the conservation law announced in the lemma, which follows from the fact that the functions F_j are real-valued. This implies global existence, and the lemma. □

Throughout this paper, we consider normalized initial data so that we have

$$\|u_1(s)\|^2_{\mathcal{H}} + \|u_2(s)\|^2_{\mathcal{H}} = 1, \quad \forall s \in \mathbb{R}. \tag{1.8}$$

We prove a scattering result for initial data which are in the range of $\mathbf{1}_{V(0)^2 \leqslant R}$ for some $R > 0$. More precisely, we introduce a cut-off operator depending on G: let θ be a smooth cut-off function , $\theta \in \mathcal{C}_0^\infty(\mathbb{R})$ with $0 \leqslant \theta \leqslant 1$, $\theta(u) = 0$ for $|u| > 1$ and $\theta(u) = 1$ for $|u| < 1/2$. Then, for $R > 0$ we set

$$\Theta_R = \mathrm{diag}\left(\theta\left(\frac{GG^*}{R^2}\right), \theta\left(\frac{G^*G}{R^2}\right)\right).$$

Because of (1.7), the operator Θ_R commutes with $V(s)$ for all $s \in \mathbb{R}$ and $\Theta_R V(s)$ is a bounded operator on $\mathcal{H}\times\mathcal{H}$ with norm $\sqrt{s^2+R^2}$. Besides, a simple computation shows that $u_R(s) = \Theta_R u(s)$ satisfies $\frac{1}{i}\partial_s u_R = V(s)u_R + F(u)u_R$ with $u_R(0) = \Theta_R u_0 = u_0$. Therefore, we have the following result.

Lemma 1.2. *Suppose $u_0 = \Theta_R u_0$ for some $R > 0$, then for all $s \in \mathbb{R}$, the solution of* (1.5) *satisfies $u(s) = \Theta_R u(s)$.*

Typically, in the physical examples presented in Section 2, the assumption $u_0 = \Theta_R u_0$ consists in saying that some physical parameter (whose value is fixed in practise) belongs to a bounded set.

Notation. For two real-valued functions $a(s)$ and $b(s)$, we write

$$a(s) = \mathcal{O}_R\left(b(s)\right), \quad s \in I,$$

whenever there exists C_R depending only on R such that

$$|a(s)| \leqslant C_R |b(s)|, \quad s \in I.$$

Similarly, for $u(s) \in \mathcal{H}$, we write $u(s) = \mathcal{O}_R\left(b(s)\right)$ if $\|u(s)\|_{\mathcal{H}} = \mathcal{O}_R\left(b(s)\right)$.

1.3. **Scattering.** We introduce the phase function φ given by

$$\varphi(s,\lambda) = \frac{s^2}{2} + \frac{\lambda}{2}\ln|s|.$$

We can describe the large time asymptotics of u. We write all the large time results in the case where $\mathcal{H}$ is a vector space of finite dimension, which implies that the unit ball of $\mathcal{H}$ is compact.

Theorem 1.3. *Assume that $u_0 = \Theta_R u_0$ for some $R > 0$. Then, there exist unique pairs $\alpha = (\alpha_1, \alpha_2) \in \mathcal{H}^2$ and $\omega = (\omega_1, \omega_2) \in \mathcal{H}^2$, such that:*
1. *As s goes to $-\infty$,*

$$u_1(s) = \mathrm{e}^{i\delta F_1(\alpha)s + i\varphi(s,GG^*)}\alpha_1 + \mathcal{O}_R\left(\frac{1}{|s|}\right),$$

$$u_2(s) = \mathrm{e}^{i\delta F_2(\alpha)s - i\varphi(s,G^*G)}\alpha_2 + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

2. *As s goes to $+\infty$,*

$$u_1(s) = \mathrm{e}^{i\delta F_1(\omega)s + i\varphi(s,GG^*)}\omega_1 + \mathcal{O}_R\left(\frac{1}{s}\right),$$

$$u_2(s) = \mathrm{e}^{i\delta F_2(\omega)s - i\varphi(s,G^*G)}\omega_2 + \mathcal{O}_R\left(\frac{1}{s}\right).$$

The above result is reminiscent of long range scattering in nonlinear Schrödinger equations, as described first in [25]: nonlinear effects are present both in the fact that the amplitude of the functions u_j undergoes a nonlinear influence (this is what happens in nonlinear scattering in general), and in the fact that oscillations are different from those of the linear case (a typical feature of long range scattering), since the linear phase φ is not enough to describe large time oscillations. An important difference though is that (1.5) is not a dispersive equation, as can be seen from (1.8).

Remark 1.4. When $\delta = 0$ and G is scalar ($G = z$), this result goes back to the 30's with the proofs of Landau and Zener [23] and [28]. The original proof is based on the use of special functions; more recently, the proof of [11] relies on the analysis of oscillatory integrals. When G is operator-valued, the theorem is proved in the linear case ($\delta = 0$) in [13, Proposition 7]. We point out that there is a slight difference with the present framework, due to nonlinear effects. In the linear case, one associates with u_0 scattering states such that the asymptotics hold true for $\Theta_R u(s)$. Here, the scattering states depend on R in a non trivial way.

Remark 1.5. If the unit ball of $\mathcal{H}$ is not compact, the proof of Section 4 gives that for all $\varepsilon > 0$, there exists $s_\varepsilon > 0$, $\omega^\varepsilon = (\omega_1^\varepsilon, \omega_2^\varepsilon) \in \mathcal{H}^2$ and some constants $(\Omega_+, \Omega_-) \in \mathbb{R}_+^2$ such that for all $s > s_\varepsilon$,

$$\left\| u_1(s) - \mathrm{e}^{is\delta f_1(\Omega^+,\Omega^-)+i\varphi(s,GG^*)}\omega_1^\varepsilon \right\|_{\mathcal{H}} \leqslant \varepsilon,$$
$$\left\| u_2(s) - \mathrm{e}^{is\delta f_2(\Omega^+,\Omega^-)-i\varphi(s,G^*G)}\omega_2^\varepsilon \right\|_{\mathcal{H}} \leqslant \varepsilon.$$

Moreover, for $j \in \{1, 2\}$, $F_j(u(s))$ goes to $f_j(\Omega_+, \Omega_-)$ as s goes to $+\infty$.

Conversely, wave operators are well-defined, as stated in the following result.

Proposition 1.6. *Let $R > 0$ and $\omega = (\omega_1, \omega_2) \in \mathcal{H}^2$ such that $\omega = \Theta_R \omega$. There exist $\phi \in [0, 2\pi)$ and a solution $u \in C(\mathbb{R}; \mathcal{H}^2)$ to (1.5) such that, as $s \to +\infty$,*

$$u_1(s) = \mathrm{e}^{i\delta F_1(\omega)s + i\varphi(s,GG^*)+i\phi}\omega_1 + \mathcal{O}_R\left(\frac{1}{s}\right),$$
$$u_2(s) = \mathrm{e}^{i\delta F_2(\omega)s - i\varphi(s,G^*G)-i\phi}\omega_2 + \mathcal{O}_R\left(\frac{1}{s}\right).$$

For a fixed ϕ, such a function u is unique.
In addition, if $F_1 = F_2$, then we may take $\phi = 0$.

Remark 1.7. A similar result holds as $s \to -\infty$.

Remark 1.8. It is not clear whether ϕ can be different from zero. It may be seen as a second order influence of the nonlinear term (recall that $\phi = 0$ if $F_1 = F_2$), the leading order term (in s) being the oscillatory factor $\mathrm{e}^{i\delta F_j(\omega)s}$. Thus, if ϕ is not trivial, it should be considered as a function of ω and $\delta(F_1 - F_2)$; the proof of Proposition 1.6 will show why $F_1 - F_2$ is involved, and not more generally (F_1, F_2).

We can therefore define a scattering operator, which may depend on ϕ. Given $\alpha \in \mathcal{H}^2$ and a suitable ϕ, Proposition 1.6 yields a solution u to (1.5), and Theorem 1.3 provides an asymptotic state $\omega \in \mathcal{H}^2$. The scattering operator maps α to ω: $\omega = S_\delta^\phi(\alpha)$.

Our final result concerning the large time behavior of solutions to (1.5) consists in describing the effect of the nonlinearity in S_δ^ϕ by comparing this operator with its linear counterpart. We denote by u^{lin} the solution of (1.4), and we associate linear scattering states with u_0 denoted by

$$\alpha^{\mathrm{lin}} = \left(\alpha_1^{\mathrm{lin}}, \alpha_2^{\mathrm{lin}}\right) \text{ and } \omega^{\mathrm{lin}} = \left(\omega_1^{\mathrm{lin}}, \omega_2^{\mathrm{lin}}\right).$$

According to Proposition 7 in [13], the linear scattering operator is given by

$$S^{\mathrm{lin}} = \begin{pmatrix} a(GG^*) & -\overline{b}(GG^*)G \\ b(G^*G)G^* & a(G^*G) \end{pmatrix}, \tag{1.9}$$

with

$$a(\lambda)=\mathrm{e}^{-\pi\lambda/2},\ \ b(\lambda)=\frac{2i\mathrm{e}^{i\pi/4}}{\lambda\sqrt{\pi}}2^{-i\lambda/2}\mathrm{e}^{-\pi\lambda/4}\,\Gamma\left(1+i\frac{\lambda}{2}\right)\sinh\left(\frac{\pi\lambda}{2}\right),$$
$$\text{and } \ a(\lambda)^2+\lambda|b(\lambda)|^2=1.$$

When $G=z$, the coefficient

$$T(z)=a(z^2)^2=\mathrm{e}^{-\pi z^2} \tag{1.10}$$

is the Landau-Zener transition coefficient which describes the ratio $|\omega_1^{\rm lin}|^2/|\alpha_1^{\rm lin}|^2$ of the energy which remains on the first component (when $\alpha_2^{\rm lin}=0$). As we shall see in the next result, the Landau-Zener transition probability remains relevant in the nonlinear regime and for small δ.

Theorem 1.9. *As δ goes to zero, we have the uniform estimate*

$$S_\delta^\phi=S^{\rm lin}+\mathcal{O}_R(\delta).$$

In particular, at leading order, S_δ^ϕ does not depend on ϕ: $\phi=\mathcal{O}_R(\delta)$.
If $F_1=F_2=\underline{F}$, we choose $\phi=0$, and we have the exact formula:

$$S_\delta(\alpha)=\mathrm{e}^{i\delta\Lambda^+}S^{\rm lin}\left(\mathrm{e}^{i\delta\Lambda^-}\alpha\right), \tag{1.11}$$

where

$$\Lambda^-=\int_{-\infty}^0\left(\underline{F}\left(u^{\rm lin}(\tau)\right)-\underline{F}\left(\alpha^{\rm lin}\right)\right)d\tau,\quad \Lambda^+=\int_0^{+\infty}\left(\underline{F}\left(u^{\rm lin}(\tau)\right)-\underline{F}\left(\omega^{\rm lin}\right)\right)d\tau.$$

In particular,

$$\left\|S_\delta-S^{\rm lin}-i\delta\left(\Lambda^++\Lambda^-\right)S^{\rm lin}\right\|_{\mathcal{L}(\mathcal{H}\times\mathcal{H})}=\mathcal{O}_R\left(\delta^2\right).$$

As expected, as $\delta\to 0$, S_δ^ϕ behaves at leading order like the linear scattering operator. Nonlinear effects show up in the $\mathcal{O}(\delta)$ corrector that can be computed explicitly in the case $F_1=F_2$ (the nonlinearity is present in the definition of Λ^- and Λ^+).

This paper is organized as follows. In Section 2, we sketch the derivation of models of the form (1.5) from cubic nonlinear Schrödinger equations used to describe Bose–Einstein Condensation. In Section 3, we present an algebraic reduction which we use to recast Theorem 1.3 in terms of another unknown function (Proposition 3.3), and we set up some technical tools needed for the large time study of (1.5). Section 4 is dedicated to the proof of the intermediary Proposition 3.3. Proposition 1.6 is proved in Section 5, and Theorem 1.9 in proved in Section 6. Finally, in Appendix A, we go back to the derivation of (1.5) from physical models, and establish rigorously that (1.5) can be interpreted as an envelope equation in the semi-classical limit.

2. Formal derivation of the model

We rapidly describe some cases where (1.5) appears as an approximation to describe the motion of a Bose–Einstein condensate.

2.1. **Condensate in an accelerated optical lattice.** As proposed in [3], and considered in e.g. [19], the motion of a Bose–Einstein condensate in an accelerated 1D optical lattice is described by the equation

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x} - \omega t\right)^2\psi + V_0\cos\left(2k_L x\right)\psi + \frac{4\pi\hbar^2 a_s}{m}|\psi|^2\psi,$$

where m is the atomic mass, k_L is the optical lattice wave number, V_0 is the strength of the periodic potential depth, ω is the inertial force, and a_s is the scattering length. After rescaling, this equation reads

$$i\frac{\partial\psi}{\partial t} = \frac{1}{2}\left(-i\frac{\partial}{\partial x} - \alpha t\right)^2\psi + v\cos(x)\psi + \epsilon|\psi|^2\psi, \tag{2.1}$$

with $\epsilon = -1$ or $+1$ according to the chemical element considered. The approach in [3] consists in substituting the ansatz

$$\psi(t,x) = a(t)\mathrm{e}^{ikx} + b(t)\mathrm{e}^{i(k-1)x} \tag{2.2}$$

into (2.1), with $k = k_L = 1/2$, corresponding to the Brillouin zone edge (this approximation amounts to considering that only the ground state and the first excited state are populated, see [19]). We compute

$$\begin{aligned}
i\partial_t\psi &= i\dot{a}\mathrm{e}^{ikx} + i\dot{b}\mathrm{e}^{i(k-1)x},\\
\left(-i\partial_x - \alpha t\right)^2\psi &= \left(k-\alpha t\right)^2 a\mathrm{e}^{ikx} + \left(k-1-\alpha t\right)^2 b\mathrm{e}^{i(k-1)x},\\
\cos(x)\psi &= \frac{1}{2}\left(a\mathrm{e}^{i(k+1)x} + b\mathrm{e}^{ikx} + a\mathrm{e}^{i(k-1)x} + b\mathrm{e}^{i(k-2)x}\right),\\
|\psi|^2\psi &= \left(|a|^2+|b|^2\right)\left(a\mathrm{e}^{ikx} + b\mathrm{e}^{i(k-1)x}\right) + |a|^2 b\mathrm{e}^{i(k-1)x} + a|b|^2\mathrm{e}^{ikx}\\
&\quad + a^2\overline{b}\mathrm{e}^{i(k+1)x} + \overline{a}b^2\mathrm{e}^{i(k-2)x}.
\end{aligned}$$

Leaving out the new harmonics (the last two exponentials) generated both by band interaction and nonlinear effects, and identifying the coefficients of e^{ikx} and $\mathrm{e}^{i(k-1)x}$, we come up with:

$$\begin{cases}
i\partial_t a = \frac{1}{2}\left(k-\alpha t\right)^2 a + \frac{v}{2}b + \epsilon\left(|a|^2+2|b|^2\right)a,\\
i\partial_t b = \frac{1}{2}\left(k-1-\alpha t\right)^2 b + \frac{v}{2}a + \epsilon\left(2|a|^2+|b|^2\right)b.
\end{cases}$$

