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ABSTRACT. We consider nonlinear Schrödinger equations with either local or nonlocal nonlinearities. In addition, we include periodic potentials as used, for example, in matter wave experiments in optical lattices. By considering the corresponding semiclassical scaling regime, we construct asymptotic solutions, which are concentrated both in space and in frequency around the effective semiclassical phase-space flow induced by Bloch's spectral problem. The dynamics of these generalized coherent states is governed by a nonlinear Schrödinger model with effective mass. In the case of nonlocal nonlinearities we establish a novel averaging type result in the critical case.

1. INTRODUCTION

Coherent states have been originally introduced in quantum mechanics to describe wave packets minimizing the uncertainty principle. This property makes coherent states highly attractive for the study of *semiclassical asymptotics*, see, e.g., [17, 15, 21]. Indeed, it can be shown that for Schrödinger equations with sub-quadratic potentials, coherent states retain their shape, providing minimum uncertainty at all time in the quadratic case [13], and up to Ehrenfest time in general [6]. Recently, extensions to weakly nonlinear situations have been studied in [8, 7]. In addition, the semiclassical dynamics of coherent states under the influence of (highly oscillatory) periodic potentials has been investigated by the authors in [10]. In the present work we *combine* the effects coming from periodic and nonlinear potentials.

To this end, we consider *nonlinear Schrödinger equations* which, after scaling into dimensionless coordinates, appear in the following semiclassical form:

$$i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon = V_{\rm per}\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon + \varepsilon^\alpha f(|\psi^\varepsilon|^2)\psi^\varepsilon, \quad \psi^\varepsilon_{|t=0} = \psi^\varepsilon_0, \tag{1.1}$$

where $t \in \mathbb{R}$, $x \in \mathbb{R}^d$, and $d \in \mathbb{N}$ denotes the spatial dimension (usually $d = 3$). Moreover, $\varepsilon \in (0, 1]$ denotes a (small) semiclassical parameter, i.e. a dimensionless rescaled Planck's constant. The factor ε^α measures the (asymptotic) strength of the nonlinearity: the larger the $\alpha > 0$, the weaker the nonlinear effects. In the following, we shall allow for two different types of *gauge invariant nonlinearities*:

- Local nonlinearities: $f(|\psi^\varepsilon|^2) = \lambda|\psi^\varepsilon|^{2\sigma}$, with $\sigma \in \mathbb{N}$ and $\lambda \in \mathbb{R}$, allowing for focusing (attractive) and defocusing (repulsive) situations.
- Nonlocal nonlinearities of convolution type: $f(|\psi^\varepsilon|^2) = K * |\psi^\varepsilon|^2$, with $K(x) \in \mathbb{R}$ a given interaction kernel.

Finally, the term $V_{\rm per}(x/\varepsilon)$ denotes a highly oscillatory periodic potential. More precisely, let $\Gamma \simeq \mathbb{Z}^d$ be some regular lattice, then we assume that for all $y \in \mathbb{R}^d$: $V_{\rm per}(y + \gamma) =$

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$V_{\rm per}(y)$ with $\gamma \in \Gamma$. In addition, we shall assume $V_{\rm per} \in C^\infty(\mathbb{R}^d)$. Equation (1.1) describes the propagation of waves on macroscopic length- and time-scales, i.e. over many periods of the periodic potential. The parameter $\varepsilon \ll 1$ consequently describes the ratio between microscopic (quantum mechanical) and the macroscopic scales.

Nonlinear Schrödinger equations with periodic potentials arise in various physical contexts: A by now classical example is the mean-field description of electrons propagating in a crystalline solid [16, 26] under the additional influence of a self-consistent electric field. The latter is usually modeled by means of a nonlocal *Hartree nonlinearity* $f(|\psi^\varepsilon|^2) = |\psi^\varepsilon|^2 * 1/|\cdot|$, see, e.g., [3] for a semiclassical study via Wigner measures. Another situation in which (1.1) applies is the description of *Bose-Einstein condensates* in so-called *optical lattices*, cf. [12]. In the regime of dilute gases, such condensates can be modeled by the Gross-Pitaevskii equation with cubic nonlinearity $\sigma = 1$, cf. [22]. Note however, that other nonlinearities also arise, see, for example, [5] where a nonlocal term is used for the description of superfluid Helium. In addition, strong magnetic confinement allows for the experimental realization of quasi-one-dimensional (cigar-shaped) condensates, or quasi two-dimensional condensates, motivating the fact that we consider (1.1) in general dimensions $d \in \mathbb{N}$, cf. [18]. A third example for the appearances of (1.1) stems from the description of wave packets propagating within nonlinear photonic crystals [24] and where the nonlinear response of the media is modeled via a *Kerr nonlinearity* $\sigma = 1$. In this case, the underlying assumption in the derivation of (1.1) is the existence of a preferred direction of propagation, implying that the appropriate model is stated in dimension $d = 1$.

In all of these situations, the joint effects of nonlinearity, periodicity and dispersion (or, quantum pressure), can lead to the existence of *stable localized states* conserving the form upon propagation and collisions. Gap solitons, discrete breathers and compactons are examples of such states. Here we shall present another possibility, which will arise from semiclassical description via coherent states. Even though the nonlinearity in our case is weaker than in the above mentioned situations (due to the fact that $\alpha > 0$), the obtained asymptotic solutions will nonetheless experience nonlinear effects in leading order, provided α is of critical size (to be made precise later on). The latter will depend on the precise form of the nonlinearity.

To present our results, we recall the classical *Bloch eigenvalue problem* [28]:

$$H(k)\chi_m(\cdot,k) = E_m(k)\chi_m(\cdot,k), \quad m \in \mathbb{N}. \tag{1.2}$$

Denoting by Y the centered fundamental domain of Γ, $E_m(k) \in \mathbb{R}$ and $\chi_m(\cdot,k)$ denote, respectively, the m-th eigenvalue/eigenvector pair of

$$H(k) = \frac{1}{2}\left(-i\nabla_y + k\right)^2 + V_{\rm per}\left(y\right), \quad y \in Y, \tag{1.3}$$

parametrized by the *crystal momentum* $k \in Y^* \simeq \mathbb{T}^d$. We shall assume that at $t = 0$,

$$\psi^\varepsilon(0,x) \underset{\varepsilon\to 0}{\sim} \varepsilon^{-d/4} u_0\left(\frac{x-q_0}{\sqrt{\varepsilon}}\right)\chi_m\left(\frac{x}{\varepsilon}, p_0\right)\mathrm{e}^{ip_0\cdot(x-q_0)/\varepsilon}, \tag{1.4}$$

where u_0 denotes some *smooth and rapidly decaying profile*. In other words, the initial data ψ_0^ε can be approximated by a highly oscillatory Bloch eigenfunction χ_m modulated by a (generalized) coherent state, i.e. a wave function which is localized both in space and in frequency.

Remark 1.1. In particular, the choice $u_0(z) = \exp(-|z|^2/2)$ yields a classical coherent state, i.e. ground state of the harmonic oscillator potential, as modulation. The states (1.4)

are more general, though, since we can allow for any $u_0 \in \mathcal{S}(\mathbb{R}^d)$, the Schwartz space of rapidly decaying, smooth functions. We also remark that the same class of initial data have recently been considered in [10], where the situation of linear Schrödinger equations with combined periodic and slowly varying external potentials has been considered (see B for more details).

