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Homogenization of the Schrödinger Equation and Effective Mass Theorems

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Abstract: We study the homogenization of a Schrödinger equation with a large periodic potential: denoting by ϵ the period, the potential is scaled as ϵ^{-2}. We obtain a rigorous derivation of so-called effective mass theorems in solid state physics. More precisely, for well-prepared initial data concentrating on a Bloch eigenfunction we prove that the solution is approximately the product of a fast oscillating Bloch eigenfunction and of a slowly varying solution of an homogenized Schrödinger equation. The homogenized coefficients depend on the chosen Bloch eigenvalue, and the homogenized solution may experience a large drift. The homogenized limit may be a system of equations having dimension equal to the multiplicity of the Bloch eigenvalue. Our method is based on a combination of classical homogenization techniques (two-scale convergence and suitable oscillating test functions) and of Bloch waves decomposition.

1. Introduction

We study the homogenization of the following Schrödinger equation

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2}c\left(\dfrac{x}{\epsilon}\right) + d\left(x, \dfrac{x}{\epsilon}\right)\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T), \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{1}$$

where $0 < T \le +\infty$ is a final time, and the unknown function u_ϵ is complex-valued. The coefficients $A(y)$, $c(y)$ and $d(x, y)$ are real and bounded functions defined for $x \in \mathbb{R}^N$ and $y \in \mathbb{T}^N$ (the unit torus). Furthermore, the matrix $A(y)$ is symmetric, uniformly positive definite, while $c(y)$ and $d(x, y)$ do not satisfy any positivity assumption. Of course, the "usual" Schrödinger equation corresponds to the choice $A(y) \equiv Id$. Other choices may be interpreted as a periodic metric. The scaling of Eq. (1) is typical of homogenization (see e.g. [3], or chapter 4 in [6]) but is different from the scaling for studying its semi-classical limit (see e.g. [12, 15–17, 27, 29]). Let us recall this different semi-classical scaling of the Schrödinger equation which is

$$i\epsilon^{-1}\frac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \epsilon^{-2}\left(c\left(\frac{x}{\epsilon}\right) + d(x)\right)u_\epsilon = 0. \tag{2}$$

There are two differences between (1) and (2). First, there is a ϵ^{-1} coefficient in front of the time derivative in (2), which implies that in (1) we consider much larger times than in the semi-classical limit. Second, the microscopic potential $c(y)$ and the macroscopic potential $d(x)$ are of the same order of magnitude in (2), on the contrary of (1) where only small macroscopic potentials are considered (of order ϵ^2 with respect to the microscopic ones). Having both potentials of the same order of magnitude implies a strong mixing of different Bloch band components, while in our case the macroscopic potential vanishes fast enough, as ϵ tends to 0, so that it does not affect the phase function but only the amplitude. (From our analysis it is clear that ϵ^2 is the critical power of ϵ for which this effect holds.) The results are thus very different in these two frameworks. In particular, our framework is somehow simpler and enough to derive effective mass theorems without taking the semi-classical limit.

The “standard” homogenization of (1) is simple as we now explain. (By standard, we mean that assumption (6) on the initial data is satisfied.) Introduce the first eigencouple of the spectral cell problem

$$-\operatorname{div}_y\left(A(y)\nabla_y\psi_1\right) + c(y)\psi_1 = \lambda_1\psi_1 \quad \text{in } \mathbb{T}^N, \tag{3}$$

which, by the Krein-Rutman theorem, is real, simple and satisfies $\psi_1(y) > 0$ in $\mathbb{T}^N$. Furthermore, by a classical regularity result, ψ_1 is also continuous. Thus, one can change the unknown by writing a so-called *factorization principle* (see e.g. [3, 5, 21, 33])

$$v_\epsilon(t,x) = e^{-i\frac{\lambda_1 t}{\epsilon^2}}\frac{u_\epsilon(t,x)}{\psi_1\left(\frac{x}{\epsilon}\right)}, \tag{4}$$

and check easily, after some algebra, that the new unknown v_ϵ is a solution of a simpler equation

$$\begin{cases} i|\psi_1|^2\left(\frac{x}{\epsilon}\right)\frac{\partial v_\epsilon}{\partial t} - \operatorname{div}\left((|\psi_1|^2A)\left(\frac{x}{\epsilon}\right)\nabla v_\epsilon\right) + (|\psi_1|^2 d)\left(x,\frac{x}{\epsilon}\right)v_\epsilon = 0 & \text{in } \mathbb{R}^N\times(0,T) \\ v_\epsilon(t=0,x) = \frac{u_\epsilon^0(x)}{\psi_1\left(\frac{x}{\epsilon}\right)} & \text{in } \mathbb{R}^N. \end{cases} \tag{5}$$

The new Schrödinger equation (5) is simple to homogenize (see e.g. [6]) since it does not contain any singularly perturbed term, and we thus obtain uniform a priori estimates for its solution.

Theorem 1.1. *Let $v^0 \in H^1(\mathbb{R}^N)$. Assume that the initial data satisfies*

$$u_\epsilon^0(x) = \psi_1\left(\frac{x}{\epsilon}\right)v^0(x). \tag{6}$$

The new unknown v_ϵ, defined by (4), converges weakly in $L^2\left((0,T);H^1(\mathbb{R}^N)\right)$ to the solution v of the following homogenized problem

$$\begin{cases} i\frac{\partial v}{\partial t} - \operatorname{div}\left(A^*\nabla v\right) + d^*(x)\,v = 0 & \text{in } \mathbb{R}^N\times(0,T), \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{7}$$

where A^* is the "usual" homogenized tensor for the periodic coefficients $(|\psi_1|^2 A)(y)$ and $d^*(x) = \int_{\mathbb{T}^N} |\psi_1|^2(y) d(x,y)\,dy$.

In other words, Theorem 1.1 gives the following asymptotic behavior for the solution of (1) :

$$u_\epsilon(t,x) \approx e^{i\frac{\lambda_1 t}{\epsilon^2}} \psi_1\left(\frac{x}{\epsilon}\right) v(t,x),$$

where v is the solution of (7). Assumption (6) can be interpreted as an hypothesis on the well-prepared character of the initial data. There are many other types of initial data for which Theorem 1.1 is not meaningful. It turns out that, according to heuristical results in solid state physics (see e.g. [25, 28, 30]), there are many other types of well-prepared initial data for which a result like Theorem 1.1 holds true, but with a different value of A^* and d^*. Such results are called *effective mass theorems*.

Let us describe briefly one example of such an effective mass theorem (many generalizations are treated in the sequel). We first introduce a variant of (3), the so-called Bloch or shifted cell problem,

$$-(\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi_n\Big) + c(y)\psi_n = \lambda_n(\theta)\psi_n \quad \text{in } \mathbb{T}^N,$$

where $\theta \in \mathbb{T}^N$ is a parameter and $(\lambda_n(\theta), \psi_n(y,\theta))$ is the n^{th} eigencouple. In physical terms, the range of $\lambda_n(\theta)$, as θ run in $\mathbb{T}^N$, is a Bloch or conduction band (also called Fermi surface). Theorem 1.1 (with its special initial data satisfying (6)) is concerned with the bottom of the first Bloch band (or ground state). Now, we focus on higher energy initial data (or excited states) and consider new well-prepared initial data of the type

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v^0(x). \tag{8}$$

Under the additional assumption (11), which means that θ^n is a critical point of the simple eigenvalue (or energy) $\lambda_n(\theta)$, we shall prove in Theorem 3.2 that the solution of (1) satisfies

$$u_\epsilon(t,x) \approx e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v(t,x),$$

where $v(t,x)$ is the unique solution of the following Schrödinger homogenized equation:

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \mathrm{div}\left(A_n^* \nabla v\right) + d_n^*(x)\, v = 0 & \text{in } \mathbb{R}^N \times (0,T), \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{9}$$

with different homogenized coefficients A_n^* and d_n^*, depending on the parameter θ^n and on the energy level n. In other words, the homogenized problem depends on the type of initial data. If A_n^* is a scalar (instead of a full matrix), its inverse value is called the effective mass of the particle. A typical effect is that the effective mass depends on the chosen energy of the particle, may be negative or zero, and even not a scalar.

Remark 1.2. A posteriori, a possible explanation of our "homogenization" scaling in (1) is the following. It is well known that the effective mass of an electron in solid state physics is a purely quantum mechanical notion, and its derivation should not involve any arguments from classical or semi-classical limits [20, 25, 30]. The small macroscopic potential in (1) has only a perturbative effect and will therefore not force the limit to be semi-classical. Instead the limit will stay in the context of quantum mechanics. Finally let us notice that the scaling of (1) was already used in the physical literature for deriving effective mass equations [28].

To obtain the homogenized limit (9) we can not follow the above simple idea, namely the factorization principle (4). Indeed, for $n > 1$ or $\theta^n \neq 0$ there is no maximum principle, and therefore no Krein-Rutman theorem, so $\psi_n(y, \theta^n)$ may change sign. Clearly we can not divide by ψ_n in a formula similar to (4). In order to homogenize (1) for initial data of the type of (8), we use a method which was first introduced in our previous work [3] for systems of parabolic equations. The main idea is to use Bloch wave theory to build adequate oscillating test functions and to pass to the limit using two-scale convergence [2, 26].

Apart from the previously quoted references in the physical literature, to the best of our knowledge effective mass theorems were addressed only in the two following mathematical papers. First, two-scale asymptotic expansions were previously performed in Sect. 4 of Chap. 4 in [6] for a slightly different version of this problem: indeed, [6] put a ϵ^{-1} scaling factor in front of the time derivative in the Schrödinger equation (which corresponds to a short time asymptotic). Second, some special cases of effective mass theorems were obtained in [29] with a different method of semi-classical measures. Let us emphasize again that the scaling of (1) is not that of the semi-classical analysis (see e.g. [12, 15–17, 27, 29]).