We notice the identity $\partial_t\left(|a|^2+|b|^2\right) = 0$, so we can write $|a|^2+|b|^2 = m_0^2 > 0$ (in [3], $m_0 = 1$). Now recalling the numerical value $k = 1/2$ and expanding the squares, we have

$$\begin{cases}
i\partial_t a = \frac{1}{8}a - \frac{\alpha t}{2}a + \frac{(\alpha t)^2}{2}a + \frac{v}{2}b + \epsilon\left(m_0^2+|b|^2\right)a,\\
i\partial_t b = \frac{1}{8}b + \frac{\alpha t}{2}b + \frac{(\alpha t)^2}{2}b + \frac{v}{2}a + \epsilon\left(m_0^2+|a|^2\right)b.
\end{cases}$$

The above system becomes

$$i\partial_t\begin{pmatrix}a\\ b\end{pmatrix} = \left(E_0 + \frac{(\alpha t)^2}{2}\right)\begin{pmatrix}a\\ b\end{pmatrix} + \frac{1}{2}\begin{pmatrix}-\alpha t & v\\ v & \alpha t\end{pmatrix}\begin{pmatrix}a\\ b\end{pmatrix} + \frac{\epsilon}{2}\operatorname{diag}\left(|b|^2,|a|^2\right)\begin{pmatrix}a\\ b\end{pmatrix},$$

with

$$E_0 = \frac{1}{8} + m_0^2\epsilon.$$

Using finally the gauge transform

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \mathrm{e}^{-iE_0 t - i\alpha^2 t^3/6} \begin{pmatrix} a \\ b \end{pmatrix},$$

we end up with

$$i\partial_t \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -\alpha t & v \\ v & \alpha t \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \frac{\epsilon}{2} \operatorname{diag}(|u_2|^2, |u_1|^2) \begin{pmatrix} u_1 \\ u_2 \end{pmatrix},$$

which is of the form (1.2)–(1.3) or (1.5) via the change of variable $s = t\sqrt{\frac{\alpha}{2}}$; we then have $G = (2\alpha)^{-1/2} v$ and $F(u) = \varepsilon(2\alpha)^{-1/2} \operatorname{diag}(|u_2|^2, |u_1|^2)$. Note that the only approximation that we have made in this computation consists in neglecting the other harmonics than $\mathrm{e}^{\pm ix/2}$, and no linearization was performed, in contrast to the computations of [3].

Theorem 1.3 gives asymptotics for the profiles a and b of the ansatz (2.2) as t goes to $\pm\infty$. Theorem 1.9 gives an information on the profiles (a_+, b_+) for $t \sim +\infty$ in terms of (a_-, b_-), those for $t \sim -\infty$. For example if for $t \sim -\infty$, we have $(a_-, b_-) = (a, 0)$, then the profiles for $t \sim +\infty$ are related via the Landau-Zener transition coefficient (1.10) for $z = (2\alpha)^{-1/2} v$: at leading order in δ, they satisfy

$$|a_+|^2 = \mathrm{e}^{-\pi v^2/(2\alpha)} |a|^2 \quad \text{and} \quad |b_+|^2 = \left(1 - \mathrm{e}^{-\pi v^2/(2\alpha)}\right) |a|^2.$$

2.2. **Condensate in a double-well potential.** As suggested in [3], and further developed in [21], nonlinear Landau–Zener tunneling may be realized in a double-well potential. We present a derivation which is different from the one presented in the above references, even on a former level. Rigorous details are presented in the appendix. Consider

$$i\frac{\partial \psi}{\partial t} + \frac{1}{2}\frac{\partial^2 \psi}{\partial x^2} = W(t,x)\psi + \epsilon |\psi|^2 \psi. \tag{2.3}$$

The potential W is of the form

$$W(t,x) = V_s(x) + \kappa t V_a(x), \tag{2.4}$$

where V_s is a symmetric double-well potential and V_a is antisymmetric. The main point to be aware of is that the lowest two eigenvalues $\lambda_+ < \lambda_-$ of the Hamiltonian $-\frac{1}{2}\partial_x^2 + V_s$ are non-degenerate, with associated eigenfunctions $\varphi_\pm$ (see Appendix A for details). The two exponential functions $\mathrm{e}^{\pm ix/2}$ of the above model are then replaced by the so-called single-well states

$$\varphi_L = \frac{1}{\sqrt{2}}\left(\varphi_+ - \varphi_-\right), \quad \varphi_R = \frac{1}{\sqrt{2}}\left(\varphi_+ + \varphi_-\right). \tag{2.5}$$

We note that this approach can be generalized to a multidimensional framework, in the spirit of [27] (see Appendix A). We sketch the computation in the simplest 1D case though, to emphasize the differences with the optical lattice case. We shall use mostly two properties of φ_L and φ_R, described more precisely in Appendix A:

- $\varphi_R(-x) = \varphi_L(x)$.
- The product $\varphi_L \varphi_R$ is negligible, because φ_L and φ_R are localized at the two distinct minima of V_s.

Seek ψ of the form

$$\psi(t,x) = a_L(t)\varphi_L(x) + a_R(t)\varphi_R(x).$$

Denoting

$$\Omega = \frac{\lambda_- + \lambda_+}{2}, \quad \omega = \frac{\lambda_- - \lambda_+}{2},$$

we compute:

$$\begin{aligned}
i\partial_t\psi &= i\dot{a}_L\varphi_L + i\dot{a}_R\varphi_R,\\
-\frac{1}{2}\partial_x^2\psi + V_s\psi &= a_L\left(\Omega\varphi_L - \omega\varphi_R\right) + a_R\left(\Omega\varphi_R - \omega\varphi_L\right)\\
&= (\Omega a_L - \omega a_R)\varphi_L + (\Omega_R - \omega a_L)\varphi_R,\\
V_a\psi &= a_L V_a\varphi_L + a_R V_a\varphi_R,\\
|\psi|^2\psi &= \left(|a_L|^2|\varphi_L|^2 + |a_R|^2|\varphi_R|^2 + 2\,\mathrm{Re}\left(\overline{a}_L a_R\overline{\varphi}_L\varphi_R\right)\right)\left(a_L\varphi_L + a_R\varphi_R\right).
\end{aligned}$$

By integrating in space and neglecting the product $\varphi_L\varphi_R$, we get:

$$\begin{cases} i\partial_t a_L = \Omega a_L - \omega a_R + \kappa t\gamma_L a_L + \epsilon_L|a_L|^2 a_L,\\ i\partial_t a_R = \Omega a_R - \omega a_L + \kappa t\gamma_R a_R + \epsilon_R|a_R|^2 a_R,\end{cases}$$

with

$$\gamma_L = \int_{\mathbb{R}} V_a\varphi_L^2, \quad \epsilon_L = \epsilon\int_{\mathbb{R}}\varphi_L^4, \quad \gamma_R = \int_{\mathbb{R}} V_a\varphi_R^2, \quad \epsilon_R = \epsilon\int_{\mathbb{R}}\varphi_R^4.$$

By symmetry, $\gamma_L = -\gamma_R$, $\epsilon_L = \epsilon_R =: \delta$, so if we set $\alpha = \kappa\gamma_L$, we come up with:

$$\begin{cases} i\partial_t a_L = \Omega a_L - \omega a_R + \alpha t a_L + \delta|a_L|^2 a_L,\\ i\partial_t a_R = \Omega a_R - \omega a_L - \alpha t a_R + \delta|a_R|^2 a_R.\end{cases}$$

Using the gauge transform

$$\begin{pmatrix}u_1\\u_2\end{pmatrix} = \begin{pmatrix}a_L\mathrm{e}^{i\Omega t}\\ a_R\mathrm{e}^{i\Omega t}\end{pmatrix},$$

we find:

$$i\partial_t\begin{pmatrix}u_1\\u_2\end{pmatrix} = \begin{pmatrix}\alpha t & -\omega\\ -\omega & -\alpha t\end{pmatrix}\begin{pmatrix}u_1\\u_2\end{pmatrix} + \delta\begin{pmatrix}|u_1|^2 & 0\\ 0 & |u_2|^2\end{pmatrix}\begin{pmatrix}u_1\\u_2\end{pmatrix},$$

which is of the form (1.5) via the change of variables $s = \sqrt{\alpha}t$ with $F_j(u) = \alpha^{-1/2}|u_j|^2$ and $G = -\omega\alpha^{-1/2}$. Therefore, Theorems 1.3 and 1.9 yield similar results as in the preceding subsection with a Landau-Zener coefficient $\mathrm{e}^{-\pi\omega^2/\alpha}$.

3. Preparation of the proof of Theorem 1.3

3.1. A useful reduction. For $u \in \mathcal{H}^2$, set

$$M(u) = \frac{\delta}{2}\left(F_1(u) + F_2(u)\right) \quad ; \quad m(u) = \frac{\delta}{2}\left(F_1(u) - F_2(u)\right), \tag{3.1}$$

where M and m are real-valued, and rewrite (1.5) as

$$-i\partial_s u = V(s)u + M(u)u + \mathrm{diag}\left(m(u), -m(u)\right)u = V\left(s + m(u)\right)u + M(u)u. \tag{3.2}$$

Since M is a scalar, the last term can be absorbed by a gauge transform:

$$v(s) := u(s)\mathrm{e}^{-i\int_0^s M(u(\tau))d\tau} \tag{3.3}$$

satisfies $\|v_j(s)\|_{\mathcal{H}} = \|u_j(s)\|_{\mathcal{H}}$ for $j \in \{1,2\}$ and

$$-i\partial_s v = V\left(s + m(u(s))\right)v = \widetilde{V}\left(s\right)v,$$

where we have introduced the notation $\widetilde{V}(s) = V\,(s + m(u(s)))$.

Remark 3.1. Note that if $F_1 = F_2$, we have $M = F_1$ and $m = 0$ in (3.1); therefore, we are reduced to the standard linear equation

$$-i\partial_s v = V\,(s)\,v,$$

for which the scattering result is known, describing the large time behavior of the solution v at leading order (see Lemma 7 in [12] or equivalently Lemma 11 in [13]). In Proposition 5.5 of [14], the remainder term is proved to be of order $\mathcal{O}(R^2 s^{-1})$.

In view of the physical models presented in Section 2, we are mainly concerned with the situation where $F_1 \neq F_2$, which is more involved mathematically. The first step of the large time study consists in proving the following proposition.

Proposition 3.2. *Let $R > 0$. For any data u_0 such that $\Theta_R u_0 = u_0$, there exist two vectors of $(\mathbb{R}^+)^2$, $\Omega = (\Omega_1, \Omega_2)$ and $A = (A_1, A_2)$ such that and for $j \in \{1, 2\}$,*

$$\|u_j(s)\|^2_{\mathcal{H}} = \Omega_j + \mathcal{O}_R\left(\frac{1}{s}\right) \text{ as } s \to +\infty,$$
$$\|u_j(s)\|^2_{\mathcal{H}} = A_j + \mathcal{O}_R\left(\frac{1}{|s|}\right) \text{ as } s \to -\infty.$$

Moreover,

$$\int_s^{+\infty} \left(\|u_j(\tau)\|^2_{\mathcal{H}} - \Omega_j\right) d\tau = \mathcal{O}_R\left(\frac{1}{s}\right) \text{ as } s \to +\infty,$$
$$\int_{-\infty}^{s} \left(\|u_j(\tau)\|^2_{\mathcal{H}} - A_j\right) d\tau = \mathcal{O}_R\left(\frac{1}{|s|}\right) \text{ as } s \to -\infty.$$

Therefore, any $\omega \in \mathcal{H}^2$ such that $\|\omega_j\|^2_{\mathcal{H}} = \Omega_j$, $j = 1, 2$, satisfies $F_j(\omega) = f_j(\Omega_1, \Omega_2)$ (f_1 and f_2 are the functions in (1.6)). Similarly, any $\alpha \in \mathcal{H}^2$ such that $\|\alpha_j\|^2_{\mathcal{H}} = A_j$, $j = 1, 2$, satisfies $F_j(\alpha) = f_j(A_1, A_2)$. We shall however use the notations ω, α until these vectors are fully determined, after Proposition 3.3 below.

Note that in view of (3.3), it is equivalent to state Proposition 3.2 for u or for v. It will be established by studying v in Section 4. In particular, this proposition implies that the complete description of the function v for large s will induce direct results on u. The analysis of the asymptotics of $v(s)$, as $s \to +\infty$, is stated in the following proposition, which in turn is established in Section 4.

Proposition 3.3. *There exist $(\nu_1, \nu_2) \in \mathcal{H}^2$ with $\|\nu_j\|^2_{\mathcal{H}} = \Omega_j$, $j = 1, 2$, such that as $s \to +\infty$,*

$$v_1(s) = \mathrm{e}^{i\varphi(s+m(\omega),GG^*)}\nu_1 + \mathcal{O}_R\left(\frac{1}{s}\right); \quad v_2(s) = \mathrm{e}^{-i\varphi(s+m(\omega),G^*G)}\nu_2 + \mathcal{O}_R\left(\frac{1}{s}\right),$$

and $(\mu_1, \mu_2) \in \mathcal{H}^2$ with $\|\mu_j\|^2_{\mathcal{H}} = A_j$, $j = 1, 2$, such that as $s \to -\infty$,

$$v_1(s) = \mathrm{e}^{i\varphi(s+m(\alpha),GG^*)}\mu_1 + \mathcal{O}_R\left(\frac{1}{|s|}\right); \quad v_2(s) = \mathrm{e}^{-i\varphi(s+m(\alpha),G^*G)}\mu_2 + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

A similar statement holds in $-\infty$.

Proposition 3.3 implies Theorem 1.3. Using (3.3) and the second part of Proposition 3.2, we obtain

$$\begin{aligned}
u_1(s) &= \mathrm{e}^{i\int_0^s M(u(\tau))d\tau + i\varphi(s+m(\omega),GG^*)}\nu_1 + \mathcal{O}_R\left(\frac{1}{s}\right)\\
&= \mathrm{e}^{isM(\omega)+i\varphi(s+m(\omega),GG^*)}\mathrm{e}^{i\int_0^{+\infty}(M(u(\tau))-M(\omega))d\tau}\nu_1 + \mathcal{O}_R\left(\frac{1}{s}\right),\\
u_2(s) &= \mathrm{e}^{i\int_0^s M(u(\tau))d\tau - i\varphi(s+m(\omega),G^*G)}\nu_2 + \mathcal{O}_R\left(\frac{1}{s}\right)\\
&= \mathrm{e}^{isM(\omega)-i\varphi(s+m(\omega),G^*G)}\mathrm{e}^{i\int_0^{+\infty}(M(u(\tau))-M(\omega))d\tau}\nu_2 + \mathcal{O}_R\left(\frac{1}{s}\right).
\end{aligned}$$

Observing the identities

$$\begin{aligned}
\varphi(s+m(\omega),\lambda) + sM(\omega) &= \varphi(s,\lambda) + s\delta F_1(\omega) + \frac{m(\omega)^2}{4} + \mathcal{O}_R\left(\frac{1}{s}\right),\\
-\varphi(s+m(\omega),\lambda) + sM(\omega) &= -\varphi(s,\lambda) + s\delta F_2(\omega) - \frac{m(\omega)^2}{4} + \mathcal{O}_R\left(\frac{1}{s}\right),
\end{aligned}$$

we obtain Theorem 1.3 for $s \gg 1$ with

$$\omega_1 = \mathrm{e}^{i\int_0^{+\infty}(M(u(\tau))-M(\omega))d\tau + im(\omega)^2/4}\nu_1; \quad \omega_2 = \mathrm{e}^{i\int_0^{+\infty}(M(u(\tau))-M(\omega))d\tau - im(\omega)^2/4}\nu_2.$$

The case $s \to -\infty$ is similar. □

Remark 3.4. If one expects the asymptotic behavior of u to be described as in Theorem 1.3, then the first step (Proposition 3.2) consists in deriving the asymptotic phase, while the role of the final step (Proposition 3.3) is to describe the amplitude. This strategy is similar to the one employed in e.g. [18] to study the long range nonlinear scattering for the one dimensional cubic Schrödinger equation and for the Hartree equation.

