SEMICLASSICAL ASYMPTOTICS FOR WEAKLY NONLINEAR BLOCH WAVES

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Abstract. 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.

1. Introduction and scaling

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

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

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 (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.*

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

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

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

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.* [**?**] 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*

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condensates (BECs) [?]. 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 [?]

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

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. 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 [?, ?]:

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

More general, non-isotropic 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 [?, ?] 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

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

where $\xi = (\xi_1, \xi_2, \xi_3)$ with $\xi_l \in \mathbb{R}$ denotes the wave vector of the laser field [?]. The sign in front of the nonlinearity in (1.5) corresponds to a *stable* (defocusing) resp. *unstable* (focusing) condensate. To rewrite the equation (1.5) into our semi-classical scaling we proceed similar to [?]. 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 "~" we find the following dimensionless equation:

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

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* [?]. 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 [?]. 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.* [?, ?]:

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

This gives: $4\pi|\bar{a}|N \approx 10^{-2}[m] \gg a_0$, hence $\varepsilon \approx 4,3 \times 10^{-3} \ll 1$ and for the wave vectors we compute $\xi_l \approx 4,6 \times 10^6[1/m]$, which is of the same order of magnitude as stated in [?]. The reference length scale in this case is $x_s = 2,1 \times 10^{-6}[m]$, which is $O(a_0)$. Finally, to motivate the choice $\sigma \geq 1$, we note that for $d < 3$ higher order nonlinearities are frequently used in the description of BECs [?, ?].

From a mathematical point of view the limit $\varepsilon \to 0$ corresponds to the simultaneous *semi-classical* (or *high-frequency*) and *adiabatic limit* (see [?, ?, ?] 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: The strongest mathematical results were obtained in recent years, using either (spatial) *adiabatic decoupling theory* [?, ?] or *Wigner measures* [?, ?, ?, ?]. A numerical study of these asymptotics can be found in [?].

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 [?].) 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 [?], which has already been successfully applied in the case of linear periodic Schrödinger equations [?, ?]. 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 [?]. (See also [?] 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 $d \geq 1$, 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*

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

where $a_I \in C_0^\infty(\mathbb{R}^d;\mathbb{C})$, $\phi_I \in C^\infty(\mathbb{R}^d;\mathbb{R})$ and $\chi_n = \chi_n(y,k)$ is a Bloch eigenfunction associated to a simple isolated Bloch band $E_n = E_n(k)$. 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 $0 < \varepsilon \leq \varepsilon_0$, the solution ψ^ε to (1.1) is defined up to time τ_0. Moreover, it satisfies the following asymptotics as $\varepsilon \to 0$,

$$\sup_{0\leq t\leq\tau_0}\left\|\psi^\varepsilon(t,x) - \frac{a_I(x)}{\sqrt{|J_t(x)|}}\chi_n\left(\frac{x}{\varepsilon}, \nabla_x\phi(t,x)\right) e^{i\omega(t,x)}e^{i\phi(t,x)/\varepsilon}\right\|_{L^2\cap L^\infty(\mathbb{R}^d)} = O(\varepsilon),$$

where ϕ solves the Hamilton–Jacobi equation (2.9), J_t is the corresponding Jacobi determinant (2.16) and ω is given by

$$\omega(t,x) := -i\int_0^t \beta(s,x)ds - |a_I(x)|^{2\sigma}\int_0^t \frac{\lambda(s)}{|J_s(x)|^\sigma}\int_Y |\chi_n\left(y, \nabla_x\phi(s,x)\right)|^{2\sigma+2} dy\, ds.$$

Here we denote by $\beta(t,x) = i\,\mathrm{Im}\,\beta$ the Berry phase (3.6), and by Y the centered fundamental domain of Γ.

Remark 1.2. Our result holds only before caustics. This must not be surprising; even in the linear case $\lambda \equiv 0$, the WKB method is effective only away from caustics.

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, originating from the interaction of the lattice and the slowly varying potential U, but the second integral in the definition of ω stems from the nonlinearity.

