Periodic homogenization and effective mass theorems for the Schrödinger equation

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Abstract

The goal of this course is to give an introduction to periodic homogenization theory with an emphasis on applications to Schrödinger equation. We shall review the formal method of two-scale asymptotic expansions, then discuss the rigorous two-scale convergence method as well as the Bloch wave decomposition. Eventually these tools will be apply to the Schrödinger equation with a periodic potential perturbed by a small macroscopic potential. The notion of effective mass for the one electron model in solid state physics will be derived. Localization effects will also be emphasized.

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1 Introduction

This set of lecture notes is an elementary introduction to periodic homogenization, two-scale convergence, Bloch waves, and their application to the Schrödinger equation with a periodic potential. In particular, the notion of effective mass which is central in solid state physics will be rigorously derived here.

Mathematically, homogenization can be defined as a theory for averaging partial differential equations and defining both effective properties and macroscopic models. Although this question of averaging and finding effective properties is very old in physics or mechanics, the mathematical theory of homogenization is quite recent, going back to the 1970's. The most general framework is known as the H-convergence, or G-convergence, introduced by Spagnolo [47], [48], and generalized by Tartar and Murat [38], [50]. Although homogenization is not restricted to periodic problems, we shall focus here on periodic homogenization which is simpler and enough for the asymptotic analysis of periodic structures. Indeed, in many fields of science and technology one has to solve boundary value problems in periodic media. If the size of the period is small compared to the size of the medium, denoting by ϵ their ratio, the complexity of the problem can be reduced by an asymptotic analysis, as ϵ goes to zero. In other words, starting from a microscopic description of a problem, one seeks a macroscopic, or effective, model. There are many textbooks on periodic homogenization, see e.g. [9], [10], [17], [31], [46].

2 Asymptotic expansions in periodic homogenization

This section is devoted to an elementary introduction to periodic homogenization using the heuristic method ot two-scale asymptotic expansions. A rigorous mathematical justification will be given in the next section on two-scale convergence.

We consider a model problem of thermal or electrical conductivity in a periodic medium (for example, an heterogeneous domain obtained by mixing periodically two different phases, one being the matrix and the other the inclusions; see Figure 1). To fix ideas, the periodic domain is called Ω (a bounded open set in $\mathbb{R}^N$ with $N \geq 1$ the space dimension), its period ϵ (a positive number which is assumed to be very small in comparison with the size of the domain), and the rescaled unit periodic cell $Y = (0,1)^N$. The conductivity in Ω is not constant, but varies periodically with period ϵ in each direction. It is a matrix (a second order tensor) $A(y)$, where $y = x/\epsilon \in Y$ is the fast periodic variable, while $x \in \Omega$ is the slow variable. Equivalently, x is also called the macroscopic variable, and y the microscopic variable. Since the component conductors do not need to be isotropic, the matrix A can be any second order tensor that is positive definite, i.e., there exists a positive constant $\alpha > 0$ such that, for any vector $\xi \in \mathbb{R}^N$ and at any point $y \in Y$,

$$\alpha |\xi|^2 \leq \sum_{i,j=1}^{N} A_{ij}(y) \xi_i \xi_j .$$

At this point, the matrix A is not necessarily symmetric (such is the case when some drift is taken into account in the diffusion process). The matrix $A(y)$ is a periodic function of y, with period Y, and it may be discontinuous in y (to model the discontinuity of conductivities from one phase to the other).

Denoting by $f(x)$ the source term (a scalar function defined in Ω), and enforcing a Dirichlet boundary condition (for simplicity), our model problem of conductivity reads

$$\begin{cases} -\mathrm{div}\left(A\left(\frac{x}{\epsilon}\right) \nabla u_\epsilon \right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega, \end{cases} \tag{1}$$

where $u_\epsilon(x)$ is the unknown function, modeling the electrical potential or the temperature.

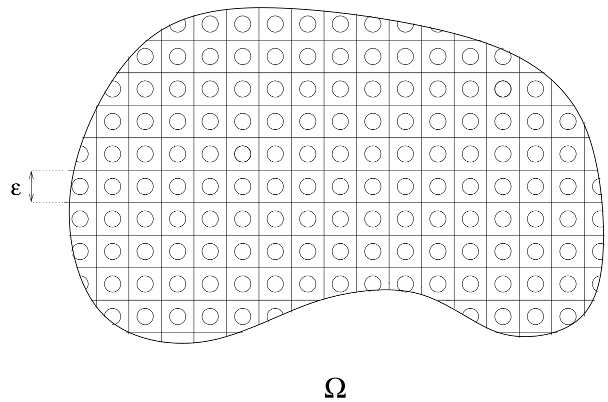

Figure 1: A periodic domain.

The domain Ω, with its conductivity $A\left(\frac{x}{\epsilon}\right)$, is highly heterogeneous with periodic heterogeneities of lengthscale ϵ. Usually one does not need the full details of the variations of the potential or temperature u_ϵ, but rather some global of averaged behavior of the domain Ω considered as an homogeneous domain. In other words, an effective or equivalent macroscopic conductivity of Ω is sought. From a numerical point of view, solving equation (1) by any method will require too much effort if ϵ is small since the number of elements (or degrees of freedom) for a fixed level of accuracy grows like $1/\epsilon^N$. It is thus preferable to average or homogenize the properties of Ω and compute an approximation of u_ϵ on a coarse mesh. Averaging the solution of (1) and finding the effective properties of the domain Ω is what we call homogenization.

The mathematical theory of homogenization works completely differently. Rather than considering a single heterogeneous medium with a fixed lengthscale, the problem is first embedded in a sequence of similar problems for which the lengthscale ϵ, becoming increasingly small, goes to zero. Then, an asymptotic analysis is performed as ϵ tends to zero, and the conductivity tensor of the limit problem is said to be the *effective* or *homogenized* conductivity. This seemingly more complex approach has the advantage of defining uniquely the homogenized properties. Further, the approximation made by using effective properties instead of the true microscopic coefficients can be rigorously justified by quantifying the resulting error.

In the case of a periodic medium Ω, this asymptotic analysis of equation (1), as the period ϵ goes to zero, is especially simple. The solution u_ϵ is written as a power series in ϵ

$$u_\epsilon = \sum_{i=0}^{+\infty} \epsilon^i u_i.$$

The first term u_0 of this series will be identified with the solution of the so-called homogenized equation whose effective conductivity A^* can be exactly computed. It turns out that A^* is a constant tensor, describing a homogeneous medium, which is independent of f and of the boundary conditions. Therefore, numerical computations on the homogenized equation do not require a fine mesh since the heterogeneities of size ϵ have been averaged out. This homogenized tensor A^* is almost never a usual average (arithmetic or harmonic) of $A(y)$. Various estimates will confirm this asymptotic analysis by telling in which sense u_ϵ is close to u_0 as ϵ tends to zero.

Remark 2.1 *From a more theoretical point of view, homogenization can be interpreted as follows. Rather than studying a single problem (1) for the physically relevant value of* ϵ*, we consider a sequence of such problems indexed by the period* ϵ*, which is now regarded as a small parameter going to zero. The question is to find the limit of this sequence of problems. The notion of limit problem is defined by considering the convergence of the sequence* $(u_\epsilon)_{\epsilon>0}$ *of solutions of (1): Denoting by* u *its limit, the limit problem is defined as the problem for which* u *is a solution. Of course,* u *will turn out to coincide with* u_0*, the first term in the series defined above, and it is therefore the solution of the homogenized equation. Section 3 is devoted to this approach. Clearly the mathematical difficulty is to define an adequate topology for this notion of convergence of problems as* ϵ *goes to zero.*

The method of two-scale asymptotic expansions is an heuristic method, which allows one to formally homogenize a great variety of models or equations posed in a periodic domain. We present it briefly and refer to the classical books [9], [10], and [46] for more detail. A mathematical justification of what follows is to be found in the next section. As already stated, the starting point is to consider the following *ansatz*, or *two-scale asymptotic expansion*, for the solution u_ϵ of e quation (1):

$$u_\epsilon(x) = \sum_{i=0}^{+\infty} \epsilon^i u_i \left(x, \frac{x}{\epsilon} \right), \tag{2}$$

where each term $u_i(x, y)$ is a function of both variables x and y, periodic in y with period $Y = (0, 1)^N$ (u_i is called a Y-periodic function with respect to y). This series is plugged into the equation, and the following derivation rule is used:

$$\nabla \left(u_i \left(x, \frac{x}{\epsilon} \right) \right) = \left(\epsilon^{-1} \nabla_y u_i + \nabla_x u_i \right) \left(x, \frac{x}{\epsilon} \right), \tag{3}$$

where ∇_x and ∇_y denote the partial derivative with respect to the first and second variable of $u_i(x, y)$. For example, one has

$$\nabla u_\epsilon(x) = \epsilon^{-1} \nabla_y u_0 \left(x, \frac{x}{\epsilon} \right) + \sum_{i=0}^{+\infty} \epsilon^i \left(\nabla_y u_{i+1} + \nabla_x u_i \right) \left(x, \frac{x}{\epsilon} \right).$$

Equation (1) becomes a series in ϵ

$$\begin{aligned}
&-\epsilon^{-2} \left[\mathrm{div}_y A \nabla_y u_0 \right] \left(x, \frac{x}{\epsilon} \right) \\
&-\epsilon^{-1} \left[\mathrm{div}_y A (\nabla_x u_0 + \nabla_y u_1) + \mathrm{div}_x A \nabla_y u_0 \right] \left(x, \frac{x}{\epsilon} \right) \\
&-\epsilon^{0} \left[\mathrm{div}_x A (\nabla_x u_0 + \nabla_y u_1) + \mathrm{div}_y A (\nabla_x u_1 + \nabla_y u_2) \right] \left(x, \frac{x}{\epsilon} \right) \\
&- \sum_{i=1}^{+\infty} \epsilon^i \left[\mathrm{div}_x A (\nabla_x u_i + \nabla_y u_{i+1}) + \mathrm{div}_y A (\nabla_x u_{i+1} + \nabla_y u_{i+2}) \right] \left(x, \frac{x}{\epsilon} \right) \\
&= f(x).
\end{aligned} \tag{4}$$

Identifying each coefficient of (4) as an individual equation yields a cascade of equations (a series of the variable ϵ is zero for all values of ϵ if each coefficient is zero). It turns out that the three first equations are enough for our purpose. The ϵ^{-2} equation is

$$-\mathrm{div}_y A(y) \nabla_y u_0(x, y) = 0,$$

which is nothing else than an equation in the unit cell Y with periodic boundary condition. In this equation, y is the variable, and x plays the role of a parameter. It can be checked (see Lemma 2.3 below) that there exists a unique solution of this equation up to a constant (i.e., a function of x independent of y since x is just a parameter). This implies that u_0 is a function that does not depend on y, i.e., there exists a function $u(x)$ such that

$$u_0(x, y) \equiv u(x).$$

Since $\nabla_y u_0 = 0$, the ϵ^{-1} equation is

$$-\mathrm{div}_y A(y) \nabla_y u_1(x, y) = \mathrm{div}_y A(y) \nabla_x u(x), \tag{5}$$

which is an equation for the unknown u_1 in the periodic unit cell Y. Again, it is a well-posed problem, which admits a unique solution up to a constant, as soon as the right hand side is known. Equation (5) allows one to compute u_1 in terms of u, and it is easily seen that $u_1(x, y)$ depends linearly on the first derivative $\nabla_x u(x)$.

Finally, the ϵ^0 equation is

$$\begin{aligned} -\mathrm{div}_y A(y) \nabla_y u_2(x, y) &= \mathrm{div}_y A(y) \nabla_x u_1 \\ &\quad + \mathrm{div}_x A(y) \left(\nabla_y u_1 + \nabla_x u \right) + f(x), \end{aligned} \tag{6}$$

which is an equation for the unknown u_2 in the periodic unit cell Y. Equation (6) admits a solution if a compatibility condition is satisfied (the so-called *Fredholm alternative*; see Lemma 2.3). Indeed, integrating the left hand side of (6) over Y, and using the periodic boundary condition for u_2, we obtain

$$\int_Y \mathrm{div}_y A(y) \nabla_y u_2(x, y) dy = \int_{\partial Y} \left[A(y) \nabla_y u_2(x, y) \right] \cdot n \, ds = 0,$$

which implies that the right hand side of (6) must have zero average over Y, i.e.,

$$\int_Y \left[\mathrm{div}_y A(y) \nabla_x u_1 + \mathrm{div}_x A(y) \left(\nabla_y u_1 + \nabla_x u \right) + f(x) \right] dy = 0,$$

which simplifies to

$$-\mathrm{div}_x \left(\int_Y A(y) \left(\nabla_y u_1 + \nabla_x u \right) dy \right) = f(x) \quad \text{in } \Omega. \tag{7}$$

Since $u_1(x, y)$ depends linearly on $\nabla_x u(x)$, equation (7) is simply an equation for $u(x)$ involving only the second order derivatives of u.

In order to compute u_1 and to simplify (7), we introduce the so-called *cell problems*. We denote by $(e_i)_{1 \le i \le N}$ the canonical basis of $\mathbb{R}^N$. For each unit vector e_i, consider the following conductivity problem in the periodic unit cell:

$$\left\{ \begin{array}{ll} -\mathrm{div}_y A(y) \left(e_i + \nabla_y w_i(y) \right) = 0 & \text{in } Y \\ y \to w_i(y) & Y\text{-periodic}, \end{array} \right. \tag{8}$$

where $w_i(y)$ is the local variation of potential or temperature created by an averaged (or macroscopic) gradient e_i. By linearity, it is not difficult to compute $u_1(x, y)$, solution of (5), in terms of $u(x)$ and $w_i(y)$

$$u_1(x, y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i(y). \tag{9}$$

In truth, $u_1(x,y)$ is merely defined up to the addition of a function $\tilde{u}_1(x)$ (depending only on x), but this does not matter since only its gradient $\nabla_y u_1(x,y)$ is used in the homogenized equation. Inserting this expression in equation (7), we obtain the homogenized equation for u that we supplement with a Dirichlet boundary condition on $\partial\Omega$,

$$\begin{cases} -\mathrm{div}_x A^* \nabla_x u(x) = f(x) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega. \end{cases} \tag{10}$$

The homogenized conductivity A^* is defined by its entries

$$A^*_{ij} = \int_Y \left[(A(y)\nabla_y w_i) \cdot e_j + A_{ij}(y) \right] dy,$$

or equivalently, after a simple integration by parts in Y,

$$A^*_{ij} = \int_Y A(y)\,(e_i + \nabla_y w_i) \cdot (e_j + \nabla w_j)\, dy. \tag{11}$$

The constant tensor A^* describes the effective or homogenized properties of the heterogeneous material $A\left(\frac{x}{\epsilon}\right)$. Note that A^* does not depend on the choice of domain Ω, source term f, or boundary condition on $\partial\Omega$.