3.2. **Technical results.** Let us now introduce notations and state technical results that can be skipped by the reader at the first reading. We set

$$J := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{ and } K := V(0) = \begin{pmatrix} 0 & G \\ G^* & 0 \end{pmatrix}, \tag{3.4}$$

thus, $V(s)$ writes

$$V(s) = sJ + K.$$

We denote by $\sigma(s)$ the function

$$\sigma(s) = s + m(u(s))$$

and we have

$$\widetilde{V}(s) = V(\sigma(s)) \text{ and } \widetilde{V}(s)^2 = \Lambda(s)^2,$$

where $\Lambda(s)$ is the diagonal operator

$$\Lambda(s) = \mathrm{diag}\left(\sqrt{\sigma(s)^2 + GG^*}, \sqrt{\sigma(s)^2 + G^*G}\right).$$

For this reason, $\Lambda(s)$ appears like a diagonalisation of $V(\sigma(s))$, all the more that if we set

$$\Pi^{\pm}(s) = \frac{1}{2}\left(\mathrm{Id} \pm \Lambda(s)^{-1}V(\sigma(s))\right),$$

then we have the following properties.

(1) $\Pi^{\pm}(s)\widetilde{V}(s) = \widetilde{V}(s)\Pi^{\pm}(s) = \pm\Lambda(s)\Pi^{\pm}(s) = \pm\Pi^{\pm}(s)\Lambda(s)$.
(2) $\Pi^{+}(s) + \Pi^{-}(s) = \mathrm{Id}$.
(3) $(\Pi^{\pm}(s))^{*} = \Pi^{\pm}(s)$.
(4) $\Pi^{\pm}(s)\Pi^{\mp}(s) = 0$ and $(\Pi^{\pm}(s))^2 = \Pi^{\pm}(s)$.

The properties (2)–(4) show that $\Pi^{\pm}(s)$ are orthogonal projectors, and the property (1) will play the role of a diagonalisation of the operator $\widetilde{V}(s)$. The fact that $\Pi^{\pm}(s)$ and $\widetilde{V}(s)$ commute with $\Lambda(s)$ is more general. In fact, $\widetilde{V}(s)$ and $\Pi^{\pm}(s)$ are in the subset $\mathcal{A}$ of $\mathcal{L}(\mathcal{H}^2)$ defined by: $A \in \mathcal{A}$ if and only if there exist smooth functions a, b, c and d such that $A = A(a, b, c, d)$ with

$$A(a, b, c, d) = \begin{pmatrix} a(GG^*) & b(GG^*)G \\ c(G^*G)G^* & d(G^*G) \end{pmatrix}. \tag{3.5}$$

A simple calculation shows that, because of the commutation property (1.7), operators of $\mathcal{A}$ commutes with $\Lambda(s)$:

$$\forall A \in \mathcal{A}, \quad \forall s \in \mathbb{R}, \quad A\Lambda(s) = \Lambda(s)A.$$

Besides $\mathcal{A}$ is an algebra, as shown by the following lemma which stems from straightforward computations

Lemma 3.5. *Let $a, b, c, d, a', b', c', d' \in \mathcal{C}^{\infty}(\mathbb{R})$. We have*

$$A(a, b, c, d)^* = A(\overline{a}, \overline{c}, \overline{b}, \overline{d}),$$
$$A(a, b, c, d)A(a', b', c', d') = A(a'', b'', c'', d''),$$

with

$$a''(\lambda) = a(\lambda)a'(\lambda) + \lambda b(\lambda)c(\lambda), \quad b''(\lambda) = a(\lambda)b'(\lambda) + b(\lambda)d'(\lambda),$$
$$d''(\lambda) = d(\lambda)d'(\lambda) + \lambda c(\lambda)b(\lambda), \quad c''(\lambda) = a'(\lambda)c(\lambda) + d(\lambda)c'(\lambda).$$

Operators of $\mathcal{A}$ will be called *diagonal* if

$$A = \Pi^{+}(s)A\Pi^{+}(s) + \Pi^{-}(s)A\Pi^{-}(s),$$

and *antidiagonal* if

$$A = \Pi^{+}(s)A\Pi^{-}(s) + \Pi^{-}(s)A\Pi^{+}(s).$$

In particular, $\widetilde{V}(s)$, $\Pi^{+}(s)$ and $\Pi^{-}(s)$ are diagonal operators of $\mathcal{A}$; on the other hand, the operators $\partial_s\Pi^{+}(s)$ and $\partial_s\Pi^{-}(s)$ are antidiagonal elements of $\mathcal{A}$. Indeed, the relation

$$\partial_s\Pi^{+}(s) = \partial_s((\Pi^{+}(s))^2) = \Pi^{+}(s)\partial_s\Pi^{+}(s) + \partial_s\Pi^{+}(s)\Pi^{+}(s)$$

implies that $\Pi^{\pm}(s)\partial_s\Pi^{+}(s)\Pi^{\pm}(s) = 0$ (and similarly for $\Pi^{-}(s)$ since $\partial_s\Pi^{-}(s) = -\partial_s\Pi^{+}(s)$).

Antidiagonal operators have interesting properties that we shall use later. Typically, they can be written as commutators with $\widetilde{V}(s)$: if $C(s) = \Pi^{\mp}(s)C(s)\Pi^{\pm}(s)$, then we have

$$C(s) = \pm\left[B(s), \widetilde{V}(s)\right],$$

with

$$B(s) = \frac{1}{2}\Lambda(s)^{-1}C(s), \tag{3.6}$$

which also belongs to $\mathcal{A}$. Because of this property, we have the following lemma.

Lemma 3.6. *Let v be a solution of* (3.2)*, $C(s) \in \mathcal{A}$ with $C(s) = \Pi^+(s)C(s)\Pi^-(s)$, and let $B(s)$ be associated with $C(s)$ as in* (3.6)*, then*

$$\langle C(s)v(s)\ ,\ v(s)\rangle_{\mathcal{H}^2} = \frac{1}{i}\frac{d}{ds}\langle B(s)v(s)\ ,\ v(s)\rangle_{\mathcal{H}^2} + i\,\langle \partial_s B(s)v(s)\ ,\ v(s)\rangle_{\mathcal{H}^2}\,. \tag{3.7}$$

Proof. We write

$$\begin{aligned}\langle C(s)v(s)\ ,\ v(s)\rangle_{\mathcal{H}^2} &= \left\langle \left[B(s)\ ,\ \widetilde{V}(s)\right] v(s)\ ,\ v(s)\right\rangle_{\mathcal{H}^2} \\ &= \left\langle B(s)\frac{1}{i}\partial_s v(s)\ ,\ v(s)\right\rangle_{\mathcal{H}^2} - \left\langle B(s)v(s)\ ,\ \frac{1}{i}\partial_s v(s)\right\rangle \\ &= \frac{1}{i}\frac{d}{ds}\langle B(s)v(s)\ ,\ v(s)\rangle_{\mathcal{H}^2} - \frac{1}{i}\langle \partial_s B(s)v(s)\ ,\ v(s)\rangle_{\mathcal{H}^2}\,,\end{aligned}$$

and the lemma follows. □

Before closing this section, we gather in a lemma some estimates on the function σ that we will use in the following. We set

$$m(v(s)) = \widetilde{m}\left(\|v_1(s)\|^2_{\mathcal{H}}, \|v_2(s)\|^2_{\mathcal{H}}\right).$$

Lemma 3.7. *Let $R > 0$, for all initial data u_0 such that $\Theta_R u_0 = u_0$, we have*

$$\dot\sigma(s) = 1 - 2\underline{m}(s)\,\mathrm{Im}\,\langle v_1(s), Gv_2(s)\rangle_{\mathcal{H}} = \mathcal{O}(R), \tag{3.8}$$

$$\ddot\sigma(s) = 4s\,\underline{m}(s)\,\mathrm{Re}\,\langle v_1(s), Gv_2(s)\rangle_{\mathcal{H}} + \mathcal{O}(R^2), \tag{3.9}$$

where $\dot\sigma(s)$ stands for $\partial_s\sigma(s)$ and where $\underline{m}$ is the bounded function:

$$\underline{m}(s) = \partial_1\widetilde{m}\left(\|v_1(s)\|^2_{\mathcal{H}}, \|v_2(s)\|^2_{\mathcal{H}}\right) - \partial_2\widetilde{m}\left(\|v_1(s)\|^2_{\mathcal{H}}, \|v_2(s)\|^2_{\mathcal{H}}\right). \tag{3.10}$$

Proof. Note first that the functions f_1 and f_2 are bounded on the unit ball, thus $m(u(s))$ and, for any multi-indices $\alpha \in \mathbb{N}^2$, $(\partial_1^{\alpha_1}\partial_2^{\alpha_2}m)(v(s))$, are bounded, uniformly in s. Besides, we have the relations

$$\begin{aligned}\partial_s(\|v_1\|^2) &= -\partial_s(\|v_2\|^2) = -2\,\mathrm{Im}\,\langle v_1, Gv_2\rangle = \mathcal{O}(R), \\ \partial_s^2(\|v_1\|^2) &= 4s\,\mathrm{Re}\,\langle v_1, Gv_2\rangle + 2\left(\|Gv_2\|^2 - \|G^*v_1\|^2\right).\end{aligned} \tag{3.11}$$

□

4. Existence of scattering states

The proof of the existence of scattering states consists of three steps.

1. We first prove that $\|\Pi^{\pm}v(s)\|_{\mathcal{H}^2}$ have a limit as s goes to $\pm\infty$.
2. We then deduce Proposition 3.2.
3. We finally prove Proposition 3.3, that is, the existence of scattering states for the function v.

Recall that Proposition 3.3 implies Theorem 1.3 as explained in Section 3.1.

4.1. Large time convergence of the norm.

In this section, we prove an auxiliary result leading to Proposition 3.2.

Proposition 4.1. *Let $R > 0$. Then for all initial data u_0 such that $u_0 = \Theta_R u_0$, there exist $\Omega^\pm, A^\pm \geqslant 0$ such that, if we set $v^\pm = \Pi^\pm v$,*

$$\|v^\pm(s)\|^2_{\mathcal{H}^2} - \Omega^\pm = \mathcal{O}_R\left(\frac{1}{s^2}\right) \quad \text{as} \quad s \to +\infty,$$

$$\|v^\pm(s)\|^2_{\mathcal{H}^2} - A^\pm = \mathcal{O}_R\left(\frac{1}{s^2}\right) \quad \text{as} \quad s \to -\infty.$$

Proof. We consider the limit $s \to +\infty$ for the $+$ mode. The limit $s \to -\infty$ and the case of the $-$ mode can be treated similarly. We are going to prove that $\|v^+(s)\|^2_{\mathcal{H}\times\mathcal{H}}$ is a Cauchy sequence as $s \to +\infty$. Note first that $v^\pm$ satisfies

$$-i\partial_s v^\pm = \pm\Lambda(s)v^\pm + \partial_s \Pi^\pm(s)v.$$

Therefore, for $0 < t < s$,

$$\|v^+(s)\|^2_{\mathcal{H}^2} - \|v^+(t)\|^2_{\mathcal{H}^2} = 2\,\mathrm{Re}\left(\int_t^s \left\langle \Pi^+(\tau)\partial_s\Pi^+(\tau)v(\tau), v(\tau)\right\rangle_{\mathcal{H}^2} d\tau\right).$$

We are going to use properties of the operator $\Pi^+(s)\partial_s\Pi^+(s)$ that we gather in the next lemma where we denote by $\mathrm{Im}\, C$ the skew adjoint part of the operator C: $\mathrm{Im}\, C = (C - C^*)/2$.

Lemma 4.2. *Let $C(s) = \Pi^+(s)\partial_s\Pi^+(s)$ and $B(s) = \frac{1}{2}\Lambda(s)^{-1}C(s)$. Then $C(s)$ and $B(s)$ are antidiagonal operators of $\mathcal{A}$ with $C(s) = \mathcal{O}_R(1/s)$ and $B(s) = \mathcal{O}_R(1/s^2)$ in $\mathcal{L}(\mathcal{H}^2)$. Moreover,*

$$\langle \partial_s(\mathrm{Im}\, B(s))v(s), v(s)\rangle = \frac{i}{8s^3}\underline{m}(s)\partial_s\left((\mathrm{Re}\,\langle v_1, Gv_2\rangle_{\mathcal{H}})^2\right) + \mathcal{O}_R(s^{-3}),$$

where the bounded function $\underline{m}(s)$ is defined in (3.10).

The proof of this lemma is postponed to the end of the section. Using Lemma 3.6, we obtain

$$\begin{aligned}
\mathrm{Re}\int_t^s & \langle C(\tau)v(\tau)\,,\; v(\tau)\rangle_{\mathcal{H}^2}\, d\sigma \\
&= \mathrm{Re}\left[i\,\langle B(\tau)v(\tau)\,,\; v(\tau)\rangle_{\mathcal{H}^2}\Big|_t^s - i\int_t^s \langle \partial_s B(\tau)v(\tau)\,,\; v(\tau)\rangle_{\mathcal{H}^2}\, d\tau\right] \\
&= i\,\langle \mathrm{Im}\, B(\tau)v(\tau)\,,\; v(\tau)\rangle_{\mathcal{H}^2}\Big|_t^s - i\int_t^s \langle \partial_s\, \mathrm{Im}\, B(\tau)v(\tau)\,,\; v(\tau)\rangle_{\mathcal{H}^2}\, d\tau \\
&= \mathcal{O}\left(\frac{1}{t^2}\right) - i\int_t^s \langle \partial_s\, \mathrm{Im}\, B(\tau)v(\tau)\,,\; v(\tau)\rangle_{\mathcal{H}^2}\, d\tau.
\end{aligned}$$

and an integration by parts allows us to conclude that

$$\mathrm{Re}\int_t^s \langle C(\tau)v(\tau)\,,\; v(\tau)\rangle_{\mathcal{H}^2}\, d\tau = \mathcal{O}_R(s^{-2})$$

since $\underline{m}(s)$ is bounded. □

Proof of Lemma 4.2. The proof relies on the computation of $C(s)$ by observing (with the notations of Section 3)

$$\partial_s\Pi^+(s) = \frac{1}{2}\left(\dot\sigma(s)\Lambda(s)^{-1}J - \partial_s\Lambda(s)^{-1}\widetilde{V}(s)\right).$$

In view of

$$\partial_s\Lambda(s) = \sigma(s)\dot\sigma(s)\Lambda(s)^{-1},$$

and since

$$\Pi^+(s)\partial_s\Pi^+(s) = \Pi^+(s)\partial_s\Pi^+(s)\Pi^-(s),$$

the operators $C(s)$ and $B(s)$ are antidiagonal and the estimates $C(s) = \mathcal{O}_R(1/s)$ and $B(s) = \mathcal{O}_R(1/s^2)$ come from Lemma 3.7 and $\Lambda(s) = \mathcal{O}_R(1/s)$.

