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High-frequency homogenization for travelling waves in periodic media

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We consider high-frequency homogenization in periodic media for travelling waves of several different equations: the wave equation for scalar-valued waves such as acoustics; the wave equation for vector-valued waves such as electromagnetism and elasticity; and a system that encompasses the Schrödinger equation. This homogenization applies when the wavelength is of the order of the size of the medium periodicity cell. The travelling wave is assumed to be the sum of two waves: a modulated Bloch carrier wave having crystal wavevector $\mathbf{k}$ and frequency ω_1 plus a modulated Bloch carrier wave having crystal wavevector $\mathbf{m}$ and frequency ω_2. We derive effective equations for the modulating functions, and then prove that there is no coupling in the effective equations between the two different waves both in the scalar and the system cases. To be precise, we prove that there is no coupling unless $\omega_1 = \omega_2$ and $(\mathbf{k}-\mathbf{m}) \odot \Lambda \in 2\pi\mathbb{Z}^d$, where $\Lambda = (\lambda_1\lambda_2\dots\lambda_d)$ is the periodicity cell of the medium and for any two vectors $a = (a_1, a_2, \dots, a_d), b = (b_1, b_2, \dots, b_d) \in \mathbb{R}^d$, the product $a \odot b$ is defined to be the vector $(a_1b_1, a_2b_2, \dots, a_db_d)$. This last condition forces the carrier waves to be equivalent Bloch waves meaning that the coupling constants in the system of effective equations vanish. We use two-scale analysis and some new weak-convergence type lemmas. The analysis is not at the same level of rigour as that of Allaire and co-workers who use two-scale convergence theory to treat the problem, but has the advantage of simplicity which will allow it to be easily extended to the case where there is degeneracy of the Bloch eigenvalue.

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1. Introduction

Periodic materials, or at least almost periodic materials abound in nature: crystals are one of the most obvious, and prevalent, examples. Opals are another example, which consist of tiny spherical particles of silica arranged in a face-centred cubic array, which act like a diffraction grating to create the beautiful colours we see [1,2]. A sea mouse has a wonderful iridescence which is caused by a hexagonal array of voids in a matrix of chitin [3]. Recently, it has been discovered that chameleons change their colour by adjusting the lattice spacing of guanine nanocrystals in their skins [4]. The word honeycomb is associated with bees, and the giant's causeway in Ireland consists of a hexagonal array of basalt columns. Many patterns of tiles are periodic. Beautiful periodic structures, now also can be tailor made using three-dimensional lithography and printing techniques [5–9] and of course two-dimensional periodic structures are even easier to produce [10–12].

There has of course been tremendous interest in the properties of periodic structures. The electronic properties of periodic structures were extensively studied (see [13]), it being realized that the band structure of the dispersion diagram for Schrödinger's equation is intimately connected with whether a material is a conductor, insulator or semiconductor, and type of semiconductor (according to whether there was a direct gap or indirect gap). Then came the realization that the same concepts of dispersion diagrams and band gaps also apply at a macroscopic scale, to electromagnetic and elastic wave propagation through periodic composite materials [14–18]). This lead to explosive growth in the area. An immense bibliography on the subject, with over 12 000 papers, approximately doubling every 2 years since 1987 (until 2008, which was when the bibliography ceased being updated) was complied by Dowling (see http://www.phys.lsu.edu/~jdowling/pbgbib.html). For an excellent review of the subject see the book by Joannopoulos *et al.* [19] (see also Gorishnyy *et al.* [20] on acoustic band gap materials).

By suitably adapting the high-frequency homogenization approach of Craster *et al.* [21], we prove that for different travelling waves in periodic medium, the effective equations in the bulk of the material for the function that modulates the wave do not *couple*, i.e. waves having wavevectors $\mathbf{k}/\epsilon$ do not couple with waves having wavevectors $\mathbf{m}/\epsilon$: here ϵ is a small parameter characterizing the length of the unit cell of periodicity, and we are looking at the homogenization limit $\epsilon \to 0$. Thus, the scaling is such that the short-scale oscillations in the waves are on the same scale as the length of the unit cell, in contrast with the usual low-frequency homogenization where the wavelength is much larger than the size of the unit cell. We assume, for simplicity, in this first analysis that the Bloch equations are non-degenerate at these wavevectors. A treatment without this assumption has been given by Brassart & Lenczner [22] for the wave equation. Then to leading order we find that for the waves $(\mathbf{k}, \omega_1)$ and $(\mathbf{m}, \omega_2)$, the field (or potential) that solves the equations takes the form

$$u(t,\mathbf{x}) \approx f_0^{(1)}(t,\mathbf{x}) V_0^{(1)}\left(\frac{\mathbf{x}}{\epsilon}\right) \mathrm{e}^{-\mathrm{i}(\mathbf{k}\cdot(\mathbf{x}/\epsilon)-\omega_1(t/\epsilon))} + f_0^{(2)}(t,\mathbf{x}) V_0^{(2)}\left(\frac{\mathbf{x}}{\epsilon}\right) \mathrm{e}^{-\mathrm{i}(\mathbf{m}\cdot(\mathbf{x}/\epsilon)-\omega_2(t/\epsilon))}, \tag{1.1}$$

here $V_0^{(1)}(\mathbf{x}/\epsilon)\,\mathrm{e}^{-\mathrm{i}(\mathbf{k}\cdot(\mathbf{x}/\epsilon)-\omega_1(t/\epsilon))}$ and $V_0^{(2)}(\mathbf{x}/\epsilon)\,\mathrm{e}^{-\mathrm{i}(\mathbf{m}\cdot(\mathbf{x}/\epsilon)-\omega_2(t/\epsilon))}$ are the Bloch solutions at the wavevectors $\mathbf{k}/\epsilon$ and $\mathbf{m}/\epsilon$, (in which $V_0^{(1)}(\mathbf{x}/\epsilon)$ and $V_0^{(2)}(\mathbf{x}/\epsilon)$ have the same unit cell of periodicity as the periodic material we are considering) and the modulating functions $f_0^{(1)}(t,\mathbf{x})$ and $f_0^{(2)}(t,\mathbf{x})$ satisfy the *homogenized equation*

$$\nabla g \cdot \nabla f_0^{(\ell)}(t,\mathbf{x}) + \frac{\partial f_0^{(\ell)}(t,\mathbf{x})}{\partial t} = 0, \quad \ell = 1,2 \tag{1.2}$$

and $\omega/\epsilon = g(\mathbf{k}/\epsilon)$ is the dispersion relation. This effective equation admits as solutions, the expected travelling waves

$$f_0^{(1)}(t,\mathbf{x}) = h_1(\mathbf{v}_1\cdot\mathbf{x} - t) \quad \text{and} \quad f_0^{(2)}(t,\mathbf{x}) = h_2(\mathbf{v}_2\cdot\mathbf{x} - t), \tag{1.3}$$

here h_1 and h_2 are arbitrary functions and $\mathbf{v}_1$ and $\mathbf{v}_2$ are the group velocities which satisfy $\mathbf{v}_i \cdot \nabla g = 1$. In the time harmonic case, where the waves are not travelling the first results on

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high-frequency homogenization are those of Birman & Suslina [23], which provides a rigorous justification of high-frequency homogenization. That paper is difficult to follow unless one is an expert in spectral theory, so in the appendix, we make the connection between the paper of Birman & Suslina [23] and that of Craster *et al.* [21]. The approach of Craster *et al.* [21] is straightforward and very reminiscent of the standard formal approach to homogenization (see Bensoussan *et al.* [24], who furthermore homogenize a Schrodinger equation at high frequency). One treats the large and small length scales as independent variables $\mathbf{X}$ and ξ that are coupled when one replaces in the governing equations any derivative $\partial/\partial x_j$ with $\partial/\partial X_j + (1/\epsilon)\partial/\partial\xi_j$. This approach is not rigorous, so will need to be supplemented at some stage, by either a rigorous analysis, or by supporting numerical calculations. Hoefer & Weinstein [25] have done a careful rigorous analysis, with error estimates, for high-frequency homogenization applied to the Schrödinger equation, where they keep higher terms in the expansion.

It is also to be emphasized that there has been extensive work by Allaire and co-workers in this area using the ideas of two-scale convergence introduced by Nguetseng [26] and Allaire [27] particularly for the acoustic equation

$$\nabla \cdot \left(\mathbf{a}\left(\frac{\mathbf{x}}{\epsilon}\right)\nabla u\right) = b\left(\frac{\mathbf{x}}{\epsilon}\right)\frac{\partial^2 u}{\partial t^2}, \quad \mathbf{x} = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d, \tag{1.4}$$

assuming ellipticity for the tensor $\mathbf{a}$, and positivity for the scalar b [22,28,29]. These assumptions are also needed in our analysis to ensure unique solvability of the Bloch equation. The work of Allaire *et al.* [29] goes further than us in that they prove the enveloping function converges to that predicted by the two-scale analysis, and that they prove the enveloping function obeys a Schrödinger type equation as expected from the paraxial approximation. At the level of our analysis the dispersion of the enveloping function is absent, so further work needs be done to account for it. We also emphasize that there is much older work in Bensoussan *et al.* [24] on high-frequency homogenization of the Schrödinger equation. Particularly, we draw the reader's attention to the effective equations (4.33) and the formulae for the effective moduli both expressed in terms of the derivatives of the dispersion formula and in terms of the solution to a cell problem (see the discussion at the bottom of p. 352). In our analysis, we treat electromagnetism and elasticity in one single stroke in §5, and we treat a general class of equations which includes the Scrödinger equation in §6. Again we note that Allaire & Piatnitski [30] treated the Schrödinger equation and Allaire *et al.* [31] treated Maxwell's equations using the tool of two-scale convergence.