The content of this paper is the following. In Sect. 2 we recall some results on Bloch theory and two-scale convergence. Section 3 is devoted to the derivation of the homogenized Schrödinger equation (9). Section 4 generalizes the previous effective mass theorem to the case when θ^n is not a critical point of an eigenvalue $\lambda_n(\theta)$, which is still assumed to be simple. This yields a large drift of the solution (of order ϵ^{-1}) in the direction of the group velocity $\nabla_\theta \lambda_n(\theta)$. The main technical tool is a variant of the notion of two-scale convergence due to [23] which takes into account this large drift. Section 5 is concerned with another generalization when θ^n is a "third order" critical point of $\lambda_n(\theta)$. In such a case, the limit equation features a fourth-order operator instead of the usual second-order one. Finally in Sect. 6 we discuss a special case of a multiple eigenvalue $\lambda_n(\theta)$. Under the strong assumption (52), which amounts to say that $\lambda_n(\theta)$ is of multiplicity $k > 1$ at $\theta = \theta^n$ and made of k smooth branches of eigenvalues and eigenvectors which all share the same value for the first order derivative $\nabla_\theta \lambda_n(\theta)$, we prove that the homogenized limit is precisely a coupled system of k equations. However, the coupling is weak since it occurs only through the macroscopic potential term $d^*(x)$ which is a full $k \times k$ tensor. It turns out that there is no coupling through the second order operator A_n^*. This result is reminiscent of a problem of modes crossing analyzed in [13, 14], but is definitely different since we assume that the drift vectors $\nabla_\theta \lambda_n(\theta)$ are equals.

2. Bloch Spectrum and Two-Scale Convergence

We assume that the coefficients $A(y)$ and $c(y)$ are real measurable bounded periodic functions, i.e. their entries belong to $L^\infty(\mathbb{T}^N)$, while $d(x, y)$ is real measurable and bounded with respect to x, and periodic continuous with respect to y, i.e. its entries belong to $L^\infty\left(\mathbb{R}^N; C(\mathbb{T}^N)\right)$ (other assumptions are possible). The tensor A is symmetric and uniformly coercive, i.e. there exists $\nu > 0$ such that for a.e. $y \in \mathbb{T}^N$,

$$A(y)\xi \cdot \xi \geq \nu |\xi|^2 \text{ for any } \xi \in \mathbb{R}^N.$$

We recall the so-called Bloch (or shifted) spectral cell equation

$$-(\operatorname{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi_n\Big) + c(y)\psi_n = \lambda_n(\theta)\psi_n \quad \text{in } \mathbb{T}^N, \tag{10}$$

which, as a compact self-adjoint complex-valued operator on $L^2(\mathbb{T}^N)$, admits a countable sequence of real increasing eigenvalues $(\lambda_n)_{n\geq 1}$ (repeated with their multiplicity) and normalized eigenfunctions $(\psi_n)_{n\geq 1}$ with $\|\psi_n\|_{L^2(\mathbb{T}^N)} = 1$. The dual parameter θ is called the Bloch frequency and it runs in the dual cell of $\mathbb{T}^N$, i.e. by periodicity it is enough to consider $\theta \in \mathbb{T}^N$.

In the sequel, we shall consider an energy level $n \geq 1$ and a Bloch parameter $\theta^n \in \mathbb{T}^N$ such that the eigenvalue $\lambda_n(\theta^n)$ satisfies some assumptions. Depending on these precise assumptions we obtain different homogenized limits for the Schrödinger equation (1). In Sect. 3 we assume that

$$\begin{cases} (i) \;\; \lambda_n(\theta^n) \text{ is a simple eigenvalue,} \\ (ii) \; \theta^n \text{ is a critical point of } \lambda_n(\theta) \text{ i.e., } \nabla_\theta \lambda_n(\theta^n) = 0. \end{cases} \tag{11}$$

In Sect. 4 we make the weaker assumption

$$\lambda_n(\theta^n) \text{ is a simple eigenvalue.} \tag{12}$$

This assumption of simplicity has two important consequences. First, if $\lambda_n(\theta^n)$ is simple, then it is infinitely differentiable in a vicinity of θ^n. Second, if $\lambda_n(\theta^n)$ is simple, then the limit problem is going to be a single Schrödinger equation. In Sect. 6 we make another assumption of a multiple eigenvalue with smooth branches. Then the homogenized limit is a system of several coupled Schrödinger equations (as many as the multiplicity).

Remark 2.1. In one space dimension $N = 1$ it is well-known that all eigenvalues $\lambda_n(\theta)$ are simple, except possibly for $\theta = 0$ or $\theta = \pm 1/2$ when there is no gap below or above the n^{th} band (the so-called co-existence case, see [22]). In higher dimensions, $\lambda_n(\theta)$ has no reason to be simple although there are some results of generic simplicity in similar contexts, see [1].

Remark 2.2. Concerning the existence of critical points of $\lambda_n(\theta)$, it is easily checked that for the first band or energy level $n = 1$ assumption (11) is always satisfied with $\theta^1 = 0$ which is a minimum point of λ_1 (see e.g. [6], [11]). In full generality, there may be or not a critical point of $\lambda_n(\theta)$. For example, in the case of constant coefficients, $\lambda_n(\theta)$ has no critical points for $n > 1$. However, in $N = 1$ space dimension it is well known (see e.g. [22, 31]) that the top and the bottom of Bloch bands are attained alternatively for $\theta^n = 0$ or $\theta^n = \pm 1/2$, and that the corresponding eigenvalue $\lambda_n(\theta^n)$ is simple if it bounds a gap in the spectrum. Therefore, the maximum point θ^n below a gap, or the minimum point θ^n above a gap, do satisfy assumption (11), which possibly holds for a non-zero value of θ^n.

Under assumption (12) it is a classical matter to prove that the n^{th} eigencouple of (10) is smooth in a neighborhood of θ^n [19]. Introducing the operator $\mathbb{A}_n(\theta)$ defined on $L^2(\mathbb{T}^N)$ by

$$\mathbb{A}_n(\theta)\psi = -(\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi\Big) + c(y)\psi - \lambda_n(\theta)\psi, \tag{13}$$

it is easy to differentiate (10). Denoting by $(e_k)_{1\leq k\leq N}$ the canonical basis of $\mathbb{R}^N$ and by $(\theta_k)_{1\leq k\leq N}$ the components of θ, the first derivative satisfies

$$\begin{aligned} \mathbb{A}_n(\theta)\frac{\partial \psi_n}{\partial \theta_k} &= 2i\pi e_k A(y)(\nabla_y + 2i\pi\theta)\psi_n + (\mathrm{div}_y + 2i\pi\theta)\left(A(y)2i\pi e_k \psi_n\right) \\ &\quad + \frac{\partial \lambda_n}{\partial \theta_k}(\theta)\psi_n, \end{aligned} \tag{14}$$

and the second derivative is

$$\begin{aligned}\mathbb{A}_n(\theta)\frac{\partial^2\psi_n}{\partial\theta_k\partial\theta_l} &= 2i\pi e_k A(y)(\nabla_y + 2i\pi\theta)\frac{\partial\psi_n}{\partial\theta_l} + (\mathrm{div}_y + 2i\pi\theta)\left(A(y)2i\pi e_k\frac{\partial\psi_n}{\partial\theta_l}\right)\\ &+2i\pi e_l A(y)(\nabla_y + 2i\pi\theta)\frac{\partial\psi_n}{\partial\theta_k} + (\mathrm{div}_y + 2i\pi\theta)\left(A(y)2i\pi e_l\frac{\partial\psi_n}{\partial\theta_k}\right)\\ &+\frac{\partial\lambda_n}{\partial\theta_k}(\theta)\frac{\partial\psi_n}{\partial\theta_l} + \frac{\partial\lambda_n}{\partial\theta_l}(\theta)\frac{\partial\psi_n}{\partial\theta_k}\\ &-4\pi^2 e_k A(y)e_l\psi_n - 4\pi^2 e_l A(y)e_k\psi_n + \frac{\partial^2\lambda_n}{\partial\theta_l\partial\theta_k}(\theta)\psi_n. \end{aligned} \tag{15}$$

Under assumption (11) we have $\nabla_\theta\lambda_n(\theta^n) = 0$, thus Eqs. (14) and (15) simplify for $\theta = \theta^n$ and we find

$$\frac{\partial\psi_n}{\partial\theta_k} = 2i\pi\zeta_k, \quad \frac{\partial^2\psi_n}{\partial\theta_k\partial\theta_l} = -4\pi^2\chi_{kl}, \tag{16}$$

where ζ_k is the solution of

$$\mathbb{A}_n(\theta^n)\zeta_k = e_k A(y)(\nabla_y + 2i\pi\theta^n)\psi_n + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_k\psi_n\right) \quad \text{in } \mathbb{T}^N, \tag{17}$$

and χ_{kl} is the solution of

$$\begin{aligned}\mathbb{A}_n(\theta^n)\chi_{kl} &= e_k A(y)(\nabla_y + 2i\pi\theta^n)\zeta_l + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_k\zeta_l\right)\\ &+e_l A(y)(\nabla_y + 2i\pi\theta^n)\zeta_k + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_l\zeta_k\right)\\ &+e_k A(y)e_l\psi_n + e_l A(y)e_k\psi_n - \frac{1}{4\pi^2}\frac{\partial^2\lambda_n}{\partial\theta_l\partial\theta_k}(\theta^n)\psi_n \quad \text{in } \mathbb{T}^N. \end{aligned}\tag{18}$$

There exists a unique solution of (17), up to the addition of a multiple of ψ_n. Indeed, the right hand side of (17) satisfies the required compatibility condition or Fredholm alternative (i.e. it is orthogonal to ψ_n) because ζ_k is just a multiple of the partial derivative of ψ_n with respect to θ_k which necessarily exists, see (14). On the same token, there exists a unique solution of (18), up to the addition of a multiple of ψ_n. The compatibility condition of (18) yields a formula for the Hessian matrix $\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$.