Provided such initial data, we shall show that the solution of (1.1) can be approximately (in a sense to be made precise) described by the following *semiclassical wave packet*:

$$\psi^\varepsilon(t,x) \underset{\varepsilon\to 0}{\sim} \varphi^\varepsilon(t,x) := \varepsilon^{-d/4} u\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\right) \chi_m\left(\frac{x}{\varepsilon}, p_0\right) e^{i\phi_m(t,x)/\varepsilon} \tag{1.5}$$

where $q(t) = q_0 + t\nabla_k E_m(p_0)$ describes the *macroscopic shift* of the centre of mass and the highly oscillatory phase function ϕ_m is

$$\phi_m(t,x) = p_0 \cdot (x - q_0) - tE_m(p_0). \tag{1.6}$$

To this end, we need to give sense to the *group velocity* $\nabla_k E_m(k)$ and thus, we have to assume from now on, that:

$$E_m(k) \text{ is a } \textit{simple eigenvalue} \text{ in the vicinity of } k = p_0. \tag{1.7}$$

(Of course, $p_0 \in \mathbb{R}^d$ has to be understood modulo Γ^* in this case.) In other words, we have to avoid that two Bloch bands cross at p_0, that is $E_m(p_0) = E_n(p_0)$, for $m \neq n$. It is known that at such crossing points $E_m(k)$ is no longer differentiable, causing the above asymptotic description (which is based on an adiabatic decoupling of the slow and fast degrees of freedom) to break down.

Remark 1.2. Clearly, the non-crossing condition given above restricts our choice for the initial wave vectors $p_0 \in \mathbb{R}^d$. It is known however that the set of band crossings has Lebesgue measure zero. For example, in the case $d = 1$, band crossings can only occur at $k = 0$ or at the boundary of the Brillouin zone.

So far, we have not said what determines the profile $u = u(t,z)$ appearing in (1.5). Its time-evolution depends on the strength of the nonlinearity, i.e. on the size of $\alpha > 0$ in the case of local nonlinearities (the situation for nonlocal ones will be described later on). We shall find that the *critical size* is $\alpha_c = 1 + d\sigma/2$ and when $\alpha = \alpha_c$, u solves the following *homogenized nonlinear Schrödinger equation*

$$i\partial_t u + \frac{1}{2}\mathrm{div}_z\left(\left(\nabla_k^2 E_m\left(p_0\right)\right)\cdot\nabla_z\right) u = \lambda_m |u|^{2\sigma} u, \quad u_{|t=0} = u_0, \tag{1.8}$$

with effective coupling constant

$$\lambda_m = \lambda \int_Y \left|\chi_m\left(y, p_0\right)\right|^{2\sigma+2} dy.$$

Note that the dispersive properties of (1.8) are determined by an *effective mass matrix* $\nabla_k^2 E_m\left(p_0\right) \in \mathbb{R}^{d\times d}$, which itself depends on the choice of the initial wave vector (cf. [14] for a recent study).

In the next section, we derive this effective mass equation from multi-scale expansion. A rigorous stability result is then proved in Section 3. The case of nonlocal nonlinearities is treated in Section 4. As we shall see, in situations where the kernel K is homogeneous, the critical value α_c depends on the degree of homogeneity (like in the case of a local nonlinearity), and the analogue of (1.8) is an envelope equation with a nonlocal nonlinearity. On the other hand, if the kernel K is a smooth function, then $\alpha_c = 1$, and in sharp contrast with the other situations studied in this paper, the analogue of (1.8) for $\alpha = \alpha_c$ is found to be a *linear* equation, see Section 4.2.

2. Multi-scale expansion

2.1. **The hierarchy of equations.** Except for the treatment of the nonlinear term, we resume the strategy followed in [10]. We seek the solution ψ^ε of (1.1) in the form

$$\psi^\varepsilon(t,x) = \varepsilon^{-d/4}\mathcal{U}^\varepsilon\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}, \frac{x}{\varepsilon}\right)\mathrm{e}^{i\phi_m(t,x)/\varepsilon}, \tag{2.1}$$

where the phase $\phi_m(t,x)$ is given by (1.6) and the function $\mathcal{U}^\varepsilon = \mathcal{U}^\varepsilon(t,z,y)$ admits an asymptotic expansion

$$\mathcal{U}^\varepsilon(t,z,y) \underset{\varepsilon\to 0}{\sim} \sum_{j\in\mathbb{N}} \varepsilon^{j/2} U_j(t,z,y) \tag{2.2}$$

with smooth profiles U_j which, in addition, are assumed to be Γ-periodic with respect to y. For ψ^ε given by the ansatz (2.1), we compute

$$\left(i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon - V_{\rm per}\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon\right) = \varepsilon^{-d/4}\mathrm{e}^{i\phi_m/\varepsilon}\sum_{j=0}^{2}\varepsilon^{j/2}b_j^\varepsilon(t,z,y)\Big|_{(z,y)=\left(\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right)}$$

with

$$\begin{aligned}
b_0^\varepsilon &= -\partial_t\phi_m\mathcal{U}^\varepsilon + \frac{1}{2}\Delta_y\mathcal{U}^\varepsilon - \frac{1}{2}|p_0|^2\mathcal{U}^\varepsilon + ip_0\cdot\nabla_y\mathcal{U}^\varepsilon - V_{\rm per}(y)\mathcal{U}^\varepsilon,\\
b_1^\varepsilon &= -i\dot q(t)\cdot\nabla_z\mathcal{U}^\varepsilon + (\nabla_y\cdot\nabla_z)\,\mathcal{U}^\varepsilon + ip_0\cdot\nabla_z\mathcal{U}^\varepsilon,\\
b_2^\varepsilon &= i\partial_t\mathcal{U}^\varepsilon + \frac{1}{2}\Delta_z\mathcal{U}^\varepsilon.
\end{aligned}$$

Using (1.6) and the fact that $\dot q(t) = \nabla_k E_m(p_0)$, we can rewrite $b_0^\varepsilon, b_1^\varepsilon$ as

$$\begin{aligned}
b_0^\varepsilon &= (E_m(p_0) - H\,(p_0))\mathcal{U}^\varepsilon,\\
b_1^\varepsilon &= i\,(p_0 - \nabla_k E_m\,(p_0))\cdot\nabla_z\mathcal{U}^\varepsilon + (\nabla_y\cdot\nabla_z)\,\mathcal{U}^\varepsilon,
\end{aligned}$$

where $H(p_0)$ is the Bloch Hamiltonian (1.3) evaluated at $k = p_0$ (again, this has to be understood modulo Γ^*). Introducing the following linear operators:

$$L_0 = E_m\,(p_0) - H\,(p_0)\,,\ L_1 = i\,(p_0 - \nabla_k E_m\,(p_0))\cdot\nabla_z + \nabla_y\cdot\nabla_z,\ L_2 = i\partial_t + \frac{1}{2}\Delta_z,$$

and expanding $\mathcal{U}^\varepsilon$ in powers of $\varepsilon\in(0,1]$, we consequently need to solve the following hierarchy of equations:

$$\begin{cases}
L_0U_0 = 0,\\
L_0U_1 + L_1U_0 = 0,\\
L_0U_2 + L_1U_1 + L_2U_0 = F(U_0),
\end{cases} \tag{2.3}$$

where, for $\alpha_c = 1 + d\sigma/2$, we find:

$$F(U_0) = \begin{cases} 0 & \text{if } \alpha > \alpha_c,\\ \lambda|U_0|^{2\sigma}U_0 & \text{if } \alpha = \alpha_c. \end{cases}$$

In the next subsection, we shall focus on the resolution of (2.3).