Remark 2.2 *This method of two-scale asymptotic expansions is unfortunately not rigorous from a mathematical point of view. In other words, it yields heuristically the homogenized equation, but it does not yield a correct proof of the homogenization process. The reason is that the ansatz (2) is usually not correct after the two first terms. For example, it does not include possible boundary layers in the vicinity of $\partial\Omega$ (for details, see, e.g., [35]). Nevertheless, it is possible to rigorously justify the above homogenization process, in particular by the method of two-scale convergence as explained below.*

Lemma 2.3 *Let $f(y) \in L^2_\#(Y)$ be a periodic function. There exists a unique solution in $H^1_\#(Y)/\mathbb{R}$ of*

$$\begin{cases} -\mathrm{div} A(y) \nabla w(y) = f & \text{in } Y \\ y \to w(y) & Y\text{-periodic}, \end{cases} \tag{12}$$

if and only if $\int_Y f(y)dy = 0$ (this is called the Fredholm alternative).

Remark 2.4 *By identifying the unit cell Y with the unit torus, equation (12) can be seen as posed in the unit torus. Since the torus has no boundary, it has the advantage of requiring no boundary conditions. In other words, the formulation of (12) in the unit torus automatically includes the periodicity of the solution.*

Proof. Due to the periodic boundary condition, a simple integration by parts yields $\int_Y (\text{div} A(y)\nabla w(y))\,dy = 0$ for any function $w \in H^1_\#(Y)$. Therefore, $\int_Y f(y)dy = 0$ is a necessary condition of existence of solutions for (12). Defining the quotient space $H^1_\#(Y)/\mathbb{R}$ of functions defined in $H^1_\#(Y)$ up to a constant, it is easily seen that $\|\nabla w\|_{L^2(Y)^N}$ is a norm for this quotient space. We check the assumptions of the Lax-Milgram lemma on the variational formulation of (12). Clearly, $\int_Y A(y)\nabla w \cdot \nabla\phi dy$ is a coercive continuous bilinear form on $H^1_\#(Y)/\mathbb{R}$. Furthermore, if $\int_Y f(y)dy = 0$, one finds

$$\int_Y f(y)w(y)dy = \int_Y f(y)\left(w(y) - \int_Y w(y)dy\right)dy,$$

which is a continuous linear form on $H^1_\#(Y)/\mathbb{R}$ thanks to the following Poincaré-Wirtinger inequality

$$\left\| w(y) - \int_Y w(y)dy \right\|_{L^2(Y)} \leq C\|\nabla w\|_{L^2(Y)^N}.$$

This proves that there exists a unique solution $w \in H^1_\#(Y)/\mathbb{R}$ of (12) if $\int_Y f(y)dy = 0$. □

3 Two-scale convergence

On the contrary of many homogenization methods, like the $\Gamma-$, $G-$, and $H-$convergence [21], [31], [51], the two-scale convergence method is devoted only to periodic homogenization problems. It is therefore a less general method, but it is also more efficient and simple in the context of periodic homogenization. Two-scale convergence has been introduced by Nguetseng [40] and Allaire [2] and is exposed in a self-content fashion below. This section is devoted to the main theoretical results which are at the root of this method. Section 4 is a detailed application of the method on a simple model problem.

Before going into the details of the method, let us give its main ideas. Two-scale convergence is a new type of convergence (see Definition 3.1) and it yields a *rigorous* justification of the first term of the ansatz (2) for any bounded sequence u_ϵ, in the sense that it asserts the existence of a *two-scale* limit $u_0(x,y)$ such that u_ϵ, tested again any periodically oscillating test function, converges to $u_0(x,y)$

$$\int_\Omega u_\epsilon(x)\varphi\left(x,\frac{x}{\epsilon}\right)dx \to \int_\Omega\int_Y u_0(x,y)\varphi(x,y)dxdy. \tag{13}$$

Two-scale convergence is an improvement over the usual weak convergence since equation (13) measures the periodic oscillations of the sequence u_ϵ. The two-scale convergence method is based on this result: it turns out that multiplying the equation satisfied by u_ϵ with an oscillating test function $\varphi\left(x,\frac{x}{\epsilon}\right)$ and passing to the *two-scale* limit automatically yields the homogenized problem.

Let us introduce some notations: Ω is an open set of $\mathbb{R}^N$ (not necessarily bounded), and $Y=(0,1)^N$ is the unit cube. We denote by $C^\infty_\#(Y)$ the space of infinitely differentiable functions in $\mathbb{R}^N$ which are periodic of period Y, and by $C_\#(Y)$ the Banach space of continuous and Y-periodic functions. Eventually, $\mathcal{D}(\Omega;C^\infty_\#(Y))$ denotes the space of infinitely smooth and compactly supported functions in Ω with values in the space $C^\infty_\#(Y)$.

Definition 3.1 *A sequence of functions u_ϵ in $L^2(\Omega)$ is said to two-scale converge to a limit $u_0(x,y)$ belonging to $L^2(\Omega\times Y)$ if, for any function $\varphi(x,y)$ in $\mathcal{D}(\Omega;C^\infty_\#(Y))$, it satisfies*

$$\lim_{\epsilon\to 0}\int_\Omega u_\epsilon(x)\varphi\left(x,\frac{x}{\epsilon}\right)dx = \int_\Omega\int_Y u_0(x,y)\varphi(x,y)dxdy.$$

This notion of “two-scale convergence” makes sense because of the next compactness theorem.

Theorem 3.2 *From each bounded sequence u_ϵ in $L^2(\Omega)$ one can extract a subsequence, and there exists a limit $u_0(x,y)\in L^2(\Omega\times Y)$ such that this subsequence two-scale converges to u_0.*

Before sketching the proof of Theorem 3.2, we give a few examples of two-scale convergences.

1. Any sequence u_ϵ which converges strongly in $L^2(\Omega)$ to a limit $u(x)$, two-scale converges to the same limit $u(x)$.

2. For any smooth function $u_0(x,y)$, being Y-periodic in y, the associated sequence $u_\epsilon(x) = u_0\left(x, \frac{x}{\epsilon}\right)$ two-scale converges to $u_0(x,y)$.

3. For the same smooth and Y-periodic function $u_0(x,y)$ the sequence defined by $v_\epsilon(x) = u_0(x, \frac{x}{\epsilon^2})$ has the same two-scale limit and weak-L^2 limit, namely $\int_Y u_0(x,y)dy$ (this is a consequence of the difference of orders in the speed of oscillations for v_ϵ and the test functions $\varphi\left(x, \frac{x}{\epsilon}\right)$). Clearly the two-scale limit captures only the oscillations which are in resonance with those of the test functions $\varphi\left(x, \frac{x}{\epsilon}\right)$.

4. Any sequence u_ϵ which admits an asymptotic expansion of the type $u_\epsilon(x) = u_0\left(x, \frac{x}{\epsilon}\right) + \epsilon u_1\left(x, \frac{x}{\epsilon}\right) + \epsilon^2 u_2\left(x, \frac{x}{\epsilon}\right) + \cdots$, where the functions $u_i(x,y)$ are smooth and Y-periodic in y, two-scale converges to the first term of the expansion, namely $u_0(x,y)$.

We now briefly give the main ideas of the proof of Theorem 3.2 (it was first proved by Nguetseng [40], but we follow the proof in [2] to which the interested reader is referred for more details). For the sake of simplicity in the exposition, we assume during the proof that Ω is a bounded set. The following elementary lemma is first required (the proof of which is left to the reader).

Lemma 3.3 *Let $B = C(\bar{\Omega}; C_\#(Y))$ be the space of continuous functions $\varphi(x,y)$ on $\bar{\Omega} \times Y$ which are Y-periodic in y. Then, B is a separable Banach space (i.e. it contains a dense countable family), is dense in $L^2(\Omega \times Y)$, and any of its elements $\varphi(x,y)$ satisfies*

$$\int_\Omega |\varphi\left(x, \frac{x}{\epsilon}\right)|^2 dx \leq C\|\varphi\|_B^2,$$

and

$$\lim_{\epsilon\to 0} \int_\Omega |\varphi\left(x, \frac{x}{\epsilon}\right)|^2 dx = \int_\Omega \int_Y |\varphi(x,y)|^2 dx dy.$$

Proof of Theorem 3.2. By Schwarz inequality, we have

$$\left|\int_\Omega u_\epsilon(x)\varphi\left(x, \frac{x}{\epsilon}\right) dx\right| \leq C \left|\int_\Omega \varphi\left(x, \frac{x}{\epsilon}\right) dx\right|^{\frac{1}{2}} \leq C\|\varphi\|_B. \tag{14}$$

This implies that the left hand side of (14) is a continuous linear form on B which can be identified to a duality product $\langle \mu_\epsilon, \varphi \rangle_{B',B}$ for some bounded sequence of measures μ_ϵ. Since B is separable, one can extract a subsequence and there exists a limit μ_0 such μ_ϵ converges to μ_0 in the weak * topology of B' (the dual of B). On the other hand, Lemma 3.3 allows us to pass to the limit in the middle term of (14). Combining these two results, yields

$$|\langle \mu_0, \varphi \rangle_{B',B}| \leq C \left| \int_\Omega \int_Y |\varphi(x,y)|^2 dxdy \right|^{\frac{1}{2}}. \tag{15}$$

Equation (15) shows that μ_0 is actually a continuous form on $L^2(\Omega \times Y)$, by density of B in this space. Thus, there exists $u_0(x,y) \in L^2(\Omega \times Y)$ such that

$$\langle \mu_0, \varphi \rangle_{B',B} = \int_\Omega \int_Y u_0(x,y)\varphi(x,y)dxdy,$$

which concludes the proof of Theorem 3.2. □

The next theorem shows that more information is contained in a two-scale limit than in a weak-L^2 limit ; some of the oscillations of a sequence are contained in its two-scale limit. When all of them are captured by the two-scale limit (condition (17) below), one can even obtain a strong convergence (a corrector result in the vocabulary of homogenization).

Theorem 3.4 *Let u_ϵ be a sequence of functions in $L^2(\Omega)$ which two-scale converges to a limit $u_0(x,y) \in L^2(\Omega \times Y)$.*

1. *Then, u_ϵ converges weakly in $L^2(\Omega)$ to $u(x) = \int_Y u_0(x,y)dy$, and we have*
$$\lim_{\epsilon \to 0} \|u_\epsilon\|^2_{L^2(\Omega)} \geq \|u_0\|^2_{L^2(\Omega\times Y)} \geq \|u\|^2_{L^2(\Omega)}. \tag{16}$$

2. *Assume further that $u_0(x,y)$ is smooth and that*
$$\lim_{\epsilon \to 0} \|u_\epsilon\|^2_{L^2(\Omega)} = \|u_0\|^2_{L^2(\Omega\times Y)}. \tag{17}$$
Then, we have
$$\|u_\epsilon(x) - u_0\left(x, \frac{x}{\epsilon}\right)\|^2_{L^2(\Omega)} \to 0. \tag{18}$$

Proof of Theorem 3.4. By taking test functions depending only on x in Definition 3.1, the weak convergence in $L^2(\Omega)$ of the sequence u_ϵ is established. Then, developing the inequality

$$\int_\Omega |u_\epsilon(x) - \varphi\left(x, \frac{x}{\epsilon}\right)|^2 dx \geq 0,$$

yields easily formula (16). Furthermore, under assumption (17), it is easily obtained that

$$\lim_{\epsilon \to 0} \int_\Omega |u_\epsilon(x) - \varphi\left(x, \frac{x}{\epsilon}\right)|^2 dx = \int_\Omega \int_Y |u_0(x, y) - \varphi(x, y)|^2 dx dy.$$

If u_0 is smooth enough to be a test function φ, it yields (18). □

Remark 3.5 *The smoothness assumption on u_0 in the second part of Theorem 3.4 is needed only to ensure the measurability of $u_0\left(x, \frac{x}{\epsilon}\right)$ (which otherwise is not guaranteed for a function of $L^2(\Omega \times Y)$). One can further check that any function in $L^2(\Omega \times Y)$ is attained as a two-scale limit (see Lemma 1.13 in [2]), which implies that two-scale limits have no extra regularity.*

So far we have only considered bounded sequences in $L^2(\Omega)$. The next Theorem investigates the case of a bounded sequence in $H^1(\Omega)$.

