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Semiclassical Asymptotics for Weakly Nonlinear Bloch Waves

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We study the simultaneous semi-classical and adiabatic asymptotics for a class of (weakly) nonlinear Schrödinger equations with a fast periodic potential and a slowly varying confinement potential. A rigorous two-scale WKB–analysis, locally in time, is performed. The main nonlinear phenomenon is a modification of the Berry phase.

KEY WORDS: Nonlinear Schrödinger equation, Bloch eigenvalue problem; WKB–asymptotics, Bose–Einstein condensate

1. INTRODUCTION AND SCALING

In this work we study the asymptotic behavior as $\varepsilon \to 0$ of the following semilinear initial value problem (IVP):

$$\begin{aligned} i\varepsilon\partial_t \psi^\varepsilon &= -\frac{\varepsilon^2}{2}\Delta\psi^\varepsilon + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon + U(x)\psi^\varepsilon + \varepsilon\lambda(t)\,|\psi^\varepsilon|^{2\sigma}\psi^\varepsilon, \\ \psi^\varepsilon\big|_{t=0} &= \psi_I^\varepsilon(x), \end{aligned} \tag{1.1}$$

where $x \in \mathbb{R}^d$, $t \in \mathbb{R}$, $\sigma \in \mathbb{N}$ and $0 < \varepsilon \ll 1$. Here and in the following ε-dependence will be denoted by the superscript ε. The external

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(confining) potential $U = U(x) \in \mathbb{R}$ is assumed to be smooth on $\mathbb{R}^d$, whereas the lattice-potential $V_\Gamma = V_\Gamma(y) \in \mathbb{R}$ is assumed to be smooth, uniformly bounded in $\mathbb{R}^d$ and *periodic* with respect to some *regular lattice* $\Gamma \simeq \mathbb{Z}^d$, generated through a basis $\{\zeta_1, \dots, \zeta_d\}$, $\zeta_l \in \mathbb{R}^d$, i.e.

$$V_\Gamma(y+\gamma) = V_\Gamma(y), \quad \forall y \in \mathbb{R}^d, \quad \gamma \in \Gamma, \tag{1.2}$$

where

$$\Gamma = \left\{ \gamma \in \mathbb{R}^d : \ \gamma = \sum_{l=1}^{d} \gamma_l \zeta_l, \ \gamma_l \in \mathbb{Z} \right\}. \tag{1.3}$$

Finally, we assume $\lambda = \lambda(t) \in \mathbb{R}$ to be a smooth coupling-function and $\psi_I^\varepsilon \in L^2(\mathbb{R}^d)$ to be normalized such that

$$\int_{\mathbb{R}^d} |\psi_I^\varepsilon(x)|^2 \, \mathrm{d}x = 1. \tag{1.4}$$

This normalization is henceforth preserved by the evolution since $\lambda(t) \in \mathbb{R}$.

Nonlinear Schrödinger equations (NLS) of type (1.1) appear in various physical situations, cf. ref. 1 for a general overview. An important example in $d = 3$ is the case $\sigma = 1$, $\lambda(t) \equiv \pm 1$, i.e. the so called *repulsive* resp. *attractive Gross–Pitaevskii equation*, a celebrated model for the description of the evolution of *Bose–Einstein condensates* (BECs).[2] In order to motivate the scaling in (1.1) we shall examine this case more closely:

In physical units, the Gross–Pitaevskii equation (for $d = 3$) is given by ref. 2

$$\mathrm{i}\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \Delta \psi + V(x)\,\psi + U_0(x)\psi \pm N\alpha(t)|\psi|^2 \psi, \tag{1.5}$$

where m is the atomic mass, $\hbar$ is the Planck constant, N is the number of atoms in the condensate and

$$\alpha(t) = \frac{4\pi \hbar^2 |a(t)|}{m}, \tag{1.6}$$

with $a(t) \in \mathbb{R}$ denoting the s-wave scattering length derived from the corresponding N-particle theory, cf. refs. 2 and 3. (The fact that $a(t)$ is chosen time-dependent is motivated by recent experiments on BEC where this has indeed be achieved by some highly sophisticated experimental techniques.) In this context the external potential $U(x)$, which traps the condensate, is usually assumed to be a harmonic confinement potential of the following form: [4,5]

$$U_0(x) = \frac{m\omega_0^2}{2}\,|x|^2, \quad \omega_0 \in \mathbb{R}, \;\; x \in \mathbb{R}^3. \tag{1.7}$$

More general, nonisotropic variants of such confinement potentials are used to create so called *disc-shaped* or *cigar-shaped*, i.e. quasi two or, resp., one dimensional, BECs (see refs. 2 and 4 and the references given therein). If in addition a periodic potential $V(x)$, which in physical experiments is generated by an intense laser field, is included, the condensates are referred to as *lattice BECs*. A particular example of V is then given by

$$V\,(x) = \sum_{l=1}^{3} \frac{\hbar^2 \xi_l^2}{2m} \sin^2\left(\xi_l x_l\right), \tag{1.8}$$

where $\xi = (\xi_1, \xi_2, \xi_3)$ with $\xi_l \in \mathbb{R}$ denotes the wave vector of the laser field.[(2)] The sign in front of the nonlinearity in (1.5) corresponds to a *stable* (defocusing) resp. *unstable* (focusing) condensate. To rewrite eqn. (1.5) into our semi-classical scaling we proceed similar to ref. 4. More precisely, we introduce dimensionless variables

$$\tilde{t} = \omega_0\, t, \qquad \tilde{x} = \frac{x}{x_s}, \qquad \tilde{\psi}(\tilde{t}, \tilde{x}) = x_s^{3/2} \psi(t, x), \tag{1.9}$$

where x_s will be determined later and $\tilde{\psi}(\tilde{t}, \tilde{x})$ is such that the normalization (1.4) is preserved for $d = 3$. Multiplying (1.5) by $1/(m\omega_0^2 x_s^2)$ and omitting again all " $\tilde{}$ " we find the following dimensionless equation:

$$\mathrm{i}\varepsilon\partial_t \psi = -\frac{\varepsilon^2}{2}\Delta\psi + V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi + U(x)\psi \pm \delta(t)\varepsilon^{5/2}|\psi|^2\psi, \tag{1.10}$$

where the potentials are defined by

$$V_\Gamma\,(y) := \frac{V(x_s \varepsilon y)}{m\omega_0^2 x_s^2}\,, \qquad U(x) := \frac{|x|^2}{2}\,, \tag{1.11}$$

and the appearing parameters ε, $\delta(t) \in \mathbb{R}_+$ are

$$\varepsilon := \frac{\hbar}{\omega_0 m x_s^2} = \left(\frac{a_0}{x_s}\right)^2, \qquad \delta(t) := \frac{N\alpha(t)}{a_0^3 \hbar\omega_0} = \frac{4\pi\,|a(t)|N}{a_0}\,, \tag{1.12}$$

with a_0 denoting the length of the harmonic oscillator ground state corresponding to $U_0(x)$, i.e.

$$a_0 := \sqrt{\frac{\hbar}{\omega_0 m}}. \tag{1.13}$$

Since we aim for $\varepsilon \ll 1$ and $\delta\varepsilon^{5/2}$ to be of the order of ε we require $\delta = O(\varepsilon^{-3/2})$, hence $4\pi|a|N \gg a_0$, which from a physical point of view corresponds to the *strong interaction regime*, also known as *Thomas–Fermi regime*.(2) Now, consider a reference value $\bar{a}$ for $a(t)$ and similarly denote by $\bar{\delta}$ the parameter δ for this reference value $\bar{a}$. Inserting (1.12) into $\bar{\delta}\varepsilon^{5/2} = \varepsilon$, we compute the *characteristic length scale*

$$x_s = (4\pi N|\bar{a}|a_0^2)^{1/3}, \tag{1.14}$$

which one needs to choose as the appropriate reference scale in our situation. In particular we shall assume $|\psi_I^\varepsilon(x)|$ to vary on this scale. The coupling function $\lambda(t)$ is then given by $\lambda(t) = \delta(t)/\bar{\delta}$. Identity (1.14) implies

$$\varepsilon = \left(\frac{a_0}{4\pi N|\bar{a}|}\right)^{2/3} \ll 1, \tag{1.15}$$

which is different from the one given in ref. 4. Moreover, having in mind (1.8), (1.11) we require for the periodic potential V_Γ

$$\varepsilon\xi_l x_s = O(1), \qquad \frac{\hbar^2\xi_l^2}{2m^2x_s^2\omega_0^2} = O(1), \quad \text{for } l = 1, 2, 3. \tag{1.16}$$

From these relations one computes

$$\xi_l \approx a_0^{-4/3}(4\pi N|\bar{a}|)^{1/3}, \quad \text{for } l = 1, 2, 3, \tag{1.17}$$

which gives the required wave vector in our regime and one checks that in this case the conditions (1.16) are satisfied. We remark that this scaling is in good agreement with some typical recent experiments. For example in the case of a lattice BEC consisting of Rb atoms we have, cf. refs. 4 and 5

$$a_0 \approx 3,4 \times 10^{-6} \ [\mathrm{m}], \qquad \bar{a} \approx 5,4 \times 10^{-9} \ [\mathrm{m}], \qquad N \approx 1,5 \times 10^5. \tag{1.18}$$

This gives: $4\pi|\bar{a}|N \approx 10^{-2}\,[\mathrm{m}] \gg a_0$, hence $\varepsilon \approx 4,3 \times 10^{-3} \ll 1$ and for the wave vectors we compute $\xi_l \approx 4,6 \times 10^6\,[1/\mathrm{m}]$, which is of the same order of magnitude as stated in ref. 6. The reference length scale in this case is

$x_s = 4,6 \times 10^{-5}$ [m]. Finally, to motivate the choice $\sigma \geqslant 1$, we note that for $d < 3$ higher-order nonlinearities are frequently used in the description of BECs.(3,7)

From a mathematical point of view the limit $\varepsilon \to 0$ corresponds to the simultaneous *semi-classical* (or *high-frequency*) and *adiabatic limit* (see refs. 8–10 for general introductions to these fields). For *linear* time-dependent Schrödinger equations (with periodic potentials) this asymptotic regime has been intensively studied by several authors, using (spatial) *adiabatic decoupling theory*(10,11) or *Wigner measures*(12–14) to mention results obtained in recent years. A numerical study of these asymptotics can be found in ref. 15.

In our scaling the nonlinearity is $o(1)$ and can thus be called *weak*, still it makes the rigorous asymptotic analysis of the given IVP considerably harder. Even without a periodic potential the semi-classical limit for NLS is still far from being completely understood. In particular, we cannot use the above mentioned mathematical techniques, which so far only work in a linear setting. (For a notable exception see ref. 16.) Thus we shall rather apply a more naive asymptotic expansion method in the spirit of the traditional *WKB–type expansions*. Due to the periodic potential, we use a so called *two-scale WKB–ansatz*, first introduced in ref. 17, which has already been successfully applied in the case of linear periodic Schrödinger equations.(18,19) Our scaling is such that the nonlinearity enters in the leading order term of the asymptotic WKB-type solutions, although the Hamilton–Jacobi equation for the phase of the wave–function is found to be the same as in the linear case. This is analogous to the *weakly nonlinear (dispersive) geometrical optics* regime discussed in ref. 20. (See also ref. 21 for an application of this scaling in another semi-classical context.) The asymptotic description is valid on *macroscopic* time-scales $t = O(1)$ but in general only for small $|t| > 0$.

