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# A NONLINEAR LANDAU-ZENER FORMULA

RÉMI CARLES AND CLOTILDE FERMANIAN-KAMMERER

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.

## 1. INTRODUCTION

1.1. **Physical motivation.** In the 30’s (see [19] and [24]), Landau and Zener have studied independently the system

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

where  $u = {}^t(u_1, u_2) \in \mathbb{C}^2$ , and the potential  $V$  is given by

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

This system is the prototype of eigenvalue crossings: 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  $z = 0$ . More recently, a nonlinear version of this system has been introduced in [3], of the form

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

with the Hamiltonian given by

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

where  $\gamma(t) = \alpha t$  denotes the level separation,  $z$  is the coupling constant between the two levels, and  $\delta$  is a nonlinear parameter describing the 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 achieved in e.g. [7]. 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. [16, 18, 17, 20]. We also show how this model can arise under the influence of a double-well potential, as in [17] (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

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background, and to study some of its properties, in particular as far as the large time regime is concerned.

**1.2. Mathematical setting.** In the linear case (1.1), classification of crossings, as performed in [5] and [6] in the one hand, and [11] on the other hand, produces the model problem

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

where  $\mathcal{H}$  is a Hilbert space and  $G$  an operator on  $\mathcal{H}$ . Equation (1.2) corresponds to  $\mathcal{H} = \mathbb{C}$  and  $G = z \in \mathbb{R}$ , as in [19] and [24] (see also [11] and [5]). Other choices of the pair  $(\mathcal{H}, G)$  are relevant:

- (1) In [6] and [14],  $G = z_1 + iz_2$  and  $\mathcal{H} = \mathbb{C}$ .
- (2) In [6] and [9],  $G = \partial_z - z$  and  $\mathcal{H} = L^2(\mathbb{R})$ .
- (3) In [14], [13] and [8],  $G = q(z)$  is a quaternion,  $z \in \mathbb{R}^4$  and  $\mathcal{H} = \mathbb{C}^2$ .
- (4) In [8] and [11],  $G$  is a semiclassical pseudodifferential operator on the space  $\mathcal{H} = L^2(\mathbb{R}^k)$ ,  $k \in \mathbb{N}^*$ .

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

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

which is the nonlinear counterpart of (1.4). The nonlinearity  $F : \mathbb{C}^2 \rightarrow \mathbb{R}^{2 \times 2}$  is of the form

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

where the functions  $F_1, F_2$  are gauge invariant, and more precisely,

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

with  $f_j \in \mathcal{C}^2(\mathbb{R}^2; \mathbb{R})$  and  $\nabla^2 f_j$  bounded. In particular, the system (1.2)–(1.3) enters into this framework. By the change of variable  $s = t\sqrt{\alpha}$ , we are left with (1.5) with  $G = z/\sqrt{\alpha}$  and  $F_j(u) = (-1)^j \delta \alpha^{-1/2} (|u_2|^2 - |u_1|^2)$  for  $j \in \{1, 2\}$ .

We make the following assumption on the operator  $G$ :

$$(1.7) \quad \chi(GG^*)G = G\chi(G^*G) \quad \text{and} \quad \chi(G^*G)G^* = G^*\chi(GG^*).$$

This assumption is satisfied in the first three examples above. The situation is more complicated in the fourth one.

We also assume that the domains of  $GG^*$  and of  $G^*G - \mathcal{D}(GG^*)$  and  $\mathcal{D}(G^*G) -$  are dense subsets of  $\mathcal{H}$ . Note that the domain of the evolution operators  $e^{i\tau GG^*}$  and  $e^{i\tau G^*G}$  are well-defined for any  $\tau \in \mathbb{R}$  with domain  $\mathcal{H}$ .

**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*

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

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

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

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

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

Local existence follows by a standard fixed point argument (Cauchy-Lipschitz), with a local existence time which depends only on  $\|u_0\|_{\mathcal{H} \times \mathcal{H}}$ . 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.  $\square$

We normalize the data so that

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

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

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

Because of (1.7), the operator  $\Theta_R$  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.

**1.3. Scattering.** We introduce the phase function  $\varphi$  given by

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

We can describe the large time asymptotics of  $u$ .

**Theorem 1.3.** *Assume that  $u_0 = \Theta_R u_0$  for some  $R > 0$ . Then, there exist  $\alpha = (\alpha_1, \alpha_2) \in \mathcal{H}^2$ ,  $\omega = (\omega_1, \omega_2) \in \mathcal{H}^2$ , such that:*

1. *As  $s$  goes to  $-\infty$ ,*

$$\begin{aligned} u_1(s) &= e^{i\delta F_1(\alpha)s + i\varphi(s, GG^*)} \alpha_1 + \mathcal{O}(R^2 s^{-1}), \\ u_2(s) &= e^{i\delta F_2(\alpha)s - i\varphi(s, G^*G)} \alpha_2 + \mathcal{O}(R^2 s^{-1}). \end{aligned}$$

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

$$\begin{aligned} u_1(s) &= e^{i\delta F_1(\omega)s + i\varphi(s, GG^*)} \omega_1 + \mathcal{O}(R^2 s^{-1}), \\ u_2(s) &= e^{i\delta F_2(\omega)s - i\varphi(s, G^*G)} \omega_2 + \mathcal{O}(R^2 s^{-1}). \end{aligned}$$

The above result is reminiscent of long range scattering in nonlinear Schrödinger equations, as described first in [21]: 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  $\varphi$  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 [19] and [24]. The original proof is based on the use of special functions; more recently, the proof of [10] relies on the analysis of oscillatory integrals. When  $G$  is operator-valued, the theorem is proved in the linear case ( $\delta = 0$ ) in [12, 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.

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

**Proposition 1.5.** *Let  $\alpha = (\alpha_1, \alpha_2) \in \mathcal{H}^2$  such that  $\alpha = \Theta_R \alpha$  for some  $R > 0$ . There exists  $C > 0$ , such that for all  $\varepsilon > 0$ , there exists a solution  $u^\varepsilon \in C(\mathbb{R}; \mathcal{H}^2)$  to (1.5) with*

$$\limsup_{s \rightarrow -\infty} \left\| u_1^\varepsilon(s) - e^{i\delta F_1(\alpha)s + i\varphi(s, GG^*)} \alpha_1 \right\|_{\mathcal{H}} + \left\| u_2^\varepsilon(s) - e^{i\delta F_2(\alpha)s - i\varphi(s, G^*G)} \alpha_2 \right\|_{\mathcal{H}} \leq C \varepsilon.$$

*Remark 1.6.* A similar result holds in  $+\infty$ .

Therefore, there exists  $\mathcal{K} \subset \mathcal{H}$  a dense subset of  $\mathcal{H}$  and an operator  $S_\delta$  with domain  $\mathcal{K}$  which is a nonlinear scattering operator mapping the scattering state at  $-\infty$ ,  $\alpha \in \mathcal{K}$ , to its counterpart  $\omega$  at  $+\infty$  given by Theorem 1.3: the scattering operator is defined by  $\omega = S_\delta \alpha$ .

Besides, if the unit ball of  $\mathcal{H}$  is a finite dimension vector space (typically,  $\mathcal{H} = \mathbb{C}$  in the case of (1.2)), one can extract from  $u^\varepsilon$  a converging sequence with limit  $u$  which solves (1.5) and admits the scattering state  $(\alpha_1, \alpha_2)$ , and the operator  $S_\delta$  is defined on  $\mathcal{H}$  ( $\mathcal{K} = \mathcal{H}$ ).

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

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

According to Proposition 7 in [12], the linear scattering operator is given by

$$(1.9) \quad S^{\text{lin}} = \begin{pmatrix} a(GG^*) & -\bar{b}(GG^*)G \\ b(G^*G)G^* & a(G^*G) \end{pmatrix},$$

with

$$a(\lambda) = e^{-\pi \frac{\lambda}{2}}, \quad b(\lambda) = \frac{2ie^{i\frac{\pi}{4}}}{\lambda\sqrt{\pi}} 2^{-i\lambda/2} e^{-\pi \frac{\lambda}{4}} \Gamma\left(1 + i\frac{\lambda}{2}\right) \sinh\left(\frac{\pi\lambda}{2}\right),$$

$$\text{and } a(\lambda)^2 + \lambda|b(\lambda)|^2 = 1.$$

When  $G = z$ , the coefficient

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

is the celebrated *Landau-Zener transition coefficient* which describes the ratio  $|\omega_1^{\text{lin}}|^2/|\alpha_1^{\text{lin}}|^2$  of the energy which remains on the first component (when  $\alpha_2^{\text{lin}} = 0$ ). As we shall see in the next result, the Landau-Zener transition probability remains relevant in the nonlinear regime and for small  $\delta$ . Let us define, for  $j = 1, 2$ ,

$$(1.11) \quad \Lambda_j^+ = \int_0^{+\infty} (F_j(u^{\text{lin}}(\tau)) - F_j(\omega^{\text{lin}})) d\tau,$$

$$(1.12) \quad \Lambda_j^- = \int_0^{-\infty} (F_j(u^{\text{lin}}(\tau)) - F_j(\alpha^{\text{lin}})) d\tau,$$

and  $\Lambda^\pm = \text{diag}(\Lambda_1^\pm, \Lambda_2^\pm)$ .