Theorem 3.6 *Let u_ϵ be a bounded sequence in $H^1(\Omega)$. Then, up to a subsequence, u_ϵ two-scale converges to a limit $u(x) \in H^1(\Omega)$, and ∇u_ϵ two-scale converges to $\nabla_x u(x) + \nabla_y u_1(x, y)$, where the function $u_1(x, y)$ belongs to $L^2(\Omega; H^1_\#(Y)/\mathbb{R})$.*

Proof. Since u_ϵ (resp. ∇u_ϵ) is bounded in $L^2(\Omega)$ (resp. $L^2(\Omega)^N$), up to a subsequence, it two-scale converges to a limit $u_0(x, y) \in L^2(\Omega \times Y)$ (resp. $\xi_0(x, y) \in L^2(\Omega \times Y)^N$). Thus for any $\vec{\psi}(x, y) \in \mathcal{D}\left(\Omega; C^\infty_\#(Y)^N\right)$, we have

$$\lim_{\epsilon \to 0} \int_\Omega \nabla u_\epsilon(x) \cdot \vec{\psi}\left(x, \frac{x}{\epsilon}\right) dx = \int_\Omega \int_Y \xi_0(x, y) \cdot \vec{\psi}(x, y) dx dy. \quad (19)$$

Integrating by parts the left hand side of (19) gives

$$\epsilon \int_\Omega \nabla u_\epsilon(x) \cdot \vec{\psi}\left(x, \frac{x}{\epsilon}\right) dx = -\int_\Omega u_\epsilon(x) \left(\mathrm{div}_y \vec{\psi}\left(x, \frac{x}{\epsilon}\right) + \epsilon \mathrm{div}_x \vec{\psi}\left(x, \frac{x}{\epsilon}\right)\right) dx. \quad (20)$$

Passing to the limit yields

$$0 = -\int_\Omega \int_Y u_0(x,y) \mathrm{div}_y \vec{\psi}(x,y) dx dy. \tag{21}$$

This implies that $u_0(x,y)$ does not depend on y. Thus there exists $u(x) \in L^2(\Omega)$, such that $u_0 = u$. Next, in (19) we choose a function $\vec{\psi}$ such that $\mathrm{div}_y \vec{\psi}(x,y) = 0$. Integrating by parts we obtain

$$\begin{aligned} \lim_{\epsilon \to 0} \int_\Omega u_\epsilon(x) \mathrm{div}_x \vec{\psi}\left(x, \frac{x}{\epsilon}\right) dx &= -\int_\Omega \int_Y \xi_0(x,y) \cdot \vec{\psi}(x,y) dx dy \\ &= \int_\Omega \int_Y u(x) \mathrm{div}_x \vec{\psi}(x,y) dx dy. \end{aligned} \tag{22}$$

If $\vec{\psi}$ does not depend on y, (22) proves that $u(x)$ belongs to $H^1(\Omega)$. Furthermore, we deduce from (22) that

$$\int_\Omega \int_Y (\xi_0(x,y) - \nabla u(x)) \cdot \vec{\psi}(x,y) dx dy = 0 \tag{23}$$

for any function $\vec{\psi}(x,y) \in \mathcal{D}\left(\Omega; C^\infty_\#(Y)^N\right)$ with $\mathrm{div}_y \vec{\psi}(x,y) = 0$. Recall that the orthogonal of divergence-free functions are exactly the gradients (this well-known result can be very easily proved in the present context by means of Fourier analysis in Y). Thus, there exists a unique function $u_1(x,y)$ in $L^2(\Omega; H^1_\#(Y)/\mathbb{R})$ such that

$$\xi_0(x,y) = \nabla u(x) + \nabla_y u_1(x,y). \square \tag{24}$$

There are many generalizations of Theorem 3.6 which gives the precise form of the two-scale limit of a sequence of functions for which some extra estimates on part of their derivatives. To obtain as much as possible informations on the two-scale limit is a key point in the application of the two-scale convergence method as described in the next subsection. For the sake of completeness we give below two examples of such generalizations of Theorem 3.6, the proofs of which may be found in [2].

Theorem 3.7 *1. Let u_ϵ be a bounded sequence in $L^2(\Omega)$ such that $\epsilon \nabla u_\epsilon$ is also bounded in $L^2(\Omega)^N$. Then, there exists a two-scale limit $u_0(x,y) \in L^2(\Omega; H^1_\#(Y)/\mathbb{R})$ such that, up to a subsequence, u_ϵ two-scale converges to $u_0(x,y)$, and $\epsilon \nabla u_\epsilon$ to $\nabla_y u_0(x,y)$.*

2. *Let u_ϵ be a bounded sequence of vector valued functions in $L^2(\Omega)^N$ such that its divergence $\mathrm{div} u_\epsilon$ is also bounded in $L^2(\Omega)$. Then, there exists a two-scale limit $u_0(x, y) \in L^2(\Omega \times Y)^N$ which is divergence-free with respect to y, i.e. $\mathrm{div}_y u_0 = 0$, has a divergence with respect to x, $\mathrm{div}_x u_0$, in $L^2(\Omega \times Y)$, and such that, up to a subsequence, u_ϵ two-scale converges to $u_0(x, y)$, and $\mathrm{div} u_\epsilon$ to $\mathrm{div}_x u_0(x, y)$.*

Remark 3.8 *It is well known that, in general, non-linear functionals are not continuous with respect to the weak topologies of $L^p(\Omega)$ spaces ($1 \le p \le +\infty$). Unfortunately, the same is true with the two-scale convergence which is also a weak-type convergence. As for the usual weak $L^p(\Omega)$ topology, we can merely establish a lower semi-continuity result for* convex *functionals of the same type than inequality (16) on the norm of the two-scale limit. For more details we refer to section 3 in [2] for details.*

4 Application to homogenization

This section shows how the notion of two-scale convergence can be used for the homogenization of partial differential equations with periodically oscillating coefficients. For simplicity we focus on the model problem of diffusion in a periodic medium, as in section 2. Of course, the principles of the two-scale convergence method are valid in many other cases with some changes, including non-linear (monotone or convex) problems.

We recall that Ω is the periodic domain (a bounded open set in $\mathbb{R}^N$), ϵ its period, and $Y = (0, 1)^N$ the rescaled unit cell. The tensor of diffusion in Ω is a $N \times N$ matrix $A\left(x, \frac{x}{\epsilon}\right)$, not necessarily symmetric, where $A(x, y)$ belongs to $C(\bar{\Omega}; L^\infty_\#(Y))^{N^2}$ and satisfies everywhere in $\Omega \times Y$

$$\alpha|\xi|^2 \le \sum_{i,j=1}^{N} A_{i,j}(x, y)\xi_i\xi_j \le \beta|\xi|^2,$$

for any vector $\xi \in \mathbb{R}^N$, α and β being two constants such that $0 < \alpha \le \beta$.

We consider the following model problem of diffusion

$$\begin{cases} -\mathrm{div}\left(A\left(x, \frac{x}{\epsilon}\right)\nabla u_\epsilon\right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega. \end{cases} \tag{25}$$

If the source term $f(x)$ belongs to $L^2(\Omega)$, equation (25) admits a unique solution u_ϵ in $H_0^1(\Omega)$ by application of Lax-Milgram lemma. Moreover, u_ϵ satisfies the following a priori estimate

$$\|u_\epsilon\|_{H_0^1(\Omega)} \leq C\|f\|_{L^2(\Omega)} \tag{26}$$

where C is a positive constant which does not depend on ϵ.

We now describe the so-called “two-scale convergence method” for homogenizing problem (25). In a **first step**, we deduce from the a priori estimate (26) the precise form of the two-scale limit of the sequence u_ϵ. By application of Theorem 3.6, there exist two functions, $u(x) \in H_0^1(\Omega)$ and $u_1(x,y) \in L^2(\Omega; H_\#^1(Y)/\mathbb{R})$, such that, up to a subsequence, u_ϵ two-scale converges to $u(x)$, and ∇u_ϵ two-scale converges to $\nabla_x u(x) + \nabla_y u_1(x,y)$. In view of these limits, u_ϵ is expected to behave as $u(x) + \epsilon u_1\left(x, \frac{x}{\epsilon}\right)$.

Thus, in a **second step**, we multiply equation (25) by a test function similar to the limit of u_ϵ, namely $\varphi(x) + \epsilon\varphi_1\left(x, \frac{x}{\epsilon}\right)$, where $\varphi(x) \in \mathcal{D}(\Omega)$ and $\varphi_1(x,y) \in \mathcal{D}(\Omega; C_\#^\infty(Y))$. This yields

$$\int_\Omega A\left(x, \frac{x}{\epsilon}\right) \nabla u_\epsilon \cdot \left(\nabla\varphi(x) + \nabla_y\varphi_1\left(x, \frac{x}{\epsilon}\right) + \epsilon\nabla_x\varphi_1\left(x, \frac{x}{\epsilon}\right)\right) dx \tag{27}$$

$$= \int_\Omega f(x)\left(\varphi(x) + \epsilon\varphi_1\left(x, \frac{x}{\epsilon}\right)\right) dx.$$

Regarding $A^t\left(x, \frac{x}{\epsilon}\right)\left(\nabla\varphi(x) + \nabla_y\varphi_1\left(x, \frac{x}{\epsilon}\right)\right)$ as a test function for the two-scale convergence (see Definition 3.1), we pass to the two-scale limit in (27) for the sequence ∇u_ϵ. Although this test function is not necessarily very smooth, as required by Definition 3.1, it belongs at least to $C\left(\bar{\Omega}; L_\#^2(Y)\right)$ which can be shown to be enough for the two-scale convergence Theorem 3.2 to hold (see [2] for details). Thus, the two-scale limit of equation (27) is

$$\int_\Omega\int_Y A(x,y)\left(\nabla u(x) + \nabla_y u_1(x,y)\right)\cdot\left(\nabla\varphi(x) + \nabla_y\varphi_1(x,y)\right) dxdy = \int_\Omega f(x)\varphi(x)dx. \tag{28}$$

In a **third step**, we read off a variational formulation for (u, u_1) in (28). Remark that (28) holds true for any (φ, φ_1) in the Hilbert space $H_0^1(\Omega) \times L^2\left(\Omega; H_\#^1(Y)/\mathbb{R}\right)$ by density of smooth functions in this space. Endowing it with the norm $\sqrt{(}\|\nabla u(x)\|^2_{L^2(\Omega)} + \|\nabla_y u_1(x,y)\|^2_{L^2(\Omega\times Y)})$, the assumptions of the Lax-Milgram lemma are easily checked for the variational formulation

(28). The main point is the coercivity of the bilinear form defined by the left hand side of (28): the coercivity of A yields

$$\int_\Omega \int_Y A(x,y)\left(\nabla\varphi(x)+\nabla_y\varphi_1(x,y)\right)\cdot\left(\nabla\varphi(x)+\nabla_y\varphi_1(x,y)\right)dxdy \geq$$

$$\alpha\int_\Omega\int_Y |\nabla\varphi(x)+\nabla_y\varphi_1(x,y)|^2 dxdy = \alpha\int_\Omega |\nabla\varphi(x)|^2 dx + \alpha\int_\Omega\int_Y |\nabla_y\varphi_1(x,y)|^2 dxdy.$$

By application of the Lax-Milgram lemma, we conclude that there exists a unique solution (u, u_1) of the variational formulation (28) in $H_0^1(\Omega) \times L^2\left(\Omega; H^1_\#(Y)/\mathbb{R}\right)$. Consequently, the entire sequences u_ϵ and ∇u_ϵ converge to $u(x)$ and $\nabla u(x)+\nabla_y u_1(x,y)$. An easy integration by parts shows that (28) is a variational formulation associated to the following system of equations, the so-called “two-scale homogenized problem”,

$$\left\{\begin{array}{ll} -\mathrm{div}_y\left(A(x,y)\left(\nabla u(x)+\nabla_y u_1(x,y)\right)\right)=0 & \text{in } \Omega\times Y \\ -\mathrm{div}_x\left(\int_Y A(x,y)\left(\nabla u(x)+\nabla_y u_1(x,y)\right)dy\right)=f(x) & \text{in } \Omega \\ y \to u_1(x,y) & Y\text{-periodic} \\ u=0 & \text{on } \partial\Omega. \end{array}\right. \tag{29}$$

At this point, the homogenization process could be considered as achieved since the entire sequence of solutions u_ϵ converges to the solution of a well-posed limit problem, namely the two-scale homogenized problem (29). However, it is usually preferable, from a physical or numerical point of view, to eliminate the microscopic variable y (one doesn't want to solve the small scale structure). In other words, we want to extract and decouple the usual homogenized and local (or cell) equations from the two-scale homogenized problem.

Thus, in a **fourth (and optional) step**, the y variable and the u_1 unknown are eliminated from (29). It is an easy exercise of algebra to prove that u_1 can be computed in terms of the gradient of u through the relationship

$$u_1(x,y)=\sum_{i=1}^N \frac{\partial u}{\partial x_i}(x)w_i(x,y), \tag{30}$$

where $w_i(x,y)$ are defined, at each point $x\in\Omega$, as the unique solutions in $H^1_\#(Y)/\mathbb{R}$ of the cell problems

$$\left\{\begin{array}{ll} -\mathrm{div}_y\left(A(x,y)\left(\vec{e}_i+\nabla_y w_i(x,y)\right)\right)=0 & \text{in } Y \\ y\to w_i(x,y) & Y\text{-periodic}, \end{array}\right. \tag{31}$$

with $(\vec{e}_i)_{1\leq i\leq N}$ the canonical basis of $\mathbb{R}^N$. Then, plugging formula (30) in (29) yields the usual homogenized problem for u

$$\left\{\begin{array}{ll} -\mathrm{div}_x\left(A^*(x)\nabla u(x)\right) = f(x) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{array}\right. \tag{32}$$

where the homogenized diffusion tensor is given by its entries

$$A^*_{ij}(x) = \int_Y A(x,y)\left(\vec{e}_i + \nabla_y w_i(x,y)\right)\cdot\left(\vec{e}_j + \nabla_y w_j(x,y)\right)dy. \tag{33}$$

Of course, all the above formulae coincide with the usual ones, obtained by using asymptotic exansions, see section 2.

Due to the simple form of our model problem the two equations of (29) can be decoupled in a microscopic and a macroscopic equation, (31) and (32) respectively, but we emphasize that it is not always possible, and sometimes it leads to very complicate forms of the homogenized equation, including integro-differential operators (see for example the double porosity model in chapter 3). Thus, the homogenized equation does not always belong to a class for which an existence and uniqueness theory is easily available, on the contrary of the two-scale homogenized system, which is in most cases of the same type as the original problem, but with a double number of variables (x and y) and unknowns (u and u_1). The supplementary microscopic variable and unknown play the role of "hidden" variables in the vocabulary of mechanics. Although their presence doubles the size of the limit problem, it greatly simplifies its structure (which could be useful for numerical purposes too), while eliminating them introduces "strange" effects (like memory or non-local effects) in the usual homogenized problem.