Although much of the work discussed thus far is analytical, it is useful to note that these types of effective media have been tested numerically and applied to interpret and design experiments [32]. The most-striking behaviour occurs when the effective equations which describe the macroscopic modulation of the waves are hyperbolic rather than elliptic: then the radiation concentrates along the characteristic lines and the star-shaped patterns predicted by high-frequency homogenization are seen in full finite-element simulations (see the figures in [33,34]).

The main factor which influences the macroscopic equations one gets is the degeneracy of the wave functions associated with the expansion point (see [35]). The simplest case, and the one first treated by Birman & Suslina [23] and Craster *et al.* [21], is when there is no degeneracy. For simplicity, and because this is the generic case, we will also assume there is no degeneracy. The next section is then the homogenization of a model equation.

2. A scalar-valued wave travelling in a periodic medium

Our first aim is to homogenize the model equation

$$\nabla \cdot \left(\mathbf{a}\left(\frac{\mathbf{x}}{\epsilon}\right)\nabla u\right) = b\left(\frac{\mathbf{x}}{\epsilon}\right)\frac{\partial^2 u}{\partial t^2}, \quad \mathbf{x} = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d, \tag{2.1}$$

where $\mathbf{a}\colon \mathbb{R}^d \to \mathbb{R}^{d\times d}$ is a symmetric matrix and $b\colon \mathbb{R}^d \to \mathbb{R}$ are also cell-periodic with the same cell of periodicity. We assume, for simplicity, that the unit cell is a rectangular prism, though of course we expect the analysis to go through for any Bravais lattice. This is the equation of acoustics when u is the pressure, $b(\mathbf{x}/\epsilon)$ is inverse of the bulk modulus of the fluid and $\mathbf{a}(\mathbf{x}/\epsilon)$ is the inverse of the density, which we allow to be anisotropic (as may be the case in metamaterials).

We rewrite the equation in the form

$$\begin{pmatrix} \dfrac{\partial}{\partial t} \\ \nabla \end{pmatrix} \cdot \mathbf{C} \begin{pmatrix} \dfrac{\partial}{\partial t} \\ \nabla \end{pmatrix} u(\mathbf{x}, t) = 0, \quad \text{where } \mathbf{C} = \begin{pmatrix} -b & 0 \\ 0 & \mathbf{a} \end{pmatrix}. \tag{2.2}$$

Denoting the new variable $x_0 = t$ and

$$\bar{\nabla} = \begin{pmatrix} \dfrac{\partial}{\partial x_0} \\ \nabla \end{pmatrix},$$

we get the equation

$$\bar{\nabla} \cdot (\mathbf{C}\bar{\nabla} u(\mathbf{x}, t)) = 0. \tag{2.3}$$

As is standard in homogenization theory we replace $\bar{\nabla}$ by $\bar{\nabla}_X + (1/\epsilon)\bar{\nabla}_\xi$, where $\mathbf{X} = (x_0, x_1, x_2, \dots, x_d)$ is the slow variable and $\boldsymbol{\xi} = (\xi_0, \xi_1, \xi_2, \dots, \xi_d) = X/\epsilon$ is the fast variable. The motivation for this is that if we have a function $g(\mathbf{x}, \mathbf{x}/\epsilon) = g(\mathbf{X}, \boldsymbol{\xi})$, then $\bar{\nabla}$ acting on $g(\mathbf{x}, \mathbf{x}/\epsilon)$ gives the same result as $\bar{\nabla}_X + (1/\epsilon)\bar{\nabla}_\xi$ acting on $g(\mathbf{X}, \boldsymbol{\xi})$, with $\boldsymbol{\xi}$ and $\mathbf{X}$ treated as independent variables. Thus, we are scaling space and time in the same way as we believe is appropriate when the dispersion diagram is such that $\partial\omega/\partial\mathbf{k}$ has a non-zero finite value. At points where $\partial\omega/\partial\mathbf{k}$ is zero we do not believe this is an appropriate scaling as indicated by Birman & Suslina [23] and later by Craster *et al.* [21]. Thus, we assume that we are in the case when $\partial\omega/\partial\mathbf{k}$ has a non-zero finite value and, therefore, making this replacement we arrive at

$$\begin{aligned} &\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi u(\mathbf{X}, \boldsymbol{\xi})) + \epsilon \bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_X u(\mathbf{X}, \boldsymbol{\xi})) \\ &\quad + \epsilon \bar{\nabla}_X \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi u(\mathbf{X}, \boldsymbol{\xi})) + \epsilon^2 \bar{\nabla}_X \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_X u(\mathbf{X}, \boldsymbol{\xi})) = 0. \end{aligned} \tag{2.4}$$

Now we choose to homogenize waves which on the short length scale look like Bloch solutions, with frequencies ω_1 and ω_2 and wavevectors $\mathbf{k}$ and $\mathbf{m}$, but which are modulated on the long length scale. Our aim is to find the macroscopic equation satisfied by the modulation. We assume that the wavenumber-frequency pairs $(\mathbf{k}, \omega_1)$ and $(\mathbf{m}, \omega_2)$ belong to the dispersion diagram. We will prove later in §3 that any two different waves do not interact (do not couple).

We have, $u(\mathbf{X}, \boldsymbol{\xi})$ is the sum of two waves,

$$u(\mathbf{X}, \boldsymbol{\xi}) = u^{(1)}(\mathbf{X}, \boldsymbol{\xi}) + u^{(2)}(\mathbf{X}, \boldsymbol{\xi}), \tag{2.5}$$

where for fixed $\mathbf{X}$ the functions $u^{(1)}(\mathbf{X}, \boldsymbol{\xi})$, $u^{(2)}(\mathbf{X}, \boldsymbol{\xi})$ as functions of $\boldsymbol{\xi}$ are Bloch functions, oscillating at frequencies ω_1 and ω_2 and having wavevectors $\mathbf{k}$ and $\mathbf{m}$, respectively. Thus, the functions $\mathrm{e}^{-\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\xi}' - \omega_1\xi_0)} u^{(1)}(\mathbf{X}, \boldsymbol{\xi})$ and $\mathrm{e}^{-\mathrm{i}(\mathbf{m}\cdot\boldsymbol{\xi}' - \omega_2\xi_0)} u^{(1)}(\mathbf{X}, \boldsymbol{\xi})$ are periodic in $\boldsymbol{\xi}' = (\xi_1, \xi_2, \dots, \xi_d)$ and independent of ξ_0. We seek a solution of equation (2.4) in the form

$$u^{(i)}(\mathbf{X}, \boldsymbol{\xi}) = u_0^{(i)}(\mathbf{X}, \boldsymbol{\xi}) + \epsilon u_1^{(i)}(\mathbf{X}, \boldsymbol{\xi}) + \epsilon^2 u_2^{(i)}(\mathbf{X}, \boldsymbol{\xi}) + \cdots, \quad i = 1, 2. \tag{2.6}$$

Plugging in the expressions of $u^{(1)}(\mathbf{X}, \boldsymbol{\xi})$ and $u^{(2)}(\mathbf{X}, \boldsymbol{\xi})$ in (2.4), we get at the zeroth order,

$$\sum_{i=1}^{2} \bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi u_0^{(i)}(\mathbf{X}, \boldsymbol{\xi})) = 0. \tag{2.7}$$

From the uniqueness of the solutions to the Bloch equations, up to a multiplicative complex constant, equation (2.7) implies that $u_0^{(1)}(\mathbf{X}, \boldsymbol{\xi})$ and $u_0^{(2)}(\mathbf{X}, \boldsymbol{\xi})$ can be separated in the fast and slow variables, i.e.

$$u_0^{(1)}(\mathbf{X},\boldsymbol{\xi}) = f_0^{(1)}(\mathbf{X})U_0^{(1)}(\boldsymbol{\xi}) \quad \text{and} \quad u_0^{(2)}(\mathbf{X},\boldsymbol{\xi}) = f_0^{(2)}(\mathbf{X})U_0^{(2)}(\boldsymbol{\xi}), \tag{2.8}$$

where $U_0^{(1)}(\boldsymbol{\xi})$ and $U_0^{(2)}(\boldsymbol{\xi})$ solve the Bloch equations

$$\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi U_0^{(i)}(\boldsymbol{\xi})) = 0, \quad i = 1, 2 \tag{2.9}$$

and $f_0^{(1)}(\mathbf{X})$ and $f_0^{(2)}(\mathbf{X})$ are the modulating functions whose governing equation we seek to find.