Let us now calculate $\partial_s \operatorname{Im} B(s)$. We have

$$\begin{aligned}\Pi^+(s)\partial_s\Pi^+(s)\Pi^-(s) &= \frac{1}{2}\dot\sigma(s)\Lambda(s)^{-1}\Pi^+(s)J\Pi^-(s)\\ &= \frac{1}{8}\dot\sigma(s)\Lambda(s)^{-1}\left(J + \Lambda(s)^{-1}[\widetilde V(s), J] - \Lambda(s)^{-2}\widetilde V(s)J\widetilde V(s)\right).\end{aligned}$$

In view of

$$[\widetilde V(s), J] = [K, J] = 2\begin{pmatrix} 0 & -G\\ G^* & 0\end{pmatrix},\quad \widetilde V(s)J\widetilde V(s) = \sigma(s)^2 J + 2\sigma(s)K + \operatorname{diag}(-GG^*, G^*G),$$

we obtain

$$C(s) = \frac{1}{4}\dot\sigma(s)\left(\Lambda(s)^{-3}\left(\operatorname{diag}(GG^*, G^*G) - \sigma(s)K\right) + \Lambda(s)^{-2}\begin{pmatrix} 0 & -G\\ G^* & 0\end{pmatrix}\right),$$

hence

$$\operatorname{Im} C(s) = \frac{1}{4}\dot\sigma(s)\Lambda(s)^{-2}\begin{pmatrix} 0 & -G\\ G^* & 0\end{pmatrix}.$$

By Lemma 3.7, we obtain

$$\begin{aligned}\partial_s \operatorname{Im} B(s) &= \frac{1}{8}\ddot\sigma(s)\Lambda(s)^{-3}\begin{pmatrix} 0 & -G\\ G^* & 0\end{pmatrix} + \mathcal{O}_R\left(1/s^3\right)\\ &= \frac{1}{2s^2}\underline{m}(s)\operatorname{Re}\langle v_1(s), Gv_2(s)\rangle_{\mathcal{H}}\begin{pmatrix} 0 & -G\\ G^* & 0\end{pmatrix} + \mathcal{O}_R\left(1/s^3\right)\end{aligned}$$

where we have used $\Lambda(s)^{-3} - s^{-3} = \mathcal{O}_R(s^{-4})$, which stems from

$$\forall m, \lambda \in \mathbb{R}^+,\ \ ((m+s)^2 + \lambda)^{-3/2} - s^{-3} = \mathcal{O}\left(\frac{m+\lambda}{s^4}\right).$$

Finally, we obtain

$$\langle \partial_s \operatorname{Im} B(s)v(s), v(s)\rangle_{\mathcal{H}^2} = \frac{i}{2s^2}\underline{m}(s)\operatorname{Re}\langle v_1(s), Gv_2(s)\rangle_{\mathcal{H}}\operatorname{Im}\langle v_1(s), Gv_2(s)\rangle_{\mathcal{H}}$$

and we conclude by observing

$$\partial_s\left(\operatorname{Re}\langle v_1(s), Gv_2(s)\rangle_{\mathcal{H}}\right) = -2s\operatorname{Im}\langle v_1(s), Gv_2(s)\rangle_{\mathcal{H}}.$$

□

4.2. **Analysis of the nonlinear term.** We are now going to prove Proposition 3.2, which allows us to describe $F(v(s))$ as s goes to $\pm\infty$. Note that, for $|s| \gg 1$, we have

$$\Lambda(s)^{-1}\Theta_R = \frac{1}{|\sigma(s)|}\left(\operatorname{Id} + \mathcal{O}_R\left(\frac{1}{s^2}\right)\right).$$

We deduce asymptotics for the operators $\Pi^\pm(s)$: for $s \gg 1$, in $\mathcal{L}(\mathcal{H}^2)$,

$$\Pi^+(s)\Theta_R = \Theta_R E_1 + \frac{1}{2}\Lambda(s)^{-1}K\Theta_R + \mathcal{O}_R\left(\frac{1}{s^2}\right), \tag{4.1}$$

$$\Pi^-(s)\Theta_R = \Theta_R E_2 - \frac{1}{2}\Lambda(s)^{-1}K\Theta_R + \mathcal{O}_R\left(\frac{1}{s^2}\right),$$

and for $s \ll -1$, in $\mathcal{L}(\mathcal{H}^2)$,

$$\Pi^+(s)\Theta_R = \Theta_R E_2 + \frac{1}{2}\Lambda(s)^{-1}K\Theta_R + \mathcal{O}_R\left(\frac{1}{s^2}\right),$$
$$\Pi^-(s)\Theta_R = \Theta_R E_1 - \frac{1}{2}\Lambda(s)^{-1}K\Theta_R + \mathcal{O}_R\left(\frac{1}{s^2}\right),$$

where $K = V(0)$ has been defined in (3.4) and

$$E_1 = \mathrm{diag}(1,0) \text{ and } E_2 = \mathrm{diag}(0,1).$$

Since $u_0 = \Theta_R u_0$ yields that for all $s \in \mathbb{R}$, $u(s) = \Theta_R u(s)$ and $v(s) = \Theta_R v(s)$ (by Lemma 1.2), we have for all $R > 0$, as $s \to +\infty$,

$$\begin{aligned}\|v_1(s)\|^2_{\mathcal{H}} &= \|v^+(s)\|^2_{\mathcal{H}^2} + \mathrm{Re}\left\langle v^+(s)\ ,\ \Lambda(s)^{-1}K\Theta_R v(s)\right\rangle_{\mathcal{H}^2} + \mathcal{O}_R\left(\frac{1}{s^2}\right)\\ &= \|v^+(s)\|^2_{\mathcal{H}^2} + \mathrm{Re}\left\langle K\Lambda(s)^{-1}\Pi^+(s)\Theta_R v(s)\ ,\ v(s)\right\rangle_{\mathcal{H}^2} + \mathcal{O}_R\left(\frac{1}{s^2}\right).\end{aligned}$$

In view of (4.1) and of the relation

$$\|\Lambda(s)^{-1}K\Theta_R\|_{\mathcal{L}(\mathcal{H}^2)} = \mathcal{O}_R(s^{-1}),$$

we have

$$\Pi^+(s)\Theta_R = E_1\Theta_R + \mathcal{O}_R(s^{-1}).$$

This implies that we can write

$$\begin{aligned}K\Lambda(s)^{-1}\Pi^+(s)\Theta_R &= K\Lambda(s)^{-1}E_1\Theta_R + \mathcal{O}_R\left(\frac{1}{s^2}\right)\\ &= E_2K\Lambda(s)^{-1}E_1\Theta_R + \mathcal{O}_R\left(\frac{1}{s^2}\right)\\ &= \Lambda(s)^{-1}\Pi^-(s)K\Theta_R\Pi^+(s) + \mathcal{O}_R\left(\frac{1}{s^2}\right),\end{aligned}$$

where we have used $E_2K = KE_1$, $\Lambda(s)^{-1}E_1 = E_1\Lambda(s)^{-1}$ and the commutation properties of $V(s)$ and $\Pi^\pm(s)$ with $\Lambda(s)^{-1}$ and Θ_R. We set

$$g_1(s) = \mathrm{Re}\left\langle \Lambda(s)^{-1}\Pi^-(s)K\Theta_R\Pi^+(s)v(s)\ ,\ v(s)\right\rangle_{\mathcal{H}^2}. \tag{4.2}$$

We obtain

$$g_1(s) = \mathcal{O}_R(s^{-1}) \text{ and } \|v_1(s)\|^2_{\mathcal{H}} = \|v^+(s)\|^2_{\mathcal{H}^2} + g_1(s) + \mathcal{O}_R\left(\frac{1}{s^2}\right).$$

Similarly, we obtain

$$\|v_2(s)\|^2_{\mathcal{H}} - \Omega^- = g_2(s) + \mathcal{O}_R\left(\frac{1}{s^2}\right), \tag{4.3}$$

with $g_2(s) = \mathcal{O}_R(s^{-1})$ and, as $s \to -\infty$,

$$\|v_1(s)\|^2_{\mathcal{H}} - A^- = \widetilde{g}_1(s) + \mathcal{O}_R\left(\frac{1}{s^2}\right), \quad \|v_2(s)\|^2_{\mathcal{H}} - A^+ = \widetilde{g}_2(s) + \mathcal{O}_R\left(\frac{1}{s^2}\right),$$

with $\widetilde{g}_j(s) = \mathcal{O}_R(|s|^{-1})$, $j = 1,2$. This yields the first part of Proposition 3.2, with

$$(\Omega_1, \Omega_2) = (\Omega^+, \Omega^-) \text{ and } (A_1, A_2) = (A^-, A^+).$$

Let us now prove that for $j \in \{1,2\}$ and $s \gg 1$,

$$\int_s^{+\infty} g_j(\tau)d\tau = \mathcal{O}_R(s^{-1}) \text{ and } \int_{-\infty}^{-s} \widetilde{g}_j(\tau)d\tau = \mathcal{O}_R(|s|^{-1}). \tag{4.4}$$

We focus on g_1; the other assertions can be proved similarly. In that purpose, we study the operator

$$\widetilde{C}(s) = \Lambda(s)^{-1}\Pi^-(s)K\Theta_R\Pi^+(s).$$

Lemma 4.3. *The operators* $\widetilde{C}(s) = \Lambda(s)^{-1}\Pi^-(s)K\Theta_R\Pi^+(s)$ *and* $\widetilde{B}(s) = \frac{1}{2}\Lambda(s)^{-1}\widetilde{C}(s)$ *are antidiagonal operators of* $\mathcal{A}$ *which satisfy*

$$\operatorname{Im}\widetilde{C}(s) = \frac{\sigma(s)}{2}\Lambda(s)^{-2}\Theta_R\begin{pmatrix} 0 & -G \\ G^* & 0\end{pmatrix}, \tag{4.5}$$

and $\widetilde{C}(s) = \mathcal{O}_R(1/s)$, $\widetilde{B}(s) = \mathcal{O}_R(1/s^2)$, $\partial_s\widetilde{B}(s) = \mathcal{O}_R(1/s^3)$ *in* $\mathcal{L}(\mathcal{H}^2)$.

Then the proof is straightforward: by Lemma 3.6, we write

$$g_1(s) = \operatorname{Re}\left(\frac{1}{i}\frac{d}{ds}\left\langle \widetilde{B}(s)v(s)\ ,\ v(s)\right\rangle_{\mathcal{H}^2}\right) + \operatorname{Re}\left(i\left\langle \partial_s\widetilde{B}(s)v(s)\ ,\ v(s)\right\rangle_{\mathcal{H}^2}\right),$$

and (4.4) follows. It remains to prove Lemma 4.3.

Proof of Lemma 4.3. We write

$$\widetilde{C}(s) = \frac{1}{4}\Lambda(s)^{-1}\left(K + \Lambda(s)^{-1}[K,\widetilde{V}(s)] - \Lambda(s)^{-2}\widetilde{V}(s)K\widetilde{V}(s)\right)\Theta_R.$$

In view of

$$[K,\widetilde{V}(s)] = 2\sigma(s)\begin{pmatrix} 0 & -G \\ G^* & 0\end{pmatrix},$$

and

$$\widetilde{V}(s)K\widetilde{V}(s) = -\sigma(s)^2K + 2\sigma(s)\operatorname{diag}(GG^*,-G^*G) + \begin{pmatrix} 0 & GG^*G \\ G^*GG^* & 0\end{pmatrix},$$

we obtain

$$\widetilde{C}(s) = \frac{1}{4}\Lambda(s)^{-1}\Big(-2\sigma(s)\Lambda(s)^{-2}\operatorname{diag}(GG^*,-G^*G) + (1+\sigma(s)^2\Lambda(s)^{-2})K$$
$$-\Lambda(s)^{-2}\begin{pmatrix} 0 & GG^*G \\ G^*GG^* & 0\end{pmatrix} + 2\sigma(s)\Lambda(s)^{-1}\begin{pmatrix} 0 & -G \\ G^* & 0\end{pmatrix}\Big)\Theta_R$$

hence (4.5) and the other properties of the lemma follow from the observation $\|Ku(s)\|_{\mathcal{H}^2} = \mathcal{O}(R)$ and from Lemma 3.7. □

4.3. Proof of Proposition 3.3.

Proof. In view of the preceding computations, we have

$$m(v(s)) = m(\omega) + g(s) + \mathcal{O}_R\left(s^{-2}\right),$$

where $\omega \in \mathcal{H}^2$ is such that $F_j(\omega) = f_j(\Omega^+,\Omega_-)$, with

$$g(s) = \mathcal{O}_R(s^{-1}) \text{ and } \int_s^{+\infty} g(\tau)d\tau = \mathcal{O}_R(s^{-1}). \tag{4.6}$$

Set $t = s + m(\omega)$ and $\check{v}(t) = v(s)$: $\check{v}$ solves

$$-i\partial_t\check{v} = V\left(t + m\left(v(t-m(\omega))\right) - m(\omega)\right)\check{v} = V\left(t+\check{g}(t)\right)\check{v}, \tag{4.7}$$

where $\check{g}$ depends on v and satisfies the same asymptotic estimates (4.6) as g. Consider the modified asymptotic phase

$$\check{\varphi}(t,\lambda) = \frac{t^2}{2} + \frac{\lambda}{2}\ln|t| - \int_t^{+\infty} \check{g}(\tau)d\tau,$$

and set, for $n \in \mathbb{N}$,

$$\check{v}^n_{\rm app}(t) = \left(\mathrm{e}^{i\check{\varphi}(t,GG^*)}\nu_1^n - \frac{G}{2t}\mathrm{e}^{-i\check{\varphi}(t,G^*G)}\nu_2^n, \mathrm{e}^{-i\check{\varphi}(t,G^*G)}\nu_2^n + \frac{G^*}{2t}\mathrm{e}^{i\check{\varphi}(t,GG^*)}\nu_1^n \right),$$

where ν_1^n and ν_2^n are to be fixed later. We compute

$$-i\partial_t \check{v}^n_{1,\rm app} = (t+\check{g}(t))\,\check{v}^n_{1,\rm app} + G\check{v}^n_{2,\rm app} + \mathcal{O}_R\left(t^{-2}\right),$$
$$-i\partial_t \check{v}^n_{2,\rm app} = -(t+\check{g}(t))\,\check{v}^n_{2,\rm app} + G^*\check{v}^n_{1,\rm app} + \mathcal{O}_R\left(t^{-2}\right),$$

hence

$$-i\partial_t \check{v}^n_{\rm app} = V\left(t+\check{g}(t)\right)\check{v}^n_{\rm app} + \mathcal{O}_R\left(t^{-2}\right). \tag{4.8}$$