Before giving a precise description, we state the typical result that we shall prove. The possibly not well-defined assumptions in the following statement will be discussed more precisely below.

Theorem 1.1. Let $d \geqslant 1$, V_Γ and U be smooth, real-valued potentials, V_Γ being Γ-periodic, U being sub-quadratic, and λ being real-valued and smooth. Assume that the initial datum ψ_I^ε is of the form

$$\psi_I^\varepsilon(x) = a_I(x)\chi_n\left(\frac{x}{\varepsilon}, \nabla\phi_I(x)\right) \mathrm{e}^{\mathrm{i}\phi_I(x)/\varepsilon} + \varepsilon\varphi_I^\varepsilon(x),$$

where $a_I \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$, $\phi_I \in C^\infty(\mathbb{R}^d;\mathbb{R})$ and $\chi_n = \chi_n(y,k)$ is a Bloch eigenfunction associated to a simple isolated Bloch band $E_n = E_n(k)$. We suppose that φ_I^ε satisfies Assumption 3.5, with $K \geq d$. Assume that no caustic is formed before time $\tau > 0$, and fix $\tau_0 \in]0, \tau[$. Then there exists $\varepsilon_0 > 0$ such that for $0 < \varepsilon \leqslant \varepsilon_0$, the solution ψ^ε to (1.1) is defined up to time τ_0. Moreover, it satisfies the following asymptotics as $\varepsilon \to 0$:

$$\begin{aligned} &\sup_{0 \leqslant t \leqslant \tau_0} \left\| \psi^\varepsilon(t) - \mathrm{v}_0^\varepsilon(t) \right\|_{L^2(\mathbb{R}^d)} = \mathcal{O}(\varepsilon), \\ &\sup_{0 \leqslant t \leqslant \tau_0} \left\| \psi^\varepsilon(t) - \mathrm{v}_0^\varepsilon(t) \right\|_{L^\infty(\mathbb{R}^d)} = \mathcal{O}\left(\varepsilon^{1-\eta}\right), \quad \text{for any } \eta > 0, \end{aligned} \tag{1.19}$$

where the approximate solution v_0^ε is given by

$$\mathrm{v}_0^\varepsilon(t, x) = \frac{a_I\left(X_t^{-1}(x)\right)}{\sqrt{J_t\left(X_t^{-1}(x)\right)}} \chi_n\left(\frac{x}{\varepsilon}, \nabla_x \phi(t, x)\right) \mathrm{e}^{\mathrm{i}\omega\left(t, X_t^{-1}(x)\right)} \mathrm{e}^{\mathrm{i}\phi(t,x)/\varepsilon}.$$

Here, ϕ solves the Hamilton–Jacobi equation (2.9), corresponding to the classical flow: $(t, x) \mapsto X_t(x)$, as defined by (2.15), J_t is the associated Jacobi determinant (2.16), and ω is given by

$$\begin{aligned} \omega(t, x) = -\mathrm{i} \int_0^t \beta\left(s, X_s(x)\right) \mathrm{d}s \\ - |a_I(x)|^{2\sigma} \int_0^t \frac{\lambda(s)}{J_s(x)^\sigma} \int_Y \left|\chi_n\left(y, \nabla_x \phi\left(s, X_s(x)\right)\right)\right|^{2\sigma+2} \mathrm{d}y\, \mathrm{d}s. \end{aligned}$$

We denote by $\beta \in \mathrm{i}\mathbb{R}$ the Berry phase (3.6), and by Y the centered fundamental domain of Γ.

Remark 1.2. Our result holds only before caustics. This should not be surprising; even in the linear case $\lambda \equiv 0$, the WKB method is effective only away from caustics. On the other hand, some techniques have proved to be efficient to overcome this difficulty in a linear framework, such as Gaussian beams (see e.g. ref. 18) or Wigner functions (see e.g. refs. 22, 23). However, adapting these techniques to a nonlinear context seems to be a challenging open question.

Remark 1.3. The assumptions on the corrector φ_I^ε for the initial data are not trivial (see Assumption 3.5). They state essentially that the initial data are well-prepared, in order to prove a nonlinear stability result. Note however that φ_I^ε is of order $\mathcal{O}(1)$ as $\varepsilon \to 0$ in any reasonable sense. The assumptions $K \geq d$ means that we have to consider (at least) d correctors to prepare the initial data. This assumption may seem surprising; the proofs we give rely on it, and it would be interesting to understand how necessary this assumption is.

The above result shows that the leading order nonlinear phenomenon is represented by the phase factor ω. The Berry phase is a linear (geometrical) feature (see (3.6)), but the second integral in the definition of ω stems from the nonlinearity. In the context of laser physics, this phenomenon is known as *phase self-modulation* (see e.g. refs. 24–26).

The paper is organized as follows. In Section 2, we start a formal asymptotic expansion, following WKB-methods. This leads us to consider the Bloch eigenvalue problem. The asymptotic expansion is considered in more detail in Section 3, where a formal approximate solution is constructed at any order. The justification of this approximation is performed in Section 4. We discuss our results and some of their possible extensions in Section 5. In Appendix A, we detail a computational step from Section 3.

2. ASYMPTOTIC EXPANSION: EMERGENCE OF BLOCH BANDS

For solutions of (1.1) we seek an asymptotic expansion of the following form

$$\psi^\varepsilon(t,x) = u^\varepsilon\left(t,x,\frac{x}{\varepsilon}\right)\mathrm{e}^{\mathrm{i}\phi(t,x)/\varepsilon}; \quad u^\varepsilon(t,x,y) \sim \sum_{j=0}^{\infty}\varepsilon^j u_j(t,x,y), \tag{2.1}$$

where we assume that both $\phi(t,x)\in\mathbb{R}$ and $u^\varepsilon(t,x,y)\in\mathbb{C}$ are sufficiently smooth. Moreover we impose

$$u^\varepsilon(\cdot,\cdot,y+\gamma) = u^\varepsilon(\cdot,\cdot,y) \qquad \forall\, y\in\mathbb{R}^d, \quad \gamma\in\Gamma.$$

We assume that the initial condition ψ_I^ε is compatible with (2.1).

Assumption 2.1. The initial wavefunction ψ_I^ε is in the Schwartz space $\mathcal{S}(\mathbb{R}^d)$, and is of WKB-type, i.e.

$$\psi_I^\varepsilon(x) = u_I\left(x,\frac{x}{\varepsilon}\right)\mathrm{e}^{\mathrm{i}\phi_I(x)/\varepsilon} + \varepsilon\varphi_I^\varepsilon(x), \tag{2.2}$$

with $\phi_I\in C^\infty(\mathbb{R}^d;\mathbb{R})$, $u_I\in\mathcal{S}(\mathbb{R}^d\times\mathbb{T}^d;\mathbb{C})$[4], $\mathbb{T}^d\equiv\mathbb{R}^d/\Gamma$. The function φ_I^ε is a corrector to be precised later on.

[4]That is, u_I is rapidly decaying w.r.t. the first variable (x), smooth w.r.t. the second one (y).

From now on we shall denote the linear part of the Hamiltonian operator by

$$H^{\varepsilon} := -\frac{\varepsilon^2}{2}\Delta + V_{\Gamma}\left(\frac{x}{\varepsilon}\right) + U(x). \tag{2.3}$$

Plugging the ansatz (2.1) into (1.1) we (formally) obtain

$$\mathrm{i}\varepsilon\partial_t\psi^{\varepsilon} - H^{\varepsilon}\psi^{\varepsilon} - \varepsilon\lambda(t)|\psi^{\varepsilon}|^{2\sigma}\psi^{\varepsilon} = b^{\varepsilon}\left(t, x, \frac{x}{\varepsilon}\right)e^{i\phi(t,x)/\varepsilon}.$$

We consequently expand the r.h.s. of this equation as

$$b^{\varepsilon}(t,x,y) \sim \sum_{j=0}^{\infty} \varepsilon^j b_j(t,x,y) \tag{2.4}$$

and choose the asymptotic amplitudes u_j in a way such that $b_j(t,x,y) \equiv 0$, $\forall j \geqslant 0$. Setting $b_0(t,x,x/\varepsilon) = 0$ yields

$$-\frac{\Delta_y u_0}{2} - \mathrm{i}\nabla_x\phi\cdot\nabla_y u_0 + \frac{|\nabla_x\phi|^2}{2}u_0 + V_{\Gamma}(y)u_0 + (U(x)+\partial_t\phi)\,u_0\Big|_{y=\frac{x}{\varepsilon}} = 0. \tag{2.5}$$

Uncorrelating the variables x and y, we shall seek a solution to the more general equation:

$$-\frac{\Delta_y u_0}{2} - \mathrm{i}\nabla_x\phi\cdot\nabla_y u_0 + \frac{|\nabla_x\phi|^2}{2}u_0 + V_{\Gamma}(y)u_0 = -\left(U(x)+\partial_t\phi\right)u_0\,. \tag{2.6}$$

Denoting by

$$H_{\Gamma}(k) := \frac{1}{2}\left(-i\nabla_y + k\right)^2 + V_{\Gamma}(y)\,, \quad k \in \mathbb{R}^d, \tag{2.7}$$

we can rewrite Eq. (2.6) in the following form:

$$H_{\Gamma}(\nabla_x\phi)u_0 = -\left(U(x)+\partial_t\phi\right)u_0. \tag{2.8}$$

We now require that for some fixed $n \in \mathbb{N}$, it holds

$$E_n(\nabla_x\phi) = -\left(U(x)+\partial_t\phi\right), \tag{2.9}$$

where $E_n(k)$, $k \in \mathbb{R}^d$, is the nth eigenvalue of the *Bloch eigenvalue problem*:[27]

$$\begin{aligned} H_\Gamma(k)\chi_n(y,k) = \;& E_n(k)\chi_n(y,k), \quad n\in\mathbb{N},\ y\in Y, \\ \chi_n(y+\gamma,k) = \;& \chi_n(y,k), \quad \text{for } \gamma\in\Gamma. \end{aligned} \tag{2.10}$$

Here and in the following, we denote by Y the centered *fundamental domain* of the lattice Γ, i.e.

$$Y := \left\{ \gamma\in\mathbb{R}^d:\ \gamma = \sum_{l=1}^{d} \gamma_l \zeta_l,\ \gamma_l \in \left[-\frac{1}{2}, \frac{1}{2}\right] \right\}, \tag{2.11}$$

whereas Y^*, denotes the corresponding basic cell of the dual lattice Γ^*. In solid state physics Y^* is called the *Brillouin zone* hence we shall denote it by $\mathcal{B}\equiv Y^*$. Let us recall some well known facts for this eigenvalue problem, cf. refs. 10, 28 and 29. Since V_Γ is smooth and periodic, we get that, for every fixed $k\in\mathcal{B}$, $H_\Gamma(k)$ is self-adjoint on $H^2(\mathbb{T}^d)$ with compact resolvent. Hence the spectrum of $H_\Gamma(k)$ is given by

$$\sigma(H_\Gamma(k)) = \left\{E_n(k);\ n\in\mathbb{N}^*\right\}, \quad E_n(k)\in\mathbb{R}.$$