2.2. **The effective mass equation.** Given the form of L_0, the equation $L_0U_0 = 0$ implies

$$U_0(t,z,y) = u(t,z)\chi_m(y,p_0). \tag{2.4}$$

By Fredholm's alternative, a necessary and sufficient condition to solve the equation $L_0U_1 + L_1U_0 = 0$, is that L_1U_0 is orthogonal to $\ker L_0$, that is:

$$\langle \chi_m, L_1U_0\rangle_{L^2(Y)} = 0. \tag{2.5}$$

Given the expression of L_1 and the formula (2.4), we compute

$$L_1U_0 = i\left(p_0 - \nabla_k E_m(p_0)\right)\cdot\nabla_z u(t,z)\chi_m(y,p_0) + \nabla_y\chi_m(y,p_0)\cdot\nabla_z u(t,z).$$

Now, we make use of the algebraic identities derived in Section A. In view of (A.2), we infer that (2.5) is automatically fulfilled. We thus obtain

$$U_1(t,z,y) = u_1(t,z)\chi_m(y,p_0) + u_1^\perp(t,z,y),$$

where $u_1^\perp$, the part of U_1 which is orthogonal to $\ker L_0$, is obtained by inverting an elliptic operator: $u_1^\perp = -L_0^{-1}L_1U_0$. Note that the formula for L_1U_0 can also be written as

$$L_1U_0 = -i\nabla_k\left(E_m(p_0) - H(p_0)\right)\chi_m(y,p_0)\cdot\nabla_z u(t,z).$$

Taking into account (A.1), this yields: $u_1^\perp(t,z,y) = -i\nabla_k\chi_m(y,p_0)\cdot\nabla_z u(t,z)$. At this stage, we shall, for simplicity, choose $u_1 = 0$, in which case U_1 becomes simply a function of u:

$$U_1(t,z,y) = -i\nabla_k\chi_m(y,p_0)\cdot\nabla_z u(t,z). \tag{2.6}$$

As a next step in the formal analysis, we must solve $L_0U_2 + L_1U_1 + L_2U_0 = F(U_0)$. By the same argument as before, we require

$$\langle \chi_m, L_1U_1 + L_2U_0 - F(U_0)\rangle_{L^2(Y)} = 0. \tag{2.7}$$

With the expression (2.6), we compute

$$L_1U_1 = \sum_{j,\ell=1}^{d}\left(\left(p_0 - \nabla_k E_m(p_0)\right)_j\partial_{k_\ell}\chi_m(y,p_0) - i\partial^2_{y_jk_\ell}\chi_m(y,p_0)\right)\partial^2_{z_jz_\ell}u,$$

and we also have

$$L_2U_0 = \left(i\partial_t + \frac{1}{2}\Delta_z\right)u(t,z)\,\chi_m(y,p_0).$$

We consequently infer

$$\begin{aligned}\langle \chi_m, L_1U_1 + L_2U_0\rangle_{L^2(Y)} &= i\partial_t u + \frac{1}{2}\Delta_z u \\ &\quad - \sum_{j,\ell=1}^{d}\left\langle \chi_m, \partial_{k_j}E_m(p_0)\,\partial_{k_\ell}\chi_m + i\partial^2_{y_jk_\ell}\chi_m\right\rangle_{L^2(Y)}\partial^2_{z_jz_\ell}u.\end{aligned}$$

In the case $\alpha = \alpha_c$, by making the last sum symmetric with respect to j and ℓ, and using (A.3), we finally obtain the nonlinear Schrödinger equation (1.8) with effective mass tensor $M = \nabla_k^2 E_m(p_0)$ and coupling constant

$$\lambda_m := \lambda\left\langle \chi_m, |\chi_m|^{2\sigma}\chi_m\right\rangle_{L^2(Y)} = \lambda\int_Y |\chi_m(y,p_0)|^{2\sigma+2}\,dy.$$

In addition, we can write

$$U_2(t,z,y) = u_2(t,z)\chi_m(y,p_0) + u_2^\perp(t,z,y), \tag{2.8}$$

where $u_2^\perp = -L_0^{-1}\left(L_1U_1 + L_2U_0\right)$. We shall also impose $u_2 \equiv 0$ and thus $U_2 = u_2^\perp$.

Assume for the moment that we can solve (1.8). Then, we have the following result, which establishes some basic regularity properties of our multi-scale expansion (where we denote by H^k the usual $L^2(\mathbb{R}^d)$ based Sobolev space).

Lemma 2.1. *Suppose* (1.7) *holds true and let* $u \in C([0,T];H^k)$*, be a solution of* (1.8) *up to some* $T>0$*. Then* $U_j \in C([0,T];H^{k-j}_z \times W^{\infty,\infty}(Y))$*, for* $j=0,1,2$*.*

Proof. First note that $(y,k) \mapsto \chi_m(y,k)$ is smooth and bounded together with all its derivatives, provided (1.7) holds true. Having this in mind, the proof follows directly from the construction of $\{U_j\}_{j=0,1,2}$ as solutions to the system (2.3). □

Remark 2.2. Note that in the case $\alpha > \alpha_c$ nonlinear effects are *absent at leading order* since we obtain, instead of (1.8), a *linear* effective mass equation:

$$i\partial_t u_{\rm lin} + \frac{1}{2}{\rm div}_z\left(\nabla_k^2 E_m\left(p_0\right)\cdot\nabla_z\right)u_{\rm lin} = 0, \quad u_{|t=0} = u_0. \tag{2.9}$$

This type of equation has been derived in [2, 25], using a different asymptotic scaling.

3. Main results

In this section we shall make the computations given above rigorous and prove a nonlinear stability result. As a first step we need to guarantee the existence of a smooth solution to (1.8), at least locally in-time.

3.1. **Construction of an approximate solution.** The dispersion relation of (1.8) is given by a real-valued symmetric matrix. Standard techniques (see, e.g., [27]) yield the existence of a unique local solution, provided that the initial datum is sufficiently smooth:

Lemma 3.1. *Let* $u_0 \in H^k$ *with* $k > d/2$*. There exists* $T_c \in (0,+\infty]$ *and a unique maximal solution* $u \in C([0,T_c);H^k)$ *to* (1.8)*, such that* $\|u(t,\cdot)\|_{L^2} = \|u_0\|_{L^2}$*. The solution is maximal in the sense that if* $T_c<\infty$*, then*

$$\lim_{t\to T_c} \|u(t,\cdot)\|_{H^k} = +\infty.$$

The solution $u(t,\cdot)$ may not exist for all times, even if $\lambda \geqslant 0$, i.e. even if the nonlinearity in the original equation (1.1) is defocusing. However, we can claim $T_c=\infty$ in either of the following cases (see e.g. [11]):

- $\nabla_k^2 E_m(p_0)$ is positive definite and $\lambda_m \geqslant 0$, or
- $\nabla_k^2 E_m(p_0)$ is negative definite and $\lambda_m \leqslant 0$.

On the contrary, if for instance $\nabla_k^2 E_m(p_0)$ is positive definite and $\lambda_m < 0$ (focusing nonlinearity), finite time blow up (that is, $T_c<\infty$) may occur, see, e.g., [27, 11]. This is the case typically if the initial datum is "too large": for any fixed profile $u_0 \in \mathcal{S}(\mathbb{R}^d)$, if one considers $u_{|t=0} = \Lambda u_0$, there exists $\Lambda_0>0$ such that for all $\Lambda \geqslant \Lambda_0$, $T_c<\infty$. Note that in other situations, where the signature of $\nabla_k^2 E_m(p_0)$ is non-trivial (hence $d\geqslant 2$), the issue of global existence *vs.* finite time blow-up is an open question.