It is often very useful to obtain so-called "corrector" results which permit to obtain strong (or pointwise) convergences instead of just weak ones by adding some extra information stemming from the local equations. Typically, in the above example we simply proved that the sequence u_ϵ converges weakly to the homogenized solution u in $H^1_0(\Omega)$. Introducing the local solution u_1, this weak convergence can be improved as follows

$$\left(u_\epsilon(x) - u(x) - \epsilon u_1\left(x, \frac{x}{\epsilon}\right)\right) \to 0 \text{ in } H^1_0(\Omega) \text{ strongly.} \tag{34}$$

This type of result is easily obtained with the two-scale convergence method. This rigorously justifies the two first term in the usual asymptotic expansion of the sequence u_ϵ. Remark first that, by standard regularity results for the solutions $w_i(x,y)$ of the cell problem (31), the term $u_1\left(x,\frac{x}{\epsilon}\right)$ does actually belong to $L^2(\Omega)$ and can be seen as a test function for the two-scale convergence. Furthermore, if the matrix A is smooth in x, say in $W^{1,\infty}(\Omega)$, then u and w_i are also smooth in x which implies that $u_1\left(x,\frac{x}{\epsilon}\right)$ belongs to $H^1(\Omega)$. Under this mild assumption we can write

$$\int_\Omega A\left(x,\frac{x}{\epsilon}\right)\left(\nabla u_\epsilon(x)-\nabla u(x)-\nabla_y u_1\left(x,\frac{x}{\epsilon}\right)\right)\cdot\left(\nabla u_\epsilon(x)-\nabla u(x)-\nabla_y u_1\left(x,\frac{x}{\epsilon}\right)\right)dx \tag{35}$$

$$= \int_\Omega f(x)u_\epsilon(x)dx$$

$$+\int_\Omega A\left(x,\frac{x}{\epsilon}\right)\left(\nabla u(x)+\nabla_y u_1\left(x,\frac{x}{\epsilon}\right)\right)\cdot\left(\nabla u(x)+\nabla_y u_1\left(x,\frac{x}{\epsilon}\right)\right)dx$$

$$-\int_\Omega A\left(x,\frac{x}{\epsilon}\right)\nabla u_\epsilon(x)\cdot\left(\nabla u(x)+\nabla_y u_1\left(x,\frac{x}{\epsilon}\right)\right)dx$$

$$-\int_\Omega A\left(x,\frac{x}{\epsilon}\right)\left(\nabla u(x)+\nabla_y u_1\left(x,\frac{x}{\epsilon}\right)\right)\cdot\nabla u_\epsilon(x)dx.$$

Using the coercivity condition for A and passing to the two-scale limit, yields

$$\alpha\lim_{\epsilon\to 0}\|\nabla u_\epsilon(x)-\nabla u(x)-\nabla_y u_1\left(x,\frac{x}{\epsilon}\right)\|^2_{L^2(\Omega)}\le\int_\Omega f(x)u(x)dx$$

$$-\int_\Omega\int_Y A(x,y)\left(\nabla u(x)+\nabla_y u_1(x,y)\right)\cdot\left(\nabla u(x)+\nabla_y u_1(x,y)\right)dxdy.$$

In view of (29), the right hand side of the above equation is equal to zero, which gives the desired result.

5 Bloch waves

The method of Bloch waves or the Bloch transform is a generalization of Fourier transform that leaves invariant periodic functions. It is also known as Floquet theory [10], [19], [45]. There are two steps in the Bloch decomposition: the first one is general (as is the Fourier transform), while the second one is specialized to a given self-adjoint partial differential equation.

The first step of the Bloch transform is the following result.

Theorem 5.1 *For any function $u(y) \in L^2(\mathbb{R}^N)$ there exists a unique function $\hat{u}(y,\theta) \in L^2(Y \times Y)$ such that*

$$u(y) = \int_Y \hat{u}(y,\theta) e^{2i\pi\theta\cdot y} d\theta. \tag{36}$$

The function $y \to \hat{u}(y,\theta)$ is Y-periodic while the function $\theta \to e^{2i\pi\theta\cdot y}\hat{u}(y,\theta)$ is Y-periodic. Furthermore, the linear map $\mathcal{B}$, called the Bloch transform and defined by $\mathcal{B}u = \hat{u}$, is an isometry from $L^2(\mathbb{R}^N)$ into $L^2(Y \times Y)$, i.e. Parseval formula holds for any $u, v \in L^2(\mathbb{R}^N)$

$$\int_{\mathbb{R}^N} u(y)\overline{v(y)}\, dy = \int_Y \int_Y \hat{u}(y,\theta)\overline{\hat{v}(y,\theta)}\, dy\, d\theta. \tag{37}$$

Remark 5.2 *In Theorem 5.1 θ plays the role of a dual variable (like for the Fourier transform). It is often called a Bloch parameter or a reduced frequency since its range is restricted to Y. Indeed, the knowledge of $\hat{u}(y,\theta)$ on the unit cubes $Y \times Y$ is enough to extend it on the whole $\mathbb{R}^N \times \mathbb{R}^N$. The physical interpretation of (36) is that any function in $L^2(\mathbb{R}^N)$ is a superposition (more precisely an integral with respect to θ) of the product of a periodic function, $y \to \hat{u}(y,\theta)$ and of a plane wave with wave number θ.*

Proof. Let $u(y)$ be a smooth compactly supported function in $\mathbb{R}^N$. We define the function $\hat{u}$ by$C_c^\infty(\mathbb{R}^N)$ and bounded on $L^2(\mathbb{R}^N)$

$$\hat{u}(y,\theta) = \sum_{k\in\mathbb{Z}^N} u(y+k)e^{-2i\pi\theta\cdot(y+k)}.$$

This sum is well defined because it has a finite number of terms sine u has compact support. It is also clearly a Y-periodic function of y. On the other hand, for $j \in \mathbb{Z}^N$, we have

$$\hat{u}(y,\theta+j) = e^{-2i\pi j\cdot y} \sum_{k\in\mathbb{Z}^N} u(y+k)e^{-2i\pi\theta\cdot(y+k)} = e^{-2i\pi j\cdot y}\hat{u}(y,\theta).$$

Thus, $\theta \to e^{2i\pi\theta\cdot y}\hat{u}(y,\theta)$ is Y-periodic. Next, we compute

$$\int_{\mathbb{T}^N} \hat{u}(y,\theta)e^{2i\pi\theta\cdot y} d\theta = \sum_{k\in\mathbb{Z}^N} u(y+k) \int_{\mathbb{T}^N} e^{-2i\pi\theta\cdot k} d\theta = u(y)$$

since all integrals vanish except for $k = 0$. Therefore (36) is proved for smoothcompactly supported functions. A similar argument works also for (37) which, in particular, shows that the Bloch transform $\mathcal{B}$ is a linear map, well defined on $C_c^\infty(\mathbb{R}^N)$ and bounded on $L^2(\mathbb{R}^N)$. Since $C_c^\infty(\mathbb{R}^N)$ is dense in $L^2(\mathbb{R}^N)$, $\mathcal{B}$ can be extended by continuity and (36), (37) holds true in $L^2(\mathbb{R}^N)$. □

We now give a Lemma showing in which sense the Bloch transform leaves invariant the periodic functions.

Lemma 5.3 *Let $a(y) \in L^\infty(\mathbb{T}^N)$ be a periodic function. For any $u(y) \in L^2(\mathbb{R}^N)$, we have*

$$\mathcal{B}(au) = a\mathcal{B}(u) \equiv a(y)\hat{u}(y,\theta).$$

We leave the proof to the reader as a simple exercise.

We now turn to the second step of the Bloch transform which relies on the choice of a self-adjoint partial differential equation. For simplicity, we consider the following second-order symmetric p.d.e.

$$-\mathrm{div}_y\Big(A(y)\nabla_y u\Big) + c(y)u = f \quad \text{ in } \mathbb{R}^N, \tag{38}$$

where the right hand side f belongs to $L^2(\mathbb{R}^N)$. We assume that the coefficients $A(y)$ and $c(y)$ are real measurable bounded periodic functions, i.e. their entries belong to $L^\infty(\mathbb{T}^N)$. The tensor A is symmetric and uniformly coercive, i.e. there exists $\nu > 0$ such that for a.e. $y \in \mathbb{T}^N$

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

Furthermore, we assume that c is uniformly positive, i.e. there exists $c_0 > 0$ such that for a.e. $y \in \mathbb{T}^N$

$$c(y) \geq c_0 > 0.$$

The variational formulation of (38) is to find $u \in H^1(\mathbb{R}^N)$ such that, for any $\phi \in H^1(\mathbb{R}^N)$,

$$\int_{\mathbb{R}^N} \Big(A(y)\nabla_y u \cdot \overline{\nabla_y \phi} + c(y)u\overline{\phi}\Big)dy = \int_{\mathbb{R}^N} f\overline{\phi}\, dy. \tag{39}$$

Thanks to our assumptions on the coefficients, a simple application of the Lax-Milgram lemma yields the existence and uniqueness of a solution of (39) and thus of (38).

A first interesting application of Theorem 5.1 is to simplify (39) which is posed on the whole space and to reduce it to a family of problems posed on the simpler compact set $\mathbb{T}^N$. To show this we need the following simple lemma, the proof of which is left to the reader as a simple exercise.

Lemma 5.4 *Let $u(y) \in H^1(\mathbb{R}^N)$. The Bloch transform of its gradient is*

$$\mathcal{B}(\nabla_y u) = (\nabla_y + 2i\pi\theta)\mathcal{B}(u) \equiv \nabla_y \hat{u}(y,\theta) + 2i\pi\theta\hat{u}(y,\theta).$$

Proposition 5.5 *The p.d.e. (38) is equivalent to the family of p.d.e.'s, indexed by $\theta \in \mathbb{T}^N$,*

$$-(\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\mathcal{B}u\Big) + c(y)\mathcal{B}u = \mathcal{B}f \quad \text{in } \mathbb{T}^N, \tag{40}$$

which admits a unique solution $y \to (\mathcal{B}u)(y,\theta) \in H^1(\mathbb{T}^N)$ for any $\theta \in \mathbb{T}^N$.

Proof. We apply Lemmas 5.3 and 5.4 to (39) and we obtain the variational formulation of (40) integrated with respect to θ which is just a parameter (there is no derivatives with respect to θ). This yields (40). □

One can still go further in the simplification of (40), and thus of (38), by using the Hilbertian basis of eigenfunctions of (40). Indeed, the Green operator for (40) is now compact (on the contrary of that for (38)). More precisely, for a given $\theta \in \mathbb{T}^N$, let us consider the Green operator $\mathcal{G}_\theta$ defined by

$$\left\{ \begin{array}{lcl} L^2(\mathbb{T}^N) & \to & L^2(\mathbb{T}^N) \\ g(y) & \to & \mathcal{G}_\theta g(y) = v(y) \end{array} \right. \tag{41}$$

where $v \in H^1(\mathbb{T}^N)$ is the unique solution of

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

Denoting by $\langle , \rangle$ the complex hilbertian product on $L^2(\mathbb{T}^N)$, the reader can easily check that

$$\langle \mathcal{G}_\theta g_1, g_2 \rangle = \int_{\mathbb{T}^N} \Big(A(y)(\nabla_y + 2i\pi\theta)v_1 \cdot \overline{(\nabla_y + 2i\pi\theta)v_2} + c(y)v_1\overline{v_2}\Big) dy = \langle g_1, \mathcal{G}_\theta g_2 \rangle.$$

Clearly, $\mathcal{G}_\theta$ is a self-adjoint compact complex-valued linear operator acting on $L^2(\mathbb{T}^N)$. As such it 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 eigenvalues and eigenfunctions depend on the dual parameter or Bloch frequency θ which runs in the dual cell of $\mathbb{T}^N$, which is again $\mathbb{T}^N$. In other words, the eigenvalues and eigenfunctions satisfy the so-called Bloch (or shifted) spectral cell equation

$$-(\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi_n\Big) + c(y)\psi_n = \lambda_n(\theta)\psi_n \quad \text{in } \mathbb{T}^N. \tag{42}$$

The second step of the Bloch transform is the following result.

Theorem 5.6 *For any function $u(y) \in L^2(\mathbb{R}^N)$ there exists a unique countable family of functions $\hat{u}_n(\theta) \in L^2(\mathbb{T}^N)$, for $n \geq 1$, such that*

$$u(y) = \sum_{n\geq 1} \int_{\mathbb{T}^N} \hat{u}_n(\theta)\psi_n(y,\theta)e^{2i\pi\theta\cdot y}d\theta. \tag{43}$$

Furthermore, the linear map $\mathcal{B}$, called the Bloch transform and defined by $\mathcal{B}u = (\hat{u}_n)_{n\geq 1}$, is an isometry from $L^2(\mathbb{R}^N)$ into $\ell_2\left(L^2(\mathbb{T}^N)\right)$, i.e. Parseval formula holds for any $u, v \in L^2(\mathbb{R}^N)$

$$\int_{\mathbb{R}^N} u(y)\overline{v(y)}\,dy = \sum_{n\geq 1} \int_{\mathbb{T}^N} \hat{u}_n(\theta)\overline{\hat{v}_n(\theta)}\,d\theta. \tag{44}$$

Proof. With the notations of Theorem 5.1 we decompose each $\hat{u}(y,\theta)$ on the corresponding eigenbasis

$$\hat{u}(y,\theta) = \sum_{n\geq 1} \hat{u}_n(\theta)\psi_n(y,\theta) \quad \text{ with } \hat{u}_n(\theta) = \int_{\mathbb{T}^N} \hat{u}(y,\theta)\overline{\psi_n(y,\theta)}dy.$$

Commuting the sum with respect to n and the integral with respect to θ is a standard Fubini type result. There is a subtle point about the measurability, with respect to θ, of the eigenfunctions $\psi_n(y,\theta)$. A special choice of their normalization (they are defined up to multiplication by a unit complex function of θ) allows to state a measurable selection result (for details, see [53]). □

Remark 5.7 *As a matter fact, our assumption on the coefficient $c(y)$ to be uniformly positive is not necessary for Theorem 5.6 to hold true. Indeed, if $c(y)$ just belongs to $L^\infty(\mathbb{T}^N)$, it is bounded from below and adding a large positive constant makes it positive, does not change the eigenfunctions and simply shifts the entire spectrum.*

We come back to our model p.d.e. (38). Applying the Bloch transform of Theorem 5.6 to the right hand side and solution of (38) we obtain an explicit algebraic formula for the solution

$$\hat{u}_n(\theta) = \frac{\hat{f}_n(\theta)}{\lambda_n(\theta)} \quad \forall n \geq 1, \forall \theta \in \mathbb{T}^N,$$

which is a generalization of a similar formula, using Fourier transform, for a constant coefficient p.d.e..