In general we can order the eigenvalues $E_n(k)$ according to their magnitude and multiplicity,

$$E_1(k)\leqslant\ldots\leqslant E_n(k)\leqslant E_{n+1}(k)\leqslant\ldots$$

Moreover every $E_n(k)$ is periodic w.r.t. Γ^* and it holds that $E_n(k) = E_n(-k)$. The set $\{E_n(k);\ k\in\mathcal{B}\}$ is called the nth-*energy band*. The associated eigenfunction, the *Bloch waves*, $\chi_n(y,k)$ form (for every fixed $k\in\mathcal{B}$) a complete orthonormal basis in $L^2(Y)$ and are smooth w.r.t. $y\in Y$. We choose the usual normalization

$$\langle\chi_n(\cdot,k), \chi_m(\cdot,k)\rangle_{L^2(Y)} \equiv \int_Y \overline{\chi_n(y,k)}\chi_m(y,k)\,\mathrm{d}y = \delta_{n,m}, \quad n,\ m\in\mathbb{N}. \tag{2.12}$$

Concerning the dependence on $k\in\mathcal{B}$, it has been shown in ref. 28 that for any $n\in\mathbb{N}$ there exists a closed subset $\mathcal{U}\subset\mathcal{B}$ such that: $E_n(k)$ are analytic, $\chi_n(\cdot,k)$ can be chosen to be analytic functions for all $k\in\Omega:=\mathcal{B}\backslash\mathcal{U}$, and

$$E_{n-1} < E_n(k) < E_{n+1}(k), \quad \forall k\in\Omega. \tag{2.13}$$

If this condition holds for all $k \in \mathcal{B}$ then $E_n(k)$ is called an *isolated Bloch band*.[10] Moreover, it is known that

$$\operatorname{meas} \mathcal{U} = \operatorname{meas}\{k \in \mathcal{B} \mid E_n(k) = E_m(k),\ n \neq m\} = 0.$$

In this set of measure zero one encounters so called *band crossings*.

Eq. (2.9) is called the nth band *Hamilton–Jacobi equation* corresponding to the *semi-classical band Hamiltonian*

$$h_n^{\mathrm{sc}}(k, x) := E_n(k) + U(x), \quad (k, x) \in \mathbb{T}^* \times \mathbb{R}^d \tag{2.14}$$

with an effective kinetic energy given by the nth eigenvalue for $k \in \mathbb{T}^* \equiv \mathbb{R}^d / \Gamma^*$. The characteristic differential equations corresponding to (2.9) are consequently given by the equations of motion:

$$\begin{aligned} \dot{x} &= \ \nabla_k E_n(k), & x\big|_{t=0} &= x_0 \in \mathbb{R}^d, \\ \dot{k} &= -\nabla_x U(x), & k\big|_{t=0} &= \nabla_x \phi_I(x_0). \end{aligned} \tag{2.15}$$

This system (locally) defines a flow map $(x, t) \mapsto X_t(x) \equiv X_t(x; \nabla_x \phi_I(x))$ in physical space. In general *caustics* will appear in this flow, which prohibits the existence of globally defined smooth solutions for (2.9). Let us denote by

$$J_t(x) := \det(\nabla_x X_t(x; \nabla_x \phi_I(x))) \tag{2.16}$$

the corresponding Jacobi determinant. We have $J_0(x) \equiv 1$. Denote by τ the time at which the first caustic appears, i.e.

$$\tau := \inf\{t > 0 \mid \exists\, x \in \mathbb{R}^d:\ J_t(x) = 0\}. \tag{2.17}$$

We thus have $J_t(x) > 0$ for $0 \leqslant t < \tau$. Standard theory implies the following.

Lemma 2.2. If $h_n^{sc}(k, x) \in C^\infty(\mathbb{T}^* \times \mathbb{R}^d)$, $\phi_I \in C^\infty(\mathbb{R}^d)$, then there exist $\tau > 0$ and a unique smooth solution $\phi \in C^\infty([0, \tau[\times \mathbb{R}^d)$ of the Hamilton–Jacobi equation

$$\partial_t \phi + h_n^{sc}(\nabla_x \phi, x) = \ 0; \quad \phi\big|_{t=0} = \ \phi_I(x).$$

To make sure that $E_n(k)$ (and hence $h_n^{\mathrm{sc}}(k, x)$) is sufficiently smooth, we shall impose the following assumption.

Assumption 2.3. The amplitude $u_I(x, y)$ is assumed to be concentrated in a single isolated Bloch band $E_n(k)$ corresponding to a simple eigenvalue of $H_\Gamma(k)$, i.e.

$$u_I(x, y) \equiv a_I(x)\chi_n(y, \nabla_x \phi_I(x)), \tag{2.18}$$

where $a_I \in \mathcal{S}(\mathbb{R}^d; \mathbb{C})$ is a given initial amplitude.

From (2.8) and (2.10) we conclude that there exists $a_0 = a_0(t, x)$ such that

$$u_0(t, x, y) = a_0(t, x)\chi_n(y, \nabla_x \phi(t, x)). \tag{2.19}$$

Remark 2.4. Note that also in the linear case, assumptions similar to Assumption 2.3 are usually imposed, cf. ref. 11 and 14. There however, the reason is largely to avoid band crossings in order to obtain global-in-time results. (The rigorous study of band crossings is quite involved and up to now established only for certain model problems, cf. refs. 30–32.

Due to caustics (and possibly additional nonlinear effects if $\lambda(t)$ is not real-valued, see Section 5), we cannot hope for such global-in-time results in our case. Assumption 2.3 therefore is only imposed for regularity reasons and could be significantly weakened, since, with some technical effort, one could modify the subsequent analysis. Indeed, all statements could be formulated locally in regions $\mathcal{U} \subseteq \mathbb{R}_t \times \mathbb{R}_x^d$ which neither contain caustics nor band crossings (in the sense that $E_n(\nabla_x \phi(t, x)) \neq E_m(\nabla_x \phi(t, x))$, for all $(t, x) \in \mathcal{U}$). In this way one could include also non-isolated bands $E_n(k)$.

We further remark that in the case $d = 1$ all band crossings can be removed through a proper analytic continuation of the bands, cf. ref. 33.

3. DERIVATION OF THE TRANSPORT EQUATIONS

To characterize the *principal amplitude* a_0, we set $b_1 = 0$ in (2.4), which yields

$$H_\Gamma(\nabla_x \phi)u_1 + (U(x) + \partial_t \phi)\, u_1 = L_1 u_0 - \lambda(t)|u_0|^{2\sigma} u_0, \tag{3.1}$$

where the linear differential operator L_1 applied to u_0 reads

$$L_1 u_0 := \mathrm{i}\partial_t u_0 + \mathrm{i}\nabla_x \phi \cdot \nabla_x u_0 + \mathrm{i}\frac{\Delta_x \phi}{2} u_0 + \mathrm{div}_x\, \nabla_y u_0. \tag{3.2}$$

We multiply Eq. (3.1) with $\overline{\chi}_n(y, \nabla_x \phi)$ and integrate over the fundamental domain Y. From (2.9), the left hand side of (3.1) is $(H_\Gamma - E_n)u_1$; since H_Γ

is self-adjoint, the integral obtained from the l.h.s. of (3.1) is identically zero, hence:

$$\int_Y \overline{\chi}_n(y, \nabla_x\phi) \left(L_1 u_0 - \lambda(t)|u_0|^{2\sigma} u_0\right) \mathrm{d}y = 0 \tag{3.3}$$

is a necessary condition such that (3.1) can be solved for u_1 in terms of u_0. This condition is known to be sufficient, from the orthogonal decomposition method (also known as "Feschbach method"), since E_n is an isolated eigenvalue. After some lengthy computations, given in the appendix, we find that (3.3) is equivalent to the following *nonlinear transport equation* for a_0:

$$\begin{aligned} \partial_t a_0 + \mathcal{L} a_0 - \beta(t,x) a_0 &= \mathrm{i}\kappa(t,x)|a_0|^{2\sigma} a_0, \\ a_0\big|_{t=0} &= a_I(x). \end{aligned} \tag{3.4}$$

Here, $\mathcal{L}$ is the usual (geometrical optics) transport operator associated to $h_n^{\mathrm{sc}}(k,x)$:

$$\mathcal{L} a_0 := \nabla_k E_n(\nabla_x\phi) \cdot \nabla_x a_0 + \frac{1}{2}\operatorname{div}_x(\nabla_k E_n(\nabla_x\phi)) a_0. \tag{3.5}$$

Moreover, we have

$$\begin{aligned} \beta(t,x) &:= \langle \chi_n(\cdot, \nabla_x\phi),\ \nabla_k \chi_n(\cdot, \nabla_x\phi)\rangle_{L^2(Y)} \cdot \nabla_x U(x) \\ &\equiv \sum_{l=1}^d \big\langle \chi_n(\cdot, \nabla_x\phi),\ \frac{\partial}{\partial k_l}\chi_n(\cdot, \nabla_x\phi)\big\rangle_{L^2(Y)} \frac{\partial}{\partial x_l} U(x) \end{aligned} \tag{3.6}$$

and

$$\kappa(t,x) := -\lambda(t) \int_Y |\chi_n\,(y, \nabla_x\phi(t,x))|^{2\sigma+2}\,\mathrm{d}y. \tag{3.7}$$

This term can be interpreted as an *effective coupling* of the selfinteraction within the nth-energy band. Note that (2.12) implies

$$\operatorname{Re}\langle \chi_n(\cdot,k),\ \nabla_k\chi_n(\cdot,k)\rangle_{L^2(Y)} \equiv 0.$$

Hence, $\beta(t,x) = i\,\operatorname{Im}\beta(t,x)$ only contributes a variation in the phase of a_0, the so called *Berry phase*.[10,34] It is due to the interaction of the lattice and the slowly varying potential U. In our case the Berry phase in addition gets modulated in a *nonlinear* way by the right hand side of (3.4).

Remark 3.1. The term $-\mathrm{i}\beta =: \mathcal{A}_n$ can be interpreted as a gauge potential, i.e. a connection in the (complex) eigenspace-bundle corresponding to $E_n(k)$, cf. ref. 10. For some particular lattice configurations (if the crystal has a center of inversion, or some other special symmetry), the curvature of the Berry connection $\Omega_n := \nabla \times \mathcal{A}_n$ is identically zero, and the Berry connection is a closed 1-form, cf. refs. 10, 34 and 35 for a broader discussion on this.

Remark 3.2. We provide a link with some already existing results. In refs. 10 and 11 the authors, roughly speaking, prove that in each isolated Bloch band $E_n(k)$ the linear Hamiltonian H^ε, defined in (2.3), can be unitarily mapped into an *effective* band Hamiltonian h_n^ε, which is the Weyl quantization of the semi-classical symbol

$$h_n^\varepsilon(k,x) \sim h_n^{\mathrm{sc}}(k,x) + \varepsilon h_1(k,x) + O(\varepsilon^2).$$

This is done by constructing an ε-dependent unitary operator, which block-diagonalizes the *Bloch–Floquet Hamiltonian* of the system, such that the relevant band decouples from the rest of the spectrum. Above the *principal symbol* $h_n^{\mathrm{sc}}(k,x)$ is defined as in (2.14) and the first order correction is such that

$$h_1(\nabla_x \phi(t,x), x) \equiv \mathrm{i}\beta(t,x).$$

Additional terms appear in $h_1(k,x)$ if one includes external magnetic fields too, cf. refs. 10 and 11.