Finally we recall the notion of two-scale convergence introduced in [2, 26].

Proposition 2.3. *Let u_ϵ be a sequence uniformly bounded in $L^2(\mathbb{R}^N)$.*

1. *There exists a subsequence, still denoted by u_ϵ, and a limit $u_0(x,y) \in L^2(\mathbb{R}^N \times \mathbb{T}^N)$ such that u_ϵ* two-scale converges *weakly to u_0 in the sense that*

$$\lim_{\epsilon\to 0}\int_{\mathbb{R}^N} u_\epsilon(x)\phi(x,\frac{x}{\epsilon})\,dx = \int_{\mathbb{R}^N}\int_{\mathbb{T}^N} u_0(x,y)\phi(x,y)\,dx\,dy$$

for all functions $\phi(x,y) \in L^2\left(\mathbb{R}^N; C_\#(\mathbb{T}^N)\right)$.

2. *Assume further that u_ϵ two-scale converges weakly to u_0 and that*

$$\lim_{\epsilon\to 0}\|u_\epsilon\|_{L^2(\mathbb{R}^N)} = \|u_0\|_{L^2(\mathbb{R}^N\times\mathbb{T}^N)}.$$

Then u_ϵ is said to two-scale converge strongly *to its limit u_0 in the sense that, if u_0 is smooth enough, e.g. $u_0 \in L^2\left(\mathbb{R}^N; C_\#(\mathbb{T}^N)\right)$, we have*

$$\lim_{\epsilon\to 0}\int_{\mathbb{R}^N}|u_\epsilon(x) - u_0(x,\frac{x}{\epsilon})|^2\,dx = 0.$$

3. *Assume that $\epsilon\nabla u_\epsilon$ is also uniformly bounded in $L^2(\mathbb{R}^N)^N$. Then there exists a subsequence, still denoted by u_ϵ, and a limit $u_0(x,y) \in L^2(\mathbb{R}^N; H^1(\mathbb{T}^N))$ such that u_ϵ two-scale converges to $u_0(x,y)$ and $\epsilon\nabla u_\epsilon$ two-scale converges to $\nabla_y u_0(x,y)$.*

Notation. for any function $\phi(x,y)$ defined on $\mathbb{R}^N \times \mathbb{T}^N$, we denote by ϕ^ϵ the function $\phi(x, \frac{x}{\epsilon})$.

3. Homogenization Without Drift

In this section we use the strong assumption (11) about the stationarity of $\lambda_n(\theta)$ at θ^n. Physically, it implies that the particle modeled by the limit wave function does not experience any drift and is a solution of an effective Schrödinger equation.

Our precise assumptions on the coefficients are that $A_{ij}(y)$ and $c(y)$ are real, measurable, bounded, periodic functions, i.e. belong to $L^\infty(\mathbb{T}^N)$, the tensor $A(y)$ is symmetric uniformly coercive, while $d(x,y)$ is real, measurable and bounded with respect to x, and periodic continuous with respect to y, i.e. belongs to $L^\infty\left(\Omega; C(\mathbb{T}^N)\right)$. Then, if the initial data u_ϵ^0 belongs to $H^1(\mathbb{R}^N)$, there exists a unique solution of the Schrödinger equation (1) in $C\left((0,T); H^1(\mathbb{R}^N)\right)$ which satisfies the following a priori estimate.

Lemma 3.1. *There exists a constant $C > 0$ that does not depend on ϵ such that the solution of (1) satisfies*

$$\begin{aligned} \|u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N))} &= \|u_\epsilon^0\|_{L^2(\mathbb{R}^N)}, \\ \epsilon\|\nabla u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N)^N)} &\le C\left(\|u_\epsilon^0\|_{L^2(\mathbb{R}^N)} + \epsilon\|\nabla u_\epsilon^0\|_{L^2(\mathbb{R}^N)^N}\right). \end{aligned} \tag{19}$$

Proof of Lemma 3.1. We multiply Eq. (1) by $\overline{u_\epsilon}$ and we take the imaginary part to obtain

$$\frac{d}{dt}\int_{\mathbb{R}^N} |u_\epsilon(t,x)|^2 dx = 0.$$

Next we multiply (1) by $\frac{\partial \overline{u_\epsilon}}{\partial t}$ and we take the real part to get

$$\frac{d}{dt}\int_{\mathbb{R}^N}\left(\epsilon^2 A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\cdot\nabla\overline{u_\epsilon} + \left(c\left(\frac{x}{\epsilon}\right) + \epsilon^2 d\left(x,\frac{x}{\epsilon}\right)\right)|u_\epsilon|^2\right)dx = 0.$$

This yields the required a priori estimates without using assumption (11). □

We obtain the following homogenized problem.

Theorem 3.2. *Assume (11) and that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ is of the form*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon},\theta^n\right) e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v^0(x), \tag{20}$$

with $v^0 \in H^1(\mathbb{R}^N)$. The solution of (1) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v_\epsilon(t,x), \tag{21}$$

where v_ϵ two-scale converges strongly to $\psi_n(y,\theta^n)v(t,x)$, i.e.

$$\lim_{\epsilon\to 0}\int_{\mathbb{R}^N}\left|v_\epsilon(t,x) - \psi_n\left(\frac{x}{\epsilon},\theta^n\right)v(t,x)\right|^2 dx = 0, \tag{22}$$

uniformly on compact time intervals in $\mathbb{R}^+$, *and* $v \in C\left((0,T); L^2(\mathbb{R}^N)\right)$ *is the unique solution of the homogenized Schrödinger equation*

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}\left(A_n^* \nabla v\right) + d_n^*(x)\, v = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{23}$$

with $A_n^* = \frac{1}{8\pi^2} \nabla_\theta \nabla_\theta \lambda_n(\theta^n)$ *and* $d_n^*(x) = \int_{\mathbb{T}^N} d(x,y)|\psi_n(y)|^2\, dy$.

In the context of quantum mechanics or solid state physics Theorem 3.2 is called an effective mass theorem [25, 28, 30]. More precisely, the inverse tensor $(A_n^*)^{-1}$ is the effective mass of an electron in the n^{th} band of a periodic crystal (characterized by the periodic metric $A(y)$ and the periodic potential $c(y)$). Since we did not assume that θ^n was a minimum point, the tensor $A_n^* = \frac{1}{8\pi^2} \nabla_\theta \nabla_\theta \lambda_n(\theta^n)$ can be neither definite nor positive, which is quite surprising for a notion of mass (but this fact is well understood in solid state physics [25, 30]).

Remark 3.3. Theorem 3.2 does not fit into the framework of G- or H-convergence (see e.g. [24, 32]). Indeed these classical theories of homogenization state that the homogenized coefficients are independent of the initial data, which is not the case here. There is no contradiction in our result since H-convergence does not apply because we lack a uniform a priori estimate in $L^2((0,T); H^1(\mathbb{R}^N))$ for the sequence of solutions u_ϵ, as required by H-convergence.

Remark 3.4. Assumption (20) can be slightly weakened for proving Theorem 3.2. For example, it still holds true if we merely assume that $u_\epsilon^0(x)e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}}$ two-scale converges strongly to $\psi_n(y,\theta^n)v^0(x)$.

On the other hand, if (20) is replaced by the even weaker assumption that $u_\epsilon^0(x)$ $e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}}$ two-scale converges weakly to $\psi_n(y,\theta^n)v^0(x)$ (which is always true up to a subsequence), then Theorem 3.2 is still valid provided that its conclusion is modified by replacing the strong two-scale convergence of v_ϵ by a weak two-scale convergence.

Remark 3.5. In the case $n = 1$ and $\theta^n = 0$ (bottom of the first Bloch band), Theorem 3.2 still holds true (with a different proof however) in the following non-linear setting. Assume that we add to the Schrödinger equation (1) a non-linear term of order ϵ^0, $g(x, \frac{x}{\epsilon}, u_\epsilon)$, where $g(x,y,\xi)$ is a Caratheodory function (i.e. measurable in $y \in \mathbb{T}^N$ and continuous in $(x,\xi) \in \mathbb{R}^N \times \mathbb{C}$) such that $g(x,y,0) = 0$, the product $g(x,y,\xi)\overline{\xi}$ is real and depends only on the modulus $|\xi|$, i.e.

$$g(x,y,\xi)\overline{\xi} = g(x,y,\xi')\overline{\xi}' \text{ for any } |\xi| = |\xi'|,$$

and g satisfies some growth condition with respect to ξ. A first example is a uniformly Lipschitz function

$$|g(x,y,\xi) - g(x,y,\xi')| \leq C|\xi - \xi'|.$$

A second example is

$$g(x,y,\xi) = g_0(x,y)|\xi|^{p-2}\xi \text{ with } g_0(x,y) \geq C > 0 \text{ and } p \geq 2.$$

In such a case, it is well-known that the non-linear Schrödinger equation admits a unique solution in $C\left((0,T); H^1(\mathbb{R}^N)\right)$ which satisfies the same a priori estimates of

Lemma 3.1 [8]. Then, Theorem 3.2 can be generalized by using the factorization principle (4) which yields Eq. (5) with an additional non-linear term $\overline{\psi}_1(\frac{x}{\epsilon}, 0)g(x, \frac{x}{\epsilon}, \psi_1(\frac{x}{\epsilon}, 0)v_\epsilon)$. Such an equation does not contain anymore a singularly perturbed term and its solution v_ϵ is easily seen to satisfy a uniform $H^1(\mathbb{R}^N)$ bound. Therefore, by a standard compactness argument it is possible to pass to the limit in the zero-order non-linear term and to obtain a non-linear homogenized equation, similar to (23) with an additional non-linear zero-order term which is

$$g^*(x, v) = \int_{\mathbb{T}^N} g(x, y, \psi_1(y, 0)v)\overline{\psi}_1(y, 0)\, dy.$$

The generalization of this result for higher order Bloch bands $n > 1$ (with a different method) is the topic of a future paper.