Remark 3.2. Clearly, for $\alpha>\alpha_c$ these issues do not occur, since the leading order profile $u_{\rm lin}$ solves the linear equation (2.9) and hence exists for all times, $T_c=+\infty$.

Lemma 3.1 provides the existence of a local-in-time solution u of the effective mass equation. In view of the multi-scale expansion given in Section 2, we can thus define an approximate solution by

$$\psi^\varepsilon_{\rm app}(t,x) := \varepsilon^{-d/4}\left(U_0+\sqrt{\varepsilon}U_1+\varepsilon U_2\right)\left(t,\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right){\rm e}^{i\phi_m(t,x)/\varepsilon}, \tag{3.1}$$

which satisfies the original equation (1.1) up to some remainder terms:

$$\left(i\varepsilon\partial_t + \frac{\varepsilon^2}{2}\Delta - V_{\rm per}\right)\psi^\varepsilon_{\rm app} - \lambda\varepsilon^\alpha|\psi^\varepsilon_{\rm app}|^{2\sigma}\psi^\varepsilon_{\rm app} = \\ \frac{\mathrm{e}^{i\phi_m/\varepsilon}}{\varepsilon^{d/4}}\varepsilon^{3/2}\left(r_1^\varepsilon + r_2^\varepsilon\right)(t,z,y)\Big|_{(z,y)=\left(\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right)} - \lambda R^\varepsilon(t,x).$$

The remainder terms are given by

$$r_1^\varepsilon(t,z,y) = L_2U_1(t,z,y), r_2^\varepsilon(t,z,y) = L_1U_2(t,z,y) + \sqrt{\varepsilon}L_2U_2(t,z,y),$$

and $R^\varepsilon = \varepsilon^\alpha|\psi^\varepsilon_{\rm app}|^{2\sigma}\psi^\varepsilon_{\rm app}$ if $\alpha > \alpha_c$, while if $\alpha = \alpha_c = 1 + d\sigma/2$,

$$R^\varepsilon = \varepsilon^{1+d\sigma/2}|\psi^\varepsilon_{\rm app}|^{2\sigma}\psi^\varepsilon_{\rm app} - \frac{\varepsilon}{\varepsilon^{d/4}}\mathrm{e}^{i\phi_m/\varepsilon}\left|U_0\left(t,\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right)\right|^{2\sigma}U_0\left(t,\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right).$$

This, together with the regularity result established in Lemma 2.1 then directly yields the following proposition.

Proposition 3.3. *Assume* (1.7) *and let* $\alpha \geqslant \alpha_c = 1 + d\sigma/2$. *Then, we can find* $\psi^\varepsilon_{\rm app}$ *such that:*
1. *For all* $T \in [0, T_c)$, $\psi^\varepsilon_{\rm app}$ *has a coherent state structure on* $[0,T]$, *in the sense that there exists* C *independent of* $\varepsilon \in (0,1]$ *such that, with* φ^ε *defined in* (1.5),

$$\text{for } \alpha = \alpha_c, \quad \sup_{t\in[0,T]}\|\psi^\varepsilon_{\rm app}(t,\cdot) - \varphi^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \leqslant C\sqrt{\varepsilon},$$
$$\text{for } \alpha > \alpha_c, \quad \sup_{t\in[0,T]}\|\psi^\varepsilon_{\rm app}(t,\cdot) - \varphi^\varepsilon_{\rm lin}(t,\cdot)\|_{L^2(\mathbb{R}^d)} \leqslant C\sqrt{\varepsilon},$$

where $\varphi^\varepsilon_{\rm lin}$ *is the approximate solution constructed from* $u_{\rm lin}$, *solving* (2.9).
2. *The function solves* (1.1) *up to a small error:*

$$i\varepsilon\partial_t\psi^\varepsilon_{\rm app} + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon_{\rm app} = V_{\rm per}\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon_{\rm app} + \lambda\varepsilon^\alpha|\psi^\varepsilon_{\rm app}|^{2\sigma}\psi^\varepsilon_{\rm app} + \varepsilon w^\varepsilon,$$

where the remainder term w^ε *satisfies: for all* $T > 0$, *with* $T < T_c$ *in the case* $\alpha = \alpha_c$, *there exists* $C > 0$ *independent of* $\varepsilon > 0$ *such that*

$$\sup_{t\in[0,T]}\|w^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)} \leqslant C\begin{cases}\varepsilon^{\min(\alpha-\alpha_c,1/2)} & \text{if } \alpha > \alpha_c,\\ \sqrt{\varepsilon} & \text{if } \alpha = \alpha_c.\end{cases}$$

Note that because of the factor ε in front of the time derivative, it is natural to represent a small error term as ε times as small term.

3.2. **Nonlinear stability.** It remains to prove nonlinear stability of the approximate solution constructed above. For the sake of simplicity we shall do so only for $\alpha = \alpha_c$ and $d = 1$. The (physically less interesting) case $\alpha > \alpha_c$ can be proved analogously and a possible generalization to higher dimensions is indicated in Remark 3.6 below. For $\varepsilon_0 > 0$, set

$$\|f^\varepsilon\|_{H^1_\varepsilon} := \sup_{0<\varepsilon\leqslant\varepsilon_0}\left(\|f^\varepsilon\|_{L^2} + \|\varepsilon\partial_x f^\varepsilon\|_{L^2}\right),$$

which is equivalent to the usual H^1-norm for every (fixed) $\varepsilon > 0$. The approach that we present is similar to the one followed in [9]: First, we need to construct a more accurate

approximate solution than the one stated in Proposition 3.3. Taking the asymptotic expansion presented in Section 2 one step further, we can gain a factor $\sqrt{\varepsilon}$ in Proposition 3.3. More precisely, we can construct $\widetilde{\psi}^\varepsilon_{\rm app}$ such that:

$$\sup_{t\in[0,T]} \left\| \psi^\varepsilon_{\rm app}(t,\cdot) - \widetilde{\psi}^\varepsilon_{\rm app}(t,\cdot) \right\|_{H^1_\varepsilon} \leqslant C\sqrt{\varepsilon}, \tag{3.2}$$

and

$$i\varepsilon\partial_t\widetilde{\psi}^\varepsilon_{\rm app} + \frac{\varepsilon^2}{2}\Delta\widetilde{\psi}^\varepsilon_{\rm app} = V_{\rm per}\left(\frac{x}{\varepsilon}\right)\widetilde{\psi}^\varepsilon_{\rm app} + \lambda\varepsilon^{1+\sigma/2}|\widetilde{\psi}^\varepsilon_{\rm app}|^{2\sigma}\widetilde{\psi}^\varepsilon_{\rm app} + \varepsilon\widetilde{w}^\varepsilon,$$

where the additional factor $\sqrt{\varepsilon}$ is reflected in the error estimate

$$\sup_{t\in[0,T]} \|\widetilde{w}^\varepsilon(t,\cdot)\|_{H^1_\varepsilon} \leqslant C\varepsilon. \tag{3.3}$$

Note that in this case the corrector U_1 is not the same for $\widetilde{\psi}^\varepsilon_{\rm app}$, since unlike what we have done in §2.2, we can no longer assume $u_1 = 0$. Rather, u_1 now solves an evolution equation, which is essentially (1.8) linearized about u, with a non-trivial source term (see [9] for more details). Therefore, the estimate (3.2) must be expected to be sharp in general.