The following lemma proves that (3.4) has a smooth solution up to caustics.

Lemma 3.3. Assume $\phi \in C^\infty([0,\tau[\times\mathbb{R}^d)$, and $a_I \in \mathcal{S}(\mathbb{R}^d;\mathbb{C})$. Then along the flow $(t,x) \mapsto X_t(x)$, (3.4) has a unique solution $a_0 \in C^\infty([0,\tau[; \mathcal{S}(\mathbb{R}^d))$, given by

$$a_0(t, X_t(x)) = \frac{a_I(x)}{\sqrt{J_t(x)}} \exp\left(\mathrm{i}|a_I(x)|^{2\sigma} \int_0^t \frac{\kappa(s, X_s(x))}{|J_s(x)|^\sigma}\,\mathrm{d}s \right. \\ \left. + \int_0^t \beta(s, X_s(x))\,\mathrm{d}s\right).$$

Proof. Using Liouville's formula,

$$\frac{\mathrm{d}}{\mathrm{d}t}\,J_t(x) = \operatorname{div}_x\Big(\nabla_k E_n\big(\nabla_x\phi\,(t,X_t(x))\big)\Big)\,J_t(x);\quad J_0(x) = 1\,,$$

we rewrite the transport equation (3.4) as an ordinary differential equation along the flow defined by the dynamical system (2.15). Let $\alpha_0(t,x) := a_0(t,X_t)$:

$$\frac{1}{\sqrt{J_t(x)}}\frac{\mathrm{d}}{\mathrm{d}t}\,(\sqrt{J_t(x)}\alpha_0) = \beta\,(t,X_t)\,\alpha_0 + \mathrm{i}\kappa\,(t,X_t)\,|\alpha_0|^{2\sigma}\alpha_0,\quad |t|<\tau.$$

If we define $\tilde{\alpha}_0 := \sqrt{J_t(x)}\alpha_0$, then the principal amplitude is determined by

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\,\tilde{\alpha}_0 &= \beta\,(t,X_t(x))\,\tilde{\alpha}_0 + \mathrm{i}\kappa\,(t,X_t(x))\,\frac{|\tilde{\alpha}_0|^{2\sigma}}{|J_t(x)|^{\sigma}}\tilde{\alpha}_0,\quad |t|<\tau,\\ \tilde{\alpha}_0\big|_{t=0} &= a_I(x).\end{aligned}\tag{3.8}$$

This implies (since $\beta(t,x)\in\mathrm{i}\mathbb{R}$ and $\kappa(t,x)\in\mathbb{R}$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\,|\tilde{\alpha}_0(t,x)|^2 = 0,\quad \text{hence } |\tilde{\alpha}_0(t,x)| \equiv |a_I(x)|\,,\quad \forall\, t\in[0,\tau[\,.$$

Define the phase shift g of $\tilde{\alpha}_0$ by $\tilde{\alpha}_0(t,x) = a_I(x)\mathrm{e}^{\mathrm{i}g(t,x)}$. Then g solves

$$\frac{\mathrm{d}}{\mathrm{d}t}g(t,x) = \operatorname{Im}\,\beta\,(t,X_t(x)) + \kappa\,(t,X_t(x))\,\frac{|\tilde{\alpha}_0(t,x)|^{2\sigma}}{|J_t(x)|^{\sigma}}$$

with $g\big|_{t=0} = 0$. Inserting $|\tilde{\alpha}_0(t,x)| = |a_I(x)|$ yields the lemma, since $x\mapsto X_t(x)$ is a diffeomorphism of $\mathbb{R}^d$ for fixed $t\in[0,\tau[$. ∎

Remark 3.4. Note that along the flow

$$\beta\,(t,X_t(x)) = \Big\langle \chi_n\,(\cdot,\nabla_x\phi\,(t,X_t(x)))\,,\,\frac{\mathrm{d}}{\mathrm{d}t}\chi_n\,(\cdot,\nabla_x\phi\,(t,X_t(x)))\Big\rangle_{L^2(Y)},$$

which is exactly the same expression as given in ref. 19, there however the authors do not distinguish between a_0 and $\tilde{\alpha}_0$.

So far we explicitly constructed an approximate solution, which solves (1.1) up to terms of order $O(\varepsilon)$, since u_1 is not fully defined yet. To obtain a better approximation we need to set the term b_2 in (2.4) equal to zero, which gives

$$\begin{aligned} &H_\Gamma(\nabla_x\phi)u_2+(U(x)+\partial_t\phi)\,u_2 \\ &\quad=L_1u_1+L_2u_0-\lambda(t)\Big((2\sigma+1)|u_0|^{2\sigma}u_1+2\sigma|u_0|^{2\sigma-2}u_0^2\overline{u}_1\Big), \end{aligned} \tag{3.9}$$

where for $u_0(t,x,y)=a_0(t,x)\chi_n(y,\nabla_x\phi)$ we define

$$L_2u_0:=\frac{1}{2}\,\Delta_x u_0.$$

Introduce the notations

$$L_0(t,x)=H_\Gamma(\nabla_x\phi)+U(x)+\partial_t\phi(t,x);\qquad F(z)=|z|^{2\sigma}z\,. \tag{3.10}$$

From (2.7), L_0 is a (t,x)-dependent operator in y, and since $\sigma\in\mathbb{N}$, F is smooth. The following projector was used to derive the transport equation (3.4):

$$\Pi_n(t,x)\left(\sum_{j=1}^{\infty}\alpha_j(t,x)\chi_j\left(y,\nabla_x\phi(t,x)\right)\right)=\alpha_n(t,x)\chi_n\left(y,\nabla_x\phi(t,x)\right). \tag{3.11}$$

Define $Q(t,x)=Id-\Pi_n(t,x)$. This operator is smooth, and a partial inverse for L_0 can be defined on its range (by elliptic inversion): $L_0^{-1}Q$ is well-defined, and smooth (up to caustics). Applying the operator Π_n to (3.9), the solvability condition reads

$$\int_Y\overline{\chi}_n(y,\nabla_x\phi)\left(L_1u_1+L_2u_0-\lambda(t)\frac{\mathrm{d}}{\mathrm{d}s}F(u_0+su_1)\Big|_{s=0}\right)\mathrm{d}y=0. \tag{3.12}$$

We decompose u_1 as

$$u_1(t,x,y)=a_1(t,x)\chi_n\left(y,\nabla_x\phi(t,x)\right)+u_1^\perp(t,x,y), \tag{3.13}$$

where a_1 is some yet unknown function and $u_1^\perp$ is such that

$$\Pi_n(t,x)u_1^\perp(t,x,\cdot)=\langle\chi_n(\cdot,\nabla_x\phi),u_1^\perp(t,x,\cdot)\rangle_{L^2(Y)}=0,\quad\forall\,(t,x)\in[0,\tau[\times\mathbb{R}^d.$$

Now, $u_1^\perp$ is determined by (3.1)

$$u_1^\perp = L_0^{-1} Q\left(L_1 u_0 - \lambda(t) F(u_0)\right), \tag{3.14}$$

which implies $u_1^\perp \in C^\infty([0,\tau[;\mathcal{S}(\mathbb{R}^d))$, since u_0 is, by Lemma 3.3. Note that this relations *imposes* a particular form for the initial perturbation φ_I^ε, that is

$$Q(0,x)\varphi_I^\varepsilon(x) = \mathrm{e}^{\mathrm{i}\frac{\phi_I(x)}{\varepsilon}} \left(L_0^{-1} Q\right)(0,x)\left(L_1 u_I - \lambda(0) F(u_I)\right) + \mathcal{O}(\varepsilon). \tag{3.15}$$

The term $\mathcal{O}(\varepsilon)$ will be defined more precisely later on. On the other hand, plugging (3.13) into (3.12) yields an inhomogeneous *linear* version of the transport equation (3.4) for a_1 (the propagating part of u_1):

$$\partial_t a_1 + \mathcal{L} a_1 - \beta(\nabla_x \phi, x) a_1 + \mathrm{i}\lambda(t) \frac{\mathrm{d}}{\mathrm{d}s} F(u_0 + s a_1)\Big|_{s=0} = \mathtt{S}(t,x),$$

where we may choose $a_1\big|_{t=0} = 0$. The complex-valued source term $\mathtt{S}(t,x)$ is given by

$$\mathtt{S}(t,x) = \mathrm{i}\Pi_n(t,x)\left(L_1 u_1^\perp + L_2 u_0\right) = \mathrm{i}\left\langle \chi_n(\cdot, \nabla_x \phi),\ L_1 u_1^\perp + L_2 u_0 \right\rangle_{L^2(Y)}. \tag{3.16}$$

By this procedure, all higher order terms $u_j(t,x,y)$, $j \geqslant 1$, of the asymptotic solution (2.1) can be obtained (recall that the nonlinearity F is smooth). Clearly we have that $u_j \in C^\infty([0,\tau[;\mathcal{S}(\mathbb{R}^d))$ for all $j \geqslant 1$. At each step however, an additional condition must be imposed recursively for the initial datum ψ_I^ε. This approach is very similar to the one followed in ref. 20, except that the Fourier modes are replaced by "Bloch modes".

Under the assumption (2.1), (2.2), we construct an approximate solution, which solves (1.1) up to a remainder $O(\varepsilon^\infty)$, provided that the initial data are well-prepared. To state precisely this property, define, for $N \geq 0$,

$$\mathrm{v}_N^\varepsilon(t,x) := \ v_N^\varepsilon\left(t,x,\frac{x}{\varepsilon}\right) \mathrm{e}^{\mathrm{i}\phi(t,x)/\varepsilon} \equiv \left(\sum_{j=0}^{N} \varepsilon^j u_j\left(t,x,\frac{x}{\varepsilon}\right)\right) \mathrm{e}^{\mathrm{i}\phi(t,x)/\varepsilon}. \tag{3.17}$$

We will use the following spaces, for $s \in \mathbb{N}$: let

$$\| f^\varepsilon \|_{X^s_\varepsilon} := \sum_{|\alpha|+|\beta| \leqslant s} \left\| x^\alpha (\varepsilon \partial)^\beta f^\varepsilon \right\|_{L^2} .$$

We define X^s_ε as

$$X^s_\varepsilon := \left\{ f^\varepsilon \in L^2(\mathbb{R}^d); \quad \sup_{0<\varepsilon\leqslant 1} \| f^\varepsilon \|_{X^s_\varepsilon} < +\infty \right\} .$$

These spaces are reminiscent of the spaces $H^s_\varepsilon(\mathbb{R}^d)$ introduced in ref. 36 (see also ref. 37). There the dependence upon ε is to recall that exactly one negative power of ε appears every time the approximate wave function is differentiated. In our case, such negative powers also appear because of the variable y and the substitution $y = x/\varepsilon$. The control of the momenta is needed because of the potential U (it would not be needed in the proof of Theorem 4.5 below with U sub-linear). We can now state precisely the assumptions on the initial data.