Now we fix ν_j^n so that $\check{v}^n_{\rm app}$ is close to $\check{v}$ for $t = n$:

$$\nu_1^n = \mathrm{e}^{-i\check{\varphi}(n,GG^*)}\check{v}_1(n) \quad ; \quad \nu_2^n = \mathrm{e}^{i\check{\varphi}(n,G^*G)}\check{v}_2(n),$$

whence $\|\check{v}(n) - \check{v}^n_{\rm app}(n)\|_{\mathcal{H}^2} = \mathcal{O}_R(n^{-1})$. Subtracting (4.8) from (4.7), the energy estimate yields

$$\frac{d}{dt}\|\check{v}(t) - \check{v}^n_{\rm app}(t)\|_{\mathcal{H}^2} = \mathcal{O}_R\left(t^{-2}\right).$$

We infer, for $t \geqslant n$,

$$\|\check{v}(t) - \check{v}^n_{\rm app}(t)\|_{\mathcal{H}^2} = \mathcal{O}_R\left(n^{-1}\right),$$

and

$$\check{v}_1(t) = \mathrm{e}^{i\check{\varphi}(t,GG^*)}\nu_1^n + \mathcal{O}_R\left(\frac{1}{t}+\frac{1}{n}\right); \quad \check{v}_2(t) = \mathrm{e}^{-i\check{\varphi}(t,G^*G)}\nu_2^n + \mathcal{O}_R\left(\frac{1}{t}+\frac{1}{n}\right).$$

Back to v, this information yields, since $v(s) = \check{v}(s+m(\omega))$,

$$v_1(s) = \mathrm{e}^{i\varphi(s+m(\omega),GG^*)}\nu_1^n + \mathcal{O}_R\left(\frac{1}{s}+\frac{1}{n}\right),$$
$$v_2(s) = \mathrm{e}^{-i\varphi(s+m(\omega),G^*G)}\nu_2^n + \mathcal{O}_R\left(\frac{1}{s}+\frac{1}{n}\right),$$

where we have used $\check{\varphi}(s,\lambda) = \varphi(s,\lambda) + \mathcal{O}_\lambda(1/s)$ by Proposition 3.2. We infer in particular

$$\left|\|v_1(s)\|^2_{\mathcal{H}} - \|\nu_1^n\|^2_{\mathcal{H}}\right| + \left|\|v_2(s)\|^2_{\mathcal{H}} - \|\nu_2^n\|^2_{\mathcal{H}}\right| \leqslant C_R\left(\frac{1}{n}+\frac{1}{s}\right).$$

Taking the lim sup as $s \to +\infty$ yields, in view of Proposition 4.1 and (4.2),

$$\left|\Omega^+ - \|\nu_1^n\|^2_{\mathcal{H}}\right| + \left|\Omega^- - \|\nu_2^n\|^2_{\mathcal{H}}\right| = \mathcal{O}_R\left(n^{-1}\right).$$

Since the unit ball of $\mathcal{H}$ is compact, one can extract a converging subsequence of ν_j^n, whose limit ν_j satisfies $\|\nu_1\|^2_{\mathcal{H}} = \Omega^+$ and $\|\nu_2\|^2_{\mathcal{H}} = \Omega^-$, as in Proposition 3.3. Uniqueness is straightforward. A similar argument allows us to define the scattering states as $s \to -\infty$. □

5. Existence of wave operators

Given an asymptotic state $\omega = (\omega_1, \omega_2) \in \mathcal{H}^2$ such that $\omega = \Theta_R \omega$, consider the expected asymptotic solution u_{app} provided by Theorem 1.3, appearing in the statement of Proposition 1.6 (up to the factor ϕ):

$$u_{1,\text{app}}(s) = \mathrm{e}^{is\delta F_1(\omega) + i\varphi(s,GG^*)}\omega_1; \quad u_{2,\text{app}}(s) = \mathrm{e}^{is\delta F_2(\omega) - i\varphi(s,G^*G)}\omega_2.$$

For $n \in \mathbb{N}$, let $u^n = \Theta_R u^n$ be the solution to (1.5) such that

$$u^n_{|s=n} = u_{\text{app}|s=n}. \tag{5.1}$$

In view of Lemma 1.1, for all $n \in \mathbb{N}$, u^n is defined globally, and $u^n \in C(\mathbb{R}; \mathcal{H}^2)$. Its initial value $u^n_{|s=0}$ is a sequence of the unit ball (in view of (1.8)) of $\mathcal{H}^2$. Since the dimension of $\mathcal{H}$ is finite, up to extracting a subsequence, we may assume that

$$u^n_{|s=0} \underset{n\to\infty}{\longrightarrow} \mathbf{u}_0 \quad \text{in } \mathcal{H}^2.$$

We denote by $\mathbf{u}$ its evolution under (1.5). Theorem 1.3 provides a unique $\widetilde{\omega} \in \mathcal{H}^2$ such that, as $s \to +\infty$,

$$\begin{aligned} \mathbf{u}_1(s) &= \mathrm{e}^{is\delta F_1(\widetilde{\omega}) + i\varphi(s,GG^*)}\widetilde{\omega}_1 + \mathcal{O}_R\left(\frac{1}{s}\right), \\ \mathbf{u}_2(s) &= \mathrm{e}^{is\delta F_2(\widetilde{\omega}) - i\varphi(s,G^*G)}\widetilde{\omega}_2 + \mathcal{O}_R\left(\frac{1}{s}\right). \end{aligned} \tag{5.2}$$

In the same spirit as to prove the existence of scattering states, we first study the norms.

Lemma 5.1. *We have* $\|\omega_j\|_{\mathcal{H}} = \|\widetilde{\omega}_j\|_{\mathcal{H}}$, $j = 1, 2$.

Proof. Suppose that the result were not true, say $\|\omega_1\|_{\mathcal{H}} \neq \|\widetilde{\omega}_1\|_{\mathcal{H}}$. We have seen in Section 4 that there exists C_R independent of u such that

$$\left| \|\mathbf{u}_1(s)\|_{\mathcal{H}} - \|\widetilde{\omega}_1\|_{\mathcal{H}} \right| \leqslant \frac{C_R}{s}, \quad \forall s \geqslant 1.$$

By assumption, there exists $\varepsilon > 0$ and $s_0 > 11$ such that

$$\left| \|\mathbf{u}_1(s)\|_{\mathcal{H}} - \|\omega_1\|_{\mathcal{H}} \right| \geqslant \varepsilon, \quad \forall s \geqslant s_0.$$

Form Theorem 1.3, for all $n \in \mathbb{N}$, there exists $\omega^n \in \mathcal{H}^2$ such that

$$\begin{aligned} u_1^n(s) - \mathrm{e}^{is\delta F_1(\omega^n) + i\varphi(s,GG^*)}\omega_1^n &= \mathcal{O}_R\left(\frac{1}{s}\right), \\ u_2^n(s) - \mathrm{e}^{is\delta F_2(\omega^n) - i\varphi(s,GG^*)}\omega_2^n &= \mathcal{O}_R\left(\frac{1}{s}\right), \end{aligned} \tag{5.3}$$

hence

$$\left| \|u_1^n(s)\|_{\mathcal{H}} - \|\omega_1^n\|_{\mathcal{H}} \right| \leqslant \frac{C_R}{s}, \quad \forall s \geqslant 1,$$

where C_R does not depend on n. This yields

$$\|\omega_1^n\|_{\mathcal{H}} = \|\omega_1\|_{\mathcal{H}} + \mathcal{O}_R\left(\frac{1}{n}\right),$$

and there exists C_R such that

$$\left| \|u_1^n(s)\|_{\mathcal{H}} - \|\omega_1\|_{\mathcal{H}} \right| \leqslant C_R\left(\frac{1}{s} + \frac{1}{n}\right), \quad \forall s \geqslant 1. \tag{5.4}$$

Fix $s \geqslant s_0$ such that $CR^2/s < \varepsilon/2$. Notice that (1.5) is locally well-posed, uniformly on all compact intervals. Indeed, if u_a and u_b are two solutions of (1.5), subtracting the two equations, using (1.8) and the energy estimate for $u_a - u_b$, Gronwall lemma yields, for some universal constant C,

$$\|u_a(s) - u_b(s)\|_{\mathcal{H}^2} \leqslant \|u_a(s_0) - u_b(s_0)\|_{\mathcal{H}^2} \mathrm{e}^{C|s-s_0|}.$$

In particular, $u_1^n(s) \to \mathbf{u}_1(s)$ as $n \to \infty$ (recall that s is fixed). Taking the lim sup in n in (5.4) yields,

$$|\|\mathbf{u}_1(s)\|_{\mathcal{H}} - \|\omega_1\|_{\mathcal{H}}| \leqslant \frac{C_R}{s} \leqslant \frac{\varepsilon}{2},$$

hence a contradiction. □

To conclude, we go back to (5.3) which yields, for $s = n$ and in view of (5.1),

$$\left\| \mathrm{e}^{in\delta F_1(\omega)}\omega_1 - \mathrm{e}^{in\delta F_1(\omega^n)}\omega_1^n \right\|_{\mathcal{H}} = \mathcal{O}_R\left(\frac{1}{n}\right),$$
$$\left\| \mathrm{e}^{in\delta F_2(\omega)}\omega_2 - \mathrm{e}^{in\delta F_2(\omega^n)}\omega_2^n \right\|_{\mathcal{H}} = \mathcal{O}_R\left(\frac{1}{n}\right).$$

Up to extracting a subsequence again, we may assume that

$$\mathrm{e}^{in\delta(F_1(\omega)-F_1(\omega^n))} \underset{n\to\infty}{\longrightarrow} \mathrm{e}^{i\phi_1} \quad \text{and} \quad \mathrm{e}^{in\delta(F_2(\omega)-F_2(\omega^n))} \underset{n\to\infty}{\longrightarrow} \mathrm{e}^{i\phi_2},$$

for some $\phi_1, \phi_2 \in [0, 2\pi)$. We infer

$$\widetilde{\omega}_1 = \mathrm{e}^{i\phi_1}\omega_1 \quad \text{and} \quad \widetilde{\omega}_2 = \mathrm{e}^{i\phi_2}\omega_2. \tag{5.5}$$

Set

$$\phi = \frac{\phi_1 - \phi_2}{2}, \quad \Phi = \frac{\phi_1 + \phi_2}{2}.$$

We see that by construction, $\phi = 0$ if $F_1 = F_2$. Let

$$u(s) = \mathrm{e}^{-i\Phi}\mathbf{u}(s).$$

Since F is gauge invariant, u solves (1.5) with $u_0 = \mathrm{e}^{-i\Phi}\mathbf{u}_0$. In view of (5.2), (5.5) and the definition of Φ, we also have

$$u_1(s) = \mathrm{e}^{is\delta F_1(\widetilde{\omega})+i\varphi(s,GG^*)-i\Phi}\widetilde{\omega}_1 + \mathcal{O}_R\left(\frac{1}{s}\right) = \mathrm{e}^{is\delta F_1(\omega)+i\varphi(s,GG^*)+i\phi}\omega_1 + \mathcal{O}_R\left(\frac{1}{s}\right),$$
$$u_2(s) = \mathrm{e}^{is\delta F_2(\widetilde{\omega})-i\varphi(s,G^*G)-i\Phi}\widetilde{\omega}_2 + \mathcal{O}_R\left(\frac{1}{s}\right) = \mathrm{e}^{is\delta F_2(\omega)-i\varphi(s,G^*G)-i\phi}\omega_2 + \mathcal{O}_R\left(\frac{1}{s}\right),$$

hence the result. Finally, uniqueness for such a solution u for a fixed ϕ stems from Theorem 1.3.

6. Analysis of the Scattering Operator

We now prove Theorem 1.9 and we take into account the dependence of the nonlinear term with respect to the parameter δ. We begin with the particular case $F_1 = F_2$, which turns out to be fairly easy, and then turn to the general case.

6.1. **The case $F_1 = F_2 = \underline{F}$.** Recall that we denote by $u^{\rm lin}$ the solution to

$$\frac{1}{i}\partial_s u^{\rm lin} = V(s)u^{\rm lin}; \quad u^{\rm lin}_{|s=0} = u_{|s=0} = u_0.$$

In view of the identity

$$\begin{aligned} u(s) &= \exp\left(i\delta\int_0^s \underline{F}(u(\tau))d\tau\right)u^{\rm lin} \\ &= \exp\left(i\delta\int_0^s (\underline{F}(u(\tau)) - \underline{F}(u(\omega)))d\tau + is\delta\underline{F}(\omega)\right)u^{\rm lin}, \end{aligned} \tag{6.1}$$

Theorem 1.3 yields

$$\omega = \exp\left(i\delta\int_0^{+\infty}\left(\underline{F}(u(\tau)) - \underline{F}(\omega)\right)d\tau\right)\omega^{\rm lin}.$$

Similarly,

$$\alpha = \exp\left(i\delta\int_0^{-\infty}\left(\underline{F}(u(\tau)) - \underline{F}(\alpha)\right)d\tau\right)\alpha^{\rm lin}.$$

In particular, we have $\underline{F}(\omega) = \underline{F}(\omega^{\rm lin})$ and $\underline{F}(\alpha) = \underline{F}(\alpha^{\rm lin})$ since

$$\|\omega_j\|_{\mathcal{H}} = \|\omega_j^{\rm lin}\|_{\mathcal{H}} \text{ and } \|\alpha_j\|_{\mathcal{H}} = \|\alpha_j^{\rm lin}\|_{\mathcal{H}} \text{ for } j\in\{1,2\}. \tag{6.2}$$

Besides, in view of (6.1), we obtain $\underline{F}(u) = \underline{F}(u^{\rm lin})$. We deduce

$$\begin{aligned} \omega &= \exp\left(i\delta\int_0^{+\infty}\left(\underline{F}(u^{\rm lin}(\tau)) - \underline{F}(\omega^{\rm lin})\right)d\tau\right)\omega^{\rm lin} = \mathrm{e}^{i\delta\Lambda^+}\omega^{\rm lin}, \\ \alpha &= \exp\left(i\delta\int_0^{-\infty}\left(\underline{F}(u^{\rm lin}(\tau)) - \underline{F}(\alpha^{\rm lin})\right)d\tau\right)\alpha^{\rm lin} = \mathrm{e}^{-i\delta\Lambda^-}\alpha^{\rm lin}, \end{aligned}$$

where $\Lambda^+ = \int_0^{+\infty}\left(F(u^{\rm lin}(\tau)) - F(\omega^{\rm lin})\right)d\tau$ and $\Lambda^- = \int_{-\infty}^0\left(F(u^{\rm lin}(\tau)) - F(\alpha^{\rm lin})\right)d\tau$. This yields the exact formula (1.11).