It is then clear that $U_0^{(1)}(\boldsymbol{\xi})$ and $U_0^{(2)}(\boldsymbol{\xi})$ have the form

$$U_0^{(1)}(\boldsymbol{\xi}) = V_0^{(1)}(\boldsymbol{\xi}')\,\mathrm{e}^{-\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\xi}'-\omega_1\xi_0)} \quad \text{and} \quad U_0^{(2)}(\boldsymbol{\xi}) = V_0^{(2)}(\boldsymbol{\xi}')\,\mathrm{e}^{-\mathrm{i}(\mathbf{m}\cdot\boldsymbol{\xi}'-\omega_2\xi_0)}, \tag{2.10}$$

where $V_0^{(1)}$ and $V_0^{(2)}$ are cell-periodic functions of $\boldsymbol{\xi}'$ solving

$$\left.\begin{aligned} &\omega_1^2 b(\boldsymbol{\xi}')V_0^{(1)}(\boldsymbol{\xi}') + (-\mathrm{i}\mathbf{k} + \bar{\nabla}_{\xi'})\cdot\mathbf{a}(\boldsymbol{\xi}')(-\mathrm{i}\mathbf{k} + \bar{\nabla}_{\xi'})V_0^{(1)}(\boldsymbol{\xi}') = 0 \\ \text{and} \quad &\omega_2^2 b(\boldsymbol{\xi}')V_0^{(2)}(\boldsymbol{\xi}') + (-\mathrm{i}\mathbf{m} + \bar{\nabla}_{\xi'})\cdot\mathbf{a}(\boldsymbol{\xi}')(-\mathrm{i}\mathbf{m} + \bar{\nabla}_{\xi'})V_0^{(2)}(\boldsymbol{\xi}') = 0. \end{aligned}\right\} \tag{2.11}$$

At the first order, we get the following equation

$$\begin{aligned} &\sum_{i=1}^{2} \bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(i)}(\mathbf{X},\boldsymbol{\xi})) \\ &\qquad = -\sum_{i=1}^{2}\left[\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_X u_0^{(i)}(\mathbf{X},\boldsymbol{\xi})) + \bar{\nabla}_X \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_0^{(i)}(\mathbf{X},\boldsymbol{\xi}))\right]. \end{aligned} \tag{2.12}$$

Next, we take the complex conjugate of equations in (2.9) to get

$$\bar{\nabla}_\xi \cdot (\mathbf{C}(\xi')\bar{\nabla}_\xi U_0^{(i)*}(\boldsymbol{\xi})) = 0, \quad i = 1, 2, \tag{2.13}$$

where z^* denotes the complex conjugate of z. Note that equation (2.12) can be written in the following way

$$\begin{aligned} &\sum_{l=1}^{2} \bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X},\boldsymbol{\xi})) \\ &\qquad = -\sum_{l=1}^{2}\sum_{i,j=0}^{d} \frac{\partial f_0^{(l)}(\mathbf{X})}{\partial X_j}\left(2C_{ij}(\boldsymbol{\xi}')\frac{\partial U_0^{(l)}(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i}U_0^{(l)}(\boldsymbol{\xi})\right). \end{aligned} \tag{2.14}$$

Assume now Q is a large rectangular cell in the coordinate system $\boldsymbol{\xi}$. Following the idea ([24, p. 307]; see also Craster *et al.* [21]), we multiply equation (2.14) by $U_0^{(p)*}$, for $p = 1, 2$ and taking the average over Q of both sides of the obtained identity we get

$$\begin{aligned} &\frac{1}{Q}\int_{|Q|}\sum_{l=1}^{2} U_0^{(p)*}\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X},\boldsymbol{\xi}))\,\mathrm{d}\boldsymbol{\xi} \\ &\quad = \sum_{l=1}^{2}\sum_{i,j=0}^{d}\frac{\partial f_0^{(l)}(\mathbf{X})}{\partial X_j}\frac{1}{|Q|}\int_Q U_0^{(p)*}\left(2C_{ij}(\boldsymbol{\xi}')\frac{\partial U_0^{(l)}(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i}U_0^{(l)}(\xi)\right)\mathrm{d}\boldsymbol{\xi}, \end{aligned} \tag{2.15}$$

where $Q = \prod_{i=0}^{d}[0, a_i]$ and $|Q|$ is the volume of Q.

Let us show the left-hand side of (2.15) goes to zero when $Q \to \infty$ by which we mean $a_i \to \infty$ for $i = 0, 1, 2, \ldots, d$. Indeed, after an integration by parts, we get

$$\int_Q \sum_{l=1}^{2} U_0^{(p)*} \bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi}))\,\mathrm{d}\boldsymbol{\xi}$$

$$= \int_{\partial Q} \sum_{l=1}^{2} U_0^{(p)*} \mathbf{n} \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi}))\,\mathrm{d}S - \int_Q \sum_{l=1}^{2} \bar{\nabla}_\xi U_0^{(p)*} \mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}, \tag{2.16}$$

where $\mathbf{n}$ is the outward unit normal to ∂Q. On the other hand, we have by multiplying (2.13) by $u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi})$ and integrating the obtained equality over Q by parts, we get

$$\int_{\partial Q} \sum_{l=1}^{2} u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi})\mathbf{n} \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi U_0^{(p)*}(\boldsymbol{\xi}))\,\mathrm{d}S - \int_Q \sum_{l=1}^{2} \bar{\nabla}_\xi U_0^{(p)*} \mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi} = 0. \tag{2.17}$$

Thus by combining (2.16) and (2.17), we get

$$\int_Q \sum_{l=1}^{2} U_0^{(p)*} \bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi}))\,\mathrm{d}\boldsymbol{\xi}$$

$$= \int_{\partial Q} \sum_{l=1}^{2} u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi})\mathbf{n} \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi U_0^{(p)*}(\boldsymbol{\xi}))\,\mathrm{d}S + \int_{\partial Q} \sum_{l=1}^{2} U_0^{(p)*} \mathbf{n} \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi}))\,\mathrm{d}S. \tag{2.18}$$

Taking into account the continuity and the periodic structure of the functions $\bar{\nabla}_\xi u_1^{(l)}$, $\bar{\nabla}_\xi U_0^{(p)*}$ and the tensor $\mathbf{C}(\boldsymbol{\xi}')$, we have the estimate

$$\left| \int_Q \sum_{l=1}^{2} U_0^{(p)*} \bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi}')\bar{\nabla}_\xi u_1^{(l)}(\mathbf{X}, \boldsymbol{\xi}))\,\mathrm{d}\boldsymbol{\xi} \right| \leq M\mathcal{H}^{d-1}(\partial Q),$$

where $\mathcal{H}^{d-1}(\partial Q)$ is the $d-1$ dimensional Hausdorff measure in $\mathbb{R}^d$, i.e. it is the surface measure, and M is a sufficiently large constant. Our claim follows now from the obvious equality

$$\lim_{Q \to \infty} \frac{\mathcal{H}^{d-1}(\partial Q)}{|Q|} = 0.$$

In other words, this condition over the supercell Q, which is the analogue of the solvability condition that was over a unit cell in Craster [21], gives us the following equations:

$$\sum_{l=1}^{2} \sum_{j=0}^{d} d_{jp}^{(l)} \frac{\partial f_0^{(l)}(\mathbf{X})}{\partial X_j} = 0, \quad \text{for } p = 1, 2, \tag{2.19}$$

where the coefficients entering these homogenized equations are given by

$$d_{jp}^{(l)} = \lim_{Q \to \infty} \sum_{i=0}^{d} \frac{1}{|Q|} \int_Q U_0^{(p)*} \left(2C_{ij}(\boldsymbol{\xi}') \frac{\partial U_0^{(l)}(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i} U_0^{(l)}(\boldsymbol{\xi}) \right) \mathrm{d}\boldsymbol{\xi},$$

$$j = 0, 1, \ldots, d, \quad p, l = 1, 2. \tag{2.20}$$

As will be seen in the §3, the formula (2.20) can be significantly simplified.

3. Wave coupling analysis

In this section, we consider the following question: is there interaction between any two different waves? Let us look to see if there is interaction in the homogenized equations between waves corresponding to points $(\mathbf{k}, \omega_1)$ and $(\mathbf{m}, \omega_2)$ on the dispersion diagram. To that end, we must analyse the coupling coefficients in the homogenized equations. We have seen in §2 that the homogenized equations are given by

$$\sum_{l=1}^{2}\sum_{j=0}^{d} d_{jp}^{(l)} \frac{\partial f_0^{(l)}(\mathbf{X})}{\partial X_j} = 0, \quad \text{for } p = 1, 2, \tag{3.1}$$

where the coefficients entering these homogenized equations are given by

$$d_{jp}^{(l)} = \lim_{Q\to\infty} \sum_{i=0}^{d} \frac{1}{|Q|} \int_Q U_0^{(p)*} \left(2C_{ij}(\boldsymbol{\xi}') \frac{\partial U_0^{(l)}(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i} U_0^{(l)}(\boldsymbol{\xi}) \right) \mathrm{d}\boldsymbol{\xi},$$
$$j = 0, 1, \ldots, d, \quad p, l = 1, 2. \tag{3.2}$$

Furthermore, we denote by $\Lambda = \prod_{i=1}^{d} [0, \lambda_i]$ the cell of periodicity and $\Lambda_{\text{diag}} = (\lambda_1, \lambda_2, \ldots, \lambda_d)$-ist diagonal. Given d-vectors, $\mathbf{k} = (k_1, k_2, \ldots, k_d)$ and $\mathbf{m} = (m_1, m_2, \ldots, m_d)$ denote

$$\mathbf{k} \odot \mathbf{m} = (k_1 m_1, k_2 m_2, \ldots, k_d m_d). \tag{3.3}$$

The next theorem gives a necessary condition for coupling between the waves u_1 and u_2.