Assumption 3.5. (well-prepared initial data). The initial data ψ^ε_I satisfy Assumptions 2.1 and 2.3, and for some $K \in \mathbb{N}$, the perturbation φ^ε_I is of the form

$$\varphi^\varepsilon_I(x) = \mathrm{e}^{\mathrm{i}\phi_I(x)/\varepsilon} \sum_{j=1}^{K} \varepsilon^{j-1} \varphi_j(x, y)\Big|_{y=x/\varepsilon} + \mathcal{O}\left(\varepsilon^K\right) , \tag{3.18}$$

where the $\mathcal{O}\left(\varepsilon^K\right)$ holds in X^s_ε for any $s \in \mathbb{N}$. The function $\mathrm{e}^{\mathrm{i}\phi_I/\varepsilon}\varphi_1$ is given by the first term of the right-hand side of (3.15), and if we denote $\varphi_0 = u_I$, $\varphi_j(x, y)$ is given recursively for $0 \le j \le K-2$ by

$$\varphi_{j+2} = \left(L_0^{-1} Q\right)(0, x) \left(L_1 \varphi_{j+1} + L_2 \varphi_j - \lambda(0) \frac{\mathrm{d}^{j+1}}{\mathrm{d}s^{j+1}} F\left(u_I + \sum_{\ell=1}^{j+1} s^\ell \varphi_\ell \right)\Big|_{s=0} \right) .$$

In the case $K = 0$, the sum in (3.18) is zero.

Remark 3.6. We chose to impose $\Pi_n(0, x)\varphi_j(x, \cdot) = 0$ for $j \ge 1$ (when we picked $a_1\big|_{t=0} = 0$ for instance). Our approach would also work with nonzero, smooth data $(\varphi_j)_{1\le j\le K}$ not necessarily satisfying this polarization property. All this approach is very similar to the one followed in ref. 38 to justify nonlinear geometric optics for hyperbolic equations (see also refs. 20, and 37 for the dispersive case).

We have the following Borel type lemma (see e.g. ref. 37):

Lemma 3.7. There exists $\widetilde{\psi}_I^\varepsilon \in \mathcal{S}(\mathbb{R}^d)$ satisfying Assumption 3.5, such that (3.18) holds for any $K \in \mathbb{N}$.

First, we will justify the asymptotics when the initial datum is given by the above lemma. We will then show how to relax this assumption. Note that the above approach is a nonlinear analog to the procedure followed in ref. 11. In ref. 11, the authors construct ε-dependent "super-adiabatic" subspaces, in order to prove higher order asymptotics in the linear case. In the present context, high order asymptotics are needed to control the nonlinear terms (see the proof of Theorem 4.5).

Proposition 3.8. Let $\widetilde{\psi}_I^\varepsilon$ as in Lemma 3.7. Let $\tau > 0$ be the time at which the first caustic is formed (if any). Then for any $N \in \mathbb{N}$, v_N^ε solves

$$\begin{aligned} i\varepsilon\partial_t \mathrm{v}_N^\varepsilon - H^\varepsilon \mathrm{v}_N^\varepsilon &= \varepsilon\lambda(t)\, |\mathrm{v}_N^\varepsilon|^{2\sigma} \mathrm{v}_N^\varepsilon + \varepsilon^{N+1} r_N^\varepsilon, \\ \mathrm{v}_N^\varepsilon\big|_{t=0} &= \widetilde{\psi}_I^\varepsilon + \varepsilon^{N+1}\rho_N^\varepsilon, \end{aligned} \tag{3.19}$$

where H^ε is defined by (2.3) and $r_N^\varepsilon \in C^\infty([0,\tau[;\, \mathcal{S}(\mathbb{R}^d))$, $\rho_N^\varepsilon \in \mathcal{S}(\mathbb{R}^d)$ are such that $r_N^\varepsilon \in L^\infty_{\rm loc}([0,\tau[;\, X_\varepsilon^s)$ and $\|\rho_N^\varepsilon\|_{X_\varepsilon^s} = \mathcal{O}(1)$ for any $s \in \mathbb{N}$.

4. NONLINEAR STABILITY OF THE APPROXIMATE SOLUTION

To prove that the above WKB-method yields a good approximation of the exact solution, a nonlinear stability result is needed. First, we make our assumptions on the potentials precise, and establish an existence result for (1.1). Next, we prove the validity of the approximation derived above.

Assumption 4.1. The potentials are smooth, real-valued: $V_\Gamma, U \in C^\infty(\mathbb{R}^d;\mathbb{R})$.

(i) V_Γ is Γ-periodic, i.e. it satisfies (1.2).

(ii) U is sub-quadratic: $\partial^\alpha U \in L^\infty(\mathbb{R}^d)$, $\quad \forall \alpha \in \mathbb{N}^d$ such that $|\alpha| \geqslant 2$.

Remark 4.2. The assumptions on U include the cases of an isotropic harmonic potential ($U(x) = |x|^2$), and of an anisotropic harmonic potential ($U(x) = \sum \omega_j^2 x_j^2$). It may also be taken equal to zero, or incorporate a linear component $E \cdot x$, modeling a constant electric field (*Stark effect*, see e.g. ref. 39).

4.1. Existence of Solutions to (1.1)

Lemma 4.3. Let Assumption 4.1 be satisfied, and let $\psi_I^\varepsilon \in \mathcal{S}(\mathbb{R}^d)$, the Schwartz space. Let $s > d/2$. Then there exists $t^\varepsilon > 0$ and a unique $\psi^\varepsilon \in C(]-t^\varepsilon, t^\varepsilon[; H^s(\mathbb{R}^d))$ solution to (1.1). Moreover, $x^\alpha \psi^\varepsilon \in C(]-t^\varepsilon, t^\varepsilon[; H^s(\mathbb{R}^d))$ for any $\alpha \in \mathbb{N}^d$, $s \in \mathbb{N}$, and the following conservation holds

$$\frac{\mathrm{d}}{\mathrm{d}t} \| \psi^\varepsilon(t) \|_{L^2} = 0 .$$

Proof. Since the dependence upon ε is irrelevant at this stage, the above statement follows from the study of

$$\mathrm{i}\partial_t \psi = -\frac{1}{2}\Delta\psi + W(x)\psi + \lambda(t)\,|\psi|^{2\sigma}\psi; \quad \psi\big|_{t=0} = \psi_I(x), \tag{4.1}$$

where

- the potential W is smooth, real-valued and sub-quadratic,
- $\lambda(t)$ is a smooth real-valued function,
- $\sigma \in \mathbb{N}$,
- $\psi_I \in \mathcal{S}(\mathbb{R}^d)$.

The dependence of the local existence time t^ε upon ε appears with scaling. Notice that the nonlinearity $z \mapsto |z|^{2\sigma} z$ is smooth, because $\sigma \in \mathbb{N}$. Since W is sub-quadratic, the Hamiltonian $-\frac{1}{2}\Delta + W$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d)$ (see for instance[40]). The assumption $s > d/2$ yields $H^s(\mathbb{R}^d) \subset L^\infty(\mathbb{R}^d)$. Therefore, local existence and uniqueness in $H^s(\mathbb{R}^d)$ follow from a fixed point argument, using Schauder's lemma (see e.g. refs. 37 and 41).

To prove higher order regularity of ψ and its momenta, one can follow the proof of ref. 42 (see also ref. 41). That article is for the case $W \equiv 0$; the proof uses Strichartz inequalities, following from dispersion estimates. When W is smooth, real-valued and sub-quadratic, the same dispersion estimates are available,[43,44] and they imply the same Strichartz inequalities.[45] Another difference with[42] is that the Galilean operator $x + \mathrm{i}t\nabla_x$ commutes with $\mathrm{i}\partial_t + 1/2\Delta$, but in general not with $\mathrm{i}\partial_t + 1/2\Delta - W$. This is not a problem in view of the above result, since

$$[x + \mathrm{i}t\nabla_x, W] = \mathrm{i}t\nabla W = \mathcal{O}(1 + |x|) .$$

Thus, ψ, $x\psi$ and $\nabla_x\psi$ solve a coupled, closed system of Schrödinger equations. A similar argument allows to treat higher order momenta and derivatives.

The conservation of the L^2-norm follows from standard arguments (see ref. 41). ∎

Remark 4.4. One cannot expect global existence in general. For instance, if $\lambda(t)$ is a negative constant and if $\sigma > 2/d$, finite time blow-up may occur (see e.g. ref. 41). On the other hand, we shall prove below that the solution ψ^ε cannot blow-up before a caustic is formed, at least for ε sufficiently small.

Notation. Let $(\alpha^\varepsilon)_{0<\varepsilon\leqslant 1}$ and $(\beta^\varepsilon)_{0<\varepsilon\leqslant 1}$ be two families of positive numbers. In the following we shall write

$$\alpha^\varepsilon \lesssim \beta^\varepsilon,$$

if there exists a $C > 0$, independent of $\varepsilon \in]0,1]$, such that

$$\alpha^\varepsilon \leqslant C\beta^\varepsilon \quad \text{for all } \varepsilon \in]0,1].$$

(The C may very well depend on other parameters.)

4.2. Accuracy of the Approximation

The main result we shall prove is the following.

Theorem 4.5. (stability result). Let $\psi_I^\varepsilon = \widetilde{\psi}_I^\varepsilon$ as in Lemma 3.7. Let $\tau > 0$ given by (2.17), and v_N^ε given by (3.17). Then for any $\tau_0 \in]0,\tau[$, there exists $\varepsilon_0 > 0$ such that for $0 < \varepsilon \leqslant \varepsilon_0$, the solution ψ^ε to (1.1) is defined up to time τ_0. Moreover, for any $N \in \mathbb{N}$ and $s \in \mathbb{N}$,

$$\sup_{0\leqslant t\leqslant\tau_0} \left\| \psi^\varepsilon(t) - \mathrm{v}_N^\varepsilon(t) \right\|_{X_\varepsilon^s} = \mathcal{O}\left(\varepsilon^{N+1}\right). \tag{4.2}$$

Proof. For $N \in \mathbb{N}$, we define the error term as $\mathtt{w}_N^\varepsilon := \psi^\varepsilon - \mathrm{v}_N^\varepsilon$. From (1.1) and (3.19), it solves

$$\begin{aligned} i\varepsilon\partial_t \mathtt{w}_N^\varepsilon &= H^\varepsilon \mathtt{w}_N^\varepsilon + \varepsilon\lambda(t)\left(|\psi^\varepsilon|^{2\sigma}\psi^\varepsilon - |\mathrm{v}_N^\varepsilon|^{2\sigma}\mathrm{v}_N^\varepsilon\right) - \varepsilon^{N+1} r_N^\varepsilon, \\ \mathtt{w}_N^\varepsilon\big|_{t=0} &= \varepsilon^{N+1}\rho_N^\varepsilon, \end{aligned} \tag{4.3}$$

where H^ε is defined by (2.3). We start with the standard energy estimate for Schrödinger equations: multiply the above equation by $\overline{\mathtt{w}_N^\varepsilon}$, integrate over $\mathbb{R}^d$ and take the imaginary part. Since H^ε is self-adjoint, this yields

$$\varepsilon\partial_t \left\| \mathtt{w}_N^\varepsilon(t) \right\|_{L^2} \lesssim \varepsilon|\lambda(t)| \left\| |\psi^\varepsilon|^{2\sigma}\psi^\varepsilon - |\mathtt{v}_N^\varepsilon|^{2\sigma}\mathtt{v}_N^\varepsilon \right\|_{L^2} + \varepsilon^{N+1} \left\| r_N^\varepsilon(t) \right\|_{L^2}.$$

Since we work on the fixed, finite interval $t \in [0, \tau_0]$, the smooth function λ is bounded, and the above estimate implies:

$$\partial_t \left\| \mathtt{w}_N^\varepsilon(t) \right\|_{L^2} \lesssim \left\| |\psi^\varepsilon|^{2\sigma}\psi^\varepsilon - |\mathtt{v}_N^\varepsilon|^{2\sigma}\mathtt{v}_N^\varepsilon \right\|_{L^2} + \varepsilon^{N} \left\| r_N^\varepsilon(t) \right\|_{L^2}. \tag{4.4}$$

The idea is now to factor out $\mathtt{w}_N^\varepsilon$ in the right hand side of the above inequality, and take advantage of the smallness of the source term. To carry out this argument, we follow the method used to justify (nonlinear) geometric optics for hyperbolic systems; we refer to ref. 37 for an expository presentation.