Having constructed such an improved approximation $\widetilde{\psi}^\varepsilon_{\rm app}$ we can state the following nonlinear stability result:

Theorem 3.4. *Let $d = 1$, $\alpha = 1 + \sigma/2$, $\sigma \in \mathbb{N}$, and Assumption* (1.7) *hold. In addition, suppose that the initial data satisfy:*

$$\left\| \psi^\varepsilon_0 - \widetilde{\psi}^\varepsilon_{\rm app|t=0} \right\|_{L^2(\mathbb{R})} = \mathcal{O}(\varepsilon), \quad \left\| \varepsilon\partial_x\left(\psi^\varepsilon_0 - \widetilde{\psi}^\varepsilon_{\rm app|t=0}\right) \right\|_{L^2(\mathbb{R})} = \mathcal{O}(1). \tag{3.4}$$

Let $T \in [0, T_c)$. Then, there exists $\varepsilon_0 = \varepsilon_0(T)$ such that for $\varepsilon \in (0, \varepsilon_0]$, the solution of (1.1) *exists on $[0, T]$. Moreover, there exists C independent of $\varepsilon \in (0, \varepsilon_0]$ such that*

$$\sup_{t\in[0,T]} \|\psi^\varepsilon(t,\cdot) - \varphi^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R})} \leqslant C\sqrt{\varepsilon}.$$

where φ^ε is defined in (1.5)*.*

Proof. The scheme of the proof is the same as the proof of Theorem 4.5 in [9], so we shall only give the main steps. Fix $T < T_c$ and let $\eta^\varepsilon = \psi^\varepsilon - \widetilde{\psi}^\varepsilon_{\rm app}$ be the error between the exact and the approximate solution. It satisfies

$$i\varepsilon\partial_t\eta^\varepsilon + \frac{\varepsilon^2}{2}\Delta\eta^\varepsilon = V_{\rm per}\left(\frac{x}{\varepsilon}\right)\eta^\varepsilon + \lambda\varepsilon^{1+\sigma/2}\left(|\psi^\varepsilon|^{2\sigma}\psi^\varepsilon - |\widetilde{\psi}^\varepsilon_{\rm app}|^{2\sigma}\widetilde{\psi}^\varepsilon_{\rm app}\right) - \varepsilon\widetilde{w}^\varepsilon,$$

with $\|\eta^\varepsilon_{|t=0}\|_{L^2} = \mathcal{O}(\varepsilon)$, $\|\varepsilon\partial_x\eta^\varepsilon_{|t=0}\|_{L^2} = \mathcal{O}(1)$ by assumption. From [23], we have:

Lemma 3.5 (Moser's lemma)**.** *Let $R > 0$, $s \in \mathbb{N}$ and $F(z) = |z|^{2\sigma}z$, $\sigma \in \mathbb{N}$. Then there exists $C = C(R, s, \sigma)$ such that if v^ε satisfies*

$$\left\| (\varepsilon\partial_x)^\beta v^\varepsilon \right\|_{L^\infty(\mathbb{R})} \leqslant R, \quad 0 \leqslant \beta \leqslant s,$$

and δ^ε satisfies $\|\delta^\varepsilon\|_{L^\infty(\mathbb{R})} \leqslant R$, then

$$\sum_{0\leqslant\beta\leqslant s} \left\| (\varepsilon\partial_x)^\beta \left(F(v^\varepsilon + \delta^\varepsilon) - F(v^\varepsilon)\right) \right\|_{L^2} \leqslant C \sum_{0\leqslant\beta\leqslant s} \left\| (\varepsilon\partial_x)^\beta \delta^\varepsilon \right\|_{L^2}.$$

We apply this lemma with $v^\varepsilon = \varepsilon^{1/4}\widetilde{\psi}^\varepsilon_{\rm app}$, and $s=0$, $s=1$ successively: there exists $R>0$ independent of $\varepsilon\in(0,1]$ such that

$$\sup_{t\in[0,T]}\sum_{\beta=0,1}\left\|(\varepsilon\partial_x)^\beta\, v^\varepsilon(t)\right\|_{L^\infty(\mathbb{R})}\leqslant R.$$

Set $\delta^\varepsilon=\varepsilon^{1/4}\eta^\varepsilon$. By assumption and the Gagliardo–Nirenberg inequality,

$$\|\delta^\varepsilon_{|t=0}\|_{L^\infty}=\varepsilon^{1/4}\|\eta^\varepsilon_{|t=0}\|_{L^\infty}\leqslant\varepsilon^{1/4}\sqrt{2}\varepsilon^{-1/2}\|\eta^\varepsilon_{|t=0}\|_{L^2}^{1/2}\|\varepsilon\partial_x\eta^\varepsilon_{|t=0}\|_{L^2}^{1/2}\leqslant C\varepsilon^{1/4}. \tag{3.5}$$

As long as $\|\delta^\varepsilon(t)\|_{L^\infty}\leqslant R$, energy estimates and Moser's lemma with $s=0$ yield

$$\|\eta^\varepsilon(t)\|_{L^2}\leqslant\|\eta^\varepsilon(0)\|_{L^2}+C\int_0^t\|\eta^\varepsilon(s)\|_{L^2}ds+\int_0^t\|\widetilde{w}^\varepsilon(s)\|_{L^2}ds,$$

where we have used the homogeneity of F. By Gronwall's Lemma, for $t\leqslant T$:

$$\|\eta^\varepsilon(t)\|_{L^2}\leqslant C(T)\left(\|\eta^\varepsilon(0)\|_{L^2}+\int_0^t\|\widetilde{w}^\varepsilon(s)\|_{L^2}ds\right)\leqslant C\varepsilon.$$

Applying the operator $\varepsilon\partial_x$ to the equation satisfied by η^ε, we infer similarly

$$\begin{aligned}\|\varepsilon\partial_x\eta^\varepsilon(t)\|_{L^2}\leqslant&\|\varepsilon\partial_x\eta^\varepsilon(0)\|_{L^2}+C\int_0^t\|\eta^\varepsilon(s)\|_{H^1_\varepsilon}ds+\int_0^t\|\varepsilon\partial_x\widetilde{w}^\varepsilon(s)\|_{L^2}ds\\&+\frac{1}{\varepsilon}\|\partial_yV_{\rm per}\|_{L^\infty}\int_0^t\|\eta^\varepsilon(s)\|_{L^2}ds,\end{aligned}$$

where the last term stems from the relation $[\varepsilon\partial_x,V_{\rm per}(x/\varepsilon)]=\partial_yV_{\rm per}(x/\varepsilon)\in L^\infty$, since $V_{\rm per}$ is smooth and periodic. Thus,

$$\|\varepsilon\partial_x\eta^\varepsilon(t)\|_{L^2}\leqslant C+C\int_0^t\|\varepsilon\partial_x\eta^\varepsilon(s)\|_{L^2}ds+Ct.$$

Gronwall's lemma now yields $\|\varepsilon\partial_x\eta^\varepsilon(t)\|_{L^2}\leqslant C(T)$. In view of the Gagliardo–Nirenberg inequality,

$$\|\delta^\varepsilon(t)\|_{L^\infty}=\varepsilon^{1/4}\|\eta^\varepsilon(t)\|_{L^\infty}\leqslant\sqrt{2}\varepsilon^{-1/4}\|\eta^\varepsilon\|_{L^2}^{1/2}\|\varepsilon\partial_x\eta^\varepsilon\|_{L^2}^{1/2}\leqslant C(T)\varepsilon^{1/4}.$$

For ε sufficiently small (depending of T), $\|\delta^\varepsilon(t)\|_{L^\infty}\leqslant R$ for all $t\in[0,T]$, and the result follows from a bootstrap argument. □

The above theorem shows nonlinear stability of the approximate solution up to times of order $\mathcal{O}(1)$, i.e. independent of ε, provided that the initial data are *well-prepared*, in the sense given in (3.4). Essentially this means that ψ_0^ε contains not only U_0, but also $\widetilde{U}_1$ associated to $\widetilde{\psi}^\varepsilon_{\rm app}$. We shall not insist further on this aspect, which is probably a technical artifact, and remark that in the linear case a stronger result is valid, see [10] where stability is proved up to the so-called *Ehrenfest time* $\mathcal{O}(\ln 1/\varepsilon)$, and no well-preparedness as in (3.4) is needed (an initial error $\mathcal{O}(\varepsilon^r)$ for *some* $r>0$ suffices).