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:

$$\left\{\begin{aligned} &\psi^\varepsilon(t,x) = u^\varepsilon\left(t,x,\frac{x}{\varepsilon}\right)e^{i\phi(t,x)/\varepsilon},\\ &u^\varepsilon(t,x,y) \sim \sum_{j=0}^\infty \varepsilon^j u_j(t,x,y), \end{aligned}\right. \tag{2.1}$$

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

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

We henceforth assume that the initial condition ψ_I^ε is compatible with our asymptotic expansion (2.1):

Assumption 2.1. *The initial wave–function ψ^ε is of WKB–type, i.e.*

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

with $\phi_I \in C^\infty(\mathbb{R}^d;\mathbb{R})$, $u_I \in L^2(\mathbb{R}^d \times \mathbb{T}^d;\mathbb{C}) \cap C^\infty(\mathbb{R}^d \times \mathbb{T}^d;\mathbb{C})$, $\mathbb{T}^d \equiv \mathbb{R}^d/\Gamma$.

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:

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

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

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

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

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

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

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

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 equation (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 n-th eigenvalue of the celebrated *Bloch eigenvalue problem* [**?**]:

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

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.* [**?**, **?**, **?**]:

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

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

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

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

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

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

Concerning the dependence on $k \in \mathcal{B}$, it has been shown [**?**] that for any $n \in \mathbb{N}$ there exists a closed subset $\mathcal{U} \subset \mathcal{B}$ such that $E_n(k)$, $\chi_n(\cdot,k)$ are 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*. Moreover, it is known that

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

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

Equation (2.9) is called the n-th band *Hamilton-Jacobi equation* corresponding to the *semi-classical band Hamiltonian*

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

with an effective kinetic energy given by the n-th 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:

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

This system (locally) defines a flow map $(x,t) \mapsto x_t(x; \nabla_x\phi_I(x))$ 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

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

the corresponding Jacobi determinant and by τ the time at which the first caustic appears, *i.e.*

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

With these preparations, standard theory implies the following lemma:

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 $\phi \in C^\infty([0,\tau[\times\mathbb{R})$ of the Hamilton-Jacobi equation*

$$\begin{cases} \partial_t\phi + h_n^{sc}(\nabla_x\phi, x) = 0, \\ \qquad\qquad \phi\big|_{t=0} = \phi_I(x). \end{cases} \tag{2.18}$$

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

Assumption 2.3. *From now on $u_I^\varepsilon(x,y)$ 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.*

$$u_I^\varepsilon(x,y) \equiv a_I(x)\chi_n(y,\nabla_x\phi_I(x)), \tag{2.19}$$

where $a_I \in C_0^\infty(\mathbb{R}^d;\mathbb{C})$ is a given initial amplitude.

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

$$u_0(t,x,y) = a_0(t,x)\chi_n(x,\nabla_x\phi(t,x)). \tag{2.20}$$

Remark 2.4. Note that also in the linear case, assumptions similar to Assumption 2.3 are usually imposed, *cf.* [**?**, **?**]. 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.* [**?**, **?**, **?**].)
Due to caustics (and possibly additional nonlinear effects if $\lambda(t)$ is not real-valued, see Sect. 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.* [**?**].

3. Derivation of the transport equations

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

$$H_\Gamma(\nabla_x\phi)u_1 + (U(x) + \partial_t\phi)\,u_1 = L_1u_0 - \lambda(t)|u_0|^{2\sigma}u_0, \tag{3.1}$$

where the linear differential operator L_1 applied to u_0 reads

$$L_1u_0 := i\partial_tu_0 + i\nabla_x\phi\cdot\nabla_xu_0 + i\frac{\Delta_x\phi}{2}u_0 + \operatorname{div}_x\nabla_yu_0. \tag{3.2}$$

We multiply equation (3.1) with $\overline{\chi}_n(y,\nabla_x\phi)$ and integrate over the fundamental domain Y. Using the fact that H_Γ is a self-adjoint operator we get that the integral obtained from the l.h.s. of (3.1) is identically zero. Hence

$$\left\langle \chi_n,\, L_1u_0 - \lambda(t)|u_0|^{2\sigma}u_0\right\rangle_{L^2(Y)} \equiv \int_Y \overline{\chi}_n(y,\nabla_x\phi)\,\left(L_1u_0 - \lambda(t)|u_0|^{2\sigma}u_0\right)\,dy = 0, \tag{3.3}$$

is a necessary and (by the Fredholm alternative) sufficient condition such that (3.1) can be solved for u_1 in terms of u_0. After some lengthy computations, given in the appendix, we find that (3.3) is equivalent to the following *nonlinear transport equation* for a_0:

$$\begin{cases} \partial_ta_0 + \mathcal{L}a_0 - \beta(t,x)a_0 = i\kappa(t,x)|a_0|^{2\sigma}a_0, \\ \qquad\qquad a_0\big|_{t=0} = a_I(x). \end{cases} \tag{3.4}$$