Following[37] (Lemma 8.1) we have the following Moser-type lemma.

Lemma 4.6. Let $R>0$, $s \in \mathbb{N}$, and $F(z) = |z|^{2\sigma}z$ for $\sigma \in \mathbb{N}$. Then there exists $C = C(R, s, \sigma, d)$ such that if $\mathtt{v}$ satisfies

$$\left\| x^\alpha (\varepsilon\partial)^\beta \mathtt{v} \right\|_{L^\infty(\mathbb{R}^d)} \leqslant R \quad \text{for all } |\alpha| + |\beta| \leqslant s,$$

and $\mathtt{w}$ satisfies $\|\mathtt{w}\|_{L^\infty(\mathbb{R}^d)} \leqslant R$, then

$$\sum_{|\alpha|+|\beta|\leqslant s} \left\| x^\alpha (\varepsilon\partial)^\beta \left(F(\mathtt{v}+\mathtt{w}) - F(\mathtt{v})\right) \right\|_{L^2(\mathbb{R}^d)} \leqslant C \sum_{|\alpha|+|\beta|\leqslant s} \left\| x^\alpha (\varepsilon\partial)^\beta \mathtt{w} \right\|_{L^2(\mathbb{R}^d)}.$$

Sketch of the proof of Lemma 4.6. When X_ε^k is replaced by H_ε^k (remove the control of the momenta), the result is exactly[37] (Lemma 8.1). The idea is to factor out $\mathtt{w}$ in the quantity $F(\mathtt{v}+\mathtt{w}) - F(\mathtt{v})$ using the fundamental theorem of calculus, then to use Leibniz' rule, to conclude with Gagliardo–Nirenberg inequalities. In the case of X_ε^k, the control of the momenta follows easily. ∎

We first notice that $\mathtt{v}_N^\varepsilon$ is uniformly bounded in $L^\infty([0, \tau_0] \times \mathbb{R}^d)$. To prove that $\mathtt{w}_N^\varepsilon$ is bounded in $L^\infty([0, \tau_0] \times \mathbb{R}^d)$, we use a continuity argument, and prove that it is actually small in that space, for N sufficiently large. This will be a consequence of the Gagliardo–Nirenberg inequalities:

$$\text{for } s > d/2, \quad \|\mathtt{w}\|_{L^\infty(\mathbb{R}^d)} \lesssim \|\mathtt{w}\|_{H^s(\mathbb{R}^d)} \lesssim \varepsilon^{-d/2} \|\mathtt{w}\|_{X_\varepsilon^s}. \tag{4.5}$$

(The scaling factor $\varepsilon^{-d/2}$ is obvious when one uses Fourier transform.)

By construction, $\mathtt{w}_N^\varepsilon(0,x)=\mathcal{O}\left(\varepsilon^{N+1}\right)$ in any space X_ε^s. We first prove the result for N sufficiently large, then show how to get rid of this assumption. From Lemma 4.3, there exists $t(\varepsilon,R)>0$ such that if $N+1>d/2$, then for ε sufficiently small,

$$\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{L^\infty(\mathbb{R}^d)}\leqslant R \tag{4.6}$$

for $t\in[0,t(\varepsilon,R)]$. As long as (4.6) holds, (4.4) and Lemma 4.6 with $s=0$ imply

$$\partial_t\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{L^2}\leqslant C\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{L^2}+C\varepsilon^N\left\|r_N^\varepsilon(t)\right\|_{L^2},$$

and from Gronwall lemma, as long as (4.6) holds for $t\leqslant\tau_0$, we get that

$$\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{L^2}\leqslant C\varepsilon^N. \tag{4.7}$$

The idea is now to obtain similar estimates for the momenta and derivatives of $\mathtt{w}_N^\varepsilon$.

Applying the operator $\varepsilon\nabla_x$ to (4.3) yields:

$$\begin{aligned}i\varepsilon\partial_t(\varepsilon\nabla_x\mathtt{w}_N^\varepsilon) &= H^\varepsilon(\varepsilon\nabla_x\mathtt{w}_N^\varepsilon)+\varepsilon\lambda(t)(\varepsilon\nabla_x)\left(F(\psi^\varepsilon)-F(\mathrm{v}_N^\varepsilon)\right)\\ &\quad+[\varepsilon\nabla,H^\varepsilon]\mathtt{w}_N^\varepsilon-\varepsilon^{N+1}\varepsilon\nabla_x r_N^\varepsilon.\end{aligned}$$

The same energy estimate as before gives:

$$\begin{aligned}\partial_t\left\|\varepsilon\nabla_x\mathtt{w}_N^\varepsilon(t)\right\|_{L^2} &\lesssim \left\|\varepsilon\nabla_x\left(F(\psi^\varepsilon)-F(\mathrm{v}_N^\varepsilon)\right)\right\|_{L^2}+\frac{1}{\varepsilon}\left\|[\varepsilon\nabla,H^\varepsilon]\mathtt{w}_N^\varepsilon\right\|_{L^2}\\ &\quad+\varepsilon^N\left\|\varepsilon\nabla_x r_N^\varepsilon\right\|_{L^2}.\end{aligned}$$

But we have

$$[\varepsilon\nabla,H^\varepsilon]=(\nabla V_\Gamma)\left(\frac{x}{\varepsilon}\right)+\varepsilon\nabla U(x).$$

Since ∇V_Γ is bounded and ∇U is sub-linear, the above estimate yields

$$\begin{aligned}\partial_t\left\|\varepsilon\nabla_x\mathtt{w}_N^\varepsilon(t)\right\|_{L^2} &\lesssim \left\|\varepsilon\nabla_x\left(F(\psi^\varepsilon)-F(\mathrm{v}_N^\varepsilon)\right)\right\|_{L^2}+\frac{1}{\varepsilon}\left\|\mathtt{w}_N^\varepsilon\right\|_{L^2}+\left\|x\mathtt{w}_N^\varepsilon\right\|_{L^2}\\ &\quad+\varepsilon^N\left\|\varepsilon\nabla_x r_N^\varepsilon\right\|_{L^2}\\ &\lesssim \left\|\varepsilon\nabla_x\mathtt{w}_N^\varepsilon\right\|_{L^2}+\left\|x\mathtt{w}_N^\varepsilon\right\|_{L^2}+\varepsilon^{N-1},\end{aligned} \tag{4.8}$$

where we have used Proposition 3.8, Lemma 4.6 with $s=1$, and (4.7). We see that when U is quadratic, we have to find a similar estimate for $\|x\mathtt{w}_N^\varepsilon\|_{L^2}$. For that, multiply (4.3) by x

$$i\varepsilon\partial_t(x\mathtt{w}_N^\varepsilon) = H^\varepsilon(x\mathtt{w}_N^\varepsilon) + \varepsilon\lambda(t)x\left(F(\psi^\varepsilon) - F(\mathtt{v}_N^\varepsilon)\right) + [x, H^\varepsilon]\mathtt{w}_N^\varepsilon - \varepsilon^{N+1}xr_N^\varepsilon.$$

Since $[x, H^\varepsilon] = -\varepsilon^2\nabla_x$, the energy estimate yields, as long as (4.6) holds

$$\begin{aligned}\partial_t \left\|x\mathtt{w}_N^\varepsilon(t)\right\|_{L^2} &\lesssim \left\|x\left(F(\psi^\varepsilon) - F(\mathtt{v}_N^\varepsilon)\right)\right\|_{L^2} + \left\|\varepsilon\nabla_x\mathtt{w}_N^\varepsilon\right\|_{L^2} + \varepsilon^N\left\|\varepsilon\nabla_x r_N^\varepsilon\right\|_{L^2} \\ &\lesssim \left\|x\mathtt{w}_N^\varepsilon(t)\right\|_{L^2} + \left\|\varepsilon\nabla_x\mathtt{w}_N^\varepsilon\right\|_{L^2} + \varepsilon^N. \end{aligned} \tag{4.9}$$

Putting (4.8) and (4.9) together, we have

$$\partial_t\left(\left\|\varepsilon\nabla_x\mathtt{w}_N^\varepsilon\right\|_{L^2} + \left\|x\mathtt{w}_N^\varepsilon(t)\right\|_{L^2}\right) \lesssim \left\|\varepsilon\nabla_x\mathtt{w}_N^\varepsilon\right\|_{L^2} + \left\|x\mathtt{w}_N^\varepsilon(t)\right\|_{L^2} + \varepsilon^{N-1},$$

and a Gronwall lemma yields, as long as (4.6) holds

$$\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{X_\varepsilon^1} \lesssim \varepsilon^{N-1}. \tag{4.10}$$

One can check by induction that for $k \geqslant 0$, so long as (4.6) holds,

$$\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{X_\varepsilon^s} \lesssim \varepsilon^{N-s}. \tag{4.11}$$

We now take advantage of the Gagliardo–Nirenberg inequality (4.5). For $s > d/2$ and as long as (4.6) holds, we get

$$\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon^{-d/2}\left\|\mathtt{w}_N^\varepsilon(t)\right\|_{X_\varepsilon^s} \lesssim \varepsilon^{N-s-d/2}.$$

Thus, if $N-s-d/2>0$, a continuity argument shows that (4.6) holds up to time τ_0 provided that ε is sufficiently small. In particular, $\mathtt{w}_N^\varepsilon$, hence ψ^ε, is well defined up to time τ_0 for $0<\varepsilon\leqslant\varepsilon(\tau_0)$. To complete the proof of Theorem 4.5, we have to prove (4.2). Fix $s, N \in \mathbb{N}$; let $s_1 \geqslant s$ such that $s_1 > d/2$, and $N_1 \geqslant s_1 + N + 1$. We infer from (4.11) that

$$\sup_{0\leqslant t\leqslant\tau_0}\left\|\mathtt{w}_{N_1}^\varepsilon(t)\right\|_{X_\varepsilon^{s_1}} \lesssim \varepsilon^{N_1-s_1} \lesssim \varepsilon^{N+1}.$$