**Theorem 1.7.** *Let  $\delta > 0$ . The nonlinear scattering operator  $S_\delta$  and the linear scattering operator  $S^{\text{lin}}$  are related by the formula*

$$S_\delta(\alpha) = e^{i\delta\Lambda^+(\alpha)} S^{\text{lin}} \left( e^{-i\delta\Lambda^-(\alpha)} \alpha \right).$$

*In addition, we have the following asymptotic behavior as  $\delta \rightarrow 0$ . There exists a constant  $C > 0$  such that for all  $R > 0$  and initial data  $u_0$  with  $\Theta_R u_0 = u_0$ , we have*

$$\|S_\delta - S^{\text{lin}} - i\delta (\Lambda^+ S^{\text{lin}} - S^{\text{lin}} \Lambda^-)\|_{\mathcal{L}(\mathcal{H} \times \mathcal{H})} \leq C R \delta^2.$$

As expected, as  $\delta \rightarrow 0$ ,  $S_\delta$  behaves at leading order like the linear scattering operator. Nonlinear effects show up in the  $\mathcal{O}(\delta)$  corrector (the nonlinearity is present in the definition of  $\Lambda^-$  and  $\Lambda^+$ ), and are described rather explicitly in terms of linear scattering and of the nonlinearity  $F$ . We note also that if  $\Lambda_1^+ \neq \Lambda_2^+$  ( $F_1 \neq F_2$ ), then  $S^{\text{lin}}$  and  $\Lambda^+$  do not commute.

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 set up some technical tools needed for the large time study of (1.5), and we prove Lemma 1.2. Theorem 1.3 is proved in Section 4, Proposition 1.5 in Section 5, and Theorem 1.7 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. [16], the motion of a Bose–Einstein condensate in an accelerated 1D optical lattice is described by the equation

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

where  $m$  is the atomic mass,  $k_L$  is the optical lattice wave number,  $V_0$  is the strength of the periodic potential depth,  $\omega$  is the inertial force, and  $a_s$  is the scattering length. The adimensionalized form of this equation reads

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

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

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

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 [16]). We compute

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

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  $e^{i(k-1)x}$ , we come up with:

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

We notice the identity  $\partial_t (|a|^2 + |b|^2) = 0$ , 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

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

The above system becomes

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

with

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

Using finally the gauge transform

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

we end up with

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

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  $F(u) = \epsilon(2\alpha)^{-1/2}\text{Diag}(|u_2|^2, |u_1|^2)$ . Note that the only approximation that we have made in this computation consists in neglecting the other harmonics than  $e^{\pm ix/2}$ , and no linearization was performed, unlike in the computations of [3].

Theorem 1.3 gives an asymptotic for the profiles  $a$  and  $b$  of the ansatz (2.2) as  $t$  goes to  $\pm\infty$ . Theorem 1.7 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  $\delta$ , they satisfy

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

**2.2. Condensate in a double-well potential.** As suggested in [3], and further developed in [17], nonlinear Landau-Zener tunneling may be realized in a double-well potential. Consider

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

The potential  $W$  is of the form

$$(2.4) \quad W(t, x) = V_s(x) + \kappa t V_a(x),$$

where  $V_s$  is symmetric and  $V_a$  is antisymmetric. In [17], we find the explicit expression

$$(2.5) \quad V_s(x) = \frac{V_0}{\cosh(\beta x)}, \quad V_a(x) = \frac{V_0 \sinh(\beta x)}{\cosh^2(\beta x)}, \quad \beta > 0.$$

Note that  $V_s$  is a double-well potential. 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  $e^{\pm ix/2}$  of the above model are then replaced by the so-called single-well states

$$(2.6) \quad \varphi_L = \frac{1}{\sqrt{2}}(\varphi_+ - \varphi_-), \quad \varphi_R = \frac{1}{\sqrt{2}}(\varphi_+ + \varphi_-).$$

We note that this approach can be generalized to a multidimensional framework, in the spirit of [23] (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  $\varphi_L$  and  $\varphi_R$ , described more precisely in Appendix A:

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

Seek  $\psi$  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:

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

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

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

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 1.7 yield similar results than in the preceding subsection with a Landau-Zener coefficient  $e^{-\pi\frac{\omega^2}{\alpha}}$ .

### 3. TECHNICAL PRELIMINARIES

In this paragraph, we introduce several operators related with  $G$  that will be useful in the following. We set

$$(3.1) \quad J := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad K := V(0) = \begin{pmatrix} 0 & G \\ G^* & 0 \end{pmatrix},$$

so that  $V(s)$  writes

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

We observe that

$$V(s)^2 = \Lambda(s)^2,$$

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

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

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

$$\Pi^\pm(s) = \frac{1}{2} (\operatorname{Id} \pm \Lambda(s)^{-1} V(s)),$$

then we have the following properties.

- (1)  $\Pi^\pm(s)V(s) = V(s)\Pi^\pm(s) = \pm\Lambda(s)\Pi^\pm(s) = \pm\Pi^\pm(s)\Lambda(s)$ .
- (2)  $\Pi^+(s) + \Pi^-(s) = \text{Id}$ .
- (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  $V(s)$ . The fact that  $\Pi^\pm(s)$  and  $V(s)$  commute with  $\Lambda(s)$  is more general. In fact,  $V(s)$  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

$$(3.2) \quad A(a, b, c, d) = \begin{pmatrix} a(GG^*) & b(GG^*)G \\ c(G^*G)G^* & d(G^*G) \end{pmatrix}.$$

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

$$\begin{aligned} A(a, b, c, d)^* &= A(\bar{a}, \bar{c}, \bar{b}, \bar{d}), \\ A(a, b, c, d)A(a', b', c', d') &= A(a'', b'', c'', d''), \end{aligned}$$

with

$$\begin{aligned} a''(\lambda) &= a(\lambda)a'(\lambda) + \lambda b(\lambda)c(\lambda), & b''(\lambda) &= a(\lambda)b'(\lambda) + b(\lambda)d'(\lambda), \\ d''(\lambda) &= d(\lambda)d'(\lambda) + \lambda c(\lambda)b(\lambda), & c''(\lambda) &= a'(\lambda)c(\lambda) + d(\lambda)c'(\lambda). \end{aligned}$$

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,  $V(s)$ ,  $\Pi^+(s)$  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

$$\partial_s\Pi^+ = \partial_s((\Pi^+)^2) = \Pi^+\partial_s\Pi^+ + \partial_s\Pi^+\Pi^+$$

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

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

$$C(s) = \pm[B(s), V(s)],$$

with

$$(3.3) \quad B(s) = \frac{1}{2}\Lambda(s)^{-1}C(s),$$

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

**Lemma 3.2.** *Let  $u$  be a solution of (1.4),  $C(s) \in \mathcal{A}$  with  $C(s) = \Pi^+(s)C(s)\Pi^-(s)$ , and let  $B(s)$  be associated with  $C(s)$  as in (3.3), then*

$$(3.4) \quad \begin{aligned} \langle C(s)u(s), u(s) \rangle_{\mathcal{H}^2} &= \frac{1}{i} \frac{d}{ds} \langle B(s)u(s), u(s) \rangle_{\mathcal{H}^2} \\ &+ i \langle \partial_s B(s)u(s), u(s) \rangle_{\mathcal{H}^2} - \langle [B(s), F(u)]u(s), u(s) \rangle_{\mathcal{H}^2}. \end{aligned}$$

*Proof.* We write

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

and the lemma follows.  $\square$

#### 4. EXISTENCE OF SCATTERING STATES

The proof of the existence of scattering states (Theorem 1.3) consists in three steps.

(1) We set

$$u^\pm(s) = \Pi^\pm(s)u(s),$$

and we first prove the existence of a limit to  $\|u^\pm(s)\|_{\mathcal{H}^2}^2$  as  $s$  goes to  $\pm\infty$ .

(2) Then, we deduce that for  $j \in \{1, 2\}$ , the functions  $F_j(u)$  have a limit that we denote by  $F_j(\omega)$  (resp.  $F_j(\alpha)$ ) as  $s$  goes to  $+\infty$  (resp.  $-\infty$ ). Besides, we prove that the functions

$$s \mapsto \int_s^{+\infty} (F_j(u(\tau) - F_j(\omega)) d\tau \quad \text{and} \quad s \mapsto \int_{-\infty}^s (F_j(u(\tau) - F_j(\alpha)) d\tau$$

are well defined and we study their behavior as  $s$  goes to  $+\infty$  or  $-\infty$ , respectively.

(3) Finally, we deduce the existence of scattering states from the scattering result for the linear equation and by using Duhamel formula to treat the nonlinearity.

If one expects the asymptotics behavior of  $u$  to be described as in Theorem 1.3, then the first two steps consist in deriving the asymptotic phase, while the goal of the final step is to describe the amplitude. This strategy is similar to the one employed in e.g. [15] to study the long range nonlinear scattering for the one dimensional cubic Schrödinger equation and for the Hartree equation.