Proof of Theorem 3.2. This proof is in the spirit of our previous work [3]. Define a sequence v_ϵ by

$$v_\epsilon(t, x) = u_\epsilon(t, x)e^{-i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}}.$$

Since $|v_\epsilon| = |u_\epsilon|$, by the a priori estimates of Lemma 3.1 we have

$$\|v_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N))} + \epsilon\|\nabla v_\epsilon\|_{L^2((0,T)\times\mathbb{R}^N)} \le C,$$

and applying the compactness of two-scale convergence (see Proposition 2.3), up to a subsequence, there exists a limit $v^*(t, x, y) \in L^2\left((0, T) \times \mathbb{R}^N; H^1(\mathbb{T}^N)\right)$ such that v_ϵ and $\epsilon\nabla v_\epsilon$ two-scale converge to v^* and $\nabla_y v^*$, respectively. Similarly, by definition of the initial data, $v_\epsilon(0, x)$ two-scale converges to $\psi_n(y, \theta^n)\, v^0(x)$.

First step. We multiply (1) by the complex conjugate of

$$\epsilon^2\phi(t, x, \frac{x}{\epsilon})e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}},$$

where $\phi(t, x, y)$ is a smooth test function defined on $[0, T) \times \mathbb{R}^N \times \mathbb{T}^N$, with compact support in $[0, T) \times \mathbb{R}^N$. Integrating by parts this yields

$$\begin{aligned} &i\epsilon^2\int_{\mathbb{R}^N} u^0_\epsilon\overline{\phi}^\epsilon e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}}dx - i\epsilon^2\int_0^T\int_{\mathbb{R}^N} v_\epsilon\frac{\partial\overline{\phi}^\epsilon}{\partial t}dt\,dx \\ &+\int_0^T\int_{\mathbb{R}^N} A^\epsilon(\epsilon\nabla + 2i\pi\theta^n)v_\epsilon\cdot(\epsilon\nabla - 2i\pi\theta^n)\overline{\phi}^\epsilon\,dt\,dx \\ &+\int_0^T\int_{\mathbb{R}^N}(c^\epsilon - \lambda_n(\theta^n) + \epsilon^2 d^\epsilon)v_\epsilon\overline{\phi}^\epsilon\,dt\,dx = 0. \end{aligned}$$

Passing to the two-scale limit yields the variational formulation of

$$-(\mathrm{div}_y + 2i\pi\theta^n)\Big(A(y)(\nabla_y + 2i\pi\theta^n)v^*\Big) + c(y)v^* = \lambda_n(\theta^n)v^* \quad \text{in } \mathbb{T}^N.$$

By the simplicity of $\lambda_n(\theta^n)$, this implies that there exists a scalar function $v(t, x) \in L^2\left((0, T) \times \mathbb{R}^N\right)$ such that

$$v^*(t, x, y) = v(t, x)\psi_n(y, \theta^n). \tag{24}$$

Second step. We multiply (1) by the complex conjugate of

$$\Psi_\epsilon = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \left(\psi_n(\frac{x}{\epsilon},\theta^n)\phi(t,x) + \epsilon\sum_{k=1}^N \frac{\partial\phi}{\partial x_k}(t,x)\zeta_k(\frac{x}{\epsilon}) \right),$$

where $\phi(t,x)$ is a smooth test function with compact support in $[0,T)\times\mathbb{R}^N$, and $\zeta_k(y)$ is the solution of (17). After some algebra we found that

$$\begin{aligned}
\int_{\mathbb{R}^N} A^\epsilon \nabla u_\epsilon\cdot\nabla\overline{\Psi}_\epsilon dx = & \int_{\mathbb{R}^N} A^\epsilon\left(\nabla + 2i\pi\frac{\theta^n}{\epsilon}\right)(\overline{\phi}v_\epsilon)\cdot\left(\nabla - 2i\pi\frac{\theta^n}{\epsilon}\right)\overline{\psi}_n^\epsilon \\
& +\epsilon\int_{\mathbb{R}^N} A^\epsilon\left(\nabla + 2i\pi\frac{\theta^n}{\epsilon}\right)\left(\frac{\partial\overline{\phi}}{\partial x_k}v_\epsilon\right)\cdot\left(\nabla - 2i\pi\frac{\theta^n}{\epsilon}\right)\overline{\zeta}_k^\epsilon \\
& -\int_{\mathbb{R}^N} A^\epsilon e_k\frac{\partial\overline{\phi}}{\partial x_k}v_\epsilon\cdot\left(\nabla - 2i\pi\frac{\theta^n}{\epsilon}\right)\overline{\psi}_n^\epsilon \\
& +\int_{\mathbb{R}^N} A^\epsilon\left(\nabla + 2i\pi\frac{\theta^n}{\epsilon}\right)\left(\frac{\partial\overline{\phi}}{\partial x_k}v_\epsilon\right)\cdot e_k\overline{\psi}_n^\epsilon \\
& -\int_{\mathbb{R}^N} A^\epsilon v_\epsilon\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot e_k\overline{\psi}_n^\epsilon \\
& -\int_{\mathbb{R}^N} A^\epsilon v_\epsilon\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot\left(\epsilon\nabla - 2i\pi\theta^n\right)\overline{\zeta}_k^\epsilon \\
& +\int_{\mathbb{R}^N} A^\epsilon\overline{\zeta}_k^\epsilon\left(\epsilon\nabla + 2i\pi\theta^n\right)v_\epsilon\cdot\nabla\frac{\partial\overline{\phi}}{\partial x_k}.
\end{aligned} \tag{25}$$

Now, for any smooth compactly supported test function Φ, we deduce from the definition of ψ_n that

$$\int_{\mathbb{R}^N} A^\epsilon\left(\nabla + 2i\pi\frac{\theta^n}{\epsilon}\right)\psi_n^\epsilon\cdot\left(\nabla - 2i\pi\frac{\theta^n}{\epsilon}\right)\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N}\left(c^\epsilon - \lambda_n(\theta^n)\right)\psi_n^\epsilon\overline{\Phi} = 0, \tag{26}$$

and from the definition of ζ_k ,

$$\begin{aligned}
&\int_{\mathbb{R}^N} A^\epsilon\left(\nabla + 2i\pi\frac{\theta^n}{\epsilon}\right)\zeta_k^\epsilon\cdot\left(\nabla - 2i\pi\frac{\theta^n}{\epsilon}\right)\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N}\left(c^\epsilon - \lambda_n(\theta^n)\right)\zeta_k^\epsilon\overline{\Phi} = \\
&\epsilon^{-1}\int_{\mathbb{R}^N} A^\epsilon\left(\nabla + 2i\pi\frac{\theta^n}{\epsilon}\right)\psi_n^\epsilon\cdot e_k\overline{\Phi} - \epsilon^{-1}\int_{\mathbb{R}^N} A^\epsilon e_k\psi_n^\epsilon\cdot\left(\nabla - 2i\pi\frac{\theta^n}{\epsilon}\right)\overline{\Phi}.
\end{aligned} \tag{27}$$

Combining (25) with the other terms of the variational formulation of (1), we easily check that the first line of its right-hand side cancels out because of (26) with $\Phi = \overline{\phi}v_\epsilon$, and the next three lines cancel out because of (27) with $\Phi = \frac{\partial\overline{\phi}}{\partial x_k}v_\epsilon$. On the other hand, we can pass to the limit in three last terms of (25). Finally, (1) multiplied by $\overline{\Psi}_\epsilon$ yields after simplification

$$
\begin{aligned}
& i \int_{\mathbb{R}^N} u_\epsilon^0 \overline{\Psi}_\epsilon(t=0) dx - i \int_0^T \int_{\mathbb{R}^N} v_\epsilon \left(\overline{\psi}_n^\epsilon \frac{\partial \overline{\phi}}{\partial t} + \epsilon \frac{\partial^2 \overline{\phi}}{\partial x_k \partial t} \overline{\zeta}_k^\epsilon \right) dt\, dx \\
& - \int_0^T \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot e_k \overline{\psi}_n^\epsilon dt\, dx \\
& - \int_0^T \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot (\epsilon \nabla - 2 i \pi \theta^n) \overline{\zeta}_k^\epsilon dt\, dx \\
& + \int_0^T \int_{\mathbb{R}^N} A^\epsilon \overline{\zeta}_k^\epsilon (\epsilon \nabla + 2 i \pi \theta^n) v_\epsilon \cdot \nabla \frac{\partial \overline{\phi}}{\partial x_k} dt\, dx \\
& + \int_0^T \int_{\mathbb{R}^N} d^\epsilon v_\epsilon \overline{\Psi}_\epsilon \, dt\, dx. \qquad = 0.
\end{aligned} \tag{28}
$$

Passing to the two-scale limit in each term of (28) gives

$$
\begin{aligned}
& i \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} \psi_n v^0 \overline{\psi}_n \overline{\phi}(t=0)\, dx\, dy - i \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} \psi_n v \overline{\psi}_n \frac{\partial \overline{\phi}}{\partial t} dt\, dx\, dy \\
& - \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} A \psi_n v \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot e_k \overline{\psi}_n dt\, dx\, dy \\
& - \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} A \psi_n v \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot (\nabla_y - 2 i \pi \theta^n) \overline{\zeta}_k dt\, dx\, dy \\
& + \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} A \overline{\zeta}_k (\nabla_y + 2 i \pi \theta^n) \psi_n v \cdot \nabla \frac{\partial \overline{\phi}}{\partial x_k} dt\, dx\, dy \\
& + \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} d(x,y) \psi_n v \overline{\psi}_n \overline{\phi}\, dt\, dx\, dy. \qquad = 0.
\end{aligned} \tag{29}
$$