It is straightforward that since $N_1 > N$,

$$\sup_{0\leqslant t\leqslant\tau_0}\left\|\mathtt{v}_N^\varepsilon(t) - \mathtt{v}_{N_1}^\varepsilon(t)\right\|_{X_\varepsilon^{s_1}} \lesssim \varepsilon^{N+1}.$$

We deduce that (4.2) holds for any $s, N \in \mathbb{N}$. ∎

Remark 4.7. A slightly shorter argument is available in the case $d \leqslant 3$, for which we have $H^2(\mathbb{R}^d) \subset L^\infty(\mathbb{R}^d)$, to prove Theorem 4.5 in the case $s=2$ only. The idea is to get an X^2_ε-estimate and use (4.5) again. Following an idea due initially to Kato,[46] consider the time derivative of the error $\mathtt{w}^\varepsilon_N$. One can prove that $\|\varepsilon\partial_t \mathtt{w}^\varepsilon_N(t)\|_{L^2} = \mathcal{O}(\varepsilon^N)$, as long as (4.6) holds. Plugging this into (4.3), we have, from (4.7) and since V_Γ is bounded and U is sub-quadratic:

$$\left\|\varepsilon^2 \Delta \mathtt{w}^\varepsilon_N(t)\right\|_{L^2} \lesssim \varepsilon^N + \left\|x^2 \mathtt{w}^\varepsilon_N(t)\right\|_{L^2}.$$

The control of $\|x^2\mathtt{w}^\varepsilon_N(t)\|_{L^2}$ is then similar to (4.9):

$$\left\|x^2 \mathtt{w}^\varepsilon_N(t)\right\|_{L^2} \lesssim \varepsilon^N + \left\|x^2 \mathtt{w}^\varepsilon_N(t)\right\|_{L^2} + \left\|\varepsilon^2 \Delta \mathtt{w}^\varepsilon_N(t)\right\|_{L^2},$$

and we can conclude as above.

Now it is easy to deduce the estimate announced in Theorem 1.1, when ψ^ε_I is as in Lemma 3.7. The L^2 estimate is (4.2) with $N=s=0$. We have an L^∞ estimate, mimicking the above proof: for $s>d/2$ and $N-d/2 \geqslant 1$, (4.2) and (4.5) yield

$$\sup_{0\leqslant t\leqslant \tau_0} \left\|\psi^\varepsilon(t) - \mathrm{v}^\varepsilon_N(t)\right\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon^{-d/2} \sup_{0\leqslant t\leqslant \tau_0} \left\|\psi^\varepsilon(t) - \mathrm{v}^\varepsilon_N(t)\right\|_{X^s_\varepsilon} \lesssim \varepsilon^{N-d/2} \lesssim \varepsilon.$$

It is straightforward that

$$\sup_{0\leqslant t\leqslant \tau_0} \left\|\mathrm{v}^\varepsilon_0(t) - \mathrm{v}^\varepsilon_N(t)\right\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon, \quad \text{hence} \quad \sup_{0\leqslant t\leqslant \tau_0} \left\|\psi^\varepsilon(t) - \mathrm{v}^\varepsilon_0(t)\right\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon.$$

Finally, we remove the assumption that ψ^ε_I is as in Lemma 3.7.

Proposition 4.8. Let $\widetilde{\psi}^\varepsilon$ be the solution to (1.1) with initial datum $\widetilde{\psi}^\varepsilon_I$ as in Lemma 3.7. Let ψ^ε_I satisfying Assumptions 2.1, 2.3 and 3.5 with $K \geq d$, and let ψ^ε be the solution to (1.1) with initial datum ψ^ε_I. Then for any $\tau_0 \in]0, \tau[$, there exists $\varepsilon_0 > 0$ such that for $0 < \varepsilon \leqslant \varepsilon_0$, ψ^ε is defined up to time τ_0. Moreover,

$$\sup_{0\leqslant t\leqslant \tau_0} \left\|\psi^\varepsilon(t) - \widetilde{\psi}^\varepsilon(t)\right\|_{X^s_\varepsilon} = \mathcal{O}\left(\varepsilon^{K+1-s}\right), \quad \text{for } s \geq 0.$$

Remark 4.9. We deduce that Theorem 1.1 holds with an $\mathcal{O}\left(\varepsilon^d\right)$ corrector in the initial datum. The L^2 estimate in Theorem 1.1 is straighforward, using Theorem 4.5. The L^∞ estimate (1.19) follows the same way, from (4.5). Notice that the larger K, the more precise asymptotics we infer; for example, if $K > d$, we can remove the restriction $\eta > 0$ in (1.19), using the above estimates and (4.5). When $s > K+1$, the above estimate does not look so good, since from Theorem 4.5, $\widetilde{\psi}^\varepsilon$ is bounded in X^s_ε. Yet, it gives some non-obvious control on ψ^ε.

Sketch of the proof of Proposition 4.8. The proof is very similar to that of Theorem 4.5, so we shall be brief. Introduce $\mathtt{w}^\varepsilon = \psi^\varepsilon - \widetilde{\psi}^\varepsilon$. It solves

$$\begin{cases} i\varepsilon\partial_t \mathtt{w}^\varepsilon = H^\varepsilon \mathtt{w}^\varepsilon + \varepsilon\lambda(t)\left(|\psi^\varepsilon|^{2\sigma}\psi^\varepsilon - |\widetilde{\psi}^\varepsilon|^{2\sigma}\widetilde{\psi}^\varepsilon\right) \\ \mathtt{w}^\varepsilon\big|_{t=0} = \mathcal{O}\left(\varepsilon^{K+1}\right) \quad \text{in } X^s_\varepsilon \text{ for any } s \in \mathbb{N}. \end{cases}$$

We can then follow the same lines as in the proof of Theorem 4.5: there is no source term (r^ε_N has disappeared), and the size of $\mathtt{w}^\varepsilon$ is determined by the size of its initial datum. We have

$$\|\mathtt{w}^\varepsilon_{|t=0}\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon^{-d/2}\|\mathtt{w}^\varepsilon_{|t=0}\|_{X^s_\varepsilon} \lesssim \varepsilon^{K+1-d/2}, \quad \text{provided that } s > \frac{d}{2}.$$

Since $K+1 > d/2$, we can start the argument of Theorem 4.5. Theorem 4.5 and Sobolev inequalities provide all the estimates we need for the "approximate" solution $\widetilde{\psi}^\varepsilon$; resuming all the arguments yields, so long as (4.6) holds,

$$\|\mathtt{w}^\varepsilon(t)\|_{X^s_\varepsilon} \lesssim \varepsilon^{K+1-s}.$$

Note that even if $K+1-s < 0$, we can apply a Gronwall argument to prove the above estimate. Since $K+1 > d$, we can choose $s > d/2$ (not necessarily an integer, but this causes no trouble, by interpolation) such that $K+1-s > d/2$. The above estimate and (4.5) show that (4.6) holds up to time τ_0, for $\varepsilon \ll 1$. ∎

5. GENERALIZATION AND CONSEQUENCES

5.1. Eigenvalue with Multiplicity

As a first generalization we remark that all given results could be extended to the case where $E_n(k)$ is an *isolated* but *m-fold degenerate* family of eigenvalues, i.e.

$$E_n(k) = E_*(k), \quad \forall n \in I \subset \mathbb{N}, \quad |I| = m.$$

Under the assumption (see ref. 28 for a discussion on this) that there exists a smooth orthonormal basis $\{\chi_l(k,y))\}_{l\in I}$ of ran $\Pi_I(k)$, where

$$\Pi_I(k) := \sum_{l=1}^{m} |\chi_l(k)\rangle\,\langle\chi_l(k)|$$

denotes the spectral projector corresponding to $E_*(k)$, the appropriate two-scale WKB–ansatz would then be

$$\psi^\varepsilon\left(t,x,\frac{x}{\varepsilon}\right) \sim \sum_{l=1}^{m} a_{0,l}(t,x)\chi_l\left(\frac{x}{\varepsilon},\nabla_x\phi(t,x)\right)\mathrm{e}^{\mathrm{i}\phi(t,x)/\varepsilon} + \mathcal{O}(\varepsilon), \quad (5.1)$$

with $\phi(t,x)$ given by the solution of the Hamilton–Jacobi equation (2.9) with $E_n(k)\equiv E_*(k)$. As in refs. 10 and 11 this would then lead to *matrix-valued* transport equations, which in our case are all coupled through the nonlinear term. The analysis of this system is analogous to the scalar case but leads to rather intricate and tedious computations, which is why we neglected this situation. Also, from the physical point of view it is known that for periodic potentials such degeneracies are rather exceptional. (For the study of a similar 2-fold degenerated situation we refer to ref. 21, where a semi-classical scaled nonlinear Dirac equation is analyzed.)

5.2. Wigner Measures

Since Theorem 4.5 yields strong asymptotics for the wave–function in $L^2(\mathbb{R}^d)$, we can compute the *Wigner measure* associated to the family $(\psi^\varepsilon)_{0<\varepsilon\leqslant 1}$. The Wigner measure of a family $(\psi^\varepsilon(t,\cdot))_{0<\varepsilon\leqslant 1}$ bounded in $L^2(\mathbb{R}^d)$ is the weak limit (up to the extraction of a subsequence) of its Wigner transform,

$$W^\varepsilon[\psi^\varepsilon(t)](x,\xi) = \int_{\mathbb{R}^d}\psi^\varepsilon\left(t,x-\frac{\varepsilon}{2}\eta\right)\overline{\psi^\varepsilon}\left(t,x+\frac{\varepsilon}{2}\eta\right)\mathrm{e}^{\mathrm{i}\xi\cdot\eta}\,\frac{\mathrm{d}\eta}{(2\pi)^d}. \quad (5.2)$$

This limit is then found to be a nonnegative Radon measure on phase space. The Wigner transform has proved to be an efficient tool in the study of semi-classical and homogenization limits (see e.g. refs. 6, 13, 14 and 22).

Corollary 5.1. Let $\psi^\varepsilon(t)$ be the unique local-time-solution of (1.1) on $[0,\tau_0]$, as guaranteed by Theorem 4.5, and let $W^\varepsilon[\psi^\varepsilon(t)]$ be its Wigner transform. Then, up to extraction of subsequences, we have

$$\lim_{\varepsilon\to 0} W^\varepsilon[\psi^\varepsilon]=\mu \quad \text{in } \mathcal{S}'([0,\tau_0)\times\mathbb{R}^d_x\times\mathbb{R}^d_\xi) \text{ weak-}\star, \tag{5.3}$$

where the Wigner measure $\mu(t)$ of $\psi^\varepsilon(t)$ is given by

$$\mu(t,x,\xi)=\frac{|a_I(x)|^2}{|J_t(x)|}\,\mathrm{d}x\otimes\sum_{\gamma^*\in\Gamma^*}\left|\int_{\mathbb{T}^d}\chi_n(y,k)\mathrm{e}^{-\mathrm{i}y\cdot\gamma^*}\frac{\mathrm{d}y}{(2\pi)^d}\right|^2\delta(\xi-k-\gamma^*), \tag{5.4}$$

with $k=\nabla_x\phi(t,x)\in\mathcal{B}$.