Definition. According to the context of Theorem 5.1 or of Theorem 5.6, a Bloch wave is either a function of the type $\psi(y)e^{2i\pi\theta\cdot y}$ where ψ is any periodic function defined on $\mathbb{T}^N$, or is precisely $\psi_n(y,\theta)e^{2i\pi\theta\cdot y}$ where ψ_n is an eigenfunction of (42).

A crucial point in the study of Bloch waves is to know the regularity of the eigenvalues $\lambda_n(\theta)$ and eigenfunctions $\psi_n(y,\theta)$ with respect to θ. Remark that the coefficients of (40) are polynomial of degree 2 in θ, so that the Green operator $\mathcal{G}_\theta$ is analytic with respect to θ. However it is well known that all eigenvalues and eigenfunctions are not as smooth, and some caution is in order [32]. Nevertheless, if an eigenvalue $\lambda_n(\theta)$ is simple at the value $\theta = \theta^n$, then it remains simple in a small neighborhood of θ^n and it is a classical matter to prove that the n-th eigencouple of (42) is analytic in this neighborhood of θ^n [32].

Remark 5.8 *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 [36]). 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]. A multiple eigenvalue corresponds to the occurence of "crossing" for smooth branches of eigenvalues, viewed as functions of θ.*

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

$$\lambda_n(\theta^n) \text{ is a simple eigenvalue.} \tag{45}$$

Under assumption (45) the n-th eigencouple of (42) is smooth in a neighborhood of θ^n [32]. Introducing the operator $\mathbb{A}_n(\theta)$ defined on $L^2(\mathbb{T}^N)$ by

$$\mathbb{A}_n(\theta)\psi = -(\mathrm{div}_y + 2i\pi\theta)\Big(A(y)(\nabla_y + 2i\pi\theta)\psi\Big) + c(y)\psi - \lambda_n(\theta)\psi, \tag{46}$$

it is easy to differentiate (42). Denoting by $(e_k)_{1\le k\le N}$ the canonical basis of $\mathbb{R}^N$ and by $(\theta_k)_{1\le k\le N}$ the components of θ, the first derivative satisfies

$$\mathbb{A}_n(\theta)\frac{\partial\psi_n}{\partial\theta_k} = 2i\pi e_k A(y)(\nabla_y+2i\pi\theta)\psi_n+(\mathrm{div}_y+2i\pi\theta)\left(A(y)2i\pi e_k\psi_n\right)+\frac{\partial\lambda_n}{\partial\theta_k}(\theta)\psi_n, \tag{47}$$

and the second derivative is

$$\begin{aligned}\mathbb{A}_n(\theta)\frac{\partial^2\psi_n}{\partial\theta_k\partial\theta_l} &= 2i\pi e_k A(y)(\nabla_y+2i\pi\theta)\frac{\partial\psi_n}{\partial\theta_l}+(\mathrm{div}_y+2i\pi\theta)\left(A(y)2i\pi e_k\frac{\partial\psi_n}{\partial\theta_l}\right)\\ &+2i\pi e_l A(y)(\nabla_y+2i\pi\theta)\frac{\partial\psi_n}{\partial\theta_k}+(\mathrm{div}_y+2i\pi\theta)\left(A(y)2i\pi e_l\frac{\partial\psi_n}{\partial\theta_k}\right)\\ &+\frac{\partial\lambda_n}{\partial\theta_k}(\theta)\frac{\partial\psi_n}{\partial\theta_l}+\frac{\partial\lambda_n}{\partial\theta_l}(\theta)\frac{\partial\psi_n}{\partial\theta_k}\\ &-4\pi^2 e_k A(y)e_l\psi_n-4\pi^2 e_l A(y)e_k\psi_n+\frac{\partial^2\lambda_n}{\partial\theta_l\partial\theta_k}(\theta)\psi_n\end{aligned} \tag{48}$$

There exists a unique solution of (47), up to the addition of a multiple of ψ_n. Indeed, since there necessarily exists a partial derivative of ψ_n with respect to θ_k, the right hand side of (47) satisfies the required compatibility condition or Fredholm alternative (i.e. it is orthogonal to ψ_n). On the same token, there exists a unique solution of (48), up to the addition of a multiple of ψ_n. The compatibility condition of (48) yields a formula for the Hessian matrix $\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$.

6 Schrödinger equation in periodic media

We study the homogenization of the following Schrödinger equation

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t}-\mathrm{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right)+\left(\epsilon^{-2}c\left(\dfrac{x}{\epsilon}\right)+d\left(x,\dfrac{x}{\epsilon}\right)\right)u_\epsilon=0 & \text{in } \mathbb{R}^N\times(0,T)\\ u_\epsilon(t=0,x)=u_\epsilon^0(x) & \text{in } \mathbb{R}^N,\end{cases} \tag{49}$$

where $0<T\le+\infty$ is a final time, and the unknown function u_ϵ is complex-valued.

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 $L^\infty\left(\Omega; C(\mathbb{T}^N)\right)$. Remark that $c(y)$ 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 equation (49) is typical of homogenization (see e.g. [3], or chapter 4 in [10]) but is different from the scaling for studying its semi-classical limit where there is a ϵ^{-1} coefficient in front of the time derivative (see e.g. [22], [27], [28], [29], [43]). In particular, this implies that in (49) we consider much larger times than in the semi-classical limit. Then, if the initial data u_ϵ^0 belongs to $H^1(\mathbb{R}^N)$, there exists a unique solution of the Schrödinger equation (49) in $C\left((0,T); H^1(\mathbb{R}^N)\right)$ which satisfies the following a priori estimate.

Lemma 6.1 *There exists a constant $C > 0$ that does not depend on ϵ such that the solution of (49) satisfies*

$$\begin{array}{lcl} \|u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N))} & = & \|u_\epsilon^0\|_{L^2(\mathbb{R}^N)}, \\ \epsilon\|\nabla u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N)^N)} & \leq & C\left(\|u_\epsilon^0\|_{L^2(\mathbb{R}^N)} + \epsilon\|\nabla u_\epsilon^0\|_{L^2(\mathbb{R}^N)^N}\right). \end{array} \tag{50}$$

Proof. We multiply equation (49) by $\overline{u_\epsilon}$ and we take the real part to obtain

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

Next we multiply (49) by $\frac{\partial \overline{u_\epsilon}}{\partial t}$ and we take the real part to get

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

This yields the required a priori estimates. □

The "standard" homogenization of (49) is simple as we now explain. (By standard, we mean that assumption (54) on the initial data is satisfied.) Introduce the first eigencouple of the spectral cell problem (which is just (42) for $n = 1$ and $\theta = 0$)

$$-\mathrm{div}_y\left(A(y)\nabla_y\psi_1\right) + c(y)\psi_1 = \lambda_1\psi_1 \quad \text{in } \mathbb{T}^N, \tag{51}$$

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], [33], [52])

$$v_\epsilon(t,x) = e^{-i\frac{\lambda_1 t}{\epsilon^2}} \frac{u_\epsilon(t,x)}{\psi_1\left(\frac{x}{\epsilon}\right)}, \tag{52}$$

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

$$\begin{cases} i|\psi_1|^2\left(\frac{x}{\epsilon}\right)\frac{\partial v_\epsilon}{\partial t} - \operatorname{div}\left((|\psi_1|^2 A)\left(\frac{x}{\epsilon}\right)\nabla v_\epsilon\right) + (|\psi_1|^2 d)\left(x,\frac{x}{\epsilon}\right) v_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v_\epsilon(t=0,x) = \frac{u_\epsilon^0(x)}{\psi_1\left(\frac{x}{\epsilon}\right)} & \text{in } \mathbb{R}^N. \end{cases} \tag{53}$$

The new Schrödinger equation (53) is simple to homogenize (see e.g. [10]) since it does not contain any singularly perturbed term, and we thus obtain uniform a priori estimates for its solution.

Theorem 6.2 *Let $v^0 \in H^1(\mathbb{R}^N)$. Assume that the initial data satisfies*

$$u_\epsilon^0(x) = \psi_1\left(\frac{x}{\epsilon}\right) v^0(x). \tag{54}$$

The new unknown v_ϵ, defined by (52), converges weakly in $L^2\left((0,T); H^1(\mathbb{R}^N)\right)$ to the solution v of the following homogenized problem

$$\begin{cases} i\frac{\partial v}{\partial t} - \operatorname{div}\left(A^*\nabla v\right) + d^*(x)\, v = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{55}$$

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 6.2 gives the following asymptotic behavior for the solution of (49)

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

where v is the solution of (55). Assumption (54) 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 6.2 is not meaningful. It turns out that, according to heuristical results in solid state physics (see e.g. [39], [42], [44]), there are many other types of well-prepared initial data for which a result like Theorem 6.2 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 replace (51) by the more general Bloch or shifted cell problem (42). Theorem 6.2 (with its special initial data satisfying (54)) 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

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0(x). \tag{56}$$

Assuming that $\lambda_n(\theta^n)$ is simple and that $\nabla\lambda_n(\theta^n) = 0$, we shall prove in Theorem 7.2 that the solution of (49) 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

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \operatorname{div}\left(A_n^* \nabla v\right) + d_n^*(x)\, v = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{57}$$

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.

To obtain the homogenized limit (57) we can not follow the above simple idea, namely the factorization principle (52). 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 (52). In order to homogenize (49) for initial data of the type of (56), we use a method based on Bloch wave theory to build adequate oscillating test functions and to pass to the limit using two-scale convergence.

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 section 4 of chapter 4 in [10] for a slightly different version of this problem: indeed, [10] 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 [43] with a different method of semi-classical measures. Let us emphasize again that the scaling of (49) is not that of the semi-classical analysis (see e.g. [22], [27], [28], [29], [43]).

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

7 Homogenization without drift

In this section we use the following strong assumption about the stationarity of $\lambda_n(\theta)$ at θ^n

$$\begin{cases} (i) & \lambda_n(\theta^n) \text{ is a simple eigenvalue,} \\ (ii) & \theta^n \text{ is a critical point of } \lambda_n(\theta) \text{ i.e., } \nabla_\theta \lambda_n(\theta^n) = 0. \end{cases} \tag{58}$$

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. 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 Section 9 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 7.1 *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 (58) is always satisfied with $\theta^1 = 0$ which is a minimum point of λ_1 (see e.g. [10], [20]). 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. [36], [45]) 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 (58), which possibly holds for a non-zero value of θ^n.*

Under assumption (58), i.e. $\nabla_\theta \lambda_n(\theta^n) = 0$, equations (47) and (48) simplify for $\theta = \theta^n$ and we find

$$\frac{\partial \psi_n}{\partial \theta_k} = 2i\pi\zeta_k, \quad \frac{\partial^2 \psi_n}{\partial \theta_k \partial \theta_l} = -4\pi^2 \chi_{kl}, \tag{59}$$

where ζ_k is the solution in $\mathbb{T}^N$ of

$$\mathbb{A}_n(\theta^n)\zeta_k = e_k A(y)(\nabla_y + 2i\pi\theta^n)\psi_n + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_k\psi_n\right), \tag{60}$$

and χ_{kl} is the solution in $\mathbb{T}^N$ of

$$\begin{aligned} \mathbb{A}_n(\theta^n)\chi_{kl} = \; & e_k A(y)(\nabla_y + 2i\pi\theta^n)\zeta_l + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_k\zeta_l\right) \\ & + e_l A(y)(\nabla_y + 2i\pi\theta^n)\zeta_k + (\mathrm{div}_y + 2i\pi\theta^n)\left(A(y)e_l\zeta_k\right) \\ & + e_k A(y) e_l \psi_n + e_l A(y) e_k \psi_n - \frac{1}{4\pi^2}\frac{\partial^2 \lambda_n}{\partial \theta_l \partial \theta_k}(\theta^n)\psi_n. \end{aligned} \tag{61}$$

We obtain the following homogenized problem.

Theorem 7.2 *Assume (58) and that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ is of the form*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi\frac{\theta^n \cdot x}{\epsilon}} v^0(x), \tag{62}$$

with $v^0 \in H^1(\mathbb{R}^N)$. The solution of (49) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n \cdot x}{\epsilon}} v_\epsilon(t,x), \tag{63}$$

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

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}^N} \left| v_\epsilon(t,x) - \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v(t,x)\right|^2 dx = 0, \tag{64}$$

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

$$\begin{cases} i\dfrac{\partial v}{\partial t} - \mathrm{div}\left(A_n^* \nabla v\right) + d_n^*(x)\, v = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{65}$$

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 7.2 is called an effective mass theorem [39], [42], [44]. 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 [39], [44]).

Remark 7.3 *Theorem 7.2 does not fit into the framework of G- or H-convergence (see e.g. [38], [48]). 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 7.4 *Assumption (62) can be slightly weakened for proving Theorem 7.2. 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 (62) 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 7.2 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 7.5 *In the case $n = 1$ and $\theta^n = 0$ (bottom of the first Bloch band), it is easy to check (by the factorization method described in Section 6) that Theorem 7.2 still holds true if we add a non-linear term of the type $g(x, \frac{x}{\epsilon}, u_\epsilon)$ where $g(x,y,\xi)$ is for example*

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

Generalizations of this nonlinear result for higher order Bloch bands $n > 1$ have been obtained by [49].