Recalling the normalization $\int_{\mathbb{T}^N} |\psi_n|^2 dy = 1$, and introducing

$$
\begin{aligned}
2 \left(A_n^* \right)_{jk} = \int_{\mathbb{T}^N} \Big(& A \psi_n e_j \cdot e_k \overline{\psi}_n + A \psi_n e_k \cdot e_j \overline{\psi}_n \\
& + A \psi_n e_j \cdot (\nabla_y - 2 i \pi \theta^n) \overline{\zeta}_k + A \psi_n e_k \cdot (\nabla_y - 2 i \pi \theta^n) \overline{\zeta}_j \\
& - A \overline{\zeta}_k (\nabla_y + 2 i \pi \theta^n) \psi_n \cdot e_j - A \overline{\zeta}_j (\nabla_y + 2 i \pi \theta^n) \psi_n \cdot e_k \Big) dy,
\end{aligned} \tag{30}
$$

and $d_n^*(x) = \int_{\mathbb{T}^N} d(x,y) |\psi_n(y)|^2\, dy$, (29) is equivalent to

$$
\begin{aligned}
& i \int_{\mathbb{R}^N} v^0 \overline{\phi} dx - i \int_0^T \int_{\mathbb{R}^N} v \frac{\partial \overline{\phi}}{\partial t} dt\, dx - \int_0^T \int_{\mathbb{R}^N} A^* v \cdot \nabla \nabla \overline{\phi} dt\, dx \\
& \quad + \int_0^T \int_{\mathbb{R}^N} d^*(x) v \overline{\phi} dt\, dx = 0
\end{aligned}
$$

which is a very weak form of the homogenized equation (23). The compatibility condition of Eq. (18) for the second derivative of ψ_n yields that the matrix A_n^*, defined by (30), is indeed equal to $\frac{1}{8\pi^2} \nabla_\theta \nabla_\theta \lambda_n(\theta^n)$, and thus is symmetric. Although, the tensor A_n^* is possibly non-coercive, the homogenized problem (23) is well posed. Indeed, by using semi-group theory (see e.g. [7] or chapter X in [31]), there exists a unique solution in $C((0,T); L^2(\mathbb{R}^N))$, although it may not belong to $L^2((0,T); H^1(\mathbb{R}^N))$. By uniqueness of the solution of the homogenized problem (23), we deduce that the entire sequence v_ϵ two-scale converges weakly to $\psi_n\,(y, \theta^n)\; v(t,x)$.

It remains to prove the strong two-scale convergence of v_ϵ. By Lemma 3.1 we have

$$\|v_\epsilon(t)\|_{L^2(\mathbb{R}^N)} = \|u_\epsilon(t)\|_{L^2(\mathbb{R}^N)} = \|u_\epsilon^0\|_{L^2(\mathbb{R}^N)} \to \|\psi_n v^0\|_{L^2(\mathbb{R}^N\times\mathbb{T}^N)} = \|v^0\|_{L^2(\mathbb{R}^N)}$$

by the normalization condition of ψ_n. From the conservation of energy of the homogenized equation (23) we have

$$\|v(t)\|_{L^2(\mathbb{R}^N)} = \|v^0\|_{L^2(\mathbb{R}^N)},$$

and thus we deduce the strong convergence (22) from Proposition 2.3. □

Remark 3.6. As we said in Sect. 2, the function $\zeta_k(y)$, which is used in the test function Ψ_ϵ, is uniquely defined up to the addition of a multiple of ψ_n (see (17)). This multiple may depend on (t, x) and therefore the homogenized system could, in principle, depend on the choice of this additive term. This is not the case as we now explain. In the homogenized system, ζ_k appears only in definition (30) of the homogenized tensor A_n^*. If we replace $\zeta_k(y)$ by $\zeta_k(y) + c_k(t, x)\psi_n(y)$, an easy calculation shows that all terms c_k cancel out because of the Fredholm alternative for ζ_k, i.e. the right-hand side of (17) is orthogonal to ψ_n.

Remark 3.7. As usual in periodic homogenization [2, 6], the choice of the test function Ψ_ϵ, in the proof of Theorem 3.2, is dictated by the formal two-scale asymptotic expansion that can be obtained for the solution u_ϵ of (1), namely

$$u_\epsilon(t, x) \approx e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \left(\psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v(t, x) + \epsilon\sum_{k=1}^N \frac{\partial v}{\partial x_k}(t, x)\zeta_k(\frac{x}{\epsilon})\right),$$

where v is the homogenized solution of (23). The purpose of the corrector ζ_k is to compensate by its second derivatives the first derivatives of ψ_n. Since ζ_k is proportional to $\partial\psi_n/\partial\theta_k$, the rule of thumb is that derivatives with respect to x correspond to derivatives with respect to θ.

Remark 3.8. Our method applies also to systems of equations (see [3]). We never use the fact that (1) is a single scalar equation.

4. Generalization with Drift

The Schrödinger equation (1) can still be homogenized when θ^n is not a critical point of $\lambda_n(\theta)$. In other words we generalize Theorem 3.2 by weakening assumption (11) that we now replace by (12), i.e. $\lambda_n(\theta^n)$ is simple. This yields a large drift in the homogenized problem associated to the group velocity

$$\mathcal{V} = \frac{1}{2\pi}\nabla_\theta\lambda_n(\theta^n). \tag{31}$$

To begin with, we shall show that assumption (12) leads to a drift of velocity $\mathcal{V}$ at the small time scale of order ϵ. Looking at such a ϵ time asymptotic is equivalent to replacing the original Schrödinger equation (1) by

$$\begin{cases} \frac{i}{\epsilon}\frac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2}c\left(\frac{x}{\epsilon}\right) + d\left(x, \frac{x}{\epsilon}\right)\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N\times(0, T), \\ u_\epsilon(t = 0, x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{32}$$

with the new ϵ^{-1} scaling in front of the time derivative (if the macroscopic potential $d(x, y)$ was of order ϵ^{-2}, this would be precisely the scaling of semi-classical analysis).

Proposition 4.1. *Assume that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ is of the form*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0(x),$$

with $v^0 \in L^2(\mathbb{R}^N)$. The solution of (32) can be written as

$$u_\epsilon(t, x) = e^{i \frac{\lambda_n(\theta^n)t}{\epsilon}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v_\epsilon(t, x),$$

where $v_\epsilon(t, x)$ two-scale converges strongly to $\psi_n(y, \theta^n) v(t, x)$ and $v \in C\big((0, T); L^2(\mathbb{R}^N)\big)$ is the unique solution of the following transport equation:

$$\begin{cases} \dfrac{\partial v}{\partial t} - \mathcal{V} \cdot \nabla v = 0 & \text{in } \mathbb{R}^N \times (0, T), \\ v(t = 0, x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{33}$$

which admits the explicit solution $v(t, x) = v^0(x + \mathcal{V}t)$, and we have

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}^N} \left| v_\epsilon(t, x) - \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v^0(x + \mathcal{V}t) \right|^2 dx = 0,$$

uniformly on compact time intervals in $\mathbb{R}^+$.

Proof. First of all, the a priori estimates of Lemma 3.1 still hold true since its proof does not depend on the assumption made on $\lambda_n(\theta^n)$ nor on the time scaling of the equation. As in the first step of the proof of Theorem 3.2 we obtain that the sequence

$$v_\epsilon(t, x) = u_\epsilon(t, x) e^{-i \frac{\lambda_n(\theta^n)t}{\epsilon}} e^{-2i\pi \frac{\theta^n \cdot x}{\epsilon}}$$

two-scale converges to a limit $\psi_n(y, \theta^n) v(t, x)$. Then, in a second step we multiply (32) by the complex conjugate of

$$\Psi_\epsilon = \epsilon\, e^{i \frac{\lambda_n(\theta^n)t}{\epsilon}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} \left(\psi_n\left(\frac{x}{\epsilon}, \theta^n\right) \phi(t, x) + \epsilon \sum_{k=1}^N \frac{\partial \phi}{\partial x_k}(t, x) \zeta_k'\left(\frac{x}{\epsilon}\right) \right), \tag{34}$$

where $\phi(t, x)$ is a smooth test function with compact support in $[0, T) \times \mathbb{R}^N$ and $\zeta_k'(y)$ is defined by

$$\frac{\partial \psi_n}{\partial \theta_k} = 2i\pi \zeta_k'.$$

Note that ζ_k' is different from ζ_k, the solution of (17), since it is a solution of

$$\begin{aligned} \mathbb{A}_n(\theta^n)\zeta_k' = {} & e_k A(y)(\nabla_y + 2i\pi\theta^n)\psi_n + (\mathrm{div}_y + 2i\pi\theta^n)(A(y)e_k\psi_n) \\ & - \frac{i}{2\pi} \frac{\partial \lambda_n}{\partial \theta_k}(\theta^n)\psi_n \quad \text{in } \mathbb{T}^N, \end{aligned} \tag{35}$$

and $\nabla_\theta \lambda_n(\theta^n) \neq 0$. After integration by parts and some algebra similar to that in the proof of Theorem 3.2 we obtain

$$
\begin{aligned}
& i \int_{\mathbb{R}^N} v^0 |\psi_n^\epsilon|^2 \overline{\phi}(t=0)\, dx - i \int_0^T \int_{\mathbb{R}^N} v_\epsilon \overline{\psi}_n^\epsilon \frac{\partial \overline{\phi}}{\partial t}\, dt\, dx \\
& - \frac{1}{2i\pi} \frac{\partial \lambda_n}{\partial \theta_k} \int_0^T \int_{\mathbb{R}^N} v_\epsilon \overline{\psi}_n^\epsilon \frac{\partial \overline{\phi}}{\partial x_k}\, dt\, dx = o(1),
\end{aligned}
\tag{36}
$$

where $o(1)$ denotes all other terms going to zero with ϵ. Passing to the two-scale limit in (36) gives a variational formulation of (33). The strong two-scale convergence is obtained as in the proof of Theorem 3.2 by using the energy conservation of the original and homogenized equations. □