**First step.** The first step of the proof relies on the following proposition.

**Proposition 4.1.** *Assume that  $u_0 = \Theta_R u_0$  for some  $R > 0$ . Then, there exist  $\Omega^\pm, A^\pm \geq 0$  such that*

$$\begin{aligned} \|u^\pm(s)\|_{\mathcal{H} \times \mathcal{H}}^2 - \Omega^\pm &= \mathcal{O}\left(\frac{R}{s^2}\right) \text{ as } s \rightarrow +\infty, \\ \|u^\pm(s)\|_{\mathcal{H} \times \mathcal{H}}^2 - A^\pm &= \mathcal{O}\left(\frac{R}{s^2}\right) \text{ as } s \rightarrow -\infty. \end{aligned}$$

*Proof.* We consider the limit  $s \rightarrow +\infty$  for the  $+$  mode. The limit  $s \rightarrow -\infty$  and the case of the  $-$  mode can be treated similarly. We are going to prove that  $\|u^+(s)\|_{\mathcal{H} \times \mathcal{H}}^2$  is a Cauchy sequence as  $s \rightarrow +\infty$ . In that purpose, we write the equation satisfied by  $u^+$

$$\frac{1}{i} \partial_s u^+ = \Lambda(s) u^+ + \frac{1}{i} \partial_s \Pi^+(s) u + F(u) u^+.$$

Therefore, for  $0 < t < s$ ,

$$\begin{aligned} (4.1) \quad & \|u^+(s)\|_{\mathcal{H}^2}^2 - \|u^+(t)\|_{\mathcal{H} \times \mathcal{H}}^2 \\ &= 2 \operatorname{Re} \left( \int_t^s \langle \Pi^+(\sigma) \partial_s \Pi^+(\sigma) u(\sigma), u(\sigma) \rangle_{\mathcal{H} \times \mathcal{H}} d\sigma \right). \end{aligned}$$

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  $\operatorname{Im} C$  the skew adjoint part of the operator  $C$ :  $\operatorname{Im} C = (C - C^*)/2$ .

**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  $C(s) = \mathcal{O}\left(\frac{1}{s}\right)$ ,  $B(s) = \mathcal{O}\left(\frac{1}{s^2}\right)$  and  $\partial_s B(s) = \mathcal{O}\left(\frac{1}{s^3}\right)$  in  $\mathcal{L}(\mathcal{H}^2)$ . Moreover,*

$$(4.2) \quad \operatorname{Im} C(s) = \frac{1}{4} \Lambda(s)^{-2} \begin{pmatrix} 0 & -G \\ G^* & 0 \end{pmatrix},$$

The proof of this lemma is postponed to the end of the section. Using Lemma 3.2, we obtain

$$\begin{aligned} & \int_t^s \langle C(\sigma) u(\sigma), u(\sigma) \rangle_{\mathcal{H}^2} d\sigma \\ &= \frac{1}{i} \langle B(\sigma) u(\sigma), u(\sigma) \rangle_{\mathcal{H} \times \mathcal{H}} \Big|_t^s \\ & \quad + i \int_t^s \langle \partial_s B(\sigma) u(\sigma), u(\sigma) \rangle_{\mathcal{H}^2} d\sigma - \int_t^s \langle [B(\sigma), F(u)] u(\sigma), u(\sigma) \rangle_{\mathcal{H}^2} d\sigma. \end{aligned}$$

A short computation gives for  $s \in \mathbb{R}$ ,

$$\operatorname{Re} \langle [B(s), F(u)] u(s), u(s) \rangle_{\mathcal{H}^2} = \operatorname{Re} \langle [\operatorname{Im} B(s), F(u)] u(s), u(s) \rangle_{\mathcal{H}^2},$$

with

$$[\operatorname{Im} B(s), F(u)] = \frac{1}{4} (F_1(u) - F_2(u)) \Lambda(s)^{-3} K.$$

Therefore,

$$\operatorname{Re} \langle [B(s), F(u)] u(s), u(s) \rangle_{\mathcal{H}^2} = \frac{1}{4} (F_1(u) - F_2(u)) \langle \Lambda(s)^{-3} K u, u \rangle_{\mathcal{H}^2}.$$

Since  $u(s) = \Theta_R u(s)$  with  $\|u(s)\|_{\mathcal{H}^2} = 1$ , we have  $\|K u\|_{\mathcal{H}^2} \leq R$ . We deduce for all  $s \in \mathbb{R}$

$$|\operatorname{Re} \langle [B(s), F(u)] u(s), u(s) \rangle_{\mathcal{H}^2}| = \mathcal{O}\left(\frac{R}{s^3}\right).$$

This observation and Lemma 4.2 yield: for  $s > t \gg 1$ ,

$$\|u^+(s)\|_{\mathcal{H} \times \mathcal{H}}^2 - \|u^+(t)\|_{\mathcal{H}^2}^2 = \mathcal{O}\left(\frac{R}{t^2}\right).$$

This implies the convergence of  $\|u^+(s)\|_{\mathcal{H} \times \mathcal{H}}$  to  $\Omega^+ \geq 0$  with

$$\|u^+(s)\|_{\mathcal{H}^2}^2 = \Omega^+ + \mathcal{O}\left(\frac{R}{s^2}\right),$$

hence the proposition.  $\square$

*Proof of Lemma 4.2.* The proof relies on the computation of  $C(s)$  by observing

$$\partial_s \Pi^+(s) = \frac{1}{2} (\Lambda(s)^{-1} J - s \Lambda(s)^{-3} V(s)),$$

where we have used  $\partial_s \Lambda(s) = s \Lambda(s)^{-1}$ . Since

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

the operators  $C(s)$  and  $B(s)$  are antidiagonal. Besides, we have

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

In view of

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

we obtain

$$C(s) = \frac{1}{4} \Lambda(s)^{-3} (\text{diag}(GG^*, G^*G) - sK) + \frac{1}{4} \Lambda(s)^{-2} \begin{pmatrix} 0 & -G \\ G^* & 0 \end{pmatrix},$$

hence (4.2). Then, the estimates

$$(4.3) \quad \begin{aligned} \|\Lambda(s)^{-1}\|_{\mathcal{L}(\mathcal{H}^2)} &\leq s^{-1}, \quad \|\partial_s \Lambda(s)^{-1}\|_{\mathcal{L}(\mathcal{H}^2)} \leq 1 \\ \|\partial_s^2 \Lambda(s)\|_{\mathcal{H}^2} &= \|\Lambda(s)^{-3} \text{diag}(GG^*, G^*G)\|_{\mathcal{H}^2} = \mathcal{O}(s^{-1}) \end{aligned}$$

allow to conclude the proof of the lemma.  $\square$

**Second step.** We study  $F(u)$  by analyzing the norm of  $u_1(s)$  and  $u_2(s)$ . Note that, for  $|s| \gg 1$ , we have

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

We deduce asymptotics for the operators  $\Pi^\pm(s)$ : for  $s > 0$ , in  $\mathcal{L}(\mathcal{H}^2)$ ,

$$(4.4) \quad \begin{aligned} \Pi^+(s) \Theta_R &= \Theta_R E_1 + \frac{1}{2} \Lambda(s)^{-1} K \Theta_R + \mathcal{O}\left(\frac{R^2}{s^2}\right), \\ \Pi^-(s) \Theta_R &= \Theta_R E_2 - \frac{1}{2} \Lambda(s)^{-1} K \Theta_R + \mathcal{O}\left(\frac{R^2}{s^2}\right), \end{aligned}$$

and for  $s < 0$ , in  $\mathcal{L}(\mathcal{H}^2)$ ,

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

where  $K = V(0)$  has been defined in (3.1),

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

This suggests that as  $s$  goes to  $+\infty$ ,  $u_1(s)$  is related to  $u^+(s)$  and  $u_2(s)$  with  $u^-(s)$  while when  $s$  goes to  $-\infty$ ,  $u_1(s)$  is related to  $u^-(s)$  and  $u_2(s)$  with  $u^+(s)$ . For this reason, we denote by  $F(\omega)$  and  $F(\alpha)$  the matrices

$$F(\omega) = F(\Omega^+, \Omega^-) \quad \text{and} \quad F(\alpha) = F(A^-, A^+).$$

We now prove that  $F(\omega)$  and  $F(\alpha)$  are the limits of  $F(u)$  as  $s$  goes to  $\pm\infty$ . More precisely, we have the following result.

**Proposition 4.3.** *If  $\Theta_R u_0 = u_0$  for some  $R > 0$ , then for  $j \in \{1, 2\}$ ,*

$$\begin{aligned}\int_s^{+\infty} (F_j(u(\tau)) - F_j(\omega)) d\tau &= \mathcal{O}\left(\frac{R^2}{s}\right) \quad \text{as } s \rightarrow +\infty, \\ \int_{-\infty}^s (F_j(u(\tau)) - F_j(\alpha)) d\tau &= \mathcal{O}\left(\frac{R^2}{|s|}\right) \quad \text{as } s \rightarrow -\infty.\end{aligned}$$

*Proof.* We first transfer the result of Proposition 4.1 on the coordinates of  $u(s)$ . Recall that  $u_0 = \Theta_R u_0$  yields that for all  $s \in \mathbb{R}$ ,  $u(s) = \Theta_R u(s)$  (by Lemma 1.2). We claim that for all  $R > 0$ , as  $s \rightarrow +\infty$ ,

$$(4.5) \quad \begin{aligned}\|u_1(s)\|_{\mathcal{H}}^2 - \Omega^+ &= g_1(s) + \mathcal{O}\left(\frac{R^2}{s^2}\right), \\ \|u_2(s)\|_{\mathcal{H}}^2 - \Omega^- &= g_2(s) + \mathcal{O}\left(\frac{R^2}{s^2}\right),\end{aligned}$$

where for  $j \in \{1, 2\}$ ,  $|g_j(s)| = \mathcal{O}(Rs^{-1})$  and  $\left|\int_s^{+\infty} g_j(\sigma) d\sigma\right| = \mathcal{O}(R^2 s^{-1})$ , and that, as  $s \rightarrow -\infty$ ,

$$\begin{aligned}\|u_1(s)\|_{\mathcal{H}}^2 - A^- &= \tilde{g}_1(s) + \mathcal{O}\left(\frac{R^2}{s^2}\right), \\ \|u_2(s)\|_{\mathcal{H}}^2 - A^+ &= \tilde{g}_2(s) + \mathcal{O}\left(\frac{R^2}{s^2}\right),\end{aligned}$$

where for  $j \in \{1, 2\}$ ,  $|\tilde{g}_j(s)| = \mathcal{O}(R|s|^{-1})$  and  $\left|\int_s^{+\infty} \tilde{g}_j(\sigma) d\sigma\right| = \mathcal{O}(R^2|s|^{-1})$ .