Proof of Theorem 7.2. This proof is based on ideas of [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 6.1 we have

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

and applying the compactness of two-scale convergence (see Theorem 3.2), 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 (49) 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

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

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

$$v^*(t,x,y) = v(t,x)\psi_n(y,\theta^n). \tag{66}$$

Second step. We multiply (49) by the complex conjugate of

$$\Psi_\epsilon = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}}e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}}\left(\psi_n(\frac{x}{\epsilon},\theta^n)\phi(t,x) + \epsilon\sum_{k=1}^N\frac{\partial\phi}{\partial x_k}(t,x)\zeta_k(\frac{x}{\epsilon})\right) \tag{67}$$

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 (60). After some algebra we found that

$$\begin{aligned}
\int_{\mathbb{R}^N} A^\epsilon \nabla u_\epsilon \cdot \nabla \overline{\Psi}_\epsilon dx = & \int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})(\overline{\phi} v_\epsilon) \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon})\overline{\psi}_n^\epsilon \\
& + \epsilon \int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})(\frac{\partial \overline{\phi}}{\partial x_k} v_\epsilon) \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon})\overline{\zeta}_k^\epsilon \\
& - \int_{\mathbb{R}^N} A^\epsilon e_k \frac{\partial \overline{\phi}}{\partial x_k} v_\epsilon \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon})\overline{\psi}_n^\epsilon \\
& + \int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})(\frac{\partial \overline{\phi}}{\partial x_k} v_\epsilon) \cdot e_k \overline{\psi}_n^\epsilon \\
& - \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot e_k \overline{\psi}_n^\epsilon \\
& - \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot (\epsilon \nabla - 2i\pi \theta^n)\overline{\zeta}_k^\epsilon \\
& + \int_{\mathbb{R}^N} A^\epsilon \overline{\zeta}_k^\epsilon (\epsilon \nabla + 2i\pi \theta^n) v_\epsilon \cdot \nabla \frac{\partial \overline{\phi}}{\partial x_k}
\end{aligned} \tag{68}$$

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

$$\int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})\psi_n^\epsilon \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon})\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N} (c^\epsilon - \lambda_n(\theta^n))\psi_n^\epsilon \overline{\Phi} = 0, \tag{69}$$

and from the definition of ζ_k

$$\begin{aligned}
\int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})\zeta_k^\epsilon \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon})\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N} (c^\epsilon - \lambda_n(\theta^n))\zeta_k^\epsilon \overline{\Phi} = \\
\epsilon^{-1}\int_{\mathbb{R}^N} A^\epsilon (\nabla + 2i\pi \frac{\theta^n}{\epsilon})\psi_n^\epsilon \cdot e_k \overline{\Phi} - \epsilon^{-1}\int_{\mathbb{R}^N} A^\epsilon e_k \psi_n^\epsilon \cdot (\nabla - 2i\pi \frac{\theta^n}{\epsilon})\overline{\Phi}.
\end{aligned} \tag{70}$$

Combining (68) with the other terms of the variational formulation of (49), we easily check that the first line of its right hand side cancels out because of (69) with $\Phi = \overline{\phi} v_\epsilon$, and the next three lines cancel out because of (70) 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 (68). Finally, (49) multiplied by $\overline{\Psi}_\epsilon$ yields after simplification

$$
\begin{aligned}
& i\int_{\mathbb{R}^N} u_\epsilon^0 \overline{\Psi}_\epsilon(t=0)dx - i\int_0^T \int_{\mathbb{R}^N} v_\epsilon \left(\overline{\psi}_n^\epsilon \frac{\partial \overline{\phi}}{\partial t} + \epsilon \frac{\partial^2 \overline{\phi}}{\partial x_k \partial t} \overline{\zeta}_k^\epsilon \right) dt\, dx \\
& - \int_0^T \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot e_k \overline{\psi}_n^\epsilon dt\, dx \\
& - \int_0^T \int_{\mathbb{R}^N} A^\epsilon v_\epsilon \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot (\epsilon \nabla - 2i\pi\theta^n) \overline{\zeta}_k^\epsilon dt\, dx \\
& + \int_0^T \int_{\mathbb{R}^N} A^\epsilon \overline{\zeta}_k^\epsilon (\epsilon \nabla + 2i\pi\theta^n) v_\epsilon \cdot \nabla \frac{\partial \overline{\phi}}{\partial x_k} dt\, dx \\
& + \int_0^T \int_{\mathbb{R}^N} d^\epsilon v_\epsilon \overline{\Psi}_\epsilon \, dt\, dx \qquad = 0.
\end{aligned}
\tag{71}
$$

Passing to the two-scale limit in each term of (71) gives

$$
\begin{aligned}
& i\int_{\mathbb{R}^N}\int_{\mathbb{T}^N} \psi_n v^0 \overline{\psi}_n \overline{\phi}(t=0)\, dx\, dy - i\int_0^T \int_{\mathbb{R}^N}\int_{\mathbb{T}^N} \psi_n v \overline{\psi}_n \frac{\partial \overline{\phi}}{\partial t} dt\, dx\, dy \\
& - \int_0^T \int_{\mathbb{R}^N}\int_{\mathbb{T}^N} A\psi_n v \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot e_k \overline{\psi}_n dt\, dx\, dy \\
& - \int_0^T \int_{\mathbb{R}^N}\int_{\mathbb{T}^N} A\psi_n v \nabla \frac{\partial \overline{\phi}}{\partial x_k} \cdot (\nabla_y - 2i\pi\theta^n) \overline{\zeta}_k dt\, dx\, dy \\
& + \int_0^T \int_{\mathbb{R}^N}\int_{\mathbb{T}^N} A\overline{\zeta}_k (\nabla_y + 2i\pi\theta^n) \psi_n v \cdot \nabla \frac{\partial \overline{\phi}}{\partial x_k} dt\, dx\, dy \\
& + \int_0^T \int_{\mathbb{R}^N}\int_{\mathbb{T}^N} d(x,y) \psi_n v \overline{\psi}_n \overline{\phi}\, dt\, dx\, dy \qquad = 0.
\end{aligned}
\tag{72}
$$

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

$$
\begin{aligned}
2\,(A_n^*)_{jk} = \int_{\mathbb{T}^N} & \Big(A\psi_n e_j \cdot e_k \overline{\psi}_n + A\psi_n e_k \cdot e_j \overline{\psi}_n \\
& + A\psi_n e_j \cdot (\nabla_y - 2i\pi\theta^n) \overline{\zeta}_k + A\psi_n e_k \cdot (\nabla_y - 2i\pi\theta^n) \overline{\zeta}_j \\
& - A\overline{\zeta}_k (\nabla_y + 2i\pi\theta^n) \psi_n \cdot e_j - A\overline{\zeta}_j (\nabla_y + 2i\pi\theta^n) \psi_n \cdot e_k \Big) dy,
\end{aligned}
\tag{73}
$$

and $d_n^*(x) = \int_{\mathbb{T}^N} d(x,y)|\psi_n(y)|^2\, dy$, (72) is equivalent to

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

which is a very weak form of the homogenized equation (65). The compatibility condition of equation (61) for the second derivative of ψ_n yields that the matrix A_n^*, defined by (73), 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 (65) is well posed. Indeed, by using semi-group theory (see e.g. [12] or chapter X in [45]), 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 (65), 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 6.1 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 (65) we have

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

and thus we deduce the strong convergence (64) from Theorem 3.4. □

Remark 7.6 *As usual in periodic homogenization, the choice of the test function Ψ_ϵ, in the proof of Theorem 7.2, is dictated by the formal two-scale asymptotic expansion that can be obtained for the solution u_ϵ of (49), 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 (65). 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 7.7 *Our method applies also to systems of equations (see [3]). We never use the fact that (49) is a single scalar equation.*

Remark 7.8 *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, if we consider

$$\begin{cases} i\epsilon^2 \dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2} c\left(\dfrac{x}{\epsilon}\right) + \epsilon^2 d\left(x, \dfrac{x}{\epsilon}\right)\right) u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{74}$$

and if we make the following assumption, instead of (58),

$$\begin{cases} (i) & \lambda_n(\theta^n) \text{ is a simple eigenvalue,} \\ (ii) & \nabla_\theta \lambda_n(\theta^n) = 0, \nabla_\theta\nabla_\theta \lambda_n(\theta^n) = 0, \nabla_\theta\nabla_\theta\nabla_\theta \lambda_n(\theta^n) = 0, \end{cases} \tag{75}$$

then, for the same type of initial data (62), we can prove that the solution of (74) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^4}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v_\epsilon(t,x), \tag{76}$$

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

$$\begin{cases} i\dfrac{\partial v}{\partial t} + \operatorname{div}\operatorname{div}\left(A_n^* \nabla\nabla v\right) + d_n^*(x)\, v = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{77}$$

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

Remark that the time scaling in (74) is not the same than that in (49): this means that we are looking for an asymptotic for longer time of order ϵ^{-2} in (74), compared to (49).

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).

8 Generalization with drift

The Schrödinger equation (49) can still be homogenized when θ^n is not a critical point of $\lambda_n(\theta)$. In other words we generalize Theorem 7.2 by weakening assumption (58) that we now replace by

$$\lambda_n(\theta^n) \text{ is a simple eigenvalue.} \tag{78}$$

This yields a large drift in the homogenized problem associated to the group velocity

$$\mathcal{V} = \frac{1}{2\pi}\nabla_\theta \lambda_n(\theta^n). \tag{79}$$

To begin with, we shall show that assumption (78) 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 replace the original Schrödinger equation (49) by

$$\begin{cases} \frac{i}{\epsilon}\frac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\frac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2}c\left(\frac{x}{\epsilon}\right) + d\left(x,\frac{x}{\epsilon}\right)\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T), \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{80}$$

with the new ϵ^{-1} scaling in front of the time derivative (this is precisely the scaling of semi-classical analysis).

Proposition 8.1 *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 (80) 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 $v \in C\left((0,T);L^2(\mathbb{R}^N)\right)$ is the unique solution of the following transport equation

$$\begin{cases} \frac{\partial v}{\partial t} - \mathcal{V}\cdot\nabla v = 0 & \text{in } \mathbb{R}^N \times (0,T), \\ v(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{81}$$

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. As in the first step of the proof of Theorem 7.2, by virtue of the a priori estimates of Lemma 6.1, a suitable subsequence of

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

two-scale converges to a limit $\psi_n(y,\theta^n)\,v(t,x)$. Then, in a second step we multiply (80) by the complex conjugate of

$$\Psi_\epsilon = \epsilon\, e^{i\frac{\lambda_n(\theta^n)t}{\epsilon}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \left(\psi_n(\frac{x}{\epsilon},\theta^n)\phi(t,x) + \epsilon \sum_{k=1}^N \frac{\partial \phi}{\partial x_k}(t,x)\zeta'_k(\frac{x}{\epsilon}) \right) \tag{82}$$

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 (60), since it is a solution of

$$\begin{aligned} \mathbb{A}_n(\theta^n)\zeta'_k = \;& e_k A(y)(\nabla_y + 2i\pi\theta^n)\psi_n + (\operatorname{div}_y + 2i\pi\theta^n)\left(A(y)e_k\psi_n\right) \\ & -\frac{i}{2\pi}\frac{\partial\lambda_n}{\partial\theta_k}(\theta^n)\psi_n \quad \text{ in } \mathbb{T}^N, \end{aligned} \tag{83}$$

and $\nabla_\theta\lambda_n(\theta^n)\neq 0$. After integration by parts and some algebra similar to that in the proof of Theorem 7.2 we obtain

$$\begin{aligned} & i\int_{\mathbb{R}^N} v^0|\psi_n^\epsilon|^2\overline{\phi}(t=0)\,dx - i\int_0^T\int_{\mathbb{R}^N} v_\epsilon\overline{\psi}_n^\epsilon\frac{\partial\overline{\phi}}{\partial t}\,dt\,dx \\ & -\frac{1}{2i\pi}\frac{\partial\lambda_n}{\partial\theta_k}\int_0^T\int_{\mathbb{R}^N} v_\epsilon\overline{\psi}_n^\epsilon\frac{\partial\overline{\phi}}{\partial x_k}\,dt\,dx \qquad = o(1), \end{aligned} \tag{84}$$

where $o(1)$ denotes all other terms going to zero with ϵ. Passing to the two-scale limit in (84) gives a variational formulation of (81). By uniqueness of the solution of (81) the entire sequence converges to this solution. The strong two-scale convergence is obtained as in the proof of Theorem 7.2 by using the energy conservation of the original and homogenized equations. □

We now come back to the original time scale of the Schrödinger equation (49)

$$\left\{ \begin{array}{ll} i\dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(\dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \left(\epsilon^{-2}c\left(\dfrac{x}{\epsilon}\right) + d\left(x,\dfrac{x}{\epsilon}\right)\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N\times(0,T), \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{array} \right. \tag{85}$$

where the macroscopic zero-order term is assumed to satisfy

$$\lim_{|x|\to+\infty} d(x,y) = d^\infty(y) \quad \text{uniformly in } \mathbb{T}^N. \tag{86}$$

Actually, assumption (86) 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], [40]), which has been introduced in [37], it is possible to homogenize (85).

Theorem 8.2 *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*

$$\lim_{\epsilon\to 0}\int_0^T\int_{\mathbb{R}^N} u_\epsilon(t,x)\phi\left(t, x+\frac{\mathcal{V}}{\epsilon}t, \frac{x}{\epsilon}\right) dt\,dx = \int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N} u_0(t,x,y)\phi(t,x,y)\,dt\,dx\,dy \tag{87}$$

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 (87) is $(0,1)^N$-periodic with respect to the y variable. Remark that Theorem 8.2 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 8.2 is similar to the proof of compactness of the usual two-scale convergence, except that it relies on the following simple lemma.

Lemma 8.3 *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 8.4 *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 converges with drift strongly *and it satisfies*

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

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 8.2 and Lemma 8.3 can be found in [37]. That of Proposition 8.4 is a simple adaptation of Theorem 1.8 in [2].

Under assumption (78) we obtain the following generalization of Theorem 7.2.