We now come back to the original time scale of the Schrödinger equation (1),

$$
\begin{cases}
i \dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2} c\left(\dfrac{x}{\epsilon}\right) + d\left(x, \dfrac{x}{\epsilon}\right)\right) u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T), \\
u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N,
\end{cases}
\tag{37}
$$

where the macroscopic zero-order term is assumed to satisfy

$$
\lim_{|x| \to +\infty} d(x,y) = d^\infty(y) \quad \text{uniformly in } \mathbb{T}^N. \tag{38}
$$

Actually, assumption (38) could be weakened by stating that the limit exists for any fixed direction in x but may vary. Using the following extension of the notion of two-scale convergence (see [2, 26]), which has been introduced in [23], it is possible to homogenize (37).

Theorem 4.2. *Let $\mathcal{V} \in \mathbb{R}^N$ be a given drift velocity. Let $(u_\epsilon)_{\epsilon>0}$ be a uniformly bounded sequence in $L^2((0,T)\times\mathbb{R}^N)$. There exists a subsequence, still denoted by ϵ, and a limit function $u_0(t,x,y) \in L^2((0,T)\times\mathbb{R}^N\times\mathbb{T}^N)$ such that u_ϵ* two-scale converges with drift *weakly to u_0 in the sense that*

$$
\begin{aligned}
\lim_{\epsilon\to 0} \int_0^T \int_{\mathbb{R}^N} u_\epsilon(t,x) \phi\left(t, x + \frac{\mathcal{V}}{\epsilon} t, \frac{x}{\epsilon}\right) dt\, dx = \\
\int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} u_0(t,x,y) \phi(t,x,y)\, dt\, dx\, dy
\end{aligned}
\tag{39}
$$

for all functions $\phi(t,x,y) \in L^2\left((0,T)\times\mathbb{R}^N; C(\mathbb{T}^N)\right)$.

Recall that, $\mathbb{T}^N$ being the unit torus, the test function ϕ in (39) is $(0,1)^N$-periodic with respect to the y variable. Remark that Theorem 4.2 does not reduce to the usual definition of two-scale convergence upon the change of variable $z = x + \frac{\mathcal{V}}{\epsilon} t$ because there is no drift in the fast variable $y = \frac{x}{\epsilon}$. The proof of Theorem 4.2 is similar to the proof of compactness of the usual two-scale convergence, except that it relies on the following simple lemma.

Lemma 4.3. *Let $\phi(t,x,y) \in L^2\left((0,T)\times\mathbb{R}^N; C(\mathbb{T}^N)\right)$. Then*

$$
\lim_{\epsilon\to 0} \int_0^T \int_{\mathbb{R}^N} \left|\phi\left(t, x + \frac{\mathcal{V}}{\epsilon} t, \frac{x}{\epsilon}\right)\right|^2 dt\, dx = \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} |\phi(t,x,y)|^2 dt\, dx\, dy.
$$

It is not difficult to check that the L^2-norm is weakly lower semi-continuous with respect to the two-scale convergence (see Proposition 1.6 in [2]), i.e., in the present setting

$$\lim_{\epsilon\to 0} \|u_\epsilon\|_{L^2((0,T)\times\mathbb{R}^N)} \geq \|u_0\|_{L^2((0,T)\times\mathbb{R}^N\times\mathbb{T}^N)}.$$

The next proposition asserts a corrector-type result when the above inequality turns out to be an equality.

Proposition 4.4. *Let $(u_\epsilon)_{\epsilon>0}$ be a sequence in $L^2((0,T)\times\mathbb{R}^N)$ which two-scale converges with drift to a limit $u_0(t,x,y) \in L^2((0,T)\times\mathbb{R}^N\times\mathbb{T}^N)$. Assume further that*

$$\lim_{\epsilon\to 0} \|u_\epsilon\|_{L^2((0,T)\times\mathbb{R}^N)} = \|u_0\|_{L^2((0,T)\times\mathbb{R}^N\times\mathbb{T}^N)}.$$

Then, it is said to **two-scale converge with drift strongly** *and it satisfies*

$$\lim_{\epsilon\to 0}\int_0^T\int_{\mathbb{R}^N}\left|u_\epsilon(t,x) - u_0\left(t, x+\frac{\mathcal{V}}{\epsilon}t, \frac{x}{\epsilon}\right)\right|^2 dx\,dt = 0,$$

if $u_0(t,x,y)$ is smooth, say $u_0(t,x,y) \in L^2\left((0,T)\times\mathbb{R}^N; C(\mathbb{T}^N)\right)$.

The proofs of Theorem 4.2 and Lemma 4.3 can be found in [23]. That of Proposition 4.4 is a simple adaptation of Theorem 1.8 in [2].

Under assumption (12) we obtain the following generalization of Theorem 3.2.

Theorem 4.5. *Assume that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ is of the form*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v^0(x), \tag{40}$$

with $v^0 \in H^1(\mathbb{R}^N)$. The solution of (37) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v_\epsilon(t,x), \tag{41}$$

where $v_\epsilon(t,x)$ converges strongly in the sense of **two-scale convergence with drift** *to $\psi_n(y,\theta^n)v(t,x)$, i.e.*

$$\lim_{\epsilon\to 0}\int_0^T\int_{\mathbb{R}^N}\left|v_\epsilon(t,x) - \psi_n\left(\frac{x}{\epsilon},\theta^n\right) v\left(t, x+\frac{\mathcal{V}}{\epsilon}t\right)\right|^2 dx\,dt = 0, \tag{42}$$

and $v \in C\left((0,T); L^2(\mathbb{R}^N)\right)$ is the unique solution of the Schrödinger homogenized problem

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}\left(A_n^*\nabla v\right) + d_n^*\, v = 0 & \text{in } \mathbb{R}^N\times(0,T),\\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{43}$$

with $A_n^* = \frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$ and $d_n^* = \int_{\mathbb{T}^N} d^\infty(y)|\psi_n(y)|^2\,dy$.

Remark 4.6. For the longer time scale of Eq. (37), the transport equation (33) can still be seen in the large drift $\mathcal{V}/\epsilon$ of formula (42).

Proof of Theorem 4.5. The proof is similar to that of Theorem 3.2 and Proposition 4.1. Nevertheless, we do not use, as before, the usual two-scale convergence but rather the two-scale convergence with drift. In a first step, by multiplying (37) by a test function

$$\epsilon^2 \phi \left(t, x + \frac{\mathcal{V}}{\epsilon} t, \frac{x}{\epsilon} \right) e^{i \frac{\lambda_n(\theta^n) t}{\epsilon^2}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}},$$

where $\phi(t, x, y)$ is a smooth test function defined on $[0, T) \times \mathbb{R}^N \times \mathbb{T}^N$, with compact support in $[0, T) \times \mathbb{R}^N$, we prove that the sequence

$$v_\epsilon(t, x) = u_\epsilon(t, x) e^{-i \frac{\lambda_n(\theta^n) t}{\epsilon^2}} e^{-2i\pi \frac{\theta^n \cdot x}{\epsilon}}$$

two-scale converges with drift to a limit $\psi_n(y, \theta^n)\, v(t, x)$. Then, in a second step we multiply (37) by the complex conjugate of

$$\Psi_\epsilon = e^{i \frac{\lambda_n(\theta^n) t}{\epsilon^2}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} \left(\psi_n(\frac{x}{\epsilon}, \theta^n) \phi(t, x + \frac{\mathcal{V}}{\epsilon} t) + \epsilon \sum_{k=1}^{N} \frac{\partial \phi}{\partial x_k}(t, x + \frac{\mathcal{V}}{\epsilon} t) \zeta'_k(\frac{x}{\epsilon}) \right),$$

which is different from the previous test function (34) by the ϵ factor, the time scale of the phase, and mostly the large drift in the macroscopic variable. Integrating by parts we perform a computation which is very similar to that in the proof of Theorem 3.2 except that new terms arise. Indeed, the time integration by parts of

$$\int_0^T \int_{\mathbb{R}^N} i \frac{\partial u_\epsilon}{\partial t} \overline{\Psi_\epsilon} dt\, dx$$

yields two new terms. The first one, of order ϵ^{-1}, corresponds to the time derivative applied to $\phi(t, x + \frac{\mathcal{V}}{\epsilon} t)$, and cancels out exactly with the additional term in Eq. (35) for ζ'_k (compared to Eq. (17) for ζ_k) which is

$$-\frac{1}{2i\pi\epsilon} \frac{\partial \lambda_n}{\partial \theta_k} \int_0^T \int_{\mathbb{R}^N} v_\epsilon \overline{\psi_n^\epsilon} \frac{\partial \overline{\phi}}{\partial x_k} dt\, dx.$$