Remark 3.6. If $x\in\mathbb{R}^d$ with $d\geqslant 2$, the proof can be easily adapted, provided an even better approximate solution is constructed. The reason is that, instead of (3.5), one needs to rely on the following Gagliardo–Nirenberg inequality

$$\|\delta^\varepsilon\|_{L^\infty(\mathbb{R}^d)}\leqslant C\varepsilon^{-d/2}\|\delta^\varepsilon\|_{L^2(\mathbb{R}^d)}^{1-d/(2s)}\,\|\,|\varepsilon\nabla|^s\delta^\varepsilon\|_{L^2(\mathbb{R}^d)}^{d/(2s)},\quad\text{for } s>d/2.$$

Thus, in order to account for the singular factor $\varepsilon^{-d/2}$, one is forced to construct an approximate solution $\widetilde{\psi}^\varepsilon_{\rm app}$ to a sufficiently high order in ε (see [9] for more details).

4. The case of nonlocal nonlinearities

In this section we shall show how to perform the same asymptotic analysis as before in the case of nonlocal nonlinearities. In other words, we consider

$$i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon = V_{\rm per}\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon + \varepsilon^\alpha(K*|\psi^\varepsilon|^2)\psi^\varepsilon \tag{4.1}$$

with $K(x)\in\mathbb{R}$ some given interaction kernel. In the following we shall focus on two particular choices of interaction kernels K which are physically relevant.

4.1. **Homogeneous kernels.**

In this subsection we shall consider functions of the form

$$K(x) = \lambda|x|^\mu,\ \lambda\in\mathbb{R},\ \text{with } \mu\in\mathbb{R}\setminus\{0\} \text{ such that } -\min(2,d) < \mu \leqslant 2.$$

For example, the choice $\mu=-1$ in $d=3$ corresponds to the classical Hartree nonlinearity, modeling a self-consistent, repulsive ($\lambda>0$) Coulomb interaction. The case $\mu>0$ has been recently studied in [19].

Like in the case of local nonlinearities, the critical exponent α_c depends on the homogeneity μ, namely $\alpha_c = 1-\mu/2$. This can be seen as follows: We plug the ansatz

$$\varphi^\varepsilon(t,x) = \varepsilon^{-d/4}u\left(t,\frac{x-q(t)}{\sqrt{\varepsilon}}\right)\chi_m\left(\frac{x}{\varepsilon},p_0\right)\mathrm{e}^{i\phi_m(t,x)/\varepsilon}$$

into the convolution term $\varepsilon^{1-\mu/2}\left(|x|^\mu * |\psi^\varepsilon|^2\right)$. This yields

$$\varepsilon^{1-\mu/2-d/2}\int_{\mathbb{R}^d}|x-\xi|^\mu\left|u\left(t,\frac{\xi-q(t)}{\sqrt{\varepsilon}}\right)\right|^2\left|\chi_m\left(\frac{\xi}{\varepsilon},p_0\right)\right|^2 d\xi.$$

We want this term to be of order $\mathcal{O}(\varepsilon)$ in our asymptotic expansion, to mimic the approach presented in §2. In this case, it will consequently appear within b_2^ε, leading to the effective mass equation. In order to show that this is indeed the case, we rewrite the initial convolution as

$$\varepsilon^{1-\mu/2-d/2}\int_{\mathbb{R}^d}|\xi|^\mu\left|u\left(t,\frac{x-\xi-q(t)}{\sqrt{\varepsilon}}\right)\right|^2\left|\chi_m\left(\frac{x-\xi}{\varepsilon},p_0\right)\right|^2 d\xi,$$

and use the substitution $z=(x-q(t))/\sqrt{\varepsilon}$ in the envelope u, and $y=x/\varepsilon$ in χ_m:

$$\varepsilon^{1-\mu/2-d/2}\int_{\mathbb{R}^d}|\xi|^\mu\left|u\left(t,z-\frac{\xi}{\sqrt{\varepsilon}}\right)\right|^2\left|\chi_m\left(y-\frac{\xi}{\varepsilon},p_0\right)\right|^2 d\xi.$$

Setting $\zeta=\xi/\sqrt{\varepsilon}$, this can be written as

$$\varepsilon\int|\zeta|^\mu\left|u\left(t,z-\zeta\right)\right|^2\left|\chi_m\left(y-\frac{\zeta}{\sqrt{\varepsilon}},p_0\right)\right|^2 d\zeta.$$

Then, the following averaging result can be proved:

Proposition 4.1. *Let* (1.7) *hold true and assume that* $\zeta\mapsto|\zeta|^\mu\left|u\left(t,z-\zeta\right)\right|^2$ *is in* $L^1(\mathbb{R}^d)$. *Then, for all* $k\in Y^*$, *it holds*

$$\int_{\mathbb{R}^d}|\zeta|^\mu\left|u\left(t,z-\zeta\right)\right|^2\left|\chi_m\left(y-\frac{\zeta}{\sqrt{\varepsilon}},k\right)\right|^2 d\zeta\underset{\varepsilon\to0}{\longrightarrow}\int_{\mathbb{R}^d}|\zeta|^\mu\left|u\left(t,z-\zeta\right)\right|^2 d\zeta.$$

In addition, if $\zeta\mapsto|\zeta|^\mu\left|u\left(t,z-\zeta\right)\right|^2$ *is in* $W^{1,1}(\mathbb{R}^d)$, *then the above convergence holds with an error of order* $\mathcal{O}(\sqrt{\varepsilon})$.

This result can be seen as a variant of the *two-scale convergence* results introduced in [20, 1], and used in [2]. The main difference here is the convolution structure.

Proof. We decompose $y \mapsto |\chi_m(y,k)|^2$ into its generalized Fourier series (recall that $\Gamma \simeq \mathbb{Z}^d$) and write

$$\int |\zeta|^\mu \left|u\left(t,z-\zeta\right)\right|^2 \left|\chi_m\left(y-\frac{\zeta}{\sqrt{\varepsilon}}\right)\right|^2 d\zeta = \sum_{\gamma\in\Gamma} \int |\zeta|^\mu \left|u\left(t,z-\zeta\right)\right|^2 c_\gamma \mathrm{e}^{i\gamma\cdot(y-\zeta/\sqrt{\varepsilon})} d\zeta$$
$$= \sum_{\gamma\in\Gamma} c_\gamma \mathrm{e}^{i\gamma\cdot y} \int |\zeta|^\mu \left|u\left(t,z-\zeta\right)\right|^2 \mathrm{e}^{-i\gamma\cdot\zeta/\sqrt{\varepsilon}} d\zeta.$$