Theorem 3.1. *For the waves* $(\mathbf{k}, \omega_1)$ *and* $(\mathbf{m}, \omega_2)$ *to couple, it is necessary, that* $\omega_1 = \omega_2$ *and* $(\mathbf{k} - \mathbf{m}) \odot \Lambda_{\text{diag}}/2\pi \in \mathbb{Z}^d$.

Proof. The proof of the theorem is based on lemma B.5. We have to show that the coefficients $d_{jp}^{(l)}$ vanish for $l \neq p$, if one of the conditions in the theorem is not satisfied. It is clear that the integrand of $d_{jp}^{(l)}$ has the form $\mathrm{e}^{\pm\mathrm{i}(\omega_1-\omega_2)\xi_0} W(\xi')$, thus the integral over the over the volume of $|Q|$ will vanish by lemma B.5, as the coefficient of the exponent $\mathrm{e}^{\pm\mathrm{i}(\omega_1-\omega_2)\xi_0}$ does not depend on ξ_0. On the other hand, if $\omega_1 = \omega_2$, then $d_{jp}^{(l)}$ will have the form $\mathrm{e}^{\pm\mathrm{i}(\mathbf{k}-\mathbf{m})\xi'} W(\xi')$, where $W(\xi')$ is a periodic function in ξ' with the cell period of that of the medium. Therefore, again, an application of lemma B.5 completes the proof. ■

Theorem 3.2. *Any two different waves* $(\mathbf{k}, \omega_1)$ *and* $(\mathbf{m}, \omega_2)$ *do not couple.*

Proof. By theorem 3.1, for the waves $(\mathbf{k}, \omega_1)$ and $(\mathbf{m}, \omega_2)$ to couple one must have $\omega_1 = \omega_2$ and $(\mathbf{k} - \mathbf{m}) \odot \Lambda_{\text{diag}}/2\pi \in \mathbb{Z}^d$. We can without loss of generality assume, making a change of variables if necessary, that the cell of periodicity Λ of the medium is an n-dimensional unit cube, i.e. $\lambda_i = 1$, for $i = 1, 2, \ldots, d$. Thus, we have $(\mathbf{k} - \mathbf{m}) \odot \Lambda_{\text{diag}}/2\pi = \mathbf{k} - \mathbf{m}/2\pi$, thus the condition $(\mathbf{k} - \mathbf{m}) \odot \Lambda_{\text{diag}}/2\pi \in \mathbb{Z}^d$ yields $k_i - m_i = 2\pi q_i$, for $i = 1, 2, \ldots, d$ and some $q_i \in \mathbb{Z}$. The last set of equations and the fact that the medium cell of periodicity is a unit cube imply the wave u_1 is a scalar multiple of u_2, which completes the proof. ■

Remark 3.3. For the coefficients $d_{jp}^{(l)}$, one has

$$d_{jp}^{(l)} = 0, \quad \text{if } l \neq p,$$

due to the non-coupling of different waves.

Combining now the above results with the result in §2, we arrive at the following:

Theorem 3.4. *The effective equation associated to* (2.1) *for the wave* $(\mathbf{k}, \omega)$ *is given by*

$$\sum_{j=0}^{d} d_j \frac{\partial f_0(\mathbf{X})}{\partial X_j} = 0, \tag{3.4}$$

where the coefficients entering this homogenized equation are given by

$$d_j = \lim_{Q\to\infty} \sum_{i=0}^{d} \frac{1}{|Q|} \int_Q U_0^* \left(2C_{ij}(\boldsymbol{\xi}') \frac{\partial U_0(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i} U_0(\boldsymbol{\xi}) \right), \quad j = 0, 1, \ldots, d \tag{3.5}$$

and U_0 *solves the Bloch equation* (2.9).

The next theorem gives a simplification of formula (3.5).

Theorem 3.5. *The formula* (3.5) *can be simplified to*

$$d_j = \sum_{i=0}^{d} \frac{1}{|\Lambda|} \int_{\Lambda} U_0^* \left(2C_{ij}(\boldsymbol{\xi}') \frac{\partial U_0(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i} U_0(\boldsymbol{\xi}) \right), \quad j = 0, 1, \ldots, d \tag{3.6}$$

and U_0 solves the Bloch equation (2.9).

Proof. The proof is a direct consequence of lemma B.5. Recalling the formula (2.10) for the function $U_0(\xi)$ and plugging in the expression of $U_0(\xi)$ into the formula (3.5) and calculating the partial derivatives, all the exponents cancel out and one is left with a function $f(\xi')$ integrated over a time–space supercell Q. The integration in time is balanced by the denominator $|Q|$ and thus we are left with the integral of $f(\xi')$ over a space supercell. Finally, an application of lemma B.5 with the value $\xi = \mathbf{0}$ completes the proof. ∎

4. The case of vector-valued waves

In this section, we allow for vector potentials $\mathbf{u}$ having n components and we consider a system of n equations in d dimensions:

$$\nabla \cdot \left(\mathbf{a} \left(\frac{\mathbf{x}}{\epsilon} \right) \nabla \mathbf{u} \right) = \mathbf{b} \left(\frac{\mathbf{x}}{\epsilon} \right) \frac{\partial^2 \mathbf{u}}{\partial t^2}, \quad \mathbf{x} = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d, \tag{4.1}$$

which reads in components as follows:

$$\sum_{j=1}^{d} \frac{\partial}{\partial x_j} \left(\sum_{k=1}^{n} \sum_{l=1}^{d} a_{ijkl} \left(\frac{\mathbf{x}}{\epsilon} \right) \frac{\partial u_k}{\partial x_l} \right) = \sum_{k=1}^{n} b_{ik} \left(\frac{\mathbf{x}}{\epsilon} \right) \frac{\partial^2 u_k}{\partial t^2}, \quad i = 1, 2, \ldots n \quad \text{and} \quad \mathbf{x} \in \mathbb{R}^d, \tag{4.2}$$

where $\mathbf{a}$ is a fourth-order tensor that has the usual symmetry $a_{ijkl} = a_{klij}$, $\mathbf{b} \in \mathbb{R}^{n \times n}$ is a symmetric matrix and $\mathbf{u}\colon \mathbb{R}^d \to \mathbb{R}^n$ is a vector field. It is assumed that $\mathbf{a}$ and $\mathbf{b}$ are cell-periodic. These equations appear most naturally in the context of elastodynamics, where $\mathbf{u}(\mathbf{x})$ is identified as the displacement field, $\mathbf{a}(\mathbf{x})$ as the elasticity tensor, having the additional symmetries $a_{ijkl} = a_{jikl} = a_{ijlk}$, and $\mathbf{b}(\mathbf{x})$ is the (possibly anisotropic) density. The three-dimensional electromagnetic equations of Maxwell can also be expressed in this form [36] with $\mathbf{u}(\mathbf{x})$ representing the electric field, $\mathbf{b}(\mathbf{x})$ the dielectric tensor and the components of $\mathbf{a}$ being related to the magnetic permeability tensor $\boldsymbol{\mu}(\mathbf{x})$ through the equations,

$$a_{ijkl} = -e_{ijp} e_{klq} \{\boldsymbol{\mu}^{-1}\}_{pq}, \tag{4.3}$$

in which e_{ijp} is the completely antisymmetric Levi–Civita tensor, taking values $+1$ or -1 according to whether ijp is an even or odd permutation of 123 and being zero otherwise.

Like in §2, we rewrite system (4.2) in the following form

$$\begin{pmatrix} \frac{\partial}{\partial t} \\ \nabla \end{pmatrix} \cdot \mathbf{C} \begin{pmatrix} \frac{\partial}{\partial t} \\ \nabla \end{pmatrix} \mathbf{u}(\mathbf{x}, t) = 0, \quad \text{where } \mathbf{C} = (C_{ijkl}), \quad 1 \le i, k \le n, \; 0 \le j, l \le d \tag{4.4}$$

and the tensor $\mathbf{C}$ derives from the tensor $\mathbf{a}$ and the matrix $\mathbf{b}$ as follows:

$$\left. \begin{aligned} C_{ijkl} &= 0 \quad \text{if } jl = 0, j + l \ge 1, \\ C_{i0k0} &= -b_{ik} \quad \text{if } 1 \le i, k \le n, \\ \text{and} \qquad C_{ijkl} &= a_{ijkl} \quad \text{if } 1 \le i, j, k, l. \end{aligned} \right\} \tag{4.5}$$

Remembering that $t = x_0$, we arrive at

$$\bar{\nabla} \cdot (\mathbf{C} \bar{\nabla} \mathbf{u}(\mathbf{x}, t)) = 0. \tag{4.6}$$