We readily infer the following expansion

$$S_\delta = S^{\rm lin} + i\delta\left(\Lambda^+ + \Lambda^-\right)S^{\rm lin} + \mathcal{O}(\delta^2\|\Lambda^+\|^2) + \mathcal{O}(\delta^2\|\Lambda^-\|^2).$$

It remains to obtain an upper bound for $\Lambda^\pm$. We write

$$\Lambda^+ = \int_0^{s_0}\left(\underline{F}(u(s)) - \underline{F}(\omega)\right)ds + \int_{s_0}^{+\infty}\left(\underline{F}(u(s)) - \underline{F}(\omega)\right)ds.$$

By the continuity of the functions f (defined in (1.6)) and because $\|u_1\|^2_{\mathcal{H}} + \|u_2\|^2_{\mathcal{H}} = \|\omega_1\|^2_{\mathcal{H}} + \|\omega_2\|^2_{\mathcal{H}} = 1$, we have

$$\left|\int_0^{s_0}\left(\underline{F}(u(s)) - \underline{F}(\omega)\right)ds\right| \leqslant 2\left(\sup_{\mathbf{S}^1}|f|\right)s_0.$$

Proposition 3.2 yields a constant C_R such that,

$$\left|\int_{s_0}^{+\infty}\left(\underline{F}(u(s,z)) - \underline{F}(\omega(z))\right)ds\right| \leqslant C_R s_0^{-1}. \tag{6.3}$$

We infer $\Lambda^+ = \mathcal{O}_R(1)$, hence Theorem 1.9 in the case $F_1 = F_2$.

6.2. **The general case.** Following for instance [15] (see also [5] for some generalizations), the most natural method to obtain an asymptotic expansion for S_δ^ϕ should consist in decomposing the nonlinear solution u as

$$u = u^{(0)} + \delta r^\delta,$$

where $u^{(0)}$ solves the linear equation (1.1) and behaves like u as $s \to -\infty$ (up to $\mathcal{O}(\delta)$). The goal would then be to prove that the remainder r^δ is uniformly bounded for $\delta \in [-\delta_0, \delta_0]$ for some $\delta_0 > 0$ possibly small. However, if suitable in the case of dispersive equations (as in [15, 5]), this approach does not seem to be successful in the present framework, because the equation satisfied by the remainder r^δ involves terms whose integrability is rather delicate. Therefore, the approach that we present follows a different path, and highly relies on structural properties related to (1.5).

Let $\alpha \in \mathcal{H}^2$, and ϕ provided by Proposition 1.6. Proposition 1.6 yields a global solution u to (1.5), and Theorem 1.3 provides an asymptotic state ω for $s \to +\infty$. Instead of considering directly u, we will work with the function v defined in (3.3) and satisfying (3.2). In terms of v, Proposition 1.6 reads

$$v_1(s) = \mathrm{e}^{is\delta F_1(\alpha)+i\varphi(s,GG^*)-isM(\alpha)+i\int_{-\infty}^0 (M(u(\tau))-M(\alpha))d\tau+i\phi}\alpha_1 + \mathcal{O}_R\left(\frac{1}{|s|}\right),$$

$$v_2(s) = \mathrm{e}^{is\delta F_2(\alpha)-i\varphi(s,G^*G)-isM(\alpha)+i\int_{-\infty}^0 (M(u(\tau))-M(\alpha))d\tau-i\phi}\alpha_2 + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

In view of the expression of φ and of the definition of m and M, we can also write

$$v_1(s) = \mathrm{e}^{i\varphi(s+m(\alpha),GG^*)+i\int_{-\infty}^0 (M(u(\tau))-M(\alpha))d\tau+i\phi-im(\alpha)^2/2}\alpha_1 + \mathcal{O}_R\left(\frac{1}{|s|}\right),$$

$$v_2(s) = \mathrm{e}^{-i\varphi(s+m(\alpha),G^*G)+i\int_{-\infty}^0 (M(u(\tau))-M(\alpha))d\tau-i\phi+im(\alpha)^2/2}\alpha_2 + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

Proposition 1.6 in the *linear* case $F_1 = F_2 = 0$ yields a unique solution $v^{\rm lin}$ to

$$\frac{1}{i}\partial_s v^{\rm lin} = V(s)\, v^{\rm lin},$$

and such that, as $s \to -\infty$,

$$v_1^{\rm lin}(s) = \mathrm{e}^{i\varphi(s,GG^*)}\alpha_1 + \mathcal{O}_R\left(\frac{1}{|s|}\right), \quad v_2^{\rm lin}(s) = \mathrm{e}^{-i\varphi(s,G^*G)}\alpha_2 + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

Therefore, $v^{\rm lin}(0)$ is the image of α under the action of the *linear* wave operator, and as $s \to +\infty$, $v^{\rm lin}$ has an asymptotic state $\omega^{\rm lin} = S^{\rm lin}(\alpha)$. Setting $v^-(s) = v^{\rm lin}(s + m(\alpha))$, we see that

$$\frac{1}{i}\partial_s v^- = V(s + m(\alpha))\, v^-,$$

and

$$v_1^-(s) = \mathrm{e}^{i\varphi(s+m(\alpha),GG^*)}\alpha_1 + \mathcal{O}_R\left(\frac{1}{|s|}\right),$$

$$v_2^-(s) = \mathrm{e}^{-i\varphi(s+m(\alpha),G^*G)}\alpha_2 + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

We note the identity

$$\|v_1(s) - v_1^-(s)\|_{\mathcal{H}} = \left|\mathrm{e}^{i\int_{-\infty}^0 (M(u(\tau))-M(\alpha))d\tau+i\phi-im(\alpha)^2/2} - 1\right| \|\alpha_1\|_{\mathcal{H}} + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

The proof of Proposition 1.6 yields $\phi = \mathcal{O}_R(\delta)$, so

$$\|v_1(s) - v_1^-(s)\|_{\mathcal{H}} = \mathcal{O}_R(\delta) + \mathcal{O}_R\left(\frac{1}{|s|}\right).$$

We infer

$$\left\| v_1\left(\frac{-1}{\delta}\right) - v_1^-\left(\frac{-1}{\delta}\right)\right\|_{\mathcal{H}} = \mathcal{O}_R(\delta).$$

We now use the following lemma the proof of which is postponed to the end of the section.

Lemma 6.1. *There exists* $\kappa^-(s)$ *such that, as* $s \to -\infty$, $\kappa^-(s) = \mathcal{O}_R(\delta s^{-2})$ *and*

$$\frac{1}{i}\partial_s\left(v - v^- + \kappa^-(s)\right) = V(s + m(\alpha))\left(v - v^- + \kappa^-(s)\right) + \mathcal{O}_R(\delta s^{-2}).$$

By integration, we infer

$$\forall s \leqslant -1, \;\; v(s) = v^-(s) + \mathcal{O}_R(\delta).$$

The Fundamental Theorem of Calculus yields the identity

$$v^{\mathrm{lin}}(s) - v^-(s) = \int_{s+m(\alpha)}^{s} \partial_s v^{\mathrm{lin}}(\tau)d\tau,$$

and since $\partial_s v^{\mathrm{lin}}$ is locally bounded (from the equation), we infer

$$v^{\mathrm{lin}}(-1) - v^-(-1) = \mathcal{O}_R\left(m(\alpha)\right) = \mathcal{O}_R(\delta).$$

On the other hand, since

$$\frac{1}{i}\partial_s\left(v - v^{\mathrm{lin}}\right) = V(s)\left(v - v^{\mathrm{lin}}\right) + m\left(u(s)\right)Jv,$$

and since v is bounded, the energy identity yields

$$\frac{d}{ds}\|v - v^{\mathrm{lin}}\|_{\mathcal{H}^2}^2 = 2\,\mathrm{Im}\left\langle m\left(u(s)\right)Jv, v - v^{\mathrm{lin}}\right\rangle = \mathcal{O}_R(\delta\|v - v^{\mathrm{lin}}\|_{\mathcal{H}^2}).$$

We infer

$$v(s) = v^{\mathrm{lin}}(s) + \mathcal{O}_R(\delta), \quad \forall s \in [-1, 1].$$

With ω the (nonlinear) asymptotic state associated to u, we define similarly

$$v^+(s) = v^{\mathrm{lin}}\left(s + m(\omega)\right).$$

For the same reason as above, $v(1) = v^+(1) + \mathcal{O}_R(\delta)$. Proceding like for $s < 0$, we can find $\kappa^+(s) \in \mathbb{R}$ so that

$$\frac{1}{i}\partial_s\left(v - v^+ + \kappa^+(s)\right) = V(s + m(\omega))\left(v - v^+ + \kappa^+(s)\right) + \mathcal{O}_R\left(\frac{\delta}{s^2}\right),$$

and we infer

$$v(s) = v^+(s) + \mathcal{O}_R(\delta), \quad \forall s \geqslant 1. \tag{6.4}$$

From the linear scattering theory, we have, as $s \to +\infty$:

$$v_1^+(s) = \mathrm{e}^{i\varphi(s+m(\omega),GG^*)}\omega_1^{\mathrm{lin}} + \mathcal{O}_R\left(\frac{1}{s}\right),$$

$$v_2^+(s) = \mathrm{e}^{-i\varphi(s+m(\omega),G^*G)}\omega_2^{\mathrm{lin}} + \mathcal{O}_R\left(\frac{1}{s}\right),$$

where $\omega^{\rm lin} = S^{\rm lin}(\alpha)$, and from Theorem 1.3 (see also Proposition 3.3), we also have (like in the case $s \to -\infty$):

$$v_1(s) = {\rm e}^{i\varphi(s+m(\omega),GG^*)-i\int_0^{+\infty}(M(u(\tau))-M(\omega))d\tau-im(\omega)^2/2}\omega_1 + \mathcal{O}_R\left(\frac{1}{s}\right),$$
$$v_2(s) = {\rm e}^{-i\varphi(s+m(\omega),G^*G)-i\int_0^{+\infty}(M(u(\tau))-M(\omega))d\tau+im(\omega)^2/2}\omega_2 + \mathcal{O}_R\left(\frac{1}{s}\right).$$

In view of these asymptotic identities and of (6.4), we infer

$$\omega = \omega^{\rm lin} + \mathcal{O}_R(\delta),$$

which is the identity $S = S^{\rm lin} + \mathcal{O}_R(\delta)$ of Theorem 1.9.

It remains to prove the intermediary result:

Proof of Lemma 6.1. In view of (3.11) and (4.4), we have

$$\|v_1(s)\|_{\mathcal{H}}^2 - \|\alpha_1\|_{\mathcal{H}}^2 = -\left(\|v_2(s)\|_{\mathcal{H}}^2 - \|\alpha_2\|_{\mathcal{H}}^2\right) \quad = \quad \int_s^{-\infty} 2\,{\rm Im}\,\langle v_1(\tau), Gv_2(\tau)\rangle\, d\tau.$$

Since

$$\partial_s\langle v_1(s), Gv_2(s)\rangle = 2is\langle v_1(s), Gv_2(s)\rangle + i\left(\|Gv_2(s)\|_{\mathcal{H}}^2 - \|Gv_1(s)\|_{\mathcal{H}}^2\right),$$

an integration by parts yields

$$\int_s^{-\infty} \langle v_1(\tau), Gv_2(\tau)\rangle = \frac{i}{2s}\langle v_1(s), Gv_2(s)\rangle$$
$$+ \int_s^{-\infty}\left(\frac{1}{2i\tau^2}\langle v_1(\tau), Gv_2(\tau)\rangle - \frac{1}{2\tau}\left(\|Gv_2(\tau)\|_{\mathcal{H}}^2 - \|G^*v_1(\tau)\|_{\mathcal{H}}^2\right)\right)d\tau,$$

whence

$${\rm Im}\int_s^{-\infty}\langle v_1(\tau), Gv_2(\tau)\rangle = {\rm Im}\left(\frac{i}{2s}\langle v_1(s), Gv_2(s)\rangle\right)$$
$$+ {\rm Im}\int_s^{-\infty}\frac{1}{2i\tau^2}\langle v_1(\tau), Gv_2(\tau)\rangle\, d\tau + \mathcal{O}_R(s^{-2}).$$

With one more integration by parts, we obtain

$$\begin{aligned} 2\,{\rm Im}\int_s^{-\infty}\langle v_1(\tau), Gv_2(\tau)\rangle &= \frac{1}{s}{\rm Re}\,\langle v_1(s), Gv_2(s)\rangle + \mathcal{O}_R(s^{-2}) \\ &= \frac{1}{2s}{\rm Re}\left\langle {\rm e}^{i\varphi(s+m(\alpha),GG^*)}\alpha_1, {\rm e}^{-i\varphi(s+m(\alpha),G^*G)}\alpha_2\right\rangle \\ &\quad + \mathcal{O}_R(s^{-2}). \end{aligned}$$

A Taylor expansion of $m(v(s))$ implies the existence of a scalar $\widehat{m}(\alpha)$ such that

$$m(v(s)) - m(\alpha) = \frac{\widehat{m}(\alpha)}{2s}{\rm Re}\left\langle {\rm e}^{i\varphi(s+m(\alpha),GG^*)}\alpha_1, {\rm e}^{-i\varphi(s+m(\alpha),G^*G)}\alpha_2\right\rangle + \mathcal{O}_R(\delta s^{-2}).$$

Therefore, there exist functions $\kappa_j(s)$ and $\tilde{\kappa}_j(s)$, $j \in \{1,2\}$ such that

$$\|\kappa_j(s)\|_{\mathcal{H}} + \|\tilde{\kappa}_j(s)\|_{\mathcal{H}} + \|\partial_s\kappa_j(s)\|_{\mathcal{H}} + \|\partial_s\tilde{\kappa}_j(s)\|_{\mathcal{H}} = \mathcal{O}_R(\delta)$$

and

$$(m(v(s)) - m(\alpha))\, Jv(s) = \frac{1}{s}\left(\mathrm{e}^{3is^2/2}\kappa_1(s) + \mathrm{e}^{-is^2/2}\tilde{\kappa}_1(s), \mathrm{e}^{-3is^2/2}\kappa_2(s) + \mathrm{e}^{is^2/2}\tilde{\kappa}_2(s)\right) + \mathcal{O}_R(\delta s^{-2}),$$

where $J = \mathrm{diag}(1, -1)$ it defined in (3.4). Define

$$\kappa_1^-(s) = -\frac{1}{2s^2}\left(\mathrm{e}^{3is^2/2}\kappa_1(s) - \mathrm{e}^{-is^2/2}\tilde{\kappa}_1(s)\right),$$
$$\kappa_2^-(s) = \frac{1}{2s^2}\left(\mathrm{e}^{-3is^2/2}\kappa_2(s) - \mathrm{e}^{is^2/2}\tilde{\kappa}_2(s)\right).$$

Then the function $\kappa^-(s) = \left(\kappa_1^-(s), \kappa_2^-(s)\right)$ satisfies

$$\frac{1}{i}\partial_s\kappa^-(s) - V\left(s + m(\alpha)\right)\kappa^-(s) = -\left(m(v(s)) - m(\alpha)\right) Jv(s) + \mathcal{O}_R(\delta s^{-2}).$$

On the other hand, we have by definition

$$\begin{aligned}\frac{1}{i}\partial_s(v - v^-) &= V\left(s + m(v(s))\right) v - V(s + m(\alpha))v^- \\ &= V(s + m(\alpha))(v - v^-) + \left(m(v) - m(\alpha)\right) Jv.\end{aligned}$$

The lemma follows by summing the last two identities. □

Appendix A. Rigorous derivation for a double-well potential

A.1. **Mathematical framework.** We give more details concerning the derivation of (1.5) in the case of a condensate in a double well. This is achieved by adapting the approach from [27], from which several intermediary results are borrowed (see also [1] for some refinements to [27] in the confining, one-dimensional case). We shall derive the model (A.3) as an envelope equation in the semi-classical limit. Rewrite (2.3) in the presence of physical constants:

$$i\hbar\frac{\partial\psi^\hbar}{\partial t} + \frac{\hbar^2}{2}\Delta\psi^\hbar = V^\hbar(t,x)\psi^\hbar + \epsilon(\hbar)|\psi^\hbar|^2\psi^\hbar, \tag{A.1}$$

where $\epsilon(\hbar)$ is a coupling constant whose value will be discussed later on. Note that we consider a slightly more general framework than in Section 2: $x \in \mathbb{R}^d$, with $d \geqslant 1$. We assume that $V^\hbar(t,x) = V_s(x) + \kappa(\hbar)tV_a(x)$, with V_s and V_a independent of $\hbar$.