Theorem 8.5 *Assume that the initial data $u_\epsilon^0\in H^1(\mathbb{R}^N)$ is of the form*

$$u_\epsilon^0(x)=\psi_n\left(\frac{x}{\epsilon},\theta^n\right)e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}}v^0(x),\tag{88}$$

with $v^0\in H^1(\mathbb{R}^N)$. The solution of (85) can be written as

$$u_\epsilon(t,x)=e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}}e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}}v_\epsilon(t,x),\tag{89}$$

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.*

$$\lim_{\epsilon\to 0}\int_0^T\int_{\mathbb{R}^N}\left|v_\epsilon(t,x)-\psi_n\left(\frac{x}{\epsilon},\theta^n\right)v\left(t,x+\frac{\mathcal{V}}{\epsilon}t\right)\right|^2dx\,dt=0,\tag{90}$$

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

$$\begin{cases} i\dfrac{\partial v}{\partial t}-\operatorname{div}\left(A_n^*\nabla v\right)+d_n^*\,v=0 & \text{in } \mathbb{R}^N\times(0,T),\\ v(t=0,x)=v^0(x) & \text{in } \mathbb{R}^N,\end{cases}\tag{91}$$

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 8.6 *For the longer time scale of equation (85), the transport equation (81) can still be seen in the large drift $\mathcal{V}/\epsilon$ of formula (90).*

Proof of Theorem 8.5. The proof is similar to that of Theorem 7.2 and Proposition 8.1. 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 (85) 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 (85) 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 (82) 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 identical to that in the proof of Theorem 7.2 except that two new terms arise and cancel out exactly, namely the term

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

which comes from the new equation (70) satisfied by ζ_k', and the same term with positive sign which arises in the integration by parts of

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

The rest of the proof is as in Theorem 7.2, 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. □

9 Homogenized system of equations

In this section we investigate the case of a Bloch eigenvalue which is not simple. Physically speaking it can be interpreted as a crossing of modes. The semi-classical limit of this problem yields the so-called Landau-Zerner formula, recently analyzed in [23], [24]. Our study is different in two respects. First our scaling is not that of semi-classical analysis. Second the crossing is tangential, i.e. the drift or velocity vectors $\nabla_\theta \lambda_n(\theta)$ are assumed to be the same for each mode. To simplify the exposition we consider an eigenvalue of multiplicity two, but the argument works through for any multiplicity. We replace assumption (58) by the following one: for $n \geq 1$, we consider a Bloch parameter $\theta^n \in \mathbb{T}^N$ such that

$$\begin{cases} (i) & \lambda_n(\theta^n) = \lambda_{n+1}(\theta^n) \neq \lambda_k(\theta^n) \quad \forall k \neq n, n+1, \\ (ii) & \text{locally near } \theta^n,\ \lambda_n(\theta) \text{ and } \lambda_{n+1}(\theta) \text{ form two} \\ & \text{smooth branches of eigenvalues with corresponding} \\ & \text{smooth eigenfunctions } \psi_n(\theta) \text{ and } \psi_{n+1}(\theta), \\ (iii) & \nabla_\theta \lambda_n(\theta^n) = \nabla_\theta \lambda_{n+1}(\theta^n) = 0. \end{cases} \tag{92}$$

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 (92) is automatically satisfied [36]. 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 [32]). Therefore, (92) is a very strong mathematical assumption which is physically not very relevant in dimension $N > 1$.

Theorem 9.1 *Assume (92) and that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ are of the form*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v_1^0(x) + \psi_{n+1}\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v_2^0(x), \tag{93}$$

with $v_1^0, v_2^0 \in H^1(\mathbb{R}^N)$. The solution of (49) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v_\epsilon(t,x), \tag{94}$$

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 $\mathbb{R}^+$,

$$\lim_{\epsilon\to 0}\int_{\mathbb{R}^N}\left|v_\epsilon(t,x)-\psi_n\left(\frac{x}{\epsilon},\theta^n\right)v_1(t,x)-\psi_{n+1}\left(\frac{x}{\epsilon},\theta^n\right)v_2(t,x)\right|^2dx=0, \quad (95)$$

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

$$\begin{cases} i\dfrac{\partial v_1}{\partial t}-\mathrm{div}\left(A_n^*\nabla v_1\right)+d_{11}^*(x)\,v_1+d_{12}^*(x)\,v_2=0 & \text{in } \mathbb{R}^N\times(0,T)\\ i\dfrac{\partial v_2}{\partial t}-\mathrm{div}\left(A_{n+1}^*\nabla v_2\right)+d_{21}^*(x)\,v_1+d_{22}^*(x)\,v_2=0 & \text{in } \mathbb{R}^N\times(0,T)\\ (v_1,v_2)(t=0,x)=(v_1^0,v_2^0)(x) & \text{in } \mathbb{R}^N, \end{cases} \quad (96)$$

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 9.2 *The main point in Theorem 9.1 is that the homogenized system is of dimension equal to the multiplicity of the eigenvalue $\lambda_n(\theta^n)$. However, the homogenized system (96) is coupled only by zero-order terms since the diffusion operator is diagonal.*

Proof of Theorem 9.1. 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 Theorem 3.2, 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 (49) 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 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

$$v^*(t,x,y) = v_1(t,x)\psi_n(y,\theta^n) + v_2(t,x)\psi_{n+1}(y,\theta^n). \tag{97}$$

Second step. We multiply (49) by the complex conjugate of

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

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 (60) 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 7.2. We also use the orthogonality property

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

to obtain

$$\begin{aligned}& i\int_{\mathbb{R}^N}\left(v_1^0\overline{\phi}_1(0) + v_2^0\overline{\phi}_2(0)\right)dx - i\int_0^T\int_{\mathbb{R}^N}\left(v_1\frac{\partial\overline{\phi}_1}{\partial t} + v_2\frac{\partial\overline{\phi}_2}{\partial t}\right)dt\,dx \\ & -\int_0^T\int_{\mathbb{R}^N}\sum_{p,q=1}^{2} A^*_{pq}v_p\cdot\nabla\nabla\overline{\phi}_q\,dt\,dx \\ & +\int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N} d(\psi_n v_1 + \psi_{n+1}v_2)(\overline{\psi}_n\overline{\phi}_1 + \overline{\psi}_{n+1}\overline{\phi}_2)\,dt\,dx\,dy \qquad = 0,\end{aligned} \tag{98}$$

where $A^*_{11} = A^*_n$ and $A^*_{22} = A^*_{n+1}$, defined by (73), and A^*_{12} is defined by

$$\begin{aligned}2\left(A^*_{12}\right)_{jk} = \int_{\mathbb{T}^N} \quad & \Big(A\psi_n e_j\cdot e_k\overline{\psi}_{n+1} + A\psi_n e_k\cdot e_j\overline{\psi}_{n+1} \\ & +A\psi_n e_j\cdot(\nabla_y - 2i\pi\theta^n)\overline{\zeta}_k^2 + A\psi_n e_k\cdot(\nabla_y - 2i\pi\theta^n)\overline{\zeta}_j^2 \\ & -A\overline{\zeta}_k^2(\nabla_y + 2i\pi\theta^n)\psi_n\cdot e_j - A\overline{\zeta}_j^2(\nabla_y + 2i\pi\theta^n)\psi_n\cdot e_k\Big)dy,\end{aligned} \tag{99}$$

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 equation (61) for the second derivative of ψ_n. This compatibility condition is obtained by multiplying (61) 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 (61) 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 (99) is equivalent to

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

by orthogonality of ψ_n and ψ_{n+1}. Thus $A^*_{12} = A^*_{21} = 0$ and (98) is a weak formulation of the limit system (96) which is thus coupled only through the zero-order terms. It is easily seen that (96) is well-posed in $C\left((0,T); L^2(\mathbb{R}^N)^2\right)$. The rest of the proof is as for Theorem 7.2. □

Remark 9.3 *Of course, Theorem 9.1 can easily be generalized in the case of a common drift $\mathcal{V} = \nabla_\theta\lambda_n(\theta^n)/2\pi = \nabla_\theta\lambda_{n+1}(\theta^n)/2\pi \neq 0$. If assumption (iii) in (92) is not satisfied, i.e. if there are two different values of the drift velocity, $\nabla_\theta\lambda_n(\theta^n) \neq \nabla_\theta\lambda_{n+1}(\theta^n)$, 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.*

10 Localization

We now come back to the scaling of semi-classical analysis and consider the following Schrödinger equation

$$\begin{cases} \dfrac{i}{\epsilon}\dfrac{\partial u_\epsilon}{\partial t} - \operatorname{div}\left(A\left(x, \dfrac{x}{\epsilon}\right)\nabla u_\epsilon\right) + \dfrac{1}{\epsilon^2}c\left(x, \dfrac{x}{\epsilon}\right)u_\epsilon = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ u_\epsilon(0,x) = u^0_\epsilon(x) & \text{in } \mathbb{R}^N. \end{cases} \qquad (100)$$

The main difference with the previous sections is that the periodic coefficients are now macroscopically modulated. The results are going to be completely different as we shall see, featuring in particular a localization phenomenon.

At least in the case when $A \equiv Id$ and $c(x,y) = c_0(x) + c_1(y)$, there is a well-known theory for the asymptotic limit of (100) when ϵ goes to zero. By using WKB asymptotic expansion or the notion of semi-classical measures (or Wigner transforms) the homogenized problem is in some sense the Liouville transport equation for a classical particle which is the limit of the wave function u_ϵ. First of all, the Bloch spectral cell problem (42) now depends on x as a parameter. In other words, (42) is replaced by

$$-(\mathrm{div}_y + 2i\pi\theta)(A(x,y)(\nabla_y + 2i\pi\theta)\psi_n) + c(x,y) = \lambda_n(x,\theta)\psi_n \qquad \text{in } \mathbb{T}^N . \tag{101}$$

For an initial data living in the n-th Bloch band and under some technical assumptions on the Bloch spectral cell problem (101), the semi-classical limit of (100) is given by the dynamic of the following Hamiltonian system in the phase space $(x,\theta) \in \mathbb{R}^N \times \mathbb{T}^N$

$$\begin{cases} \dot{x} = \nabla_\theta \lambda_n(x,\theta) \\ \dot{\theta} = -\nabla_x \lambda_n(x,\theta) \end{cases} \tag{102}$$

where the Hamiltonian $\lambda_n(x,\theta)$ is precisely the n-th Bloch eigenvalue of (101) (see [14], [22], [27], [28], [29], [30], [41], [43] for more details).

Our approach to (100) is different since we consider special initial data that are monochromatic, have zero group velocity and zero applied force. Namely the initial data is concentrating at a point (x^n, θ^n) of the phase space where $\nabla_\theta \lambda_n(x^n,\theta^n) = \nabla_x \lambda_n(x^n,\theta^n) = 0$. In such a case, the previous Hamiltonian system (102) degenerates (its solution is constant) and is unable to describe the precise dynamic of the wave function u_ϵ. We exhibit another limit problem which is again a Schrödinger equation with quadratic potential. In other words we build a sequence of approximate solutions of (100) which are the product of a Bloch wave and of the solution of an homogenized Schrödinger equation. Furthermore, if the full Hessian tensor of the Bloch eigenvalue $\lambda_n(x,\theta)$ is positive definite at (x^n,θ^n), we prove that all the eigenfunctions of an homogenized Schrödinger equation are exponentially decreasing at infinity. In other words, we exhibit a localization phenomenon for (100) since we build a sequence of approximate solutions that decay exponentially fast away from x^n. The root of this localization phenomenon is the macroscopic modulation (i.e. with respect to x) of the periodic coefficients which is similar in spirit to the randomness that causes Anderson's localization (see [15] and references therein).

Our main assumptions are that there exist $x^n \in \mathbb{R}^N$ and $\theta^n \in \mathbb{T}^N$ such that

$$\begin{array}{rl} (i) & x \to A(x,y), c(x,y) \text{ are } C^2 \text{ in a neighborhood of } x^n, \\ (ii) & \lambda_n(x^n,\theta^n) \text{ is a simple eigenvalue}, \\ (iii) & (x^n,\theta^n) \text{ is a critical point of } \lambda_n(x,\theta), i.e. \\ & \nabla_x \lambda_n(x^n,\theta^n) = \nabla_\theta \lambda_n(x^n,\theta^n) = 0. \end{array} \tag{103}$$

Notations. We introduce a new intermediate scale variable z, defined by

$$z := \sqrt{\epsilon}(y - y^n) \equiv \frac{x - x^n}{\sqrt{\epsilon}}.$$

Theorem 10.1 *Under assumption (103) and for an initial data*

$$u_\epsilon^0(x) = \psi_n\Big(x^n, \frac{x}{\epsilon}, \theta^n\Big) e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v^0\Big(\frac{x - x^n}{\sqrt{\epsilon}}\Big), \tag{104}$$

the solution of (100) can be written as

$$u_\epsilon(t,x) = e^{i\frac{\lambda_n t}{\epsilon}} e^{2i\pi \frac{\theta^n \cdot x}{\epsilon}} v_\epsilon\Big(t, \frac{x - x^n}{\sqrt{\epsilon}}\Big), \tag{105}$$

where $v_\epsilon(t,z)$ two-scale converges strongly to $\psi_n(y)v(t,z)$, i.e.

$$\lim_{\epsilon \to 0} \int_{\mathbb{R}^N} \left| v_\epsilon(t,z) - \psi_n\left(\frac{z}{\sqrt{\epsilon}}\right) v(t,z) \right|^2 dz = 0, \tag{106}$$

uniformly on compact time intervals in $\mathbb{R}^+$, and v is the unique solution of the homogenized Schrödinger equation

$$\left\{ \begin{array}{ll} i\dfrac{\partial v}{\partial t} - \operatorname{div}(A^* \nabla v) + \operatorname{div}(v B^* z) + c^* v + v D^* z \cdot z = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ v(0,z) = v^0(z) & \text{in } \mathbb{R}^N \end{array} \right. \tag{107}$$

where

$$A^* = \frac{1}{8\pi^2} \nabla_\theta \nabla_\theta \lambda_n(x^n,\theta^n), \ B^* = \frac{1}{2i\pi} \nabla_\theta \nabla_x \lambda_n(x^n,\theta^n), \ D^* = \frac{1}{2} \nabla_x \nabla_x \lambda_n(x^n,\theta^n),$$

and c^* is given by

$$
\begin{aligned}
c^* = \ & \int_{\mathbb{T}^N} \Big[A(\nabla_y + 2i\pi\theta^n)\psi_n \cdot \frac{\partial \bar{\psi}_n}{\partial x_k} e_k - A(\nabla_y - 2i\pi\theta^n) \frac{\partial \bar{\psi}_n}{\partial x_k} \cdot \psi_n \, e_k \\
& - \frac{\partial A}{\partial x_k}(x^n, y)(\nabla_y - 2i\pi\theta^n)\bar{\psi}_n \cdot \psi_n e_k \Big] dy \, .
\end{aligned}
\tag{108}
$$

Notice that even if the tensor A^* might be non-coercive, the homogenized problem (107) is well posed. Indeed the operator $\mathbb{A}^* : L^2(\mathbb{R}^N) \to L^2(\mathbb{R}^N)$ defined by

$$
\mathbb{A}^*\phi = -\mathrm{div}\,(A^*\nabla\phi) + \mathrm{div}(\phi B^* z) + c^*\phi + \phi D^* z \cdot z \tag{109}
$$

is self-adjoint by virtue of Proposition 10.2 below and therefore by using semi-group theory (see *e.g.* [12] or Chapter X in [45]), one can show that there exists a unique solution in $C(\mathbb{R}^+; L^2(\mathbb{R}^N))$, although it may not belong to $L^2(\mathbb{R}^+; H^1(\mathbb{R}^N))$. The next result establishes the conservation of the L^2-norm for the solution v of the homogenized equation (107) and the self-adjointness of the operator $\mathbb{A}^*$.