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Replacing now $\bar{\nabla}$ with $\bar{\nabla}_X + (1/\epsilon)\bar{\nabla}_\xi$, where $\mathbf{X} = (X_0, X_1, \ldots, X_d)$ is the slow variable and $\boldsymbol{\xi} = (\xi_0, \xi_1, \ldots, \xi_d)$ is the fast variable, we arrive at the system of equations

$$\begin{aligned}\bar{\nabla}_\xi \cdot (\mathbf{C}(\xi)\bar{\nabla}_\xi \mathbf{u}(\mathbf{X},\boldsymbol{\xi})) + \epsilon\bar{\nabla}_\xi \cdot (\mathbf{C}(\xi)\bar{\nabla}_X \mathbf{u}(\mathbf{X},\boldsymbol{\xi}))\\ + \epsilon\bar{\nabla}_X \cdot (\mathbf{C}(\xi)\bar{\nabla}_\xi \mathbf{u}(\mathbf{X},\boldsymbol{\xi})) + \epsilon^2\bar{\nabla}_X \cdot (\mathbf{C}(\xi)\bar{\nabla}_X \mathbf{u}(\mathbf{X},\boldsymbol{\xi})) = 0.\end{aligned} \tag{4.7}$$

We adopt the same strategy as in §2, but with a slight difference: as we already know, that there is no coupling between two different waves, we seek the solution to (4.7) in the form of one wave (rather than the two of (2.5)) corresponding to the pair $(\mathbf{m}, \omega)$ on the dispersion diagram:

$$\mathbf{u}(\mathbf{X},\boldsymbol{\xi}) = \mathbf{u}(\mathbf{X},\boldsymbol{\xi}), \tag{4.8}$$

where the vector $\mathrm{e}^{-\mathrm{i}(\mathbf{m}\cdot\boldsymbol{\xi}' - \omega\xi_0)}\mathbf{u}(\mathbf{X},\boldsymbol{\xi})$ is periodic in $\boldsymbol{\xi}' = (\xi_1, \xi_2, \ldots, \xi_d)$ and independent of ξ_0. Next, we assume that the vector $\mathbf{u}$ has the expansion

$$\mathbf{u}(\mathbf{X},\boldsymbol{\xi}) = \mathbf{u}_0(\mathbf{X},\boldsymbol{\xi}) + \epsilon\mathbf{u}_1(\mathbf{X},\boldsymbol{\xi}) + \epsilon^2\mathbf{u}_2(\mathbf{X},\boldsymbol{\xi}) + \cdots. \tag{4.9}$$

At the zeroth order, we get the system

$$\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi \mathbf{u}_0(\mathbf{X},\boldsymbol{\xi})) = 0.$$

This has the solution $\mathbf{u}_0(\mathbf{X},\boldsymbol{\xi}) = f_0(\mathbf{X})\mathbf{U}_0(\boldsymbol{\xi})$, where f_0 is a scalar and $\mathbf{U_0}: \mathbb{R}^{d+1} \to \mathbb{R}^n$ is a vector such that $\mathrm{e}^{-\mathrm{i}(\mathbf{m}\cdot\boldsymbol{\xi}' - \omega\xi_0)}\mathbf{U_0}(\boldsymbol{\xi})$ is periodic in $\boldsymbol{\xi}' = (\xi_1, \xi_2, \ldots, \xi_d)$ and independent of ξ_0, and that the vector $\mathbf{U_0}$ solves the system of the Bloch equations:

$$\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi \mathbf{U}_0(\boldsymbol{\xi})) = 0. \tag{4.10}$$

At the first order, we get the following system

$$\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}y_\xi \mathbf{u}_1(\mathbf{X},\boldsymbol{\xi})) = -[\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_X \mathbf{u}_0(\mathbf{X},\boldsymbol{\xi})) + \bar{\nabla}_X \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi \mathbf{u}_0(\mathbf{X},\boldsymbol{\xi}))]. \tag{4.11}$$

We can then calculate

$$\bar{\nabla}_X(f_0(\mathbf{X})\mathbf{U}_0(\boldsymbol{\xi})) = \left(\frac{\partial f_0(\mathbf{X})}{\partial X_l}U_0^k(\boldsymbol{\xi})\right)_{lk},$$

thus

$$\begin{aligned}\bar{\nabla}_X \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi \mathbf{u}_0(\mathbf{X},\boldsymbol{\xi})) &= \sum_{j=0}^{d}\frac{\partial}{\partial\xi_j}\left(\sum_{l=0}^{d}\sum_{k=1}^{n}C_{ijkl}(\boldsymbol{\xi})\frac{\partial f_0(\mathbf{X})}{\partial X_l}U_0^k(\boldsymbol{\xi})\right)\\ &= \sum_{j,l=0}^{d}\frac{\partial f_0(\mathbf{X})}{\partial X_l}\sum_{k=1}^{n}\left(\frac{\partial C_{ijkl}(\boldsymbol{\xi})}{\partial\xi_j}U_0^k(\boldsymbol{\xi}) + C_{ijkl}(\boldsymbol{\xi})\frac{\partial U_0^k(\boldsymbol{\xi})}{\partial\xi_j}\right).\end{aligned} \tag{4.12}$$

We have similarly

$$\bar{\nabla}_X \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi \mathbf{u}_0(\mathbf{X},\boldsymbol{\xi})) = \sum_{j,l=0}^{d}\frac{\partial f_0(\mathbf{X})}{\partial X_l}\sum_{k=1}^{n}C_{ilkj}(\boldsymbol{\xi})\frac{\partial U_0^k(\boldsymbol{\xi})}{\partial\xi_j}, \tag{4.13}$$

thus we finally obtain

$$\begin{aligned}&\bar{\nabla}_\xi \cdot (\mathbf{C}(\boldsymbol{\xi})\bar{\nabla}_\xi \mathbf{u}_1(\mathbf{X},\boldsymbol{\xi}))\\ &\quad = \sum_{j,l=0}^{d}\frac{\partial f_0(\mathbf{X})}{\partial X_l}\sum_{k=1}^{n}\left(\frac{\partial C_{ijkl}(\boldsymbol{\xi})}{\partial_{\xi_j}}U_0^k(\boldsymbol{\xi}) + (C_{ijkl}(\boldsymbol{\xi}) + C_{ilkj}(\boldsymbol{\xi}))\frac{\partial U_0^k(\boldsymbol{\xi})}{\partial\xi_j}\right),\quad i = 1, 2, \ldots, n.\end{aligned} \tag{4.14}$$

Proceeding like in §2, we multiply the system (4.14) by the field $\mathbf{U_0^*}$ and then integrate the obtained identity over the cell Q to eliminate the vector $\mathbf{u_1}$. This gives the following result:

Theorem 4.1. *By the analogy of theorem 3.5, the system (4.1) homogenizes to the following equation:*

$$\sum_{l=0}^{d} d_l \frac{\partial f_0(\mathbf{X})}{\partial X_l} = 0, \tag{4.15}$$

where the coefficients d_l entering the homogenized equation are given by the formulae:

$$\begin{aligned} d_l = \frac{1}{|\Lambda|} \int_\Lambda \sum_{j=0}^{d} \sum_{i,k=1}^{n} \Bigg[& \frac{\partial C_{ijkl}(\boldsymbol{\xi})}{\partial \xi_j} U_0^k(\boldsymbol{\xi}) U_0^{i*}(\boldsymbol{\xi}) \\ & + (C_{ijkl}(\boldsymbol{\xi}) + C_{ilkj}(\boldsymbol{\xi})) \frac{\partial U_0^k(\boldsymbol{\xi})}{\partial \xi_j} U_0^{i*}(\boldsymbol{\xi}) \Bigg] \mathrm{d}\boldsymbol{\xi}, \quad l = 1, 2, \ldots, d. \end{aligned} \tag{4.16}$$

5. A general case applicable to the Schrödinger equation

Let $\mathbf{x} = (x_0, x_1, \ldots, x_d)$ and $\mathbf{x}' = (x_1, x_2, \ldots, x_d)$. Here x_0 could represent the time, and $\mathbf{x}'$ the remaining spatial coordinates. We aim to homogenize the problem

$$\begin{pmatrix} \mathbf{G} \\ \nabla \cdot \mathbf{G} \end{pmatrix} = \mathbf{L}_\epsilon \left(\frac{\mathbf{x}'}{\epsilon} \right) \begin{pmatrix} \nabla u \\ u \end{pmatrix}, \tag{5.1}$$

where $u(\mathbf{x}) \colon \mathbb{R}^{d+1} \to \mathbb{R}$ is the unknown, $\mathbf{L}_\epsilon(\mathbf{x}') \colon \mathbb{R}^d \to \mathbb{R}^{(d+2)(d+2)}$ is a Hermitian matrix that is cell-periodic in $\mathbf{x}' \in \mathbb{R}^d$.