Then, one concludes as follows: for  $\tau > 0$  and  $j \in \{1, 2\}$ , we write

$$\begin{aligned}F_j(u(\tau)) - F_j(\omega) &= \nabla f_j(\Omega^+, \Omega^-) \cdot (g_1(\tau), g_2(\tau)) \\ &+ \int_0^1 \nabla^2 f_j(\Omega^+ + \sigma g_1(\tau), \Omega^- + \sigma g_2(\tau)) [g_1(\tau), g_2(\tau)]^2 (1 - \sigma) d\sigma + \mathcal{O}(R^2 s^{-2}),\end{aligned}$$

where the  $f_1, f_2$  are the functions of (1.6). Recall that, for  $j \in \{1, 2\}$ ,  $\nabla^2 f_j$  are bounded,  $\nabla f_j$  are continuous and  $\Omega_j^\pm \leq 1$  from (1.8). Therefore, the fact that

$|g_j(s)| = \mathcal{O}(Rs^{-1})$  and  $\left| \int_s^{+\infty} g_j(\tau) \right| = \mathcal{O}(R^2s^{-1})$  for all  $j \in \{1, 2\}$  yields the lemma for  $s \rightarrow +\infty$  (one argues similarly in  $-\infty$ ).

Let us now prove (4.5). Indeed, by Lemma 4.1, there exists  $\Omega^+$  such that as  $s \rightarrow +\infty$ ,

$$\|u^+(s)\|_{\mathcal{H}^2}^2 = \Omega^+ + \mathcal{O}(Rs^{-2}).$$

By (4.4), we can write

$$\begin{aligned} \|u_1(s)\|_{\mathcal{H}}^2 &= \|u^+(s)\|_{\mathcal{H}^2}^2 + \operatorname{Re} \langle u^+(s), \Lambda(s)^{-1} K \Theta_R u(s) \rangle_{\mathcal{H}^2} + \mathcal{O}\left(\frac{R^2}{s^2}\right) \\ &= \|u^+(s)\|_{\mathcal{H}^2}^2 + \operatorname{Re} \langle K \Lambda(s)^{-1} \Pi^+(s) \Theta_R u(s), u(s) \rangle_{\mathcal{H}^2} + \mathcal{O}\left(\frac{R^2}{s^2}\right). \end{aligned}$$

In view of (4.4) and of the relation

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

we have

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

This implies that we can write

$$\begin{aligned} K \Lambda(s)^{-1} \Pi^+(s) \Theta_R &= K \Lambda(s)^{-1} E_1 \Theta_R + \mathcal{O}\left(\frac{R^2}{s^2}\right) \\ &= E_2 K \Lambda(s)^{-1} E_1 \Theta_R + \mathcal{O}\left(\frac{R^2}{s^2}\right) \\ &= \Lambda(s)^{-1} \Pi^-(s) K \Theta_R \Pi^+(s) + \mathcal{O}\left(\frac{R^2}{s^2}\right) \end{aligned}$$

where we have used  $E_2 K = K E_1$ ,  $\Lambda(s)^{-1} E_1 = E_1 \Lambda(s)^{-1}$  and the commutation properties of  $V(s)$  and  $\Pi^\pm(s)$  with  $\Lambda(s)^{-1}$  and  $\Theta_R$ . We set

$$g_1(s) = \operatorname{Re} \langle \Lambda(s)^{-1} \Pi^-(s) K \Theta_R \Pi^+(s) u(s), u(s) \rangle_{\mathcal{H}^2}.$$

We obtain

$$(4.6) \quad g_1(s) = \mathcal{O}(Rs^{-1}) \quad \text{and} \quad \|u_1(s)\|_{\mathcal{H}}^2 = \|u^+(s)\|_{\mathcal{H}^2}^2 + g_1(s) + \mathcal{O}\left(\frac{R^2}{s^2}\right).$$

In order to prove the integrability properties of  $g_1$ , we study the operator

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

**Lemma 4.4.** *The operators  $\tilde{C}(s) = \Lambda(s)^{-1} \Pi^-(s) K \Theta_R \Pi^+(s)$  and  $\tilde{B}(s) = \frac{1}{2} \Lambda(s)^{-1} \tilde{C}(s)$  are antidiagonal operators of  $\mathcal{A}$  which satisfy*

$$(4.7) \quad \operatorname{Im} \tilde{C}(s) = \frac{s}{2} \Lambda(s)^{-2} \Theta_R \begin{pmatrix} 0 & -G \\ G^* & 0 \end{pmatrix},$$

and  $\tilde{C}(s) = \mathcal{O}\left(\frac{R}{s}\right)$ ,  $\tilde{B}(s) = \mathcal{O}\left(\frac{R}{s^2}\right)$ ,  $\partial_s \tilde{B}(s) = \mathcal{O}\left(\frac{R^2}{s^3}\right)$  in  $\mathcal{L}(\mathcal{H}^2)$ .

We postpone the proof of this lemma. By Lemma 3.2, we write

$$\begin{aligned} g_1(s) &= \operatorname{Re} \left( \frac{1}{i} \frac{d}{ds} \langle \tilde{B}(s) u(s), u(s) \rangle_{\mathcal{H}^2} \right) + \operatorname{Re} \left( i \langle \partial_s \tilde{B}(s) u(s), u(s) \rangle_{\mathcal{H}^2} \right) \\ &\quad - \operatorname{Re} \langle [\tilde{B}(s), F(u)] u(s), u(s) \rangle_{\mathcal{H}^2} + \mathcal{O}\left(\frac{R^2}{s^2}\right). \end{aligned}$$

In view of

$$[\operatorname{Im} B(s), F(u)] = \frac{s}{4}(F_1(u) - F_2(u))\Lambda(s)^{-3}K,$$

we obtain

$$\begin{aligned} g_1(s) &= \operatorname{Re} \left( \frac{1}{i} \frac{d}{ds} \left\langle \tilde{B}(s)u(s), u(s) \right\rangle_{\mathcal{H}^2} \right) + \operatorname{Re} \left( i \left\langle \partial_s \tilde{B}(s)u(s), u(s) \right\rangle_{\mathcal{H}^2} \right) \\ &\quad + \frac{s}{4}(F_1(u) - F_2(u)) \operatorname{Re} \left\langle \Lambda(s)^{-3}Ku(s), u(s) \right\rangle_{\mathcal{H}^2} + \mathcal{O} \left( \frac{R^2}{s^2} \right). \end{aligned}$$

By (4.6) and using that  $s\Lambda(s)^{-3} \leq s^{-2}$ ,  $\|Ku(s)\|_{\mathcal{H}^2} \leq R$  and  $\|u(s)\|_{\mathcal{H}^2}$  for all  $s \in \mathbb{R}$ , we infer (4.5) with the properties stated for  $g_1(s)$ . The other assertions of the claim can be proved similarly.  $\square$

It remains to prove Lemma 4.4.

*Proof of Lemma 4.4.* We write

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

In view of

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

and

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

we obtain

$$\begin{aligned} \tilde{C}(s) &= \frac{1}{4}\Lambda(s)^{-1} \left( -2s\Lambda(s)^{-2} \operatorname{diag}(GG^*, -G^*G) + (1 + s^2\Lambda(s)^{-2})K \right. \\ &\quad \left. - \Lambda(s)^{-2} \begin{pmatrix} 0 & GG^*G \\ G^*GG^* & 0 \end{pmatrix} + 2s\Lambda(s)^{-1} \begin{pmatrix} 0 & -G \\ G^* & 0 \end{pmatrix} \right) \Theta_R \end{aligned}$$

hence (4.7) and the other properties of the Lemma follow from the observation  $\|Ku(s)\|_{\mathcal{H}^2} = \mathcal{O}(R)$  and from the properties of  $\Lambda(s)$  stated in (4.3).  $\square$

**Third step.** We are now able to prove the existence of scattering states and to conclude the proof of Theorem 1.3.

*Proof of Theorem 1.3.* Let us focus on the case  $s \rightarrow +\infty$ . Because of Lemma 4.3, we can define  $v(s) = (v_1(s), v_2(s))$  with for  $j = 1, 2$ ,

$$v_j(s) = u_j(s) \exp \left( -is\delta F_j(\omega) - i\delta \int_0^s (F_j(u(\tau)) - F_j(\omega)) d\tau \right).$$