The second new term, of order ϵ^0, corresponds to the time derivative applied to $\epsilon \frac{\partial \phi}{\partial x_k}(t, x + \frac{\mathcal{V}}{\epsilon} t)$, and cancels out exactly with the additional term in the Fredholm alternative of Eq. (15) for $\frac{\partial^2 \psi_n}{\partial \theta_k \partial \theta_l}$ (compared to Eq. (18) for χ_{kl}). In any case we still obtain that the homogenized matrix A_n^* is proportional to the Hessian matrix $\nabla_\theta \nabla_\theta \lambda_n(\theta^n)$. The rest of the proof is as in Theorem 3.2, provided the usual two-scale convergence is replaced by the two-scale convergence with drift which relies on test functions having a large drift in the macroscopic variable. □

5. Fourth Order Homogenized Problem

By changing the main assumption on the Bloch spectrum it is possible to obtain a fourth order homogenized equation instead of the usual Schrödinger equation. Specifically we consider

$$\begin{cases} i\epsilon^2 \frac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon \right) + \left(\epsilon^{-2} c\left(\frac{x}{\epsilon}\right) + \epsilon^2 d\left(x, \frac{x}{\epsilon}\right) \right) u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0, T) \\ u_\epsilon(t = 0, x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N. \end{cases} \tag{44}$$

Remark that the time scaling in (44) is not the same as that in (1): this means that we are looking for an asymptotic for longer time of order ϵ^{-2} in (44), compared to (1). Instead of (11), we now make the following assumption:

$$\begin{cases} (i) \;\; \lambda_n(\theta^n) \text{ is a simple eigenvalue,} \\ (ii) \;\; \nabla_\theta \lambda_n(\theta^n) = 0,\, \nabla_\theta\nabla_\theta \lambda_n(\theta^n) = 0,\, \nabla_\theta\nabla_\theta\nabla_\theta \lambda_n(\theta^n) = 0, \end{cases} \tag{45}$$

which means that θ^n is a "third order" critical point of $\lambda_n(\theta)$. We do not know if assumption (45) is satisfied for any practical example but it seems "reasonable". Under assumption (45) the first eigencouple of (10) is smooth at θ^n. Recall that, for $\theta = \theta^n$, the two first derivatives of ψ_n are given by

$$\frac{\partial \psi_n}{\partial \theta_k} = 2i\pi\zeta_k, \qquad \frac{\partial^2 \psi_n}{\partial \theta_k \partial \theta_l} = -4\pi^2 \chi_{kl}, \tag{46}$$

where ζ_k is the solution of (17) and χ_{kl} is the solution of (18) (remark that this last equation simplifies since $\nabla_\theta\nabla_\theta\lambda_n(\theta^n) = 0$). Similarly, the third derivative is

$$\frac{\partial^3 \psi_n}{\partial \theta_j \partial \theta_k \partial \theta_l} = -8i\pi^3 \xi_{jkl}, \tag{47}$$

where

$$\begin{aligned} \mathbb{A}(\theta^n)\xi_{jkl} = \; & e_j A(y)(\nabla_y + 2i\pi\theta^n)\chi_{kl} + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_j\chi_{kl}\right) \\ & + e_k A(y)(\nabla_y + 2i\pi\theta^n)\chi_{jl} + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_k\chi_{jl}\right) \\ & + e_l A(y)(\nabla_y + 2i\pi\theta^n)\chi_{kj} + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_l\chi_{kj}\right) \\ & + e_k A(y)e_l\zeta_j + e_j A(y)e_l\zeta_k + e_k A(y)e_j\zeta_l. \end{aligned} \tag{48}$$

There exists a unique solution of (48), up to the addition of a multiple of ψ_n. Indeed, the right hand side of (48) satisfies the required compatibility condition (i.e. it is orthogonal to ψ_n) because all derivatives of $\lambda_n(\theta)$, up to third order, are zero at $\theta = \theta^n$.

Theorem 5.1. *Assume that the initial data $u_\epsilon^0 \in L^2(\mathbb{R}^N)$ are of the form*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v^0(x), \tag{49}$$

with $v^0 \in H^1(\mathbb{R}^N)$. The solution of (44) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^4}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v_\epsilon(t,x), \tag{50}$$

where v_ϵ converges strongly in the sense of two-scale convergence to $\psi_n(y,\theta^n)v(t,x)$ and $v \in C\left((0,T); L^2(\mathbb{R}^N)\right)$ is the solution of the fourth-order homogenized problem

$$\begin{cases} i\dfrac{\partial v}{\partial t} + \mathrm{div}\,\mathrm{div}\left(A_n^*\nabla\nabla v\right) + d_n^*(x)\,v = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{51}$$

with $A_n^* = \frac{1}{(2\pi)^4 4!}\nabla_\theta\nabla_\theta\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$ and $d_n^*(x) = \int_{\mathbb{T}^N} d(x,y)|\psi_n(y)|^2\,dy$.

Proof. The proof is similar to that of Theorem 3.2 since we have the same a priori estimates as in Lemma 3.1. The first step is identical: the sequence

$$v_\epsilon = u_\epsilon e^{-i\frac{\lambda_n(\theta^n)t}{\epsilon^4}} e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}},$$

two-scale converges to a limit $v(t,x)\psi_n(y,\theta^n)$. In the second step, we multiply (44) by the complex conjugate of

$$\Psi_\epsilon = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^4}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \Bigg(\psi_n(\frac{x}{\epsilon},\theta^n)\phi(t,x) + \epsilon\sum_{k=1}^N \frac{\partial\phi}{\partial x_k}(t,x)\zeta_k(\frac{x}{\epsilon})$$
$$+\epsilon^2\sum_{k,l=1}^N \frac{\partial^2\phi}{\partial x_k\partial x_l}(t,x)\chi_{kl}(\frac{x}{\epsilon}) + \epsilon^3\sum_{j,k,l=1}^N \frac{\partial^3\phi}{\partial x_j\partial x_k\partial x_l}(t,x)\xi_{jkl}(\frac{x}{\epsilon})\Bigg),$$

where $\phi(t,x)$ is a smooth test function with compact support in $[0,T)\times\mathbb{R}^N$, $\zeta_k(y)$ is the solution of (17), $\chi_{kl}(y)$ is the solution of (18), and $\xi_{jkl}(y)$ is the solution of (48). After some tedious algebra we can pass to the two-scale limit and find a variational formulation of (51) (see [3] where a similar computation is done for a parabolic system). We obtain a fourth-order homogenized tensor which is (up to symmetrization)

$$\left(A_n^*\right)_{jklm} = \int_{\mathbb{T}^N}\Big(- A\psi_n e_m\cdot e_k\overline{\chi}_{jl} - A\psi_n e_m\cdot(\nabla_y - 2i\pi\theta^n)\overline{\eta}_{jkl}$$
$$+A\overline{\eta}_{jkl}(\nabla_y + 2i\pi\theta^n)\psi_n\cdot e_m\Big)dy.$$

The compatibility condition of the equation giving the fourth derivative of ψ_n shows that this tensor A^* is actually equal to $\frac{1}{(2\pi)^4 4!}\nabla_\theta\nabla_\theta\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$. □

Remark 5.2. Similarly we could derive a third-order homogenized problem, if we replace assumption (45) by the hypothesis that θ^n is a "second order" critical point of $\lambda_n(\theta)$, and if we change the time scale in (44) by writing the time derivative as $i\epsilon\frac{\partial u_\epsilon}{\partial t}$. More generally, any p-order critical point of $\lambda_n(\theta)$ yields a p-order (in space) homogenized equation. This is a well-known consequence of the duality between derivatives in the physical space and multiplication by Fourier variables (or more precisely here Bloch variables).

6. Homogenized System of Equations

In this section we investigate the case of a Bloch eigenvalue which is not simple. To simplify the exposition we consider an eigenvalue of multiplicity two, but the argument works through for any multiplicity. We replace assumption (11) by the following one: for $n\geq 1$, we consider a Bloch parameter $\theta^n\in\mathbb{T}^N$ such that

$$\begin{cases} (i) & \lambda_n(\theta^n) = \lambda_{n+1}(\theta^n) \neq \lambda_k(\theta^n) \quad \forall k\neq n, n+1, \\ (ii) & \text{locally near } \theta^n,\ \lambda_n(\theta) \text{ and } \lambda_{n+1}(\theta) \text{ form two} \\ & \text{smooth branches of eigenvalues with corresponding} \\ & \text{smooth eigenfunctions } \psi_n(\theta) \text{ and } \psi_{n+1}(\theta), \\ (iii) & \nabla_\theta\lambda_n(\theta^n) = \nabla_\theta\lambda_{n+1}(\theta^n) = 0. \end{cases} \tag{52}$$

By a convenient abuse of language we still denote by $\lambda_n(\theta)$ and $\lambda_{n+1}(\theta)$ the two smooth (local) branches of eigenvalues passing through θ^n (this is equivalent to a pointwise relabeling of these two eigenvalues, not necessarily following the usual increasing order). In dimension $N = 1$ a double eigenvalue can only occur when there is no gap between two consecutive Bloch bands and assumption (52) is automatically satisfied [22]. However, in dimension $N > 1$ it is not even clear that, near a double eigenvalue, one can find two smooth branches because θ is a vector-valued parameter (see [19]). Therefore, (52) is a very strong mathematical assumption which is physically not very relevant in dimension $N > 1$.