By Riemann–Lebesgue lemma, for each term with $\gamma \neq 0$, the limit, as $\varepsilon \to 0$, is zero. Then only the term corresponding to $\gamma = 0$ remains, with

$$c_0(k) = \int_Y \left|\chi_m\left(y,k\right)\right|^2 dy = 1,$$

since the eigenfunctions $\chi_m(\cdot,k)$ form an orthonormal basis of $L^2(Y)$. By the Dominated Convergence Theorem, we can exchange the sum over $\gamma \in \Gamma$ and the limit $\varepsilon \to 0$ in the above computation provided that $\zeta \mapsto |\zeta|^\mu \left|u\left(t,z-\zeta\right)\right|^2$ is in L^1 (with an error $o(1)$). In the case where the function is in $W^{1,1}$ we obtain an error $\mathcal{O}(\sqrt{\varepsilon})$. The reason is that the coefficients $(c_\gamma)_{\gamma\in\Gamma}$ decrease rapidly for large $|\gamma|$, since $y \mapsto |\chi_m(y,k)|^2$ is smooth, provided Assumption (1.7) holds true and thus we can perform an integration by parts, and use dominated convergence again. □

Assuming that u is sufficiently smooth and decaying, we can use the above averaging result and perform the same asymptotic expansion as given in Section 2 to arrive at the effective nonlinear Schrödinger equation

$$i\partial_t u + \frac{1}{2}\mathrm{div}_z\left(\left(\nabla_k^2 E_m\left(p_0\right)\right)\cdot\nabla_z\right)u = \lambda(|z|^\mu * |u|^2)u, \quad u_{|t=0} = u_0. \tag{4.2}$$

For $\mu < 0$, existence of a smooth solution $u \in C([0,T_c), H^k)$, locally in time, can be proved along the same lines as in [11] and hence, a result analogous to the one stated in Proposition 3.3 is straightforward. In the case $\mu > 0$ one can follow the arguments of [19], using a functional framework which is more intricate, however (the Sobolev spaces H^k are not sufficient but have to be intersected with weighted L^2 spaces), and we shall not do so here. In a similar spirit, stability in the sense of Theorem 3.4 follows from an adaptation of Lemma 3.5, which we leave out.

4.2. **Smooth kernels.** If in (4.1) the interaction kernel $K(x)$ is a given smooth function, bounded as well as its derivative, then $\alpha_c = 1$ (corresponding *formally* to the case $\mu = 0$). Such a situation appears for example in [5], where

$$K(x) = \left(a_1 + a_2|x|^2 + a_3|x|^4\right)\mathrm{e}^{-A^2|x|^2} + a_4\mathrm{e}^{-B^2|x|^2},$$

with constants $a_1, a_2, a_3, a_4 \in \mathbb{R}$, $A, B > 0$. Resuming the above computations in this context, we find:

$$K * |\psi^\varepsilon|^2 = \varepsilon^{-d/2}\int_{\mathbb{R}^d} K(\xi)\left|u\left(t,\frac{x-\xi-q(t)}{\sqrt{\varepsilon}}\right)\right|^2\left|\chi_m\left(\frac{x-\xi}{\varepsilon},p_0\right)\right|^2 d\xi$$
$$= \int_{\mathbb{R}^d} K(\zeta\sqrt{\varepsilon})\left|u\left(t,z-\zeta\right)\right|^2\left|\chi_m\left(y-\frac{\zeta}{\sqrt{\varepsilon}},p_0\right)\right|^2 d\zeta$$
$$\underset{\varepsilon\to 0}{\longrightarrow} K(0)\int_{\mathbb{R}^d}\left|u\left(t,z-\zeta\right)\right|^2 d\zeta = K(0)\|u(t)\|_{L^2}^2 = K(0)\|u_0\|_{L^2}^2,$$

due to mass conservation, along with an $\mathcal{O}(\sqrt{\varepsilon})$ convergence rate under suitable assumptions. In particular, this shows that, as $\varepsilon \to 0$, the nonlinear effects become *negligible*. Indeed, in this case the envelope equation becomes

$$i\partial_t u + \frac{1}{2}\mathrm{div}_z\left(\left(\nabla_k^2 E_m\left(p_0\right)\right)\cdot\nabla_z\right)u = K(0)\|u_0\|_{L^2}^2 u, \quad u_{|t=0} = u_0.$$

The right hand side involves a constant potential term, which can be *gauged away* via

$$v(t,x) = u(t,x)\mathrm{e}^{itK(0)\|u_0\|_{L^2}^2}.$$

The remaining amplitude $v(t,x)$ then solves a *free* Schrödinger equation with effective mass tensor $\nabla_k^2 E_m\left(p_0\right)$.

Appendix A. Some useful algebraic identities

For the derivation of the effective mass equation (1.8) we shall rely on several algebraic identities, which can be derived from Bloch's spectral problem (for more details see, e.g., [4]): First, taking the gradient w.r.t. to k of (1.2), we have

$$\nabla_k\left(H(k)-E_m\right)\chi_m + \left(H(k)-E_m\right)\nabla_k\chi_m = 0 \tag{A.1}$$

and, by taking the in $L^2(Y)$-scalar product with χ_m, we obtain

$$\nabla_k E_m = \left\langle\chi_m, \nabla_k H(k)\chi_m\right\rangle_{L^2(Y)} + \left\langle\chi_m, \left(H(k)-E_m\right)\nabla_k\chi_m\right\rangle_{L^2(Y)}.$$

Since $H(k)$ is self-adjoint, the last term is zero, thanks to (1.2). We infer

$$\nabla_k E_m(k) = \left\langle\chi_m, \left(-i\nabla_y + k\right)\chi_m\right\rangle_{L^2(Y)}. \tag{A.2}$$

Differentiating (A.1) again, we have, for all $j,\ell\in\{1,\ldots,d\}$:

$$\begin{aligned}\partial^2_{k_jk_\ell}\left(H(k)-E_m\right)\chi_m + \partial_{k_j}\left(H(k)-E_m\right)\partial_{k_\ell}\chi_m + \partial_{k_\ell}\left(H(k)-E_m\right)\partial_{k_j}\chi_m \\ + \left(H(k)-E_m\right)\partial^2_{k_jk_\ell}\chi_m = 0.\end{aligned}$$

Taking the scalar product with χ_m, we have:

$$\begin{aligned}\partial^2_{k_jk_\ell}E_m(k) = \delta_{j\ell} + \left\langle\left(-i\partial_{y_j}+k_j\right)\partial_{k_\ell}\chi_m + \left(-i\partial_{y_\ell}+k_\ell\right)\partial_{k_j}\chi_m, \chi_m\right\rangle_{L^2(Y)} \\ - \left\langle\partial_{k_\ell}E_m\partial_{k_j}\chi_m + \partial_{k_j}E_m\partial_{k_\ell}\chi_m, \chi_m\right\rangle_{L^2(Y)}.\end{aligned} \tag{A.3}$$

Appendix B. Adding an additional, slowly varying potential

As a possible extension of our study, one might want to consider the case where the wave function is not only under the influence of the nonlinearity and the periodic potential, but also add an additional *slowly varying* external potential $V(t,x)$, i.e.

$$i\varepsilon\partial_t\psi^\varepsilon + \frac{1}{2}\Delta\psi^\varepsilon = V_{\mathrm{per}}\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon + V(t,x)\psi^\varepsilon + \varepsilon^\alpha f(|\psi^\varepsilon|^2)\psi^\varepsilon.$$

At least formally, this can be done by combining our analysis with the results given in [10]: To this end, we define the semi-classical band Hamiltonian

$$h_m^{\mathrm{sc}}(k,x) = E_m(k) + V(t,x), \quad (k,x)\in Y^*\times\mathbb{R}^d,$$

and denote the corresponding semiclassical phase space trajectories by

$$\begin{cases}\dot q(t) = \nabla_k E_m\left(p(t)\right), & q(0) = q_0,\\ \dot p(t) = -\nabla_x V\left(t,q(t)\right), & p(0) = p_0.\end{cases} \tag{B.1}$$

This system is the analogue of the classical Hamiltonian phase space flow, in the presence of an additional periodic potential V_{per}. In order to make sure that the system (B.1) is

well-defined, it is sufficient to assume that $E_m(p(t))$ is a simple eigenvalue ($|E_m(p(t)) - E_n(k)| \neq 0$ for all $n \neq m$, $t \in \mathbb{R}$, $k \in Y^*$); see e.g. [10], where examples of such situations are given.