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

$$\mathcal{L}a_0 := \nabla_kE_n(\nabla_x\phi)\cdot\nabla_xa_0 + \frac{1}{2}\operatorname{div}_x(\nabla_kE_n((\nabla_x\phi))a_0. \tag{3.5}$$

Moreover, we have

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

and

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

This term can be interpreted as an *effective coupling* of the self-interaction 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* [**?**, **?**]. 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 reader may expect the other sign for the Berry phase. Note that the scalar product we use on $L^2(Y)$ is anti-linear with respect to the first argument (see (3.3)), while it is anti-linear with respect to the second argument in [**?**].

Remark 3.2. It is known that for some particular lattice configurations (including additional symmetries for example) one can achieve $\operatorname{Im}\beta(t,x)\equiv 0$ by performing a smooth gauge transformation $\chi_n(y,k)\to e^{i\theta(y)}\chi_n(y,k)$, *cf.* [**?**, **?**, **?**] for a broader discussion on this.

To provide a link with some already existing results, we remark that in [**?**, **?**] 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 (by applying the so called *Bloch-Floquet transformation*) into an *effective* band Hamiltonian h_n^ε, which is the *Weyl quantization* of the following semi-classical symbol

$$h_n^\varepsilon(k,x) \sim h_n^{sc}(k,x) + \varepsilon h_1(k,x) + O(\varepsilon^2). \tag{3.8}$$

Here the *principal symbol* $h_n^{sc}(k,x)$ is defined as in (2.14) and the first order correction is such that

$$ih_1(\nabla_x\phi(t,x),x) \equiv \beta(t,x). \tag{3.9}$$

Additional terms appear in $h_1(k,x)$ if one includes external magnetic fields too, *cf.* [**?**].

Multiplying (3.4) by $2\overline{a}_0$ and taking the real part of the resulting expression, gives the usual conservation law for the intensity

$$\partial_t|a_0|^2 + \operatorname{div}_x\left(\nabla_k E_n(\nabla_x\phi)|a_0|^2\right) = 0. \tag{3.10}$$

Clearly, this implies

$$\int_{\mathbb{R}^d}|a_0(t,x)|^2dx = \int_{\mathbb{R}^d}|a_I(x)|^2dx. \tag{3.11}$$

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 $a_I\in C_0^\infty(\mathbb{R}^d;\mathbb{R})$. Then there exists a unique smooth solution $a_0\in C^\infty([0,\tau[;C_0^\infty(\mathbb{R}^d))$ of (3.4), given by*

$$a_0(t,x) = \frac{a_I(x)}{\sqrt{|J_t(x)|}}\exp\left(i|a_I(x)|^{2\sigma}\int_0^t\frac{\kappa(s,x)}{|J_s(x)|^\sigma}\,ds + \int_0^t\beta(s,x)\,ds\right). \tag{3.12}$$

Proof. Using Liouville's formula (to simplify the notation we shall only use $x_t \in [0,\tau[\times\mathbb{R}^d$ as a new coordinate),

$$\frac{d}{dt}\,J_t(x_t) = \operatorname{div}_x\left(\nabla_k E_n\left(\nabla_x\phi(x_t)\right)\right) J_t(x_t) \quad ; \quad J_0(x) = 1\,,$$

we rewrite the transport equation (3.4) as an ordinary differential equation along the flow defined by the dynamical system (2.15):

$$\frac{1}{\sqrt{J_t}}\frac{d}{dt}\,(\sqrt{J_t}a_0) = \beta(x_t)a_0 + i\kappa(x_t)|a_0|^{2\sigma}a_0, \quad |t|<\tau.$$

If we define $\tilde{a}_0 := \sqrt{J_t}a_0$, then, locally away from caustics, the principal amplitude is determined by

$$\left\{\begin{aligned} \frac{d}{dt}\,\tilde{a}_0 =&\beta(x_t)\tilde{a}_0 + \ i\kappa(x_t)\frac{|\tilde{a}_0|^{2\sigma}}{|J_t|^{\sigma}}\,\tilde{a}_0, \quad |t|<\tau,\\ \tilde{a}_0\big|_{t=0} =&\ a_I(x). \end{aligned}\right. \tag{3.13}$$