Proof. We have to compute

$$\lim_{\varepsilon\to 0}\int_{\mathbb{R}^{2d}} f(x,\xi)W^\varepsilon[\psi^\varepsilon(t)](x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi=\int_{\mathbb{R}^{2d}} f(x,\xi)\mu(t,\mathrm{d}x,\mathrm{d}\xi)$$

for any smooth test-function (observable) $f\in\mathcal{S}(\mathbb{R}^d_x\times\mathbb{R}^d_\xi)$. To this end, we plug the approximation v^ε_0 into the left hand side of this relation (that is, we use the strong L^2 convergence stated in Theorem 1.1). Since $\chi_n(y,k)$ is Γ-periodic w.r.t. $y\in\mathbb{R}^d$, we can rewrite it in form of a Fourier series:

$$\chi_n(y,k)=\frac{1}{(2\pi)^d}\sum_{\gamma^*\in\Gamma^*}\mathrm{e}^{\mathrm{i}y\cdot\gamma^*}\int_{\mathbb{T}^d}\chi_n(z,k)\mathrm{e}^{-\mathrm{i}z\cdot\gamma^*}\,\mathrm{d}z.$$

Using this representation, a non-stationary phase argument shows that all "non-diagonal" terms in (5.2) vanish in the limit $\varepsilon\to 0$ and hence (5.4) is obtained from a straightforward computation. ∎

In our case, the strong convergence stated in Theorem 4.5 shows that the Wigner measure of $(\psi^\varepsilon(t,\cdot))_{0<\varepsilon\leqslant 1}$ is the same as in the linear case (see ref. 14 [Section 5.1]), since the main nonlinear effect appears as an order $\mathcal{O}(1)$ phase ω, defined in Theorem 1.1. In other words, the Wigner measure does not "see" the nonlinearity. This can be compared with the Wigner measures studied in ref. 47, for equations similar to (1.1), without potential. For the same scaling as in (1.1), the main nonlinear effect was a "slowly" varying phase, which was invisible to the Wigner measure. It only appears as the first order correction in the Wigner transform.

5.3. Complex-valued Coupling Factor

When the coupling factor $\lambda(t)$ is not real-valued, the analysis may be completely different; the approximate solution may blow up before the caustic. The first hint is that the L^2–norm of ψ^ε is not formally conserved. Multiply (1.1) by $\overline{\psi^\varepsilon}$, integrate over $\mathbb{R}^d$ and take the imaginary part:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\|\psi^\varepsilon(t)\right\|_{L^2}^2 = 2\ \mathrm{Im}\,\lambda(t)\left\|\psi^\varepsilon(t)\right\|_{L^{2\sigma+2}}^{2\sigma+2}.$$

On the other hand, the formal analysis of Sections 2 and 3 still yields the transport equation (3.4), which can also be written as (3.8). Multiply (3.8) by $\overline{\tilde{a}_0}$ and take the real part:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}|\tilde{a}_0(X_t)|^2 &= -\,\mathrm{Im}\,\kappa(X_t)\frac{|\tilde{a}_0(X_t)|^{2\sigma+2}}{|J_t|^\sigma}\\ &\equiv \mathrm{Im}\,\lambda(t)\frac{|\tilde{a}_0(X_t)|^{2\sigma+2}}{|J_t|^\sigma}\int_Y |\chi_n(y,\nabla_x\phi)|^{2\sigma+2}\,\mathrm{d}y.\end{aligned}$$

The solution of this ordinary differential equation may blow up in finite time before a caustic is formed, and the WKB-analysis breaks down at blow-up time. The above equation for the evolution of $\|\psi^\varepsilon(t)\|_{L^2}^2$ suggests that the exact solution may also blow up. In that case, the limitation for the validity of the WKB-expansion would not be a drawback of the method (as it is in the case of caustics), but a genuine nonlinear effect.

APPENDIX A. DERIVATION OF THE LEADING ORDER TRANSPORT EQUATION

For the benefit of the reader, we shall discuss here in more detail how to pass from (3.3) to (3.4).

First, it will be convenient to rewrite (3.2) in a more symmetric form

$$L_1 u_0 = \mathrm{i}\partial_t u_0 - \frac{1}{2}\left[D_x\cdot(D_y+\nabla_x\phi)+(D_y+\nabla_x\phi)\cdot D_x\right]u_0,$$

where from now on $D_x := -\mathrm{i}\nabla_x$. Then, inserting

$$u_0(t,x,y) = a_0(t,x)\chi_n(y,\nabla_x\phi),$$

and denoting

$$g_n(t, x, y) = \chi_n\left(y, \nabla_x \phi(t, x)\right),$$

the solvability condition (3.3) can be written as

$$\partial_t a_0 + \langle g_n,\, \partial_t g_n \rangle_{L^2(Y)}\, a_0 + \frac{1}{2}\left\langle g_n,\, \nabla_x \cdot (D_y + \nabla_x \phi)\,(a_0 g_n)\right\rangle_{L^2(Y)}$$
$$+ \frac{1}{2}\left\langle g_n,\, (D_y + \nabla_x \phi) \cdot \nabla_x (a_0 g_n)\right\rangle_{L^2(Y)} - \mathrm{i}\kappa(t, x)|a_0|^{2\sigma} a_0 = 0. \quad \text{(A.1)}$$

Here we have used definition (3.7) and the fact that $\langle \chi_n,\, \chi_n \rangle_{L^2(Y)} = 1$. Differentiating the eigenvalue equation (2.10) w.r.t. to k yields

$$(\nabla_k H_\Gamma(k) - \nabla_k E_n(k))\chi_n + (H_\Gamma(k) - E_n(k))\nabla_k \chi_n = 0. \quad \text{(A.2)}$$

Taking in this identity the scalar product with χ_n we obtain

$$\langle \chi_n,\, \nabla_k H_\Gamma(k)\chi_n \rangle_{L^2(Y)} \equiv \left\langle \chi_n,\, (D_y + k)\chi_n \right\rangle_{L^2(Y)} = \nabla_k E_n(k), \quad \text{(A.3)}$$

since H_Γ is self-adjoint. From (A.3) we deduce that (A.1) can be written as

$$\partial_t a_0 + \langle g_n,\, \partial_t g_n \rangle_{L^2(Y)}\, a_0 + \nabla_k E_n(\nabla_x \phi) \cdot \nabla_x a_0 + f(t, x)\, a_0$$
$$= \mathrm{i}\kappa(t, x)|a_0|^{2\sigma} a_0, \quad \text{(A.4)}$$

where

$$f(t, x) = \frac{1}{2}\left\langle g_n,\, (D_y + \nabla_x \phi) \cdot \nabla_x g_n \right\rangle_{L^2(Y)} + \frac{1}{2}\left\langle g_n,\, \nabla_x \cdot (D_y + \nabla_x \phi) g_n \right\rangle_{L^2(Y)}.$$

Next, we substitute χ_n by g_n in (A.3) and differentiate w.r.t. $x \in \mathbb{R}^d$:

$$\left\langle \nabla_x g_n,\, (D_y + \nabla_x \phi) g_n \right\rangle_{L^2(Y)} + \left\langle g_n,\, \nabla_x \cdot (D_y + \nabla_x \phi) g_n \right\rangle_{L^2(Y)}$$
$$= \operatorname{div}_x \nabla_k E_n(\nabla_x \phi).$$

Since D_y is self-adjoint and $\nabla_x \phi$ is real, we have

$$\alpha :\, = \left\langle g_n,\, (D_y + \nabla_x \phi) \cdot \nabla_x g_n \right\rangle_{L^2(Y)} = \left\langle (D_y + \nabla_x \phi) g_n,\, \nabla_x g_n \right\rangle_{L^2(Y)},$$

and we infer from above that

$$\alpha + \Delta_x \phi + \overline{\alpha} = \operatorname{div}_x \nabla_k E_n(\nabla_x \phi).$$

Therefore,

$$\begin{aligned} f(t,x) &= \alpha + \frac{1}{2}\Delta_x\phi = \text{Re}\ \alpha + \frac{1}{2}\Delta_x\phi + \text{i Im}\ \alpha \\ &= \frac{1}{2}\,\text{div}_x\ \nabla_k E_n(\nabla_x\phi) + \text{i Im}\ \alpha. \end{aligned} \tag{A.5}$$

We simplify the last term. From (A.2), with $k = \nabla_x\phi$, we obtain

$$\begin{aligned} &\big((D_y + \nabla_x\phi) - \nabla_k E_n(\nabla_x\phi)\big)\, g_n \\ &\quad + (H_\Gamma(\nabla_x\phi) - E_n(\nabla_x\phi))\, \nabla_k\chi_n\,(y, \nabla_x\phi) = 0. \end{aligned}$$

Taking the $L^2(Y)$-scalar product by

$$\partial_{x_j} g_n = \sum_{l=1}^{d} \partial^2_{x_j x_l}\phi\, \partial_{k_l}\chi_n\,(y, \nabla_x\phi)$$

and taking the imaginary part, we have, since $\langle \chi_n, \nabla_x\chi_n\rangle_{L^2(Y)} \in \text{i}\mathbb{R}$:

$$\begin{aligned} \text{Im}\ \alpha = &-\text{i}\nabla_k E_n(\nabla_x\phi)\cdot\langle g_n, \nabla_x g_n\rangle_{L^2(Y)} \\ &- \sum_{j=1}^{d} \text{Im}\Big\langle (H_\Gamma(\nabla_x\phi) - E_n(\nabla_x\phi))\ \partial_{k_j}\chi_n, \sum_{l=1}^{d} \partial^2_{x_j x_l}\phi\ \partial_{k_l}\chi_n\Big\rangle. \end{aligned} \tag{A.6}$$

The last sum also reads:

$$\sum_{1\leqslant j,l\leqslant d} \partial^2_{x_j x_l}\phi \quad \text{Im}\big\langle (H_\Gamma(\nabla_x\phi) - E_n(\nabla_x\phi))\ \partial_{k_j}\chi_n,\ \partial_{k_l}\chi_n\big\rangle.$$

Since H_Γ is self-adjoint, this term is zero. Hence, (A.4) together with (A.5) and (A.6) give the following equation for the principal amplitude:

$$\begin{aligned} &\partial_t a_0 + \langle g_n,\ \partial_t g_n\rangle_{L^2(Y)}\ a_0 + \mathcal{L}a_0 + \nabla_k E_n(\nabla_x\phi)\cdot\langle g_n,\ \nabla_x g_n\rangle\, a_0 \\ &\quad = \text{i}\kappa(t,x)|a_0|^{2\sigma} a_0, \end{aligned}$$

where $\mathcal{L}$ is defined as in (3.5). Finally, using the Hamilton-Jacobi equation (2.9), a straightforward calculation shows

$$\langle g_n,\ \partial_t g_n\rangle_{L^2(Y)} + \nabla_k E_n(\nabla_x\phi)\cdot\langle g_n,\ \nabla_x g_n\rangle = -\beta(t,x) \tag{A.7}$$

and we conclude that a_0 satisfies the nonlinear transport equation (3.4).

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