The approximate solution under the form of a coherent state within the m-th Bloch band is then given by:

$$\varphi^\varepsilon(t,x) = \varepsilon^{-d/4} u\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\right) \chi_m\left(\frac{x}{\varepsilon}, p(t)\right) \mathrm{e}^{i\Phi_m(t,x)/\varepsilon}$$

with $q(t), p(t)$ obtained from (B.1). The highly oscillatory phase takes the form $\Phi_m(t,x) = S_m(t) + p(t)\cdot(x-q(t))$, where $S_m(t) \in \mathbb{R}$ is the (purely time-dependent) semi-classical action

$$S_m(t) = \int_0^t p(s)\cdot\nabla E_m(p(s)) - h_m^{\mathrm{sc}}\left(p(s), q(s)\right)\, ds.$$

Note that Φ_m simplifies to (1.6) in the case where $V(t,x) = 0$. In this case, the governing equation for the leading profile $u(t,z)$ is found to be a nonlinear Schrödinger equation with time-dependent quadratic potential, time-dependent effective mass $\nabla_k^2 E_m(p(t))$ and coupling constant $\lambda_m(t)$, see [10] for more details. These features make it difficult to give sufficient conditions under which where the solution $u(t,z)$ is global, i.e. $T_c = \infty$. Indeed, the signature of $\nabla_k^2 E_m(p(t))$ may change, and the existence of Strichartz estimates for the linear part is a non-trivial issue. Moreover, $\lambda_m(t)$ may also change sign, making the analysis even more delicate.

REFERENCES

[1] G. ALLAIRE, *Homogenization and two-scale convergence*, SIAM J. Math. Anal., 23 (1992), pp. 1482–1518.

[2] G. ALLAIRE AND A. PIATNITSKI, *Homogenization of the Schrödinger equation and effective mass theorems*, Comm. Math. Phys., 258 (2005), pp. 1–22.

[3] P. BECHOUCHE, N. MAUSER, AND F. POUPAUD, *Semiclassical limit for the Schrödinger-Poisson equation in a crystal*, Comm. Pure Appl. Math., 54 (2001), pp. 851–890.

[4] A. BENSOUSSAN, J.-L. LIONS, AND G. PAPANICOLAOU, *Asymptotic analysis for periodic structures*, vol. 5 of Studies in Mathematics and its Applications, North-Holland Publishing Co., Amsterdam, 1978.

[5] N. G. BERLOFF, *Nonlocal nonlinear Schroedinger equations as models of superfluidity*, J. Low Temp. Phys., 116 (1999), pp. 1–2.

[6] A. BOUZOUINA AND D. ROBERT, *Uniform semiclassical estimates for the propagation of quantum observables*, Duke Math. J., 111 (2002), pp. 223–252.

[7] R. CARLES AND C. FERMANIAN-KAMMERER, *A nonlinear adiabatic theorem for coherent states*, Nonlinearity, 24 (2011), pp. 2143–2164.

[8] ———, *Nonlinear coherent states and Ehrenfest time for Schrödinger equations*, Commun. Math. Phys., 301 (2011), pp. 443–472.

[9] R. CARLES, P. A. MARKOWICH, AND C. SPARBER, *Semiclassical asymptotics for weakly nonlinear Bloch waves*, J. Statist. Phys., 117 (2004), pp. 343–375.

[10] R. CARLES AND C. SPARBER, *Semiclassical wave packet dynamics in Schrödinger equations with periodic potentials*. Preprint. `http://arxiv.org/abs/1101.3136`, 2011.

[11] T. CAZENAVE, *Semilinear Schrödinger equations*, vol. 10 of Courant Lecture Notes in Mathematics, New York University Courant Institute of Mathematical Sciences, New York, 2003.

[12] D. CHOI AND Q. NIU, *Bose-Einstein condensates in an optical lattice*, Phys. Rev. Lett., 82 (1999), pp. 2022–2025.

[13] M. COMBESCURE AND D. ROBERT, *Quadratic quantum Hamiltonians revisited*, Cubo, 8 (2006), pp. 61–86.

[14] Z. DUAN, M. J. STEEL, X. A., AND W. ZHANG, *Effective mass approach for a Bose-Einstein condensate in an optical lattice*, Chinese Science Bulletin, 54 (2009), pp. 4182–4196.

[15] E. FAOU, V. GRADINARU, AND C. LUBICH, *Computing semiclassical quantum dynamics with Hagedorn wavepackets*, SIAM J. Sci. Comput., 31 (2009), pp. 3027–3041.

[16] J.-C. GUILLOT, J. RALSTON, AND E. TRUBOWITZ, *Semiclassical asymptotics in solid state physics*, Comm. Math. Phys., 116 (1988), pp. 401–415.

[17] G. A. HAGEDORN, *Semiclassical quantum mechanics. I. The $\hbar \to 0$ limit for coherent states*, Comm. Math. Phys., 71 (1980), pp. 77–93.
[18] E. B. KOLOMEISKY, T. J. NEWMAN, J. P. STRALEY, AND X. QI, *Low-dimensional Bose liquids: Beyond the Gross-Pitaevskii approximation*, Phys. Rev. Lett., 85 (2000), pp. 1146–1149.
[19] S. MASAKI, *Analysis of Hartree equation with an interaction growing at the spatial infinity*. Preprint, `http://arxiv.org/abs/1103.3083`.
[20] G. NGUETSENG, *A general convergence result for a functional related to the theory of homogenization*, SIAM J. Math. Anal., 20 (1989), pp. 608–623.
[21] T. PAUL, *Semi-classical methods with emphasis on coherent states*, in Quasiclassical methods (Minneapolis, MN, 1995), vol. 95 of IMA Vol. Math. Appl., Springer, New York, 1997, pp. 51–88.
[22] L. PITAEVSKII AND S. STRINGARI, *Bose-Einstein condensation*, vol. 116 of International Series of Monographs on Physics, The Clarendon Press Oxford University Press, Oxford, 2003.
[23] J. RAUCH AND M. KEEL, *Lectures on geometric optics*, in Hyperbolic equations and frequency interactions (Park City, UT, 1995), Amer. Math. Soc., Providence, RI, 1999, pp. 383–466.
[24] R. E. SLUSHER AND B. J. EGGLETON, eds., *Nonlinear Photonic Crystals*, Springer-Verlag, Berlin, 2003.
[25] C. SPARBER, *Effective mass theorems for nonlinear Schrödinger equations*, SIAM J. Appl. Math., 66 (2006), pp. 820–842.
[26] H. SPOHN, *Long time asymptotics for quantum particles in a periodic potential*, Phys. Rev. Lett., 77 (1996), pp. 1198–1201.
[27] T. TAO, *Nonlinear dispersive equations*, vol. 106 of CBMS Regional Conference Series in Mathematics, Published for the Conference Board of the Mathematical Sciences, Washington, DC, 2006. Local and global analysis.
[28] C. H. WILCOX, *Theory of Bloch waves*, J. Analyse Math., 33 (1978), pp. 146–167.

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