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

$$\frac{d}{dt}\,|\tilde{a}_0(x_t)|^2 = 0,$$

hence: $|\tilde{a}_0(x_t)| = |\tilde{a}_I(x)| \equiv |a_I(x)|$, $\forall\, t\in[0,\tau[$. Define the phase shift g of a_0 by $a_0(x_t) = a_I(x_t)e^{ig(x_t)}$, then g solves

$$\frac{d}{dt}\,g(x_t) = \operatorname{Im}\beta(x_t) + \kappa(x_t)\frac{|\tilde{a}_0(x_t)|^{2\sigma}}{|J_t|^{\sigma}},$$

with $g\big|_{t=0} = 0$. Inserting $|\tilde{a}_0(x_t)| = |a_I(x)|$ yields (3.12). ☐

Remark 3.4. Note that along the flow

$$\beta(x_t) = \left\langle \chi_n(\cdot,\nabla_x\phi(x_t)),\, \frac{d}{dt}\chi_n(\cdot,\nabla_x\phi(x_t))\right\rangle_{L^2(Y)}, \tag{3.14}$$

which is exactly the same expression as given in [**?**], there however the authors do not distinguish between a_0 and $\tilde{a}_0$.

So far we explicitly constructed an approximate solution, which solves (1.1) up to terms of order $O(\varepsilon^2)$. To obtain a better approximation we need to set the term b_2 in (2.4) equal to zero, which gives

$$\begin{aligned} H_\Gamma(\nabla_x\phi)u_2 + \left(U(x)+\partial_t\phi\right)u_2 = L_1u_1 + L_2u_0 -& \\ - \lambda(t)\Big((2\sigma+1)|u_0|^{2\sigma}u_1 + 2\sigma|u_0|^{2\sigma-2}u_0^2\overline{u}_1\Big)&, \end{aligned} \tag{3.15}$$

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

$$L_2u_0 := \frac{1}{2}\,\Delta_x u_0 = \frac{1}{2}\,\chi_n\Delta_x a + \nabla_x a_0\cdot\nabla_x\chi_n + \frac{1}{2}\,a_0\Delta_x\chi_n. \tag{3.16}$$

Consequently, the corresponding solvability condition reads

$$\begin{aligned} \int_Y \overline{\chi}_n(y,\nabla_x\phi)\,\Big(L_1u_1 + L_2u_0 -& \\ - \lambda(t)\left((2\sigma+1)|u_0|^{2\sigma}u_1 + 2\sigma|u_0|^{2\sigma-2}u_0^2\overline{u}_1\,\right)\Big)\,dy = 0&. \end{aligned} \tag{3.17}$$

We decompose u_1 as

$$u_1(t,x,y) = a_1(t,x)\chi_n(y,k) + u_1^{\perp}(t,x,y), \quad k = \nabla_x\phi(t,x), \tag{3.18}$$

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

$$\left\langle \chi_n(\cdot, \nabla_x \phi),\, u_1^\perp(t,x,\cdot) \right\rangle_{L^2(Y)} = 0, \quad \forall\, (t,x) \in [0,\tau[\times \mathbb{R}^d. \tag{3.19}$$

Now, $u_1^\perp$ is determined by (3.1), which implies $u_1^\perp \in C^\infty([0,\tau[; C_0^\infty(\mathbb{R}^d))$, since u_0 is, by Lemma 3.3. On the other hand plugging (3.18) into (3.17) yields a inhomogeneous *linear* version of the transport equation (3.4) for a_1 (the propagating part of u_1):

$$\partial_t a_1 + \mathcal{L} a_1 - \beta(\nabla_x \phi, x) a_1 + i\lambda(t) \left((2\sigma+1)|u_0|^{2\sigma} a_1 + 2\sigma |u_0|^{2\sigma-2} u_0^2 \overline{a}_1 \right) = \rho(t,x),$$
$$a_1\big|_{t=0} = 0.$$

The complex-valued source term $\rho(t,x)$ is given by

$$\rho(t,x) = i \left\langle \chi_n(\cdot, \nabla_x\phi),\, L_1 u_1^\perp + L_2 u_0 \right\rangle_{L^2(Y)} . \tag{3.20}$$

By this procedure all higher order terms $u_j(t,x,y)$, $j \geq 1$, of the asymptotic solution (2.1) can be obtained (recall that $\sigma \in \mathbb{N}$, hence $z \mapsto |z|^{2\sigma} z$ is smooth). Clearly we have that $u_j \in C^\infty([0,\tau[; C_0^\infty(\mathbb{R}^d))$ for all $j \geq 1$.