We first describe the assumptions performed on the potential V_s and discuss the first consequences.

Assumption A.1 (Symmetric potential)**.** *The potential $V_s \in \mathcal{C}^\infty(\mathbb{R}^d)$ is a smooth real-valued function such that:*

(1) *The potential V_s is at most quadratic,*

$$\partial^\alpha V_s \in L^\infty(\mathbb{R}^d), \quad \forall |\alpha| \geqslant 2.$$

(2) *V_s is symmetric with respect to the first coordinate:*

$$V_s(-x_1, x_2, \ldots, x_d) = V_s(x_1, x_2, \ldots, x_d), \quad \forall x \in \mathbb{R}^d.$$

(3) *V_s admits two minima at $x = x_\pm$, where x_- and x_+ are distinct and symmetric with respect to the first axis. Moreover,*

$$V_s(x) > V_s^{\min} = V(x_\pm), \quad \forall x \in \mathbb{R}^d,\ x \neq x_\pm,$$

and

$$V_s^{\min} < \liminf_{|x|\to\infty} V_s(x) =: V_\infty^-.$$

(4) *The minima x_+ and x_- are non-degenerate critical points: $\nabla V(x_\pm) = 0$ and $\nabla^2 V(x_\pm) > 0$.*

Remark A.2. As noted in [27], the last assumption (non-degeneracy) is not crucial.

We denote by

$$H_0 = -\frac{\hbar^2}{2}\Delta + V_s.$$

The operator H_0 admits a self-adjoint realization (still denoted by H_0) on $L^2(\mathbb{R}^d)$ (see e.g. [26]). Let $\sigma(H_0) = \sigma_d \cup \sigma_{\rm ess}$ be the spectrum of the self-adjoint operator H_0, where σ_d denotes the discrete spectrum and $\sigma_{\rm ess}$ denotes the essential spectrum. It follows that

$$\sigma_d \subset (V_s^{\min}, V_\infty^-) \quad \text{and} \quad \sigma_{\rm ess} = [V_\infty^-, +\infty).$$

Furthermore, the following two lemmas hold, which follow from [2]:

Lemma A.3 (Lemma 1 from [27]). *For any $\hbar \in (0, \hbar^*]$, for some $\hbar^*$ fixed, it follows that:*

(i) *σ_d is not empty and, in particular, it contains two eigenvalues at least.*

(ii) *The lowest two eigenvalues $\lambda_\pm^\hbar$ of H_0 are non-degenerate, in particular, $\lambda_+^\hbar < \lambda_-^\hbar$. There exists $C > 0$, independent of $\hbar$, such that*

$$\lambda_\pm^\hbar = V_s^{\min} + \mathcal{O}(\hbar); \qquad \inf_{\lambda \in \sigma(H_0)\setminus[\lambda_+^\hbar, \lambda_-^\hbar]} \left(\lambda - \lambda_\pm^\hbar\right) \geqslant C\hbar.$$

Lemma A.4 ([2], and Lemma 2 from [27]). *Let $\varphi_\pm^\hbar$ be the normalized eigenvectors associated to $\lambda_\pm^\hbar$, then:*

(i) *$\varphi_\pm^\hbar$ can be chosen to be real-valued functions such that*

$$\varphi_\pm^\hbar(-x_1, x_2, \dots, x_d) = \pm\varphi_\pm^\hbar(x_1, x_2, \dots, x_d).$$

(ii) *$\varphi_\pm^\hbar \in \Sigma \cap L^\infty(\mathbb{R}^d)$, where*

$$\Sigma = \{f \in H^1(\mathbb{R}^d),\ x \mapsto |x| f(x) \in L^2(\mathbb{R}^d)\}.$$

(iii) *There exists C independent of $\hbar$ such that for all $\hbar \in (0, \hbar*]$,*

$$\|\varphi_\pm^\hbar\|_{L^p(\mathbb{R}^d)} \leqslant C\hbar^{-\frac{d}{2}\left(\frac{1}{2}-\frac{1}{p}\right)}, \quad \forall p \in [2, \infty],$$
$$\|\nabla\varphi_\pm^\hbar\|_{L^2(\mathbb{R}^d)} \leqslant C\hbar^{-1/2}, \quad \|x\varphi_\pm^\hbar\|_{L^2(\mathbb{R}^d)} \leqslant C.$$

The single-well states are then defined as in (2.5). They satisfy:

- $\varphi_R^\hbar(-x_1, x_2, \dots, x_d) = \varphi_L^\hbar(x_1, x_2, \dots, x_d)$.
- $\|\varphi_L^\hbar \varphi_R^\hbar\|_{L^\infty} = \mathcal{O}\left(\mathrm{e}^{-c/\hbar}\right)$ for all $c < \Gamma$, where Γ denotes the Agmon distance between the two wells

$$\Gamma = \inf_{\gamma \text{ connecting the two wells}} \int_\gamma \sqrt{V_s(x) - V_s^{\min}}\,dx > 0.$$

- For any $r > 0$, there exists $C > 0$ such that

$$\int_{B(x_+,r)} |\varphi_R^\hbar(x)|^2 dx = 1 + \mathcal{O}\left(\mathrm{e}^{-C/\hbar}\right), \quad \int_{B(x_-,r)} |\varphi_L^\hbar(x)|^2 dx = 1 + \mathcal{O}\left(\mathrm{e}^{-C/\hbar}\right).$$

We denote by

$$\Pi_c^\hbar = 1 - \left(\left\langle \varphi_+^\hbar, \cdot \right\rangle \varphi_+^\hbar + \left\langle \varphi_-^\hbar, \cdot \right\rangle \varphi_-^\hbar\right)$$

the projection onto the eigenspace orthogonal to the bi-dimensional space associated to $\lambda_\pm^\hbar$. Finally, we define the splitting between the lowest two eigenvalues

$$\omega^\hbar = \frac{\lambda_-^\hbar - \lambda_+^\hbar}{2}. \tag{A.2}$$

Then for all $c < \Gamma$, $\omega^\hbar = \mathcal{O}\left(\mathrm{e}^{-c/\hbar}\right)$.

We now describe the assumptions made on the potential V_a.

Assumption A.5 (Antisymmetric potential)**.** *The potential $V_a \in \mathcal{C}^\infty(\mathbb{R}^d)$ is a smooth real-valued function such that:*

(1) *The potential V_a is bounded, as well as its derivatives,*

$$\partial^\alpha V_a \in L^\infty(\mathbb{R}^d), \quad \forall |\alpha| \geqslant 0.$$

(2) *V_a is antisymmetric with respect to the first coordinate:*

$$V_a(-x_1, x_2, \dots, x_d) = -V_a(x_1, x_2, \dots, x_d), \quad \forall x \in \mathbb{R}^d.$$

A.2. **An approximation result.** In this section, we prove:

Proposition A.6. *Let $d \leqslant 2$. Let $V^\hbar$ be as in Section A.1, with*

$$\kappa = \kappa(\hbar) = \eta \frac{(\omega^\hbar)^2}{\hbar},$$

for some $\eta \in \mathbb{R}$ independent of $\hbar$. Suppose that $\epsilon(\hbar)$ is given by

$$\epsilon(\hbar) = \delta \omega^\hbar \hbar^{d/2},$$

where $\delta \geqslant 0$ does not depend on $\hbar$. Suppose also that the initial datum is of the form

$$\psi^\hbar(0,x) = \alpha_L \varphi_L^\hbar(x) + \alpha_R \varphi_R^\hbar(x), \quad \alpha_L, \alpha_R \in \mathbb{C} \text{ independent of } \hbar.$$

Define the approximation solution ψ_{app} by

$$\psi_{\mathrm{app}}^\hbar(t,x) = a_L\left(\frac{\omega^\hbar t}{\hbar}\right)\varphi_L^\hbar(x) + a_R\left(\frac{\omega^\hbar t}{\hbar}\right)\varphi_R^\hbar(x),$$

where $(a_L, a_R) = (a_L(\tau), a_R(\tau))$ solves

$$\begin{cases} i\partial_\tau a_L = \eta\tau a_L - a_R + \delta^\hbar |a_L|^2 a_L; & a_{L|\tau=0} = \alpha_L, \\ i\partial_\tau a_R = -\eta\tau a_R - a_L + \delta^\hbar |a_R|^2 a_R; & a_{R|\tau=0} = \alpha_R, \end{cases} \tag{A.3}$$

and

$$\delta^\hbar = \delta \hbar^{d/2} \int_{\mathbb{R}^d} \varphi_L^4 = \delta \hbar^{d/2} \int_{\mathbb{R}^d} \varphi_R^4$$

is uniformly bounded in $\hbar \in (0, \hbar^*]$. Then we have the following error estimate: there exist c, C independent of $\hbar$ such that for all $\gamma < \Gamma$,

$$\sup_{|t| \leqslant c\sqrt{\hbar}/\omega^\hbar} \|\psi^\hbar(t) - \mathrm{e}^{-it(\lambda_-^\hbar + \lambda_+^\hbar)/(2\hbar)} \psi_{\mathrm{app}}^\hbar(t)\|_{L^2} \leqslant C\mathrm{e}^{-\gamma/\hbar}.$$

Remark A.7. The case $d=1$ and $\delta<0$ could be considered as well, leading to the same result. Considering this case would just make the proof a bit longer, and we refer to [27] for the adaptation.

Remark A.8. Since the range for the slow time $\tau=\omega^\hbar t/\hbar$ is $-c/\sqrt{\hbar}\leqslant\tau\leqslant c/\sqrt{\hbar}$, the above approximation result is a large time result, which is consistent with the large time study of (A.3), or, more generally, of (1.5) to which one reduces thanks to the change of variables $s=\sqrt{\eta}\tau$ (we then have $G=-\eta^{-1/2}$ and $\delta F(u)=\eta^{-1/2}\delta^\hbar\mathrm{diag}(|u_1|^2,|u_2|^2)$). When $\hbar$ is small, Theorem 1.3 gives asymptotics for the profiles a_L and a_R of $\psi^\hbar_{\rm app}$ for large times ($|t|\leqslant c\sqrt{\hbar}/\omega^\hbar$) and the connexion between the profiles for $t<0$ and $t>0$ involves the Landau-Zener transition coefficient $\mathrm{e}^{-\frac{\pi}{\eta^2}}$ (at leading order when $\hbar$ goes to 0).

Proof. For simplicity, we write the proof for $t\geqslant 0$ and it naturally extends to $t\leqslant 0$.
Step 1: Preliminaries. We begin by proving estimates on $\psi^\hbar$, then we perform the rescaling suggested by the form of the approximation solution. First, it follows from Lemma A.4 and [4] that for fixed $\hbar>0$, (A.1) has a unique, global solution $\psi^\hbar\in C(\mathbb{R};\Sigma)$ (Σ is defined in Lemma A.4). In addition, if we set

$$\text{Mass: } M^\hbar(t)=\|\psi^\hbar(t)\|^2_{L^2},$$
$$\text{Energy: } E^\hbar(t)=\frac{1}{2}\|\hbar\nabla\psi^\hbar(t)\|^2_{L^2}+\frac{\epsilon(\hbar)}{2}\|\psi^\hbar(t)\|^4_{L^4}+\int_{\mathbb{R}^d}V(t,x)|\psi^\hbar(t,x)|^2dx,$$

then we have the *a priori* estimates:

$$\frac{dM^\hbar}{dt}=0,$$
$$\frac{dE^\hbar}{dt}=\int_{\mathbb{R}^d}\partial_tV(t,x)|\psi^\hbar(t,x)|^2dx=\kappa(\hbar)\int_{R^d}V_a(x)|\psi^\hbar(t,x)|^2dx,$$

where we have used (2.4) for the last equality. Note that (A.1) is not a Hamiltonian equation, unlike the one studied in [1], where the Hamiltonian structure is crucial. The conservation of mass and the form of the initial data yield

$$M^\hbar(t)=\|\psi^\hbar(t)\|_{L^2}=\|\psi^\hbar(0)\|_{L^2}=M^\hbar(0)\leqslant C,$$

for some C independent of $\hbar$. We have

$$E^\hbar(0)=\left\langle\alpha_L\varphi^\hbar_L+\alpha_R\varphi^\hbar_R,\alpha_LH_0\varphi^\hbar_L+\alpha_RH_0\varphi^\hbar_R\right\rangle+\frac{\epsilon(\hbar)}{2}\|\alpha_L\varphi^\hbar_L+\alpha_R\varphi^\hbar_R\|^4_{L^4}.$$

Introduce $\Omega^\hbar=(\lambda^\hbar_-+\lambda^\hbar_+)/2$ and notice that $\Omega^\hbar=V_s^{\min}+\mathcal{O}(\hbar)$ by Lemma A.3. Noting the identities

$$H_0\varphi^\hbar_L=\Omega^\hbar\varphi^\hbar_L-\omega^\hbar\varphi^\hbar_R;\quad H_0\varphi^\hbar_R=\Omega^\hbar\varphi^\hbar_R-\omega^\hbar\varphi^\hbar_L,\tag{A.4}$$

we infer from Lemma A.3 and Lemma A.4 that

$$E^\hbar(0)=V_s^{\min}M^\hbar(0)+\mathcal{O}(\hbar).$$

Therefore, since V_a is bounded,

$$\begin{aligned}\|\hbar\nabla\psi^\hbar(t)\|^2_{L^2}&\leqslant 2E^\hbar(t)-2V_s^{\min}M^\hbar(t)+C\kappa(\hbar)tM^\hbar(t)\\&\leqslant 2E^\hbar(0)-2V_s^{\min}M^\hbar(0)+2\kappa(\hbar)\int_0^t\int_{R^d}V_a(x)|\psi^\hbar(t,x)|^2dx+C\kappa(\hbar)t\\&\leqslant C\hbar+C\frac{(\omega^\hbar)^2}{\hbar}t.\end{aligned}$$

Next, as in [27], we consider the slow time

$$\tau = \frac{\omega^\hbar t}{\hbar} \geqslant 0,$$

and the new unknown function

$$\Psi^\hbar(\tau, x) = \psi^\hbar(t, x) e^{i\Omega^\hbar t/\hbar} = \psi^\hbar(t, x) e^{i\Omega^\hbar \tau/\omega^\hbar}.$$