Theorem 6.1. *Assume (52) and that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ are of the form*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v_1^0(x) + \psi_{n+1}\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v_2^0(x), \tag{53}$$

with $v_1^0, v_2^0 \in H^1(\mathbb{R}^N)$. The solution of (1) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v_\epsilon(t,x), \tag{54}$$

where v_ϵ two-scale converges strongly to $\psi_n(y,\theta^n)v_1(t,x) + \psi_{n+1}(y,\theta^n)v_2(t,x)$, i.e., uniformly on compact time intervals in $\mathbb{R}^+$,

$$\lim_{\epsilon\to 0}\int_{\mathbb{R}^N}\left|v_\epsilon(t,x) - \psi_n\left(\frac{x}{\epsilon},\theta^n\right)v_1(t,x) - \psi_{n+1}\left(\frac{x}{\epsilon},\theta^n\right)v_2(t,x)\right|^2 dx = 0, \tag{55}$$

and $(v_1, v_2) \in C\left((0,T); L^2(\mathbb{R}^N)^2\right)$ is the unique solution of the homogenized Schrödinger system of two equations

$$\begin{cases} i\dfrac{\partial v_1}{\partial t} - \operatorname{div}\left(A_n^*\nabla v_1\right) + d_{11}^*(x)\, v_1 + d_{12}^*(x)\, v_2 = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ i\dfrac{\partial v_2}{\partial t} - \operatorname{div}\left(A_{n+1}^*\nabla v_2\right) + d_{21}^*(x)\, v_1 + d_{22}^*(x)\, v_2 = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ (v_1, v_2)(t=0,x) = (v_1^0, v_2^0)(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{56}$$

with $A_n^* = \frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$, $A_{n+1}^* = \frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_{n+1}(\theta^n)$ and

$$\begin{pmatrix} d_{11}^*(x) & d_{12}^*(x) \\ d_{21}^*(x) & d_{22}^*(x) \end{pmatrix} = \int_{\mathbb{T}^N} d(x,y)\begin{pmatrix} \psi_n(y)\overline{\psi}_n(y) & \psi_n(y)\overline{\psi}_{n+1}(y) \\ \psi_{n+1}(y)\overline{\psi}_n(y) & \psi_{n+1}(y)\overline{\psi}_{n+1}(y) \end{pmatrix} dy.$$

Remark 6.2. The main point in Theorem 6.1 is that the homogenized system is of dimension equal to the multiplicity of the eigenvalue $\lambda_n(\theta^n)$. However, the homogenized system (56) is coupled only by zero-order terms since the diffusion operator is diagonal.

Remark 6.3. Part (iii) of assumption (52) means that the two Bloch modes λ_n and λ_{n+1} are tangent at θ_n. The fact that the derivatives are zero is not essential and (52)-(iii) can be replaced by $\mathcal{V} = \nabla_\theta\lambda_n(\theta^n)/2\pi = \nabla_\theta\lambda_{n+1}(\theta^n)/2\pi$. In such a case, Theorem 6.1 can easily be generalized and both components of the homogenized solution are subject to a large common drift $\epsilon^{-1}\mathcal{V} \neq 0$.

However, if assumption (iii) in (52) is not satisfied, i.e. if there are two different group velocities, $\nabla_\theta\lambda_n(\theta^n) \neq \nabla_\theta\lambda_{n+1}(\theta^n)$, then we obtain an uncoupled limit system, i.e. each branch of eigenfunctions yields a different homogenized Schrödinger equation (we safely leave the details to the reader). Physically speaking, this last situation can be interpreted as a crossing of modes, whereas (52) is just a case of tangential modes. The semi-classical limit of the crossing of modes yields the so-called Landau-Zerner formula, recently analyzed in [13], [14]. Our study is very different since it leads to a non-trivial limit only in the case of tangential modes.

Proof of Theorem 6.1. Introducing a sequence v_ϵ defined by

$$v_\epsilon(t,x) = u_\epsilon(t,x) e^{-i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}},$$

which satisfies the same a priori estimates as u_ϵ, and applying Proposition 2.3, there exists a limit $v^*(t,x,y) \in L^2\left((0,T)\times\mathbb{R}^N; H^1(\mathbb{T}^N)\right)$ such that, up to a subsequence, v_ϵ and $\epsilon\nabla v_\epsilon$ two-scale converge to v^* and $\nabla_y v^*$, respectively.

First step. We multiply (1) by the complex conjugate of

$$\epsilon^2\phi\left(t,x,\frac{x}{\epsilon}\right) e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}},$$

where $\phi(t,x,y)$ is a smooth test function defined on $[0,T)\times\mathbb{R}^N\times\mathbb{T}^N$, with compact support in $[0,T)\times\mathbb{R}^N$. Integrating by parts and passing to the two-scale limit yields the variational formulation of

$$-(\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)v^*\Big) + c(y)v^* = \lambda_n(\theta^n)v^* \quad \text{in } \mathbb{T}^N.$$

Since $\lambda_n(\theta^n) = \lambda_{n+1}(\theta^n)$ is of multiplicity 2, there exist two scalar functions $v_1(t,x), v_2(t,x) \in L^2\left((0,T)\times\mathbb{R}^N\right)$ such that

$$v^*(t,x,y) = v_1(t,x)\psi_n(y,\theta^n) + v_2(t,x)\psi_{n+1}(y,\theta^n). \tag{57}$$

Second step. We multiply (1) by the complex conjugate of

$$\Psi_\epsilon = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \Bigg(\psi_n(\frac{x}{\epsilon},\theta^n)\phi_1(t,x) + \psi_{n+1}(\frac{x}{\epsilon},\theta^n)\phi_2(t,x) + \epsilon\sum_{k=1}^N \left(\frac{\partial\phi_1}{\partial x_k}(t,x)\zeta_k^1(\frac{x}{\epsilon}) + \frac{\partial\phi_2}{\partial x_k}(t,x)\zeta_k^2(\frac{x}{\epsilon})\right)\Bigg),$$

where ϕ_1,ϕ_2 are two smooth test functions with compact support in $[0,T)\times\mathbb{R}^N$, and $\zeta_k^1(y)$ is the solution of (17) with ψ_n in the right hand side (respectively, $\zeta_k^2(y)$ with ψ_{n+1}). Note that at this point we strongly use the assumption on the smoothness of the eigenfunctions since $\zeta_k^1(y)$ (respectively, $\zeta_k^2(y)$) is defined as the partial derivative of ψ_n (respectively, ψ_{n+1}) with respect to θ_k. We integrate by parts and we pass to the two-scale limit using the same algebra as in the proof of Theorem 3.2. We also use the orthogonality property

$$\int_{\mathbb{T}^N} \psi_n\overline{\psi}_{n+1}\,dy = 0,$$

to obtain

$$
\begin{aligned}
& i \int_{\mathbb{R}^N} \left(v_1^0 \overline{\phi}_1(0) + v_2^0 \overline{\phi}_2(0) \right) dx - i \int_0^T \int_{\mathbb{R}^N} \left(v_1 \frac{\partial \overline{\phi}_1}{\partial t} + v_2 \frac{\partial \overline{\phi}_2}{\partial t} \right) dt\, dx \\
& - \int_0^T \int_{\mathbb{R}^N} \sum_{p,q=1}^{2} A^*_{pq} v_p \cdot \nabla \nabla \overline{\phi}_q \, dt\, dx \\
& + \int_0^T \int_{\mathbb{R}^N} \int_{\mathbb{T}^N} d(\psi_n v_1 + \psi_{n+1} v_2)(\overline{\psi}_n \overline{\phi}_1 + \overline{\psi}_{n+1} \overline{\phi}_2)\, dt\, dx\, dy = 0, \qquad (58)
\end{aligned}
$$

where $A^*_{11} = A^*_n$ and $A^*_{22} = A^*_{n+1}$, defined by (30), and A^*_{12} is defined by

$$
\begin{aligned}
2 \left(A^*_{12} \right)_{jk} = \int_{\mathbb{T}^N} \Big(& A \psi_n e_j \cdot e_k \overline{\psi}_{n+1} + A \psi_n e_k \cdot e_j \overline{\psi}_{n+1} \\
& + A \psi_n e_j \cdot (\nabla_y - 2i\pi\theta^n) \overline{\zeta}^2_k + A \psi_n e_k \cdot (\nabla_y - 2i\pi\theta^n) \overline{\zeta}^2_j \\
& - A \overline{\zeta}^2_k (\nabla_y + 2i\pi\theta^n) \psi_n \cdot e_j - A \overline{\zeta}^2_j (\nabla_y + 2i\pi\theta^n) \psi_n \cdot e_k \Big) dy, \qquad (59)
\end{aligned}
$$

with a symmetric formula for A^*_{21}. Recall that $A^*_n = \frac{1}{8\pi^2} \nabla_\theta \nabla_\theta \lambda_n(\theta^n)$ because of the compatibility condition of Eq. (18) for the second derivative of ψ_n. This compatibility condition is obtained by multiplying (18) by ψ_n and remarking that

$$
\int_{\mathbb{T}^N} \mathbb{A}_n(\theta^n) \chi_{kl} \overline{\psi}_n \, dy = \int_{\mathbb{T}^N} \chi_{kl} \overline{\mathbb{A}_n(\theta^n) \psi_n} \, dy = 0
$$

because $\mathbb{A}_n(\theta^n)\psi_n = 0$. However, the same holds true if we multiply (18) by ψ_{n+1} ,

$$
\int_{\mathbb{T}^N} \mathbb{A}_n(\theta^n) \chi_{kl} \overline{\psi}_{n+1} \, dy = 0,
$$

because $\mathbb{A}_n(\theta^n)\psi_{n+1} = 0$. Therefore, we deduce that (59) is equivalent to

$$
2 \left(A^*_{12} \right)_{lk} = \int_{\mathbb{T}^N} \frac{1}{4\pi^2} \frac{\partial^2 \lambda_n}{\partial \theta_l \partial \theta_k} (\theta^n) \psi_n \overline{\psi}_{n+1} \, dy = 0
$$

by orthogonality of ψ_n and ψ_{n+1}. Thus $A^*_{12} = A^*_{21} = 0$ and (58) is a weak formulation of the limit system (56) which is thus coupled only through the zero-order terms. It is easily seen that (56) is well-posed in $C\left((0,T); L^2(\mathbb{R}^N)^2\right)$. The rest of the proof is as for Theorem 3.2. □

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