Under the assumption (2.1), (2.3), we have constructed an approximate solution, which solves our IVP (1.1) up to a remainder $O(\varepsilon^\infty)$. To state precisely this property, define, for $N \geq 0$,

$$\mathtt{v}_N^\varepsilon(t,x) := \ v_N^\varepsilon\left(t, x, \frac{x}{\varepsilon}\right) e^{i\phi(t,x)/\varepsilon} \equiv \left(\sum_{j=0}^N \varepsilon^j u_j \left(t,x,\frac{x}{\varepsilon}\right) \right) e^{i\phi(t,x)/\varepsilon} . \tag{3.21}$$

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

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

We define X_ε^s as:

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

These spaces are reminiscent of the spaces $H_\varepsilon^s(\mathbb{R}^d)$ introduced in [**?**] (see also [**?**]). 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 result provided by the above WKB–method:

Proposition 3.5. *Let ψ_I^ε satisfying Assumptions 2.1 and 2.3, and let $\tau > 0$ be the time at which the first caustic is formed (if any). Then for any $N \in \mathbb{N}$, $\mathtt{v}_N^\varepsilon$ solves*

$$\begin{cases} i\varepsilon \partial_t \mathtt{v}_N^\varepsilon - H^\varepsilon \mathtt{v}^\varepsilon = \varepsilon\lambda(t)\, |\mathtt{v}_N^\varepsilon|^{2\sigma} \mathtt{v}_N^\varepsilon + \varepsilon^{N+1} r_N^\varepsilon, \\ \qquad \mathtt{v}_N^\varepsilon\big|_{t=0} = \psi_I^\varepsilon(x), \end{cases} \tag{3.22}$$

where H^ε is defined by (2.3) and $r_N^\varepsilon \in C^\infty([0,\tau[; C_0^\infty(\mathbb{R}^d))$ is such that $r_N^\varepsilon \in L^\infty_{\mathrm{loc}}([0,\tau[; X_\varepsilon^s)$ 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* $|\alpha| \geq 2$.

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.* [**?**]).

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:*

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

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

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

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

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 [**?**]). 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.* [**?**, **?**]).

To prove higher order regularity of ψ and its momenta, one can follow the proof of [**?**] (see also [**?**]). 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 ([**?**, **?**]), and they imply the same Strichartz inequalities ([**?**]). Another difference with [**?**] is that the Galilean operator $x + it\nabla_x$ commutes with $i\partial_t + \frac{1}{2}\Delta$, but in general not with $i\partial_t + \frac{1}{2}\Delta - W$. This is not a problem in view of the above result, since

$$[x + it\nabla_x, W] = it\nabla W = O\left(1 + |x|\right)\,.$$

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 [**?**]). $\square$

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.* [**?**]). 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 $(\alpha^\varepsilon)_{0<\varepsilon\leq 1}$ and $(\beta^\varepsilon)_{0<\varepsilon\leq 1}$ be two families of positive numbers. In the following we shall frequently write

$$\alpha^\varepsilon \lesssim \beta^\varepsilon, \tag{4.2}$$

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

$$\alpha^\varepsilon \leq C\beta^\varepsilon, \quad \text{for all } \varepsilon \in]0,1]. \tag{4.3}$$

(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 ψ_I^ε satisfy Assumptions 2.1 and 2.3, $\tau > 0$ given by* (2.17)*, and $\mathtt{v}_N^\varepsilon$ given by* (3.21)*. Then for any $\tau_0 \in]0,\tau[$, there exists $\varepsilon_0 > 0$ such that for $0 < \varepsilon \leq \varepsilon_0$, the solution ψ^ε to* (1.1) *is defined up to time τ_0. Moreover, the following asymptotics holds: for any $N \in \mathbb{N}$ and $s \in \mathbb{N}$,*

$$\sup_{0\leq t\leq\tau_0} \|\psi^\varepsilon(t) - \mathtt{v}_N^\varepsilon(t)\|_{X_\varepsilon^s} = O\left(\varepsilon^{N+1}\right). \tag{4.4}$$