We have

$$(4.8) \quad \frac{1}{i} \partial_s v = V(s)v; \quad v|_{s=0} = u_0.$$

The linear scattering result of [12, Proposition 7] can then be applied to  $v$ . This gives the existence of  $\tilde{\omega} = (\tilde{\omega}_1, \tilde{\omega}_2)$  (independent of  $R$ ) such that

$$\begin{aligned} v_1(s) &= e^{i\varphi(s, GG^*)} \theta(GG^*/R^2) \tilde{\omega}_1 + o(1), \\ v_2(s) &= e^{-i\varphi(s, G^*G)} \theta(G^*G/R^2) \tilde{\omega}_2 + o(1), \end{aligned}$$

where  $\theta$  is the smooth cut-off function used for defining the operator  $\Theta_R$ . Besides, the rest term  $o(1)$  which comes from the  $o(1)$  in Lemma 7 in [12] (or equivalently



Lemma 11 in [11]) has been studied in the proof of Proposition 5.5 of [13] and proved to be  $\mathcal{O}(R^2 s^{-1})$ . Therefore, we have

$$\begin{aligned} v_1(s) &= e^{i\varphi(s, GG^*)} \theta(GG^*/R^2) \tilde{\omega}_1 + \mathcal{O}(R^2 s^{-1}), \\ v_2(s) &= e^{-i\varphi(s, G^*G)} \theta(G^*G/R^2) \tilde{\omega}_2 + \mathcal{O}(R^2 s^{-1}), \end{aligned}$$

Note that  $v$  does not need to be truncated by  $\Theta_R$  since it is associated with a initial data which is already truncated by  $\Theta_R$  ( $u_0 = \Theta_R u_0$ ). Again by Lemma 4.3, we have

$$\exp\left(i\delta \int_s^{+\infty} (F_j(u(\tau)) - F_j(\omega)) d\tau\right) = 1 + \mathcal{O}\left(\frac{R^2}{s}\right).$$

Therefore,

$$\begin{aligned} u_1(s) &= e^{is\delta F_1(\omega)} v_1(s) = e^{is\delta F_1(\omega) + i\varphi(s, GG^*)} \omega_1 + \mathcal{O}(R^2 s^{-1}), \\ u_2(s) &= e^{is\delta F_2(\omega)} v_2(s) = e^{is\delta F_2(\omega) - i\varphi(s, G^*G)} \omega_2 + \mathcal{O}(R^2 s^{-1}), \end{aligned}$$

with

$$(4.9) \quad \begin{aligned} \omega_1 &= \exp\left[i\delta \int_0^{+\infty} (F_1(u(\tau)) - F_1(\omega))\right] \theta(GG^*/R^2) \tilde{\omega}_1, \\ \omega_2 &= \exp\left[i\delta \int_0^{+\infty} (F_2(u(\tau)) - F_2(\omega))\right] \theta(G^*G/R^2) \tilde{\omega}_2, \end{aligned}$$

and the existence of scattering states in  $+\infty$  is proved. We point out that

$$\|u_1(s)\|_{\mathcal{H}}^2 = \|v_1(s)\|_{\mathcal{H}}^2, \quad \|u_2(s)\|_{\mathcal{H}}^2 = \|v_2(s)\|_{\mathcal{H}}^2,$$

so that we have

$$\begin{aligned} \Omega^+ &= \|\theta(GG^*/R^2) \tilde{\omega}_1\|_{\mathcal{H}}^2 = \|\omega_1\|_{\mathcal{H}}^2, \\ \Omega^- &= \|\theta(G^*G/R^2) \tilde{\omega}_2\|_{\mathcal{H}}^2 = \|\omega_2\|_{\mathcal{H}}^2, \end{aligned}$$

which justifies the notation  $F(\omega) = F(\Omega^+, \Omega^-)$ .

A similar argument allows to define the scattering states in  $-\infty$ .  $\square$

## 5. EXISTENCE OF WAVE OPERATORS

In this section, we prove Proposition 1.5. Let  $\alpha = (\alpha_1, \alpha_2) \in \mathcal{H}^2$  such that  $\alpha_1 \in \mathcal{D}(GG^*)$  and  $\alpha_2 \in \mathcal{D}(G^*G)$  with

$$\|\alpha_1\|_{\mathcal{H}}^2 + \|\alpha_2\|_{\mathcal{H}}^2 \leq 1 \quad \text{and} \quad \|GG^* \alpha_1\|_{\mathcal{H}} + \|G^*G \alpha_2\|_{\mathcal{H}} \leq R^2$$

for some  $R > 0$ . This assumption implies that  $\|G^* \alpha_1\|_{\mathcal{H}} + \|G \alpha_2\|_{\mathcal{H}} \leq R$ .

The strategy is the following. We first introduce an *ansatz* which solves (1.5) up to an integrable source term. Then, for  $\varepsilon > 0$ , we infer the existence of an exact solution which is at distance  $\varepsilon > 0$  of this *ansatz* as  $s \rightarrow -\infty$ . We conclude by noticing that the *ansatz* is an  $\mathcal{O}(1/|s|)$  perturbation of the expected reference solution.

**Step 1. Construction of the *ansatz*.** We consider a continuous function from  $\mathbb{R}$  to  $\mathcal{H}^2$ ,  $\tilde{u}(s) = (\tilde{u}_1(s), \tilde{u}_2(s))$ , with

$$\begin{aligned} \tilde{u}_1(s) &= e^{i\theta_1(s)} \alpha_1 + e^{i\tilde{\theta}_2(s)} \left( \frac{\beta_1}{s} + \frac{\gamma_1}{s^2} \right) + e^{-is^2/2} \frac{\kappa_1(s)}{s^2} + e^{3is^2/2} \frac{\tilde{\kappa}_1(s)}{s^2}, \\ \tilde{u}_2(s) &= e^{i\theta_2(s)} \alpha_2 + e^{i\tilde{\theta}_1(s)} \left( \frac{\beta_2}{s} + \frac{\gamma_2}{s^2} \right) + e^{is^2/2} \frac{\kappa_2(s)}{s^2} + e^{-3is^2/2} \frac{\tilde{\kappa}_2(s)}{s^2}. \end{aligned}$$

The phase operators  $\theta_1$  and  $\theta_2$  correspond to the phases obtained in the previous section, and are given by

$$\begin{aligned}\theta_1(s) &= \frac{s^2}{2} + \phi_1(s), \quad \phi_1(s) = \frac{1}{2}(\ln|s|)GG^* + \delta s F_1(\alpha), \\ \theta_2(s) &= -\frac{s^2}{2} + \phi_2(s), \quad \phi_2(s) = -\frac{1}{2}(\ln|s|)G^*G + \delta s F_2(\alpha).\end{aligned}$$

Similarly, we define

$$\begin{aligned}\tilde{\theta}_1(s) &= \frac{s^2}{2} + \frac{1}{2}(\ln|s|)G^*G + \delta s F_1(\alpha), \\ \tilde{\theta}_2(s) &= -\frac{s^2}{2} - \frac{1}{2}(\ln|s|)GG^* + \delta s F_2(\alpha),\end{aligned}$$

so that we have

$$(5.1) \quad \begin{aligned}e^{i\tilde{\theta}_1}G^* &= G^*e^{i\theta_1} \quad \text{and} \quad Ge^{i\tilde{\theta}_1} = e^{i\theta_1}G, \\ e^{i\tilde{\theta}_2}G &= Ge^{i\theta_2} \quad \text{and} \quad G^*e^{i\tilde{\theta}_2} = e^{i\theta_2}G^*.\end{aligned}$$

The coefficients  $\beta_j$ ,  $\gamma_j$  and  $\kappa_j$ ,  $j \in \{1, 2\}$  satisfy

$$\begin{aligned}\beta_2 &= \frac{1}{2}G^*\alpha_1, \quad \beta_1 = -\frac{1}{2}G\alpha_2, \\ \gamma_1 &= \frac{\delta}{2}(F_2(\alpha) - F_1(\alpha))\beta_1, \quad \gamma_2 = \frac{\delta}{2}(F_2(\alpha) - F_1(\alpha))\beta_2, \\ \kappa_1(s) &= -\frac{\delta}{2}e^{i\psi_1}\alpha_1 \left( \partial_1 f_1(\alpha) \left\langle \beta_1, e^{i(\ln|s|)GG^*}\alpha_1 \right\rangle_{\mathcal{H}} + \partial_2 f_1(\alpha) \left\langle e^{-i(\ln|s|)G^*G}\alpha_2, \beta_2 \right\rangle_{\mathcal{H}} \right), \\ \kappa_2(s) &= \frac{\delta}{2}e^{i\psi_2}\alpha_2 \left( \partial_1 f_2(\alpha) \left\langle e^{i(\ln|s|)GG^*}\alpha_1, \beta_1 \right\rangle_{\mathcal{H}} + \partial_2 f_2(\alpha) \left\langle \beta_2, e^{-i(\ln|s|)G^*G}\alpha_2 \right\rangle_{\mathcal{H}} \right), \\ \tilde{\kappa}_1(s) &= \frac{\delta}{2}e^{i\tilde{\psi}_1}\alpha_1 \left( \partial_1 f_1(\alpha) \left\langle e^{i(\ln|s|)GG^*}\alpha_1, \beta_1 \right\rangle_{\mathcal{H}} + \partial_2 f_1(\alpha) \left\langle \beta_2, e^{-i(\ln|s|)G^*G}\alpha_2 \right\rangle_{\mathcal{H}} \right), \\ \tilde{\kappa}_2(s) &= -\frac{\delta}{2}e^{i\tilde{\psi}_2}\alpha_2 \left( \partial_1 f_2(\alpha) \left\langle \beta_1, e^{i(\ln|s|)G^*G}\alpha_1 \right\rangle_{\mathcal{H}} + \partial_2 f_2(\alpha) \left\langle e^{-i(\ln|s|)G^*G}\alpha_2, \beta_2 \right\rangle_{\mathcal{H}} \right),\end{aligned}$$