To see the connection with the Schrödinger equation, we assume $\psi(\mathbf{x})$ denotes the wave function, where $\mathbf{x} = (x_0, \mathbf{x}')$ and $x_0 = t$ denote the time coordinate while $\mathbf{x}'$ the spatial coordinate, $V(\mathbf{x}')$ the time independent electrical potential, $\boldsymbol{\Phi}(\mathbf{x}') = (\Phi_1(\mathbf{x}'), \Phi_2(\mathbf{x}'), \Phi_3(\mathbf{x}'))$ the time independent magnetic potential, with $\mathbf{b} = \nabla \times \boldsymbol{\Phi}$ the magnetic induction, e the charge on the electron, and m its mass. Using the Lorentz gauge, and noting that $V(\mathbf{x}')$ is independent of time, $\boldsymbol{\Phi}(\mathbf{x}')$ can be taken to have zero divergence. Let us also choose units so that $\hbar$, which is Planck's constant divided by 2π, has the value 1. We assume both $V(\mathbf{x}')$ and $\boldsymbol{\Phi}(\mathbf{x}')$ are periodic functions of $\mathbf{x}'$ with the same unit cell. Following Milton [37], the Schrödinger equation in a magnetic field can be written in the form

$$\begin{pmatrix} q_t \\ \mathbf{q}_x \\ \dfrac{\partial q_t}{\partial t} + \nabla' \cdot \mathbf{q}_x \end{pmatrix} = \begin{pmatrix} 0 & 0 & -\dfrac{\mathrm{i}}{2} \\ 0 & \dfrac{-\mathbf{I}}{2m} & \dfrac{\mathrm{i}e\boldsymbol{\Phi}}{2m} \\ +\dfrac{\mathrm{i}}{2} & \dfrac{-\mathrm{i}e\boldsymbol{\Phi}}{2m} & -eV \end{pmatrix} \begin{pmatrix} \dfrac{\partial \psi}{\partial t} \\ \nabla' \psi \\ \psi \end{pmatrix}, \tag{5.2}$$

where $q_t(t, \mathbf{x})$ is a scalar field and $\mathbf{q}_x(t, \mathbf{x}')$ a vector field, and where ∇', and $\nabla' \cdot$ are the gradient and divergence with respect to $\mathbf{x}'$. Expanding out this in matrix form gives

$$\left.\begin{aligned} & q_t = -\frac{\mathrm{i}}{2}\psi, \\ & \mathbf{q}_x = -\frac{1}{2m}\nabla'\psi + \frac{\mathrm{i}e\boldsymbol{\Phi}}{2m}\psi, \\ \text{and} \quad & \frac{\partial q_t}{\partial t} + \nabla' \cdot \mathbf{q}_x = -\frac{(\nabla')^2\psi}{2m} + \frac{\mathrm{i}\nabla' \cdot (e\boldsymbol{\Phi}\psi)}{2m} - \frac{\mathrm{i}}{2}\frac{\partial \psi}{\partial t} = -\frac{\mathrm{i}e\boldsymbol{\Phi}}{2m}\nabla'\psi + \frac{\mathrm{i}}{2}\frac{\partial \psi}{\partial t} - eV\psi, \end{aligned}\right\} \tag{5.3}$$

where $(\nabla')^2$ is the Laplacian with respect to $\mathbf{x}'$. Upon eliminating $\mathbf{q}_x$ and q_t, these imply the familiar form for Schrödinger's equation in a magnetic field:

$$\mathrm{i}\frac{\partial \psi}{\partial t} = \frac{1}{2m}[\mathrm{i}\nabla' + e\boldsymbol{\Phi}]^2\psi + eV\psi. \tag{5.4}$$

Setting $\mathbf{G} = (q_t, \mathbf{q}_x)$, $\nabla = (\partial/\partial t, \nabla')$ and $u = \psi$, we see that Schrödinger's equation in a magnetic field can be expressed in the form

$$\begin{pmatrix} \mathbf{G} \\ \nabla \cdot \mathbf{G} \end{pmatrix} = \mathbf{L}(\mathbf{x}') \begin{pmatrix} \nabla u \\ u \end{pmatrix}, \quad \text{with } \mathbf{L}(\mathbf{x}') = \begin{pmatrix} \mathbf{a} & \mathbf{b}(\mathbf{x}') \\ (\mathbf{b}(\mathbf{x}'))^{T*} & c(\mathbf{x}') \end{pmatrix}, \tag{5.5}$$

where

$$\mathbf{a} = \begin{pmatrix} 0 & 0 \\ 0 & \dfrac{-\mathbf{I}}{2m} \end{pmatrix}, \quad \mathbf{b}(\mathbf{x}') = \begin{pmatrix} -\dfrac{\mathrm{i}}{2} \\ \dfrac{\mathrm{i}e\boldsymbol{\Phi}(\mathbf{x}')}{2m} \end{pmatrix}, \quad c(\mathbf{x}') = -\mathbf{e}V(\mathbf{x}'). \tag{5.6}$$

With appropriate scaling, this is of the form (5.1).

Equation (5.1) will be called a constitutive relation, as it relates u and its gradient ∇u to $\mathbf{G}$ and its divergence $\nabla \cdot \mathbf{G}$ through the matrix $\mathbf{L}_\epsilon$. Let $\mathbf{X} = (X_0, X_1, \ldots, X_d)$ be the slow variable and let $\boldsymbol{\xi} = \mathbf{X}/\epsilon$ be the fast variable. Furthermore, we denote $\boldsymbol{\xi}' = (\xi_1, \xi_2, \ldots, \xi_d)$. We assume that the matrix $\mathbf{L}_\epsilon$ has the form

$$\mathbf{L}_\epsilon = \begin{pmatrix} \mathbf{a}(\boldsymbol{\xi}') & \dfrac{\mathbf{b}(\boldsymbol{\xi}')}{\epsilon} \\ \dfrac{(\mathbf{b}(\boldsymbol{\xi}'))^{T*}}{\epsilon} & \dfrac{c(\boldsymbol{\xi}')}{\epsilon^2} \end{pmatrix},$$

where we assume that $\mathbf{a} \in \mathbb{R}^{(d+1)\times(d+1)}$ is a real symmetric matrix, $\mathbf{b} \in \mathbb{C}^{(d+1)\times 1}$ is a complex divergence free field and $c \in \mathbb{R}$ is a real function. With our choice of the Lorentz gauge, $\mathbf{b}(\mathbf{x})$ is divergence free for the Schrödinger equation in a magnetic field.

Next, we expand u and $\mathbf{G}$ in powers of ϵ :

$$\left.\begin{aligned} \mathbf{G} &= \mathbf{G}_0 + \epsilon \mathbf{G}_1 + \epsilon^2 \mathbf{G}_2 + \cdots \\ \text{and} \qquad u &= u_0 + \epsilon u_1 + \epsilon^2 u_2 + \cdots . \end{aligned}\right\} \tag{5.7}$$

After replacing ∇ by $\nabla_X + (1/\epsilon)\nabla_\xi$ and equating the coefficients of the same power of ϵ on both sides of (5.1), we obtain the following equations in orders of ϵ^{-1} and ϵ^0, respectively:

— [Order ϵ^{-1}].

$$\begin{aligned} \mathbf{G}_0(\mathbf{X}, \boldsymbol{\xi}) &= \mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_0(\mathbf{X}, \boldsymbol{\xi}) + \mathbf{b}(\boldsymbol{\xi}')u_0(\mathbf{X}, \boldsymbol{\xi}) \\ \nabla_\xi \cdot \mathbf{G}_0 &= c(\boldsymbol{\xi}')u_0(\mathbf{X}, \boldsymbol{\xi}) + (\mathbf{b}(\boldsymbol{\xi}'))^* \nabla_\xi u_0(\mathbf{X}, \boldsymbol{\xi}) \end{aligned}$$

from which we get the Bloch equation for u_0 :

$$\nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_0) + (\mathbf{b}(\boldsymbol{\xi}') - (\mathbf{b}(\boldsymbol{\xi}'))^*) \cdot \nabla_\xi u_0 - c(\boldsymbol{\xi}')u_0 = 0. \tag{5.8}$$

— [Order ϵ^0]. In the zeroth order, we get the following system

$$\begin{aligned} \mathbf{G}_1(\mathbf{X}, \boldsymbol{\xi}) &= \mathbf{a}(\boldsymbol{\xi}')(\nabla_X u_0(\mathbf{X}, \boldsymbol{\xi}) + \nabla_\xi u_1(\mathbf{X}, \boldsymbol{\xi})) + \mathbf{b}(\boldsymbol{\xi}')u_1(\mathbf{X}, \boldsymbol{\xi}) \\ \nabla_x \cdot \mathbf{G}_0 + \nabla_\xi \cdot \mathbf{G}_1 &= (\mathbf{b}(\boldsymbol{\xi}'))^*(\nabla_x u_0(\mathbf{X}, \boldsymbol{\xi}) + \nabla_\xi u_1(\mathbf{X}, \boldsymbol{\xi})) + c(\boldsymbol{\xi}')u_1(\mathbf{X}, \boldsymbol{\xi}), \end{aligned}$$

from where we get by eliminating $\mathbf{G}_0$ and $\mathbf{G}_1$,

$$\begin{aligned} &\nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_1) + (\mathbf{b}(\boldsymbol{\xi}') - (\mathbf{b}(\boldsymbol{\xi}'))^*) \cdot \nabla_\xi u_1 - c(\boldsymbol{\xi}')u_1 \\ &\quad = -\nabla_X \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_0) - \nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_x u_0) - \nabla_X \cdot (\mathbf{b}(\boldsymbol{\xi}')u_0) + (\mathbf{b}(\boldsymbol{\xi}'))^* \cdot \nabla_X u_0. \end{aligned} \tag{5.9}$$