Proof. For $N \in \mathbb{N}$, we define the error term as $\mathtt{w}_N^\varepsilon := \psi^\varepsilon - \mathtt{v}_N^\varepsilon$. From (1.1) and (3.22), it solves

$$\begin{cases} i\varepsilon\partial_t \mathtt{w}_N^\varepsilon = H^\varepsilon \mathtt{w}_N^\varepsilon + \varepsilon\lambda(t)\left(|\psi^\varepsilon|^{2\sigma}\psi^\varepsilon - |\mathtt{v}_N^\varepsilon|^{2\sigma}\mathtt{v}_N^\varepsilon\right) - \varepsilon^{N+1} r_N^\varepsilon\,, \\ \mathtt{w}_N^\varepsilon\big|_{t=0} = 0\,, \end{cases} \tag{4.5}$$

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

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

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

$$\partial_t \|\mathtt{w}_N^\varepsilon(t)\|_{L^2} \lesssim \left\||\psi^\varepsilon|^{2\sigma}\psi^\varepsilon - |\mathtt{v}_N^\varepsilon|^{2\sigma}\mathtt{v}_N^\varepsilon\right\|_{L^2} + \varepsilon^{N}\|r_N^\varepsilon(t)\|_{L^2}\,. \tag{4.6}$$

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 [**?**] for an expository presentation.

Following [**?**, 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*

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

and $\mathtt{w}$ satisfies

$$\|\mathtt{w}\|_{L^\infty(\mathbb{R}^d)} \leq R\,,$$

then

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

Sketch of the proof of Lemma 4.6. When X^k_ε is replaced by H^k_ε (remove the control of the momenta), the result is exactly [?, 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^k_ε, the control of the momenta follows easily. □

We first notice that $\mathtt{v}^\varepsilon_N$ is uniformly bounded in $L^\infty([0,\tau_0]\times\mathbb{R}^d)$. To prove that $\mathtt{w}^\varepsilon_N$ 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 Gagliardo–Nirenberg inequalities:

$$\text{for } s>d/2,\qquad \|\mathtt{w}\|_{L^\infty(\mathbb{R}^d)}\lesssim \|\mathtt{w}\|_{H^s(\mathbb{R}^d)}\lesssim \varepsilon^{-d/2}\|\mathtt{w}\|_{X^s_\varepsilon}\,. \tag{4.7}$$

(The scaling factor $\varepsilon^{-d/2}$ is obvious when one uses Fourier transform.)
By construction, $\mathtt{w}^\varepsilon_N(0,x)\equiv 0$. From Lemma 4.3, there exists $t(\varepsilon,R)>0$ such that

$$\|\mathtt{w}^\varepsilon_N(t)\|_{L^\infty(\mathbb{R}^d)}\leq R \tag{4.8}$$

for $t\in[0,t(\varepsilon,R)]$. As long as (4.8) holds, (4.6) and Lemma 4.6 with $s=0$ imply

$$\partial_t\|\mathtt{w}^\varepsilon_N(t)\|_{L^2}\leq C\,\|\mathtt{w}^\varepsilon_N(t)\|_{L^2}+C\varepsilon^N\,\|r^\varepsilon_N(t)\|_{L^2}\ ,$$

and from Gronwall lemma, as long as (4.8) holds for $t\leq\tau_0$, we get that

$$\|\mathtt{w}^\varepsilon_N(t)\|_{L^2}\leq C\varepsilon^N\,. \tag{4.9}$$

The idea is now to obtain similar estimates for the momenta and derivatives of $\mathtt{w}^\varepsilon_N$. Applying the operator $\varepsilon\nabla_x$ to (4.5) yields:

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

The same energy estimate as before gives:

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

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

$$\begin{aligned}\partial_t\|\varepsilon\nabla_x\mathtt{w}^\varepsilon_N(t)\|_{L^2}\lesssim&\,\|\varepsilon\nabla_x\left(F(\psi^\varepsilon)-F(\mathtt{v}^\varepsilon_N)\right)\|_{L^2}+\frac{1}{\varepsilon}\,\|\mathtt{w}^\varepsilon_N\|_{L^2}+\|x\mathtt{w}^\varepsilon_N\|_{L^2}\\&+\varepsilon^N\,\|\varepsilon\nabla_x r^\varepsilon_N\|_{L^2}\\\lesssim&\,\|\varepsilon\nabla_x\mathtt{w}^\varepsilon_N\|_{L^2}+\|x\mathtt{w}^\varepsilon_N\|_{L^2}+\varepsilon^{N-1}\,,\end{aligned}\tag{4.10}$$

where we have used Proposition 3.5, Lemma 4.6 with $s=1$, and (4.9). We see that when U is quadratic, we have to find a similar estimate for $\|x\mathtt{w}^\varepsilon_N\|_{L^2}$. For that, multiply (4.5) by x:

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

Since $[x,H^\varepsilon]=-\varepsilon^2\nabla_x$, the energy estimate yields, as long as (4.8) holds:

$$\begin{aligned}\partial_t\|x\mathtt{w}^\varepsilon_N(t)\|_{L^2}\lesssim&\,\|x\left(F(\psi^\varepsilon)-F(\mathtt{v}^\varepsilon_N)\right)\|_{L^2}+\|\varepsilon\nabla_x\mathtt{w}^\varepsilon_N\|_{L^2}+\varepsilon^N\,\|\varepsilon\nabla_x r^\varepsilon_N\|_{L^2}\\\lesssim&\,\|x\mathtt{w}^\varepsilon_N(t)\|_{L^2}+\|\varepsilon\nabla_x\mathtt{w}^\varepsilon_N\|_{L^2}+\varepsilon^N\,.\end{aligned}\tag{4.11}$$

Putting (4.10) and (4.11) together, we have:

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

and a Gronwall lemma yields, as long as (4.8) holds:

$$\|\mathtt{w}_N^\varepsilon(t)\|_{X_\varepsilon^1} \lesssim \varepsilon^{N-1} . \tag{4.12}$$

One can check by induction that for $k \geq 0$, so long as (4.8) holds,

$$\|\mathtt{w}_N^\varepsilon(t)\|_{X_\varepsilon^s} \lesssim \varepsilon^{N-s} . \tag{4.13}$$

We now take advantage of Gagliardo–Nirenberg inequality (4.7). For $s > d/2$ and as long as (4.8) holds, we get

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

Thus, if $N - s - d/2 > 0$, a continuity argument shows that (4.8) 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 $0 < \varepsilon \leq \varepsilon(\tau_0)$. To complete the proof of Theorem 4.5, we have to prove (4.4). Fix $s, N \in \mathbb{N}$; let $s_1 \geq s$ such that $s_1 > d/2$, and $N_1 \geq s_1 + N + 1$. We infer from (4.13) that

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

It is straightforward that since $N_1 > N$,

$$\sup_{0\leq t\leq \tau_0} \left\|\mathtt{v}_N^\varepsilon(t) - \mathtt{v}_{N_1}^\varepsilon(t)\right\|_{X_\varepsilon^{k_1}} \lesssim \varepsilon^{N+1} .$$

We deduce that (4.4) holds for any $s, N \in \mathbb{N}$. $\square$

Remark 4.7. A slightly shorter argument is available in the case $d \leq 3$, 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_ε^2-estimate and use (4.7) again. Following an idea due initially to T. Kato [**?**], consider the time derivative of the error $\mathtt{w}_N^\varepsilon$. One can prove that $\|\varepsilon\partial_t \mathtt{w}_N^\varepsilon(t)\|_{L^2} = O(\varepsilon^N)$, as long as (4.8) holds. Plugging this into (4.5), we have, from (4.9) and since V_Γ is bounded and U is sub-quadratic:

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

The control of $\|x^2 \mathtt{w}_N^\varepsilon(t)\|_{L^2}$ is then similar to (4.11):

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

and we can conclude as above.

Now it is easy to deduce the estimate announced in Theorem 1.1. The L^2 estimate is (4.4) with $N = s = 0$, since $\mathtt{v}_0^\varepsilon$ is known explicitly. For the L^∞ estimate, mimic the above proof: for $s > d/2$ and $N - d/2 \geq 1$, (4.4) and (4.7) yield

$$\sup_{0\leq t\leq \tau_0} \|\psi^\varepsilon(t) - \mathtt{v}_N^\varepsilon(t)\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon^{-d/2} \sup_{0\leq t\leq \tau_0} \|\psi^\varepsilon(t) - \mathtt{v}_N^\varepsilon(t)\|_{X_\varepsilon^s} \lesssim \varepsilon^{N-d/2} \lesssim \varepsilon .$$

It is straightforward that

$$\sup_{0\leq t\leq \tau_0} \|\mathtt{v}_0^\varepsilon(t) - \mathtt{v}_N^\varepsilon(t)\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon ,$$

hence,

$$\sup_{0\leq t\leq \tau_0} \|\psi^\varepsilon(t) - \mathtt{v}_0^\varepsilon(t)\|_{L^\infty(\mathbb{R}^d)} \lesssim \varepsilon .$$