with

$$\begin{aligned}\psi_1 &= \phi_1 - \delta s(F_1(\alpha) - F_2(\alpha)) = \frac{1}{2}(\ln|s|)GG^* + \delta s F_2(\alpha), \\ \tilde{\psi}_1 &= \phi_1 + \delta s(F_1(\alpha) - F_2(\alpha)) = \frac{1}{2}(\ln|s|)GG^* + \delta s(2F_1(\alpha) - F_2(\alpha)),\end{aligned}$$

and

$$\begin{aligned}\psi_2 &= \phi_2 + \delta s(F_1(\alpha) - F_2(\alpha)) = -\frac{1}{2}(\ln|s|)G^*G + \delta s F_1(\alpha), \\ \tilde{\psi}_2 &= \phi_2 - \delta s(F_1(\alpha) - F_2(\alpha)) = -\frac{1}{2}(\ln|s|)G^*G + \delta s(2F_2(\alpha) - F_1(\alpha)).\end{aligned}$$

We have denoted by  $\partial_i f_j(\alpha)$  the real-number  $\partial_i f_j(\|\alpha_1\|_{\mathcal{H}}^2, \|\alpha_2\|_{\mathcal{H}}^2)$ .

We observe that for  $j \in \{1, 2\}$ ,

$$(5.2) \quad \begin{aligned}\|\beta_j\|_{\mathcal{H}} &= \mathcal{O}(R) \quad \text{and} \quad \|\gamma_j\|_{\mathcal{H}} = \mathcal{O}(R), \\ \|\kappa_j(s)\|_{\mathcal{H}} + \|\tilde{\kappa}_j(s)\|_{\mathcal{H}} &= \mathcal{O}(R) \quad \text{and} \quad \|\partial_s \kappa_j(s)\|_{\mathcal{H}} + \|\partial_s \tilde{\kappa}_j(s)\|_{\mathcal{H}} = \mathcal{O}(R^3 s^{-1}).\end{aligned}$$

We begin by studying each term of the equation (1.5):  $s$ -derivatives, linear term, nonlinear term. Then we project on each family of oscillations generated by the operator-valued phases.

*Derivatives.* Using (5.2), we get

$$\begin{aligned} -i\partial_s \tilde{u}_1 &= e^{i\theta_1} \left( s + \frac{1}{2s} GG^* + \delta F_1(\alpha) \right) \alpha_1 + e^{i\tilde{\theta}_2} \left( -\beta_1 + \frac{\delta}{s} F_2(\alpha) \beta_1 - \frac{\gamma_1}{s} \right) \\ &\quad - \frac{1}{s} e^{-i\frac{s^2}{2}} \kappa_1(s) + \frac{3}{s} e^{3i\frac{s^2}{2}} \tilde{\kappa}_1(s) + \mathcal{O}(R^3 s^{-2}), \\ -i\partial_s \tilde{u}_2 &= e^{i\theta_2} \left( -s - \frac{1}{2s} G^* G + \delta F_2(\alpha) \right) \alpha_2 + e^{i\tilde{\theta}_1} \left( \beta_2 + \frac{\delta}{s} F_1(\alpha) \beta_2 + \frac{\gamma_2}{s} \right) \\ &\quad + \frac{1}{s} e^{i\frac{s^2}{2}} \kappa_2(s) - \frac{3}{s} e^{-3i\frac{s^2}{2}} \tilde{\kappa}_2(s) + \mathcal{O}(R^3 s^{-2}). \end{aligned}$$

*Linear part.* Using (5.1) and (5.2), we get

$$\begin{aligned} s\tilde{u}_1 + G\tilde{u}_2 &= e^{i\theta_1} \left( s\alpha_1 + \frac{1}{s} G\beta_2 \right) + e^{i\theta_2} \left( \beta_1 + \frac{1}{s} \gamma_1 + G\alpha_2 \right) \\ &\quad + \frac{1}{s} e^{-i\frac{s^2}{2}} \kappa_1(s) + \frac{1}{s} e^{3i\frac{s^2}{2}} \tilde{\kappa}_1(s) + \mathcal{O}(R^2 s^{-2}), \\ -s\tilde{u}_2 + G^*\tilde{u}_1 &= e^{i\theta_2} \left( -s\alpha_2 + \frac{1}{s} G^*\beta_1 \right) + e^{i\theta_1} \left( -\beta_2 - \frac{1}{s} \gamma_2 + G^*\alpha_1 \right) \\ &\quad - \frac{1}{s} e^{i\frac{s^2}{2}} \kappa_2(s) - \frac{1}{s} e^{-3i\frac{s^2}{2}} \tilde{\kappa}_2(s) + \mathcal{O}(R^2 s^{-2}). \end{aligned}$$

*Nonlinear part.* We begin by expanding  $F_j(\tilde{u}) = f_j(\|\tilde{u}_1\|_{\mathcal{H}}^2, \|\tilde{u}_2\|_{\mathcal{H}}^2)$  for  $j \in \{1, 2\}$ . We observe

$$\begin{aligned} \|\tilde{u}_1\|_{\mathcal{H}}^2 &= \|\alpha_1\|_{\mathcal{H}}^2 + \frac{2}{s} \operatorname{Re} \left\langle e^{i\theta_1} \alpha_1, e^{i\tilde{\theta}_2} \beta_1 \right\rangle_{\mathcal{H}} + \mathcal{O}(R^2 s^{-2}), \\ \|\tilde{u}_2\|_{\mathcal{H}}^2 &= \|\alpha_2\|_{\mathcal{H}}^2 + \frac{2}{s} \operatorname{Re} \left\langle e^{i\theta_2} \alpha_2, e^{i\tilde{\theta}_1} \beta_2 \right\rangle_{\mathcal{H}} + \mathcal{O}(R^2 s^{-2}). \end{aligned}$$

We deduce

$$\begin{aligned} (5.3) \quad F_j(\tilde{u}) &= F_j(\alpha) + \frac{2}{s} \partial_1 f_j(\alpha) \operatorname{Re} \left\langle e^{i\theta_1} \alpha_1, e^{i\tilde{\theta}_2} \beta_1 \right\rangle_{\mathcal{H}} \\ &\quad + \frac{2}{s} \partial_2 f_j(\alpha) \operatorname{Re} \left\langle e^{i\theta_2} \alpha_2, e^{i\tilde{\theta}_1} \beta_2 \right\rangle_{\mathcal{H}} + \mathcal{O}(R^2 s^{-2}). \end{aligned}$$

Note that

$$\begin{aligned} (5.4) \quad e^{-i\tilde{\theta}_2} e^{i\theta_1} &= e^{is^2 + i\delta s(F_1(\alpha) - F_2(\alpha))} e^{i(\ln|s|)GG^*}, \\ e^{-i\tilde{\theta}_1} e^{i\theta_2} &= e^{-is^2 - i\delta s(F_1(\alpha) - F_2(\alpha))} e^{-i(\ln|s|)G^*G}. \end{aligned}$$

Finally, we have

$$\begin{aligned} F_1(\tilde{u})\tilde{u}_1 &= F_1(\alpha) e^{i\theta_1} \alpha_1 + \frac{1}{s} F_1(\alpha) e^{i\tilde{\theta}_2} \beta_1 \\ &\quad + \frac{1}{s} e^{-i\frac{s^2}{2} + i\psi_1} \alpha_1 \left( \partial_1 f_1(\alpha) \left\langle \beta_1, e^{i(\ln|s|)GG^*} \alpha_1 \right\rangle_{\mathcal{H}} + \partial_2 f_1(\alpha) \left\langle e^{-i(\ln|s|)G^*G} \alpha_2, \beta_2 \right\rangle_{\mathcal{H}} \right) \\ &\quad + \frac{1}{s} e^{3i\frac{s^2}{2} + i\tilde{\psi}_1} \alpha_1 \left( \partial_1 f_1(\alpha) \left\langle e^{i(\ln|s|)GG^*} \alpha_1, \beta_1 \right\rangle_{\mathcal{H}} + \partial_2 f_1(\alpha) \left\langle \beta_2, e^{-i(\ln|s|)G^*G} \alpha_2 \right\rangle_{\mathcal{H}} \right) \\ &\quad + \mathcal{O}(R^2 s^{-2}). \end{aligned}$$