It solves

$$i\partial_\tau \Psi^\hbar = \frac{1}{\omega^\hbar}\left(H_0 - \Omega^\hbar\right)\Psi^\hbar + \eta\tau V_a \Psi^\hbar + \delta\hbar^{d/2}|\Psi^\hbar|^2\Psi^\hbar, \tag{A.5}$$

and in view of the above estimates,

$$\|\Psi^\hbar(\tau)\|_{L^2} = \|\Psi^\hbar(0)\|_{L^2} = \mathcal{O}(1); \quad \|\nabla\Psi^\hbar(\tau)\|_{L^2}^2 \leqslant C\left(\frac{1}{\hbar} + \frac{\omega^\hbar}{\hbar^2}\tau\right). \tag{A.6}$$

We decompose $\Psi^\hbar$ as

$$\Psi^\hbar = \varphi^\hbar + \psi_c^\hbar, \quad \psi_c^\hbar = \Pi_c^\hbar \Psi^\hbar, \tag{A.7}$$

so we can write $\varphi^\hbar$ as

$$\varphi^\hbar(\tau, x) = \mathtt{a}_L^\hbar(\tau)\varphi_L^\hbar(x) + \mathtt{a}_R^\hbar(\tau)\varphi_R^\hbar(x),$$

for some complex-valued coefficients $\mathtt{a}_L^\hbar$ and $\mathtt{a}_R^\hbar$. Projecting (A.5), and using (A.4), we find:

$$\begin{aligned}
i\dot{\mathtt{a}}_L^\hbar &= -\mathtt{a}_R^\hbar + \eta\tau\int_{\mathbb{R}^d} V_a \Psi^\hbar \varphi_L^\hbar + \delta\hbar^{d/2}\int_{\mathbb{R}^d}|\Psi^\hbar|^2\Psi^\hbar\varphi_L^\hbar,\\
i\dot{\mathtt{a}}_R^\hbar &= -\mathtt{a}_L^\hbar + \eta\tau\int_{\mathbb{R}^d} V_a \Psi^\hbar \varphi_R^\hbar + \delta\hbar^{d/2}\int_{\mathbb{R}^d}|\Psi^\hbar|^2\Psi^\hbar\varphi_R^\hbar,\\
i\partial_\tau\psi_c^\hbar &= \frac{1}{\omega^\hbar}\left(H_0 - \Omega^\hbar\right)\psi_c^\hbar + \eta\tau\Pi_c^\hbar\left(V_a\Psi^\hbar\right) + \delta\hbar^{d/2}\Pi_c^\hbar\left(|\Psi^\hbar|^2\Psi^\hbar\right).
\end{aligned}$$

The proof of Proposition A.6 consists in showing that $\mathtt{a}_{L/R}^\hbar$ are close to $a_{L/R}$, and that $\psi_c^\hbar$ is small. This is achieved in two more steps.

Step 2. *A priori* estimates on $\mathtt{a}_R^\hbar$, $\mathtt{a}_L^\hbar$ and $\psi_c^\hbar$. By definition, we have $\mathtt{a}_L^\hbar = \int_{\mathbb{R}^d}\Psi^\hbar\varphi_L^\hbar$, so Cauchy–Schwarz inequality yields

$$\|\varphi^\hbar(\tau)\|_{L^2}^2 = |\mathtt{a}_L^\hbar(\tau)|^2 + |\mathtt{a}_R^\hbar(\tau)|^2 \leqslant \left(M^\hbar\right)^2\left(\|\varphi_L^\hbar\|_{L^2}^2 + \|\varphi_R^\hbar\|_{L^2}^2\right) \leqslant 2\left(M^\hbar\right)^2.$$

Decompose the nonlinearity acting on $\Psi^\hbar$ as

$$|\Psi^\hbar|^2\Psi^\hbar = |\varphi^\hbar|^2\varphi^\hbar + \mathtt{R}^\hbar.$$

Using the *a priori* estimates on $\mathtt{a}^\hbar$ and Lemma A.4, we have

$$\left\||\varphi^\hbar|^2\varphi^\hbar\right\|_{L^2} \leqslant \|\varphi^\hbar\|_{L^\infty}^2\|\varphi^\hbar\|_{L^2} \leqslant C\left(\|\varphi_L^\hbar\|_{L^\infty}^2 + \|\varphi_R^\hbar\|_{L^\infty}^2\right) \leqslant C\hbar^{-d/2}.$$

Since we have the pointwise estimate

$$|\mathtt{R}^\hbar| \leqslant C\left(|\varphi^\hbar|^2|\psi_c^\hbar| + |\psi_c^\hbar|^3\right),$$

we infer

$$\|\mathtt{R}^\hbar\|_{L^2} \leqslant C\left(\hbar^{-d/2}\|\psi_c^\hbar\|_{L^2} + \|\psi_c^\hbar\|_{L^6}^3\right),$$

and Gagliardo–Nirenberg inequality yields ($d \leqslant 2$)

$$\|\psi_c^\hbar\|_{L^6(\mathbb{R}^d)}^3 \leqslant C\|\psi_c^\hbar\|_{L^2(\mathbb{R}^d)}^{3-d}\|\nabla\psi_c^\hbar\|_{L^2(\mathbb{R}^d)}^d.$$

Since $d \leqslant 2$, we can factor out $\|\psi_c^\hbar\|_{L^2(\mathbb{R}^d)}$, and (A.6) gives

$$\|\psi_c^\hbar\|^3_{L^6(\mathbb{R}^d)} \leqslant C\|\psi_c^\hbar\|_{L^2(\mathbb{R}^d)}\hbar^{-d/2}\left(1+\left(\frac{\omega^\hbar\tau}{\hbar}\right)^{d/2}\right).$$

Therefore,

$$\|\mathtt{R}^\hbar\|_{L^2} \leqslant C\hbar^{-d/2}\left(1+\left(\frac{\omega^\hbar\tau}{\hbar}\right)^{d/2}\right)\|\psi_c^\hbar\|_{L^2}, \tag{A.8}$$

and $|\Psi^\hbar|^2\Psi^\hbar$ satisfies a similar estimate. We infer

$$\left|\dot{\mathtt{a}}_L^\hbar(\tau)\right| + \left|\dot{\mathtt{a}}_R^\hbar(\tau)\right| \leqslant C\left(1+\tau\right) + C\left(1+\left(\frac{\omega^\hbar\tau}{\hbar}\right)^{d/2}\right).$$

Since $d \leqslant 2$ and $\omega^\hbar = \mathcal{O}(\mathrm{e}^{-c/\hbar})$, we can simplify the above estimate:

$$\left|\dot{\mathtt{a}}_L^\hbar(\tau)\right| + \left|\dot{\mathtt{a}}_R^\hbar(\tau)\right| \leqslant C\left(1+\tau\right), \quad \forall \tau \geqslant 0.$$

From this we infer

$$\left\|\partial_\tau\varphi^\hbar\right\|_{L^2} \leqslant \left|\dot{\mathtt{a}}_L^\hbar(\tau)\right|\|\varphi_L^\hbar\|_{L^2} + \left|\dot{\mathtt{a}}_R^\hbar(\tau)\right|\|\varphi_R^\hbar\|_{L^2} \leqslant C(1+\tau), \tag{A.9}$$

and, again from Lemma A.4,

$$\left\|\partial_\tau\left(|\varphi^\hbar|^2\varphi^\hbar\right)\right\|_{L^2} \leqslant 3\|\varphi^\hbar\|^2_{L^\infty}\left\|\partial_\tau\varphi^\hbar\right\|_{L^2} \leqslant C\hbar^{-d/2}(1+\tau). \tag{A.10}$$

Step 3. Stability estimates. In view of (A.7), we first prove that $\psi_c^\hbar$ is small. Since $\psi^\hbar_{c|\tau=0} = 0$, Duhamel's formula yields

$$\begin{aligned}\psi_c^\hbar(\tau) = &-i\eta\int_0^\tau \mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\left(s\Pi_c^\hbar\left(V_a\Psi^\hbar\right)(s)\right)ds \\ &- i\delta\hbar^{d/2}\int_0^\tau \mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\Pi_c^\hbar\left(|\Psi^\hbar|^2\Psi^\hbar\right)(s)ds.\end{aligned} \tag{A.11}$$

Each term is treated in a similar fashion: when $\Psi^\hbar$ is replaced by $\varphi^\hbar$, we perform an integration by parts, and for the remaining term, we use directly the *a priori* estimates. For the first part of (A.11), we write

$$\Pi_c^\hbar\left(V_a\Psi^\hbar\right) = \Pi_c^\hbar\left(V_a\varphi^\hbar\right) + \Pi_c^\hbar\left(V_a\psi_c^\hbar\right),$$

and set

$$\begin{aligned}I_1^\hbar(\tau) &= \int_0^\tau \mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\left(s\Pi_c^\hbar\left(V_a\varphi^\hbar\right)(s)\right)ds, \\ I_2^\hbar(\tau) &= \int_0^\tau \mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\left(s\Pi_c^\hbar\left(V_a\psi_c^\hbar\right)(s)\right)ds.\end{aligned}$$

Integrating by parts,

$$\begin{aligned}I_1^\hbar(\tau) = &-i\omega^\hbar\mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\left(H_0-\Omega^\hbar\right)^{-1}\Pi_c^\hbar\left(sV_a\varphi^\hbar\right)(s)\Big|_0^\tau \\ &+i\omega^\hbar\int_0^\tau \mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\left(H_0-\Omega^\hbar\right)^{-1}\left(\Pi_c^\hbar\left(V_a\varphi^\hbar\right)+s\Pi_c^\hbar\left(V_a\partial_\tau\varphi^\hbar\right)\right)(s)ds.\end{aligned}$$

From Lemma A.3, there exists C independent of $\hbar \in (0,\hbar^*]$ such that

$$\left\|\hbar\left(H_0-\Omega^\hbar\right)^{-1}\Pi_c^\hbar\right\|_{L^2\to L^2} \leqslant C.$$

We infer, using (A.9),

$$|I_1^\hbar(\tau)| \leqslant C\frac{\omega^\hbar}{\hbar}\left(\tau+\tau^3\right).$$

For $I_2^\hbar$, we have directly

$$|I_2^\hbar(\tau)| \leqslant C\int_0^\tau s\|\psi_c^\hbar(s)\|_{L^2}ds.$$

For the nonlinear term in Duhamel's formula (the second term of (A.11)), we also write

$$\Pi_c^\hbar(|\Psi^\hbar|^2\Psi^\hbar) = \Pi_c^\hbar(|\varphi^\hbar|^2\varphi^\hbar) + \Pi_c^\hbar \mathtt{R}^\hbar,$$

and set

$$I_3^\hbar(\tau) = \hbar^{d/2}\int_0^\tau \mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\Pi_c^\hbar\left(|\varphi^\hbar|^2\varphi^\hbar\right)(s)ds,$$
$$I_4^\hbar(\tau) = \hbar^{d/2}\int_0^\tau \mathrm{e}^{-i(H_0-\Omega^\hbar)(\tau-s)/\omega^\hbar}\Pi_c^\hbar \mathtt{R}^\hbar(s)ds.$$

We have, directly from (A.8),

$$|I_4^\hbar(\tau)| \leqslant C\int_0^\tau \left(1+\left(\frac{\omega^\hbar s}{\hbar}\right)^{d/2}\right)\|\psi_c^\hbar(s)\|_{L^2}ds,$$

and performing an integration by parts for $I_3^\hbar$, using (A.10), we have

$$|I_3^\hbar(\tau)| \leqslant C\frac{\omega^\hbar}{\hbar}\left(1+\tau^2\right).$$

Since $d \leqslant 2$ and $\omega^\hbar$ decays exponentially, we come up with:

$$\|\psi_c^\hbar(\tau)\|_{L^2} \leqslant C\left(\frac{\omega^\hbar}{\hbar}\left(1+\tau^3\right)+\int_0^\tau(1+s)\|\psi_c^\hbar(s)\|_{L^2}ds\right).$$

Gronwall lemma yields

$$\|\psi_c^\hbar(\tau)\|_{L^2} \leqslant C\frac{\omega^\hbar}{\hbar}(1+\tau^3)\mathrm{e}^{C(\tau+\tau^2)}.$$

Recalling again that $\omega^\hbar$ decays exponentially, we can write that for all $c_0 < \Gamma$ (the Agmon distance between the two wells),

$$\|\psi_c^\hbar(\tau)\|_{L^2} \leqslant C(1+\tau^3)\mathrm{e}^{C(\tau+\tau^2)-c_0/\hbar}.$$

This is small as $\hbar \to 0$, provided that $\tau^2 \ll /\hbar$. More precisely, there exist $c_1, c_2 > 0$ independent of $\hbar$ such that

$$\|\psi_c^\hbar(\tau)\|_{L^2} \leqslant C\mathrm{e}^{-c_1/\hbar}, \quad 0 \leqslant \tau \leqslant \frac{c_2}{\sqrt{\hbar}}. \tag{A.12}$$

To conclude the proof of the proposition, set

$$\mathtt{w}_L^\hbar = \mathtt{a}_L^\hbar - a_L; \quad \mathtt{w}_R^\hbar = \mathtt{a}_R^\hbar - a_R.$$

Subtracting the equation for a_L from the equation for $\mathtt{a}_L^\hbar$, we have

$$i\dot{\mathtt{w}}_L^\hbar = -\mathtt{w}_R^\hbar + \eta\tau\int_{\mathbb{R}^d} V_a\left(\Psi^\hbar - a_L\varphi_L^\hbar\right)\varphi_L^\hbar$$
$$+ \delta\hbar^{d/2}\int_{\mathbb{R}^d}\left(|\Psi^\hbar|^2\Psi^\hbar - |a_L|^2 a_L|\varphi_L^\hbar|^2\varphi_L^\hbar\right)\varphi_L^\hbar.$$

We have

$$\int_{\mathbb{R}^d} V_a \left(\Psi^\hbar - a_L\varphi_L^\hbar\right)\varphi_L^\hbar = \int_{\mathbb{R}^d} V_a \left(\mathtt{a}_R^\hbar\varphi_R^\hbar + \psi_c^\hbar + \mathtt{w}_L^\hbar\varphi_L^\hbar\right)\varphi_L^\hbar,$$

therefore, since the product $\varphi_L^\hbar\varphi_R^\hbar$ decays exponentially in $\hbar$,

$$\left|\int_{\mathbb{R}^d} V_a \left(\Psi^\hbar - a_L\varphi_L^\hbar\right)\varphi_L^\hbar\right| \leqslant C\left(\mathrm{e}^{-c/\hbar} + \|\psi_c^\hbar\|_{L^2} + |\mathtt{w}_L^\hbar|\right).$$

A similar estimate can be established for the other source term in the equation for $\mathtt{w}_L^\hbar$. The equation for $\mathtt{w}_R^\hbar$ is handled in the same fashion, and using (A.12), we end up with:

$$|\dot{\mathtt{w}}_L^\hbar(\tau)| + |\dot{\mathtt{w}}_R^\hbar(\tau)| \leqslant C\left(|\mathtt{w}_L^\hbar(\tau)| + |\mathtt{w}_R^\hbar(\tau)| + \mathrm{e}^{-c/\hbar}\right), \quad 0 \leqslant \tau \leqslant \frac{c_2}{\sqrt{\hbar}}.$$

Gronwall lemma and (A.12) then yield Proposition A.6. □

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