5. Discussion and consequences

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

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

Under the assumption (see *e.g.* [**?**] for a discussion on this) that there exists a smooth orthonormal basis $\{\chi_l(k,y))\}_{l\in I}$ of $\operatorname{ran}\Pi_I(k)$, 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

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

with $\phi(t,x)$ given by the solution of the Hamilton-Jacobi equation (2.9) with $E_n(k) \equiv E_*(k)$. As in [**?**, **?**] 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 [**?**], 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 $(\psi^\varepsilon)_{0<\varepsilon\leq 1}$. The Wigner measure of a family $(\psi^\varepsilon(t,\cdot))_{0<\varepsilon\leq1}$ bounded in $L^2(\mathbb{R}^d)$ is the weak limit (up to the extraction of a subsequence) of its Wigner transform,

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

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 for *linear* problems (see *e.g.* [**?**, **?**, **?**, **?**, **?**]).

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*

$$\lim_{\varepsilon\to0} W^\varepsilon[\psi^\varepsilon] = \mu \quad \text{in } \mathcal{S}'([0,\tau_0)\times\mathbb{R}^d_x\times\mathbb{R}^d_\xi) \text{ weak-}\star, \tag{5.3}$$

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

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

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

Proof. We have to compute

$$\lim_{\varepsilon\to0}\int_{\mathbb{R}^{2d}} f(x,\xi)W^\varepsilon\left[\psi^\varepsilon(t)\right](x,\xi)dx\,d\xi = \int_{\mathbb{R}^{2d}} f(x,\xi)\mu(t,dx,d\xi),$$

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 $\mathtt{v}_0^\varepsilon$ 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:

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

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. $\square$

In our case, the strong convergence stated in Theorem 4.5 shows that the Wigner measure of $(\psi^\varepsilon(t,\cdot))_{0<\varepsilon\leq 1}$ is the same as in the linear case (see [**?**, Sect. 5.1]), since the main nonlinear effect appears as an order $O(1)$ phase ω, defined in Theorem 1.1. In other words, the Wigner measure (resp. the Wigner transform) does not "see" the nonlinearity. This can be compared with the Wigner measures studied in [**?**], 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:

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

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 (3.13). Multiply (3.13) by $\overline{\tilde{a}_0}$ and take the real part:

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

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 $\|\psi^\varepsilon(t)\|^2_{L^2}$ 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 truly nonlinear effect.

Appendix A. Derivation of the leading order transport equation

We shall discuss here in more detail how to pass from (3.3) to (3.4) (we found some inconsistent derivations in the so far existing literature [**?**, **?**, **?**, **?**]).

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

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

where from now on $D_x := -i\nabla_x$. 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

$$\begin{aligned}\partial_t a_0 + \langle g_n,\, \partial_t g_n\rangle_{L^2(Y)}\, a_0 + \frac{1}{2}\left\langle g_n,\, \nabla_x\cdot\left(D_y+\nabla_x\phi\right)(a_0 g_n)\right\rangle_{L^2(Y)} \\ + \frac{1}{2}\left\langle g_n,\, (D_y+\nabla_x\phi)\cdot\nabla_x(a_0g_n)\right\rangle_{L^2(Y)} - i\kappa(t,x)|a_0|^{2\sigma}a_0 = 0.\end{aligned} \tag{A.1}$$

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

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

Taking in this identity the scalar product with χ_n we obtain

$$\begin{aligned}\langle\chi_n,\, \nabla_k H_\Gamma(k)\chi_n\rangle_{L^2(Y)} &\equiv \langle\chi_n,\, (D_y+k)\chi_n\rangle_{L^2(Y)} \\ &= \nabla_k E_n(k),\end{aligned} \tag{A.3}$$

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

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

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. $x\in\mathbb{R}^d$:

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

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

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

and we infer from above that

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

Therefore

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

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

$$\left((D_y+\nabla_x\phi) - \nabla_k E_n(\nabla_x\phi)\right)g_n + \left(H_\Gamma(\nabla_x\phi) - E_n(\nabla_x\phi)\right)\nabla_k\chi_n\left(y,\nabla_x\phi\right) = 0.$$

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

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

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

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

The last sum also reads:

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

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:

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

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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