Proposition 10.2 *Let $v \in C(\mathbb{R}^+; L^2(\mathbb{R}^N))$ be solution to (107). Then*

$$
||v(t,\cdot)||_{L^2(\mathbb{R}^N)} = ||v^0||_{L^2(\mathbb{R}^N)} \quad \forall\, t \in \mathbb{R}^+ \, . \tag{110}
$$

Moreover the operator $\mathbb{A}^*$ defined in (109) is self-adjoint.

Proof. We multiply the equation (107) by $\bar{v}$ and take the imaginary part to obtain

$$
\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}^N} |v|^2 \, dz = \mathrm{Im}\left(\int_{\mathbb{R}^N} v B^* z \cdot \nabla \bar{v} - c^* |v|^2 \, dz \right) . \tag{111}
$$

After integrating by parts one finds that the right hand side of (111) equals

$$
-\Big(\frac{1}{2i} \mathrm{tr}\, B^* + \mathrm{Im} c^* \Big) \int_{\mathbb{R}^N} |v|^2 \, dz
$$

and therefore (110) is proved as soon as we show that

$$
\frac{1}{2i}\mathrm{tr}\, B^* + \mathrm{Im} c^* = 0 \, . \tag{112}
$$

Actually, (112) is a conseqence of the Fredholm alternatives for the derivatives, with respect to x and θ, of the cell spectral equation (101) (for details, see [6]).

In order to prove the self-adjointness of the operator $\mathbb{A}^*$, one first checks that $\mathbb{A}^*$ is symmetric, which easily follows by (112) and the fact that $\overline{B}^* = -B^*$, and then observes that up to addition of a multiple of the identity the operator $\mathbb{A}^*$ is monotone (see *e.g.* [13], Chapter VII). $\square$

In the next proposition we will denote by $\nabla\nabla\lambda_n$ the Hessian matrix of the function $\lambda_n(x, \theta)$ evaluated at the point (x^n, θ^n), namely

$$\nabla\nabla\lambda_n = \begin{pmatrix} \nabla_x\nabla_x\lambda_n & \nabla_\theta\nabla_x\lambda_n \\ \nabla_\theta\nabla_x\lambda_n & \nabla_\theta\nabla_\theta\lambda_n \end{pmatrix} (x^n, \theta^n)\,.$$

Proposition 10.3 *Assume that the matrix $\nabla\nabla\lambda_n$ is positive definite. Then there exists an orthonormal basis $\{\phi_n\}_{n\geq 1}$ of eigenfunctions of $\mathbb{A}^*$; moreover for each n there exists a real constant $\gamma_n > 0$ such that*

$$e^{\gamma_n|z|}\phi_n\,,\ e^{\gamma_n|z|}\nabla\phi_n \in L^2(\mathbb{R}^N)\,. \tag{113}$$

Proof. Up to shifting the spectrum of the operator $\mathbb{A}^*$, we may assume that $\mathrm{Re}(c^*) = 0$. In order to prove the existence of an orthonormal basis of eigenfunctions we introduce the inverse operator of $\mathbb{A}^*$, denoted by G^*

$$\begin{array}{ll} G^* : L^2(\mathbb{R}^N) & \to L^2(\mathbb{R}^N) \\ f & \to \phi \text{ unique solution in } H^1(\mathbb{R}^N) \text{ of} \\ & \qquad \mathbb{A}^*\phi = f \quad \text{in } \mathbb{R}^N \end{array} \tag{114}$$

and we show that G^* is compact. Indeed multiplication of (114) by $\bar{\phi}$ yields

$$\int_{\mathbb{R}^N} [A^*\nabla\phi\cdot\nabla\bar{\phi} - iB^*\mathrm{Im}(\phi z\cdot\nabla\bar{\phi}) + D^*z\cdot z|\phi|^2]\,dz = \int_{\mathbb{R}^N} f\bar{\phi}\,dz\,. \tag{115}$$

Upon defining the $2N$-dimensional vector-valued function Φ

$$\Phi := \begin{pmatrix} 2i\pi z\phi \\ \nabla\phi \end{pmatrix}$$

we rewrite (115) in agreement with this block notation

$$\int_{\mathbb{R}^N} \frac{1}{8\pi^2}\nabla\nabla\lambda_n\Phi\cdot\overline{\Phi}\,dz = \int_{\mathbb{R}^N} f\bar{\phi}\,dz\,.$$

By the positivity assumption on the matrix $\nabla\nabla\lambda_n$ it follows that there exists a positive constant c_0 such that

$$c_0\Big(||\nabla\phi||^2_{L^2(\mathbb{R}^N)} + ||z\phi||^2_{L^2(\mathbb{R}^N)}\Big) \le ||f||_{L^2(\mathbb{R}^N)}||\phi||_{L^2(\mathbb{R}^N)}\,,$$

which implies by a standard argument

$$||\phi||^2_{L^2(\mathbb{R}^N)} + ||\nabla\phi||^2_{L^2(\mathbb{R}^N)} + ||z\phi||^2_{L^2(\mathbb{R}^N)} \le C||f||^2_{L^2(\mathbb{R}^N)},$$

from which we deduce the compactness of G^* in $L^2(\mathbb{R}^N)$-strong. Thus there exists an infinite countable number of eigenvalues for $\mathbb{A}^*$.

We are left to prove the exponential decay of the eigenfunctions. Let ϕ_n be an eigenfunction and let σ_n be the associated eigenvalue

$$\mathbb{A}^*\phi_n = \sigma_n\phi_n\,. \tag{116}$$

Let $R_0 > 0$ and $\rho \in C^\infty(\mathbb{R})$ be a real function such that $0 \le \rho \le 1$, $\rho(s) = 0$ for $s \le R_0$ and $\rho(s) = 1$ for $s \ge R_0 + 1$ and for every positive integer k define $\rho_k \in C^\infty(\mathbb{R}^N)$ in the following way

$$\rho_k(z) := \rho(|z| - k).$$

We now multiply (116) by $\bar\phi_n\rho_k^2$ to get

$$\int_{\mathbb{R}^N} \rho_k^2\left(A^*\nabla\phi_n\cdot\nabla\bar\phi_n - iB^*\mathrm{Im}(\phi_n z\cdot\nabla\bar\phi_n) + D^*z\cdot z|\phi_n|^2 - \sigma_n|\phi_n|^2\right)dz =$$

$$\int_{\mathbb{R}^N}\left(\rho_k|\phi_n|^2B^*z\cdot\nabla\rho_k - 2\rho_k\,\bar\phi_nA^*\nabla\phi_n\cdot\nabla\rho_k\right)dz\,. \tag{117}$$

Next remark that since the left hand side of (117) is real the right hand side must be also real and therefore it is equal to

$$\int_{\mathbb{R}^N} -2\rho_k\,\mathrm{Re}(\bar\phi_nA^*\nabla\phi_n)\cdot\nabla\rho_k\,dz\,. \tag{118}$$

Let B_k denote the ball of radius R_0+k and center $z=0$ and observe that the support of $\nabla\rho_k$ is contained in $B_{k+1}\setminus B_k$. Then putting up together (117) and (118) and using again the positive definiteness of the matrix $\nabla\nabla\lambda_n$ we obtain for R_0 sufficiently large ($\sqrt{R_0} > \sigma_n$ does the job)

$$||\phi_n||^2_{H^1(\mathbb{R}^N\setminus B_{k+1})} \le c_1\Big(||\phi_n||^2_{H^1(\mathbb{R}^N\setminus B_k)} - ||\phi_n||^2_{H^1(\mathbb{R}^N\setminus B_{k+1})}\Big)$$

where c_1 is a positive constant independent of k. Thus we deduce that

$$||\phi_n||^2_{H^1(\mathbb{R}^N\setminus B_{k+1})} \leq \left(\frac{c_1}{1+c_1}\right)^k ||\phi_n||^2_{H^1(\mathbb{R}^N\setminus B_0)} . \tag{119}$$

Upon defining a positive constant $\gamma_0 > 0$ by

$$\left(\frac{c_1}{1+c_1}\right)^k = e^{-2\gamma_0(k+R_0)}$$

it is finally seen that (119) implies the estimate (113) for any exponent $0 < \gamma_n < \gamma_0$. $\Box$

Proof of Theorem 10.1. We content ourselves in giving a sketch of it. The main idea is to rescale the space variable by introducing

$$z = \frac{x - x^n}{\sqrt{\epsilon}} ,$$

and to perform a Taylor expansion in the coefficients for z close to the origin. We define a sequence v_ϵ by

$$v_\epsilon(t,z) := e^{-i\frac{\lambda_n t}{\epsilon}} e^{-2i\pi\frac{\theta^n \cdot x}{\epsilon}} u_\epsilon(t,x) . \tag{120}$$

The a priori estimates of Lemma 6.1 (which are still valid here) implies that $v_\epsilon(t,z)$ satisfies

$$||v_\epsilon||_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^N))} + \sqrt{\epsilon}||\nabla v_\epsilon||_{L^\infty(\mathbb{R}^+;L^2(\mathbb{R}^N))} \leq C.$$

We apply the compactness of two-scale convergence (see Theorem 3.2) with test functions oscillating periodically in z with period $\sqrt{\epsilon}$ (instead of ϵ as before). Therefore, up to a subsequence, there exists a limit $v^*(t,z,y) \in L^2\left(\mathbb{R}^+ \times \mathbb{R}^N; H^1(\mathbb{T}^N)\right)$ such that v_ϵ and $\sqrt{\epsilon}\nabla v_\epsilon$ two-scale converge to v^* and $\nabla_y v^*$, respectively. Similarly, by definition of the initial data, $v_\epsilon(0,z)$ two-scale converges to $\psi_n(y)v^0(z)$.

Although v_ϵ is the unknown which will pass to the limit in the sequel, it is simpler to write an equation for another function, namely

$$w_\epsilon(t,z) := e^{2i\pi\frac{\theta^n \cdot z}{\sqrt{\epsilon}}} v_\epsilon(t,z) = e^{-i\frac{\lambda_n t}{\epsilon}} u_\epsilon(t,x) . \tag{121}$$

Upon this change of unknown and of variable, it can be checked that w_ϵ solves the following equation

$$\begin{cases} i\dfrac{\partial w_\epsilon}{\partial t} - \operatorname{div}[A\left(\sqrt{\epsilon}z, z/\sqrt{\epsilon}\right)\nabla w_\epsilon] + \dfrac{1}{\epsilon}[c(\sqrt{\epsilon}z, z/\sqrt{\epsilon}) - \lambda_n]w_\epsilon = 0 & \text{in } \mathbb{R}^N \times \mathbb{R}^+ \\ w_\epsilon(0,z) = u_\epsilon^0(\sqrt{\epsilon}z) & \text{in } \mathbb{R}^N \end{cases} \tag{122}$$

where the differential operators div and ∇ act with respect to the new variable z.

First step. As usual we multiply the equation (122) by the complex conjugate of

$$\epsilon\phi\Big(t, z, \frac{z}{\sqrt{\epsilon}}\Big)e^{2i\pi\frac{\theta^n\cdot z}{\sqrt{\epsilon}}}$$

where $\phi(t,z,y)$ is a smooth test function defined on $\mathbb{R}^+ \times \mathbb{R}^N \times \mathbb{T}^N$, with compact support in $\mathbb{R}^+ \times \mathbb{R}^N$. Since this test function has compact support (fixed with respect to ϵ), the effect of the non-periodic variable in the coefficients is negligible for sufficiently small ϵ. Therefore we can replace the value of each coefficient at $(\sqrt{\epsilon}z, z/\sqrt{\epsilon})$ by its Taylor expansion of order two about the point $(0, z/\sqrt{\epsilon})$. Passing to the two-scale limit we get the variational formulation of

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

The simplicity of λ_n implies that there exists a scalar function $v(t,z) \in L^2\left(\mathbb{R}^+ \times \mathbb{R}^N\right)$ such that

$$v^*(t,z,y) = v(t,z)\psi_n(y). \tag{123}$$

Second step. We multiply (122) by the complex conjugate of

$$\Psi_\epsilon(t,z) = e^{2i\pi\theta^n\cdot\frac{z}{\sqrt{\epsilon}}}\Big[\psi_n^\epsilon\phi(t,z) + \sqrt{\epsilon}\sum_{k=1}^N \Big(\frac{1}{2i\pi}\frac{\partial\psi_n^\epsilon}{\partial\theta_k}\frac{\partial\phi}{\partial z_k}(t,z) + z_k\frac{\partial\psi_n^\epsilon}{\partial x_k}\phi(t,z)\Big)\Big], \tag{124}$$

where $\phi(t,z)$ is a smooth test function with compact support in $\mathbb{R}^+ \times \mathbb{R}^N$. Remark the new terms depending linearly on z in (124), new with respect to (67). Nevertheless a similar computation (see [6] for details) allows us to pass to the scale limit and obtain a weak formulation of (107). □

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