Next we assume, $u_j(\mathbf{X}, \boldsymbol{\xi})$ is such that the functions $\mathrm{e}^{\mathrm{i}(k\boldsymbol{\xi}' - \omega\xi_0)}u_j(\mathbf{X}, \boldsymbol{\xi})$ are periodic in $\boldsymbol{\xi}'$ and do not depend on ξ_0. We, furthermore, assume that $u_0(\mathbf{X}, \boldsymbol{\xi})$ solves the Bloch equation

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(5.8) and thus is separable in the fast and slow variables, namely we get

$$u_0(\mathbf{X}, \boldsymbol{\xi}) = U_0(\boldsymbol{\xi}')f_0(\mathbf{X}). \tag{5.10}$$

We have that

$$-\nabla_x \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_0) - \nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_x u_0) - \nabla_X \cdot (\mathbf{b}(\boldsymbol{\xi}')u_0) + (\mathbf{b}(\boldsymbol{\xi}'))^* \cdot \nabla_X u_0 =$$
$$= -\sum_{i,j=0}^{d} \frac{\partial f_0(\mathbf{X})}{\partial X_j}\left(2C_{ij}(\boldsymbol{\xi}')\frac{\partial U_0(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i}U_0(\boldsymbol{\xi}) - (b_j(\xi') + (b_j(\xi'))^*)U_0\right).$$

Thus, we get combining with (5.10),

$$\nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_1) + (\mathbf{b}(\boldsymbol{\xi}') - (\mathbf{b}(\boldsymbol{\xi}'))^*) \cdot \nabla_\xi u_1 - c(\boldsymbol{\xi}')u_1$$
$$= -\sum_{i,j=0}^{d} \frac{\partial f_0(\mathbf{X})}{\partial X_j}\left(2C_{ij}(\boldsymbol{\xi}')\frac{\partial U_0(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i}U_0(\boldsymbol{\xi}) - (b_j(\xi') + (b_j(\xi'))^*)U_0\right). \tag{5.11}$$

Next, we multiply equation (5.11) by U_0^* and integrate over $\bar{Q}$ to eliminate u_1 and obtain the effective equation. We proceed by the analogy of (2.14)–(2.20). First, by taking the complex conjugate of Bloch equation (5.8), we get

$$\nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi U_0^*) - (\mathbf{b}(\boldsymbol{\xi}') - (\mathbf{b}(\boldsymbol{\xi}'))^*) \cdot \nabla_\xi U_0^* - c(\boldsymbol{\xi}')U_0^* = 0, \tag{5.12}$$

thus by multiplying equation (5.12) by u_1 and integrating over a rectangle Q by parts and using the divergence-free property of $\mathbf{b}$, we get

$$0 = \int_Q u_1(\nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi U_0^*) - (\mathbf{b}(\boldsymbol{\xi}') - (\mathbf{b}(\boldsymbol{\xi}'))^*) \cdot \nabla_\xi U_0^* - c(\boldsymbol{\xi}'))U_0^*)\,\mathrm{d}\boldsymbol{\xi}$$
$$= \int_Q U_0^*(\nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_1) + U_0^*(\mathbf{b}(\boldsymbol{\xi}') - (\mathbf{b}(\boldsymbol{\xi}'))^*) \cdot \nabla_\xi u_1 - c(\boldsymbol{\xi}')u_1)\mathrm{d}\boldsymbol{\xi}$$
$$+ \text{surface term}, \tag{5.13}$$

thus by the analogy of (2.14)–(2.20), we get

$$\lim_{Q\to\infty} \frac{1}{|Q|}\int_Q U_0^*(\nabla_\xi \cdot (\mathbf{a}(\boldsymbol{\xi}')\nabla_\xi u_1) + U_0^*(\mathbf{b}(\boldsymbol{\xi}') - (\mathbf{b}(\boldsymbol{\xi}'))^*) \cdot \nabla_\xi u_1 - c(\boldsymbol{\xi}')u_1)\,\mathrm{d}\boldsymbol{\xi} = 0. \tag{5.14}$$

Finally, combining (5.14) and (5.11) we arrive at the effective equation

$$\sum_{j=0}^{d} d_j \frac{\partial f_0(\mathbf{X})}{\partial X_j} = 0, \tag{5.15}$$

where by the analogy of theorem 3.5, one has

$$d_j = \sum_{i=0}^{d} \frac{1}{|\Lambda|}\int_\Lambda U_0^*\left(2C_{ij}(\boldsymbol{\xi}')\frac{\partial U_0(\boldsymbol{\xi})}{\partial \xi_i} + \frac{\partial C_{ij}(\boldsymbol{\xi}')}{\partial \xi_i}U_0(\boldsymbol{\xi}) - (b_j(\xi') + (b_j(\xi'))^*)U_0\right)\mathrm{d}\boldsymbol{\xi}. \tag{5.16}$$

6. Simplifying the effective equation

In this section, we relate the dispersion relation $\omega = g(\mathbf{k})$ and the effective coefficients.

(a) The scalar case

Assume we have the effective equation (3.4) for a single wave $(\mathbf{k}, \omega)$. Identifying $X_0, X_1, \ldots X_d$ with $t, x_1, \ldots x_d$, we can rewrite it in the following way:

$$\mathbf{a}_1 \cdot \nabla f_0(t, \mathbf{x}) + b_1 \frac{\partial f_0(t, \mathbf{x})}{\partial t} = 0. \tag{6.1}$$

Assume $\epsilon > 0$ is small enough, and suppose the pair $(\mathbf{k} + \epsilon\delta\mathbf{k}, \omega + \epsilon\delta\omega)$ also lies on the dispersion relation. Since $g(\mathbf{k} + \epsilon\delta\mathbf{k}) = g(\mathbf{k}) + \epsilon\delta\mathbf{k} \cdot \nabla g(\mathbf{k}) + \mathcal{O}(\epsilon^2)$, we have $\delta\omega = \delta\mathbf{k} \cdot \nabla g(\mathbf{k}) + \mathcal{O}(\epsilon)$. We know one solution of the wave equation is the Bloch solution

$$u(\mathbf{x}, t) = \mathrm{e}^{\mathrm{i}[(\mathbf{k}+\epsilon\delta\mathbf{k})\cdot(\mathbf{x}/\epsilon) - (\omega\epsilon\delta\omega)(t/\epsilon)]} V_\epsilon\left(\frac{\mathbf{x}}{\epsilon}\right), \tag{6.2}$$

where with $\mathbf{x}/\epsilon = \boldsymbol{\xi}'$, $V_\epsilon(\boldsymbol{\xi}')$ satisfies Bloch equations

$$(\omega + \epsilon\delta\omega)^2 b(\boldsymbol{\xi}') V_\epsilon(\boldsymbol{\xi}') + (-\mathrm{i}(\mathbf{k} + \epsilon\delta\mathbf{k}) + \bar{\nabla}_{\xi'}) \cdot \mathbf{a}(\boldsymbol{\xi}')(-\mathrm{i}(\mathbf{k} + \epsilon\delta\mathbf{k}) + \bar{\nabla}_{\xi'}) V_\epsilon(\boldsymbol{\xi}') = 0 \tag{6.3}$$

and $V_\epsilon(\boldsymbol{\xi})$ is periodic in $\boldsymbol{\xi}$. With appropriate normalizations to ensure this has a unique solution for $V_\epsilon(\boldsymbol{\xi}')$, we can write

$$V_\epsilon(\boldsymbol{\xi}') = V_0(\boldsymbol{\xi}') + \left.\frac{\partial V_\epsilon(\boldsymbol{\xi}')}{\partial \epsilon}\right|_{\epsilon=0} \epsilon + \mathcal{O}(\epsilon^2). \tag{6.4}$$

So (6.2) has the expansion

$$u(\mathbf{x}, t) = f(t, \mathbf{x}) U_0(\boldsymbol{\xi}') + \mathcal{O}(\epsilon), \quad \text{with } f(t, \mathbf{x}) = \mathrm{e}^{\mathrm{i}(\delta\mathbf{k}\cdot\mathbf{x} - \delta\omega t)}. \tag{6.5}$$

Then it is clear that the function $f_0 = \mathrm{e}^{\mathrm{i}(\delta\mathbf{k}\cdot\mathbf{x} - \delta\omega t)}$ must solve equation (6.1) from which we get

$$\mathrm{i}(\mathbf{a}_1 \cdot \delta\mathbf{k} - b_1 \nabla g(\mathbf{k}) \cdot \delta\mathbf{k}) = 0, \quad \text{for all } \delta\mathbf{k} \in \mathbb{R}^d,$$

from where we get

$$\mathbf{a}_1 = b_1 \nabla g(\mathbf{k}). \tag{6.6}$$

Thus, the effective equation becomes

$$\nabla g \cdot \nabla f_0(t, \mathbf{x}) + \frac{\partial f_0(t, \mathbf{x})}{\partial t} = 0, \tag{6.7}$$

Note that the solution of this equation is the travelling wave packet

$$f_0(t, \mathbf{x}) = h(\mathbf{v} \cdot \mathbf{x} - t)),$$

where h is an arbitrary function that has first partial derivatives, and $\mathbf{v}$ is the group velocity which satisfies $\mathbf{v} \cdot \nabla g = 1$. As mentioned in the introduction this effective equation fails to capture dispersion which is captured in the approach of Allaire *et al.* [29].