Similarly, we obtain

$$\begin{aligned} F_2(\tilde{u})\tilde{u}_2 &= F_2(\alpha)e^{i\theta_2}\alpha_2 + \frac{1}{s}F_2(\alpha)e^{i\tilde{\theta}_1}\beta_2 \\ &\quad + \frac{1}{s}e^{i\frac{s^2}{2}+i\psi_2}\alpha_2 \left( \partial_1 f_2(\alpha) \left\langle e^{i(\ln|s|)GG^*} \alpha_1, \beta_1 \right\rangle_{\mathcal{H}} + \partial_2 f_2(\alpha) \left\langle \beta_2, e^{-i(\ln|s|)G^*G} \alpha_2 \right\rangle_{\mathcal{H}} \right) \\ &\quad + \frac{1}{s}e^{-3i\frac{s^2}{2}+i\tilde{\psi}_2}\alpha_2 \left( \partial_1 f_2(\alpha) \left\langle \beta_1, e^{i(\ln|s|)G^*G} \alpha_1 \right\rangle_{\mathcal{H}} + \partial_2 f_2(\alpha) \left\langle e^{-i(\ln|s|)G^*G} \alpha_2, \beta_2 \right\rangle_{\mathcal{H}} \right) \\ &\quad + \mathcal{O}(R^2 s^{-2}). \end{aligned}$$

By the definition of  $\beta_j$ ,  $\gamma_j$ ,  $\kappa_j$  and  $\tilde{\kappa}_j$  for  $j \in \{1, 2\}$ , one gets that  $\tilde{u}(s)$  satisfies

$$-i\partial_s \tilde{u} = V(s)\tilde{u} + F(\tilde{u})\tilde{u} + \mathcal{O}(R^3 s^{-2}).$$

**Step 2. Existence of an exact solution with prescribed behavior.** We first prove the result in the linear setting. Consider

$$v_-(s) = \begin{pmatrix} e^{is^2/2+i(\ln|s|)GG^*/2}\alpha_1 \\ e^{-is^2/2-i(\ln|s|)G^*G/2}\alpha_2 \end{pmatrix},$$

$s_0 \in \mathbb{R}^+$  such that  $R^3 s_0^{-1} \leq \varepsilon$ ,  $\tilde{v}_0 = \tilde{u}_{\delta=0}$  and  $v^\varepsilon = (v_1^\varepsilon, v_2^\varepsilon)$  solution to the linear equation

$$-i\partial_s v^\varepsilon = V(s)v^\varepsilon; \quad v_{|s=-s_0}^\varepsilon = v_-(s_0).$$

Then, by step 1,

$$\frac{d}{ds} \|\tilde{v}_0(s) - v^\varepsilon(s)\|_{\mathcal{H}^2} = \mathcal{O}(R^3 s^{-2}).$$

Therefore, there exists  $C > 0$  such that for  $s < -s_0$ ,

$$\|\tilde{v}_0(s) - v^\varepsilon(s)\|_{\mathcal{H}^2} \leq C\varepsilon.$$

Consequently,

$$(5.5) \quad \|v_-(s) - v^\varepsilon(s)\|_{\mathcal{H}^2} \leq C\varepsilon.$$

In particular, this implies that the scattering states  $(\alpha_1^{\text{lin},\varepsilon}, \alpha_2^{\text{lin},\varepsilon})$  associated with  $v_\varepsilon$  satisfy  $\|\alpha_j^{\text{lin},\varepsilon} - \alpha_j\|_{\mathcal{H}} \leq C\varepsilon$  for  $j \in \{1, 2\}$ .

Let us now study the nonlinear case. We set

$$\tilde{\Phi}_j(s) = \int_{-\infty}^s (F_j(\tilde{u}(t)) - F_j(\alpha)) dt.$$

This integral is well-defined, in view of (5.3)–(5.4), since integration by parts yields

$$\tilde{\Phi}_j(s) = \mathcal{O}\left(\frac{1}{|s|}\right) \text{ as } s \rightarrow -\infty.$$

Define  $\tilde{v}$  by  $\tilde{v}_j = e^{-i\delta s F_j(\alpha) - i\delta \tilde{\Phi}_j(s)} \tilde{u}_j(s)$ . In view of the first step, it satisfies

$$-i\partial_s \tilde{v} = V(s)\tilde{v} + \mathcal{O}(R^3 s^{-2}).$$

Moreover, by construction,

$$\|\tilde{v}(s) - v_-(s)\|_{\mathcal{H}^2} \xrightarrow{s \rightarrow -\infty} 0,$$

so in view of

$$\frac{d}{ds} \|v^\varepsilon(s) - \tilde{v}(s)\|_{\mathcal{H}^2} = \mathcal{O}(R^3 s^{-2}),$$

there exists a constant  $C > 0$  such that, for  $s < -s_0$ ,

$$\|v(s) - \tilde{v}(s)\|_{\mathcal{H}^2} \leq C\varepsilon.$$

Now set

$$u_j^\varepsilon(s) = v_j^\varepsilon(s) e^{i\delta s F_j(\alpha) + i\delta \Phi_j(s)}, \quad \Phi_j(s) = \int_{-\infty}^s (F_j(v^\varepsilon(t)) - F_j(\alpha)) dt.$$

Then  $u^\varepsilon$  solves (1.5), and since  $F$  is gauge invariant,

$$\Phi_j(s) = \int_{-\infty}^s (F_j(u^\varepsilon(t)) - F_j(\alpha)) dt = \mathcal{O}\left(\frac{1}{|s|}\right) \text{ as } s \rightarrow -\infty.$$

We infer

$$(5.6) \quad \exists C > 0, \quad \forall s < -s_0, \quad \|u^\varepsilon(s) - \tilde{u}(s)\| < C\varepsilon$$

and the scattering states  $(\alpha_1^\varepsilon, \alpha_2^\varepsilon)$  associated with  $u_\varepsilon$  satisfy  $\|\alpha_j^\varepsilon - \alpha_j\|_{\mathcal{H}} \leq C\varepsilon$  for  $j \in \{1, 2\}$ .

Finally, if the unit ball of  $\mathcal{H}$  is compact, we can extract from  $u^\varepsilon$  a converging sequence which still solves (1.5) and whose scattering states are  $(\alpha_1, \alpha_2)$ .

## 6. ANALYSIS OF THE SCATTERING OPERATOR

We now prove Proposition 1.7 and we take into account the dependence of the nonlinear term with respect to the parameter  $\delta$ . Because of (4.9), we have  $\omega^{\text{lin}} = \Theta_R \tilde{\omega}$  and

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

Similarly,

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

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

$$(6.1) \quad \|\omega_j\|_{\mathcal{H}} = \|\omega_j^{\text{lin}}\|_{\mathcal{H}} \quad \text{and} \quad \|\alpha_j\|_{\mathcal{H}} = \|\alpha_j^{\text{lin}}\|_{\mathcal{H}} \quad \text{for } j \in \{1, 2\}.$$

Besides, in view of

$$u(s) = \exp\left(i\delta \int_0^s F(u(\tau)) d\tau\right) u^{\text{lin}},$$

we obtain  $F(u) = F(u^{\text{lin}})$ . We deduce

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

where  $\Lambda^\pm = \text{diag}(\Lambda_1^\pm, \Lambda_2^\pm)$ , and  $\Lambda_j^\pm$  are defined in (1.11) and (1.12), respectively. Therefore, the nonlinear scattering operator  $S_\delta = S_\delta(\alpha)$  such that  $\omega = S_\delta \alpha$  satisfies

$$(6.2) \quad S_\delta(\alpha) = e^{i\delta \Lambda^+(\alpha)} S^{\text{lin}}\left(e^{-i\delta \Lambda^-(\alpha)} \alpha\right),$$

and the scattering operator  $S_\delta$  has the following expansion

$$S_\delta = S^{\text{lin}} + i\delta (\Lambda^+ S^{\text{lin}} - S^{\text{lin}} \Lambda^-) + \mathcal{O}_R(\delta^2)$$

where  $\mathcal{O}_R(\delta^2) = \sum_{j \in \{1, 2\}} (\mathcal{O}(\delta^2 \|\Lambda_j^+\|^2) + \mathcal{O}(\delta^2 \|\Lambda_j^-\|^2))$ .

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

$$\Lambda_j^+ = \int_0^{s_0} (F_j(u(s)) - F_j(\omega)) ds + \int_{s_0}^{+\infty} (F_j(u(s)) - F_j(\omega)) ds.$$

By the continuity of the functions  $f_1$  and  $f_2$  (defined in (1.6)) and because of  $\|u_1\|_{\mathcal{H}}^2 + \|u_2\|_{\mathcal{H}}^2 = \|\omega_1\|_{\mathcal{H}}^2 + \|\omega_2\|_{\mathcal{H}}^2 = 1$ , we have

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

Lemma 4.3 gives the existence of a constant  $C$  such that,

$$(6.3) \quad \left| \int_{s_0}^{+\infty} (F_j(u(s, z)) - F_j(\omega(z))) ds \right| \leq CR^2 s_0^{-1}.$$

In order to optimize the upper bound, we choose  $s_0 = R$  whence

$$\mathcal{O}_R(\delta^2) = \mathcal{O}(R\delta^2),$$

which completes the proof of Theorem 1.7.

#### 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 [23], from which several intermediary results are borrowed (see also [1] for some refinements to [23] 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:

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

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  $d \geq 1$ . 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  $V_s \in C^\infty(\mathbb{R}^d)$  is a smooth real-valued function such that:*

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

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

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

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

- (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,*

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

and

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

- (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 [23], 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. [22]). Let  $\sigma(H_0) = \sigma_d \cup \sigma_{\text{ess}}$  be the spectrum of the self-adjoint operator  $H_0$ , where  $\sigma_d$  denotes the discrete spectrum and  $\sigma_{\text{ess}}$  denotes the essential spectrum. It follows that

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

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

**Lemma A.3** (Lemma 1 from [23]). *For any  $\hbar \in (0, \hbar^*]$ , for some  $\hbar^*$  fixed, it follows that:*

- (i)  $\sigma_d$  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

$$\lambda_\pm^\hbar = V_s^{\min} + \mathcal{O}(\hbar); \quad \inf_{\lambda \in \sigma(H_0) \setminus \{\lambda_+^\hbar, \lambda_-^\hbar\}} (\lambda - \lambda_\pm^\hbar) \geq C\hbar.$$

**Lemma A.4** ([2], and Lemma 2 from [23]). *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  $\hbar \in (0, \hbar^*]$ ,

$$\begin{aligned} \|\varphi_\pm^\hbar\|_{L^p(\mathbb{R}^d)} &\leq C\hbar^{-\frac{d}{2}(\frac{1}{2}-\frac{1}{p})}, \quad \forall p \in [2, \infty], \\ \|\nabla \varphi_\pm^\hbar\|_{L^2(\mathbb{R}^d)} &\leq C\hbar^{-1/2}, \quad \|\varphi_\pm^\hbar\|_{L^2(\mathbb{R}^d)} \leq C. \end{aligned}$$

The single-well states are then defined as in (2.6). They satisfy:

- $\varphi_R^\hbar(-x_1, x_2, \dots, x_d) = \varphi_L^\hbar(x_1, x_2, \dots, x_d)$ .
- $\|\varphi_L^\hbar \varphi_R^\hbar\|_{L^\infty} = \mathcal{O}(e^{-c/\hbar})$  for all  $c < \Gamma$ , where  $\Gamma$  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

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

We denote by

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

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

$$(A.2) \quad \omega^\hbar = \frac{\lambda_-^\hbar - \lambda_+^\hbar}{2}.$$

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

We now describe the assumptions made on the potential  $V_a$ .

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

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

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

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

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

*Remark A.6.* We note that Assumption A.1 and A.5 are satisfied in the case (2.5) borrowed from [17].

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

**Proposition A.7.** *Let  $d \leq 2$ . 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  $\delta \geq 0$  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  $\psi_{\text{app}}$  by*

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

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

$$(A.3) \quad \begin{cases} i\partial_\tau a_L = \eta \tau a_L - a_R + \delta^{\hbar} |a_L|^2 a_L; & a_L|_{\tau=0} = \alpha_L, \\ i\partial_\tau a_R = -\eta \tau a_R - a_L + \delta^{\hbar} |a_R|^2 a_R; & a_R|_{\tau=0} = \alpha_R, \end{cases}$$

*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  $\gamma < \Gamma$ ,*

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

*Remark A.8.* 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 [23] for the adaptation.

*Remark A.9.* Since the range for the slow time  $\tau = \omega^{\hbar} t / \hbar$  is  $-c/\sqrt{\hbar} \leq \tau \leq c/\sqrt{\hbar}$ , 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  $\delta F(u) = \eta^{-1/2} \delta^{\hbar} \text{Diag}(|u_1|^2, |u_2|^2)$ ). When  $\hbar$  is small, Theorem 1.3 gives asymptotics for the profiles  $a_L$  and  $a_R$  of  $\psi_{\text{app}}^{\hbar}$  for large times ( $|t| \leq c\sqrt{\hbar}/\omega^{\hbar}$ ) and the connexion between



the profiles for  $t < 0$  and  $t > 0$  involves the Landau-Zener transition coefficient  $e^{-\frac{\pi}{\eta^2}}$  (at leading order when  $\hbar$  goes to 0).

*Proof.* For simplicity, we write the proof for  $t \geq 0$  and it naturally extends to  $t \leq 0$ .

**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  $\psi^\hbar \in C(\mathbb{R}; \Sigma)$  ( $\Sigma$  is defined in Lemma A.4). In addition, if we set

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

then we have the *a priori* estimates:

$$\begin{aligned} \frac{dM^\hbar}{dt} &= 0, \\ \frac{dE^\hbar}{dt} &= \int_{\mathbb{R}^d} \partial_t V(t, x) |\psi^\hbar(t, x)|^2 dx = \kappa(\hbar) \int_{\mathbb{R}^d} V_a(x) |\psi^\hbar(t, x)|^2 dx, \end{aligned}$$

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

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

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

$$E^\hbar(0) = \langle \alpha_L \varphi_L^\hbar + \alpha_R \varphi_R^\hbar, \alpha_L H_0 \varphi_L^\hbar + \alpha_R H_0 \varphi_R^\hbar \rangle + \frac{\epsilon(\hbar)}{2} \|\alpha_L \varphi_L^\hbar + \alpha_R \varphi_R^\hbar\|_{L^4}^4.$$

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

$$(A.4) \quad H_0 \varphi_L^\hbar = \Omega^\hbar \varphi_L^\hbar - \omega^\hbar \varphi_R^\hbar; \quad H_0 \varphi_R^\hbar = \Omega^\hbar \varphi_R^\hbar - \omega^\hbar \varphi_L^\hbar,$$

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,

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

Next, as in [23], we consider the slow time

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

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

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

and in view of the above estimates,

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

We decompose  $\Psi^{\hbar}$  as

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

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

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

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

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

The proof of Proposition A.7 consists in showing that  $\mathbf{a}_{L/R}^{\hbar}$  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  $\mathbf{a}_R^{\hbar}$ ,  $\mathbf{a}_L^{\hbar}$  and  $\psi_c^{\hbar}$ .** By definition, we have  $\mathbf{a}_L^{\hbar} = \int_{\mathbb{R}^d} \Psi^{\hbar} \varphi_L^{\hbar}$ , so Cauchy-Schwarz inequality yields

$$\|\varphi^{\hbar}(\tau)\|_{L^2}^2 = |\mathbf{a}_L^{\hbar}(\tau)|^2 + |\mathbf{a}_R^{\hbar}(\tau)|^2 \leq (M^{\hbar})^2 (\|\varphi_L^{\hbar}\|_{L^2}^2 + \|\varphi_R^{\hbar}\|_{L^2}^2) \leq 2(M^{\hbar})^2.$$

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

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

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

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

Since we have the pointwise estimate

$$|\mathbf{R}^{\hbar}| \leq C (|\varphi^{\hbar}|^2 |\psi_c^{\hbar}| + |\psi_c^{\hbar}|^3),$$

we infer

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

and Gagliardo-Nirenberg inequality yields ( $d \leq 2$ )

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

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

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

Therefore,

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

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

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

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

$$|\dot{\mathbf{a}}_L^{\hbar}(\tau)| + |\dot{\mathbf{a}}_R^{\hbar}(\tau)| \leq C(1 + \tau), \quad \forall \tau \geq 0.$$

From this we infer

$$(A.9) \quad \|\partial_{\tau}\varphi^{\hbar}\|_{L^2} \leq |\dot{\mathbf{a}}_L^{\hbar}(\tau)| \|\varphi_L^{\hbar}\|_{L^2} + |\dot{\mathbf{a}}_R^{\hbar}(\tau)| \|\varphi_R^{\hbar}\|_{L^2} \leq C(1 + \tau),$$

and, again from Lemma A.4,

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

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

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

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

$$\Pi_c^{\hbar}(V_a\Psi^{\hbar}) = \Pi_c^{\hbar}(V_a\varphi^{\hbar}) + \Pi_c^{\hbar}(V_a\psi_c^{\hbar}),$$

and set

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

Integrating by parts,

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

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

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

We infer, using (A.9),

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

For  $I_2^{\hbar}$ , we have directly

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

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

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

and set

$$\begin{aligned} I_3^{\hbar}(\tau) &= \hbar^{d/2} \int_0^\tau e^{-i(H_0 - \Omega^{\hbar})(\tau-s)/\omega^{\hbar}} \Pi_c^{\hbar} (|\varphi^{\hbar}|^2 \varphi^{\hbar})(s) ds, \\ I_4^{\hbar}(\tau) &= \hbar^{d/2} \int_0^\tau e^{-i(H_0 - \Omega^{\hbar})(\tau-s)/\omega^{\hbar}} \Pi_c^{\hbar} \mathbf{R}^{\hbar}(s) ds. \end{aligned}$$

We have, directly from (A.8),

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

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

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

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

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

Gronwall lemma yields

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

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

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

This is small as  $\hbar \rightarrow 0$ , provided that  $\tau^2 \ll 1/\hbar$ . More precisely, there exist  $c_1, c_2 > 0$  independent of  $\hbar$  such that

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

To conclude the proof of the proposition, set

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

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

$$\begin{aligned} i\dot{\mathbf{w}}_L^{\hbar} &= -\mathbf{w}_R^{\hbar} + \eta\tau \int_{\mathbb{R}^d} V_a (\Psi^{\hbar} - a_L \varphi_L^{\hbar}) \varphi_L^{\hbar} \\ &\quad + \delta \hbar^{d/2} \int_{\mathbb{R}^d} (|\Psi^{\hbar}|^2 \Psi^{\hbar} - |a_L|^2 a_L |\varphi_L^{\hbar}|^2 \varphi_L^{\hbar}) \varphi_L^{\hbar}. \end{aligned}$$

We have

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

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

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

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

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

Gronwall lemma and (A.12) then yield Proposition A.7.  $\square$

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