(b) The vector case

As effective equations (4.15) in the vector case are exactly the same as in the scalar case, then we get the same relation as in the scalar case.

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Appendix A

Here we make the connection between the results of Birman & Suslina [23] and those of Craster *et al.* [21]. The first thing that is relevant is eqn (1.12) of Birman & Suslina [23], where they expand at the edge E_s of a band-gap (where E_s may represent an energy or frequency) a minimum or maximum of the dispersion diagram as a quadratic form, involving quadratic functions $b^{(\pm)}$. These quadratic functions determine the 'effective coefficients' that enter the homogenized equations of Craster *et al.* [21]. In that formula (1.12), the $\xi^{(\pm)}$ is the wave vector $\mathbf{k}=\xi$, one expands around. (They assume there may be $j=1,2,\ldots m_{\pm}$ such wavevectors attaining the same energy E_s, but here, for simplicity, we assume there is just one.) The $\psi_{s\pm}(\mathbf{x},\boldsymbol{\xi})$ at the top of p. 3685 is the eigenfunction, or Bloch function, associated with E_s. The main result is that the resolvent (2.1) approaches (2.2). The connection is clearer if one writes out what this means. Let us suppose there is a source term $g(\mathbf{x})$. Then if you are interested in solving $[A-(\lambda-\epsilon^2\kappa^2)]u=g$, where κ is chosen so $(\lambda-\kappa^2)$ is in the gap, and $\epsilon\in(0,1]$, the solution is $u=S(\epsilon)g$, where $S(\epsilon)$ is the resolvent. Birman and Suslina say that when ϵ is small, the result is approximately the same as solving $u=S^0(\epsilon)g$, i.e.

$$[b_j(D)+\epsilon^2]\left(\frac{u}{\psi_{s\pm}}\right)=\left(\frac{g}{\psi_{s\pm}}\right). \tag{A 1}$$

Here $u/\psi_{s\pm}$ can be identified with the modulating function f of Craster *et al.* [21], $b_j(D)$ is the effective operator, D is the operator $-\mathrm{i}\nabla$ (see point 3 in introduction). Thus the analysis of Birman & Suslina [23] applies even when there are source terms $g\neq 0$ and allows for expansion points $\xi^{(\pm)}$ which are not necessarily at $\mathbf{k}=\xi^{(\pm)}=0$ or at the edge of the Brillouin zone. The reason Birman & Suslina [23] assume one is in the gap is to make sure the solution is localized, which is easier for the mathematical analysis.

Appendix B

Definition B.1. Assume $Q=\prod_{i=1}^{d}[a_i,b_i]\subset\mathbb{R}^d$ is a rectangle. Then we write $Q\to\infty$ if $b_i-a_i\to\infty$, for all $i\in\{1,2,\ldots,d\}$.

The next two lemmas will be crucial in the process of homogenization.

Lemma B.2. *Assume $f:\mathbb{R}\to\mathbb{R}$ is periodic with a period $T>0$ and $f\in L^2(0,T)$. Then for any $b\neq 0$ there holds*:

$$\left.\begin{aligned}&\lim_{a\to\infty}\frac{1}{a}\int_0^a f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x=0, \quad \textit{if } \frac{Tb}{2\pi}\notin\mathbb{Z}\\ \textit{and}\quad &\lim_{a\to\infty}\frac{1}{a}\int_0^a f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x=\frac{1}{T}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x, \quad \textit{if } \frac{Tb}{2\pi}\in\mathbb{Z}.\end{aligned}\right\} \tag{B 1}$$

Proof. Note that if $a=mT+r$, where $0\le r<T$ and $m\in\mathbb{Z},\ m\ge 0$, then we have

$$\begin{aligned}\frac{1}{a}\int_0^a f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x&=\frac{1}{a}\int_0^{mT+r} f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x\\ &=\frac{1}{a}\int_{mT}^{mT+r} f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x+\frac{1}{mT+r}\sum_{j=0}^{m-1}\int_{jT}^{(j+1)T} f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x\\ &=\frac{1}{a}\int_{mT}^{mT+r} f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x+\frac{1}{mT+r}\sum_{j=0}^{m-1}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}b(x+jT)}\,\mathrm{d}x\\ &=\frac{1}{a}\int_{mT}^{mT+r} f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x+\frac{1}{mT+r}\sum_{j=0}^{m-1}\mathrm{e}^{\mathrm{i}bTj}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x.\end{aligned} \tag{B 2}$$

We have by the Schwartz inequality that

$$\left|\frac{1}{a}\int_{mT}^{mT+r} f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x\right| \le \frac{1}{a}\int_0^T |f(x)|\,\mathrm{d}x \le \frac{\sqrt{T}}{a}\|f\|_{L^2(0,T)} \to 0, \quad \text{as } a\to\infty. \tag{B 3}$$

On the other hand, we have

$$\left.\begin{aligned} &\frac{1}{mT+r}\sum_{j=0}^{m-1}\mathrm{e}^{\mathrm{i}bTj}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x = \frac{m}{mT+r}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x, \quad \text{if } bT=2\pi l\\ \text{and}\quad &\frac{1}{mT+r}\sum_{j=0}^{m-1}\mathrm{e}^{\mathrm{i}bTj}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x = \frac{(1-\mathrm{e}^{\mathrm{i}bTm})}{(mT+r)(1-\mathrm{e}^{\mathrm{i}bT})}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x, \quad \text{if } bT\neq 2\pi l. \end{aligned}\right\} \tag{B 4}$$

In the first case, we get

$$\begin{aligned} \lim_{a\to\infty}\frac{1}{a}\int_0^a f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x &= \lim_{m\to\infty}\frac{m}{mT+r}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x\\ &= \frac{1}{T}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x, \end{aligned} \tag{B 5}$$

In the second case, we have again by the Schwartz inequality that

$$\left|\frac{(1-\mathrm{e}^{\mathrm{i}bTm})}{(mT+r)(1-\mathrm{e}^{\mathrm{i}bT})}\int_0^T f(x)\,\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x\right| \le \frac{2\sqrt{T}\|f\|_{L^2(0,T)}}{a|1-\mathrm{e}^{\mathrm{i}bT}|}, \tag{B 6}$$

thus we get

$$\lim_{a\to\infty}\frac{1}{a}\int_0^a f(x)\mathrm{e}^{\mathrm{i}bx}\,\mathrm{d}x = 0.$$

■

The next lemma is generalization of lemma B.2.

Lemma B.3. *Let the functions $f,g\colon \mathbb{R}\to\mathbb{R}$ have periods $T_1,T_2>0$ respectively. Assume that $f\in L^2(0,T_1)$ and $g\in L^2(0,T_2)$ and*

$$\int_0^{T_1} f(x)\,\mathrm{d}x = 0. \tag{B 7}$$

Then one has:

$$\left.\begin{aligned} &\lim_{a\to\infty}\frac{1}{a}\int_0^a f(x)g(x)\,\mathrm{d}x = 0, \quad \textit{if } \frac{T_1}{T_2}\notin\mathbb{Q}\\ \textit{and}\quad &\lim_{a\to\infty}\frac{1}{a}\int_0^a f(x)g(x)\,\mathrm{d}x = \frac{1}{nT_1}\int_0^{nT_1} f(x)g(x)\,\mathrm{d}x, \quad \textit{if } \frac{T_1}{T_2}=\frac{m}{n}, \quad m,n\in\mathbb{Z}. \end{aligned}\right\} \tag{B 8}$$

Proof. Assume first that $T_1/T_2=m/n$, where $m,n\in\mathbb{N}$, thus $nT_1=mT_2$. We have for any $a>nT_1$, that $a=knT_1+r$, where $0\le r<nT_1$ and $k\in\mathbb{N}$. Then we have by the periodicity of f and g that

$$\begin{aligned} \frac{1}{a}\int_0^a f(x)g(x)\,\mathrm{d}x &= \frac{1}{knT_1+r}\int_0^{knT_1} f(x)g(x)\,\mathrm{d}x + \frac{1}{knT_1+r}\int_{knT_1}^{knT_1+r} f(x)g(x)\,\mathrm{d}x\\ &= \frac{k}{knT_1+r}\int_0^{nT_1} f(x)g(x)\,\mathrm{d}x + \frac{1}{knT_1+r}\int_{knT_1}^{knT_1+r} f(x)g(x)\,\mathrm{d}x. \end{aligned} \tag{B 9}$$

It is clear that

$$\begin{aligned} \lim_{a\to\infty}\frac{k}{knT_1+r}\int_0^{nT_1} f(x)g(x)\,\mathrm{d}x &= \lim_{k\to\infty}\frac{k}{knT_1+r}\int_0^{nT_1} f(x)g(x)\,\mathrm{d}x\\ &= \frac{1}{nT_1}\int_0^{nT_1} f(x)g(x)\,\mathrm{d}x, \end{aligned}$$

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and by the Schwartz inequality

$$\left|\frac{1}{knT_1+r}\int_{knT_1}^{knT_1+r} f(x)g(x)\,\mathrm{d}x\right| \le \frac{1}{knT_1}\int_0^{nT_1}|f(x)g(x)|\,\mathrm{d}x$$
$$\le \frac{1}{knT_1}\|f(x)\|_{L^2(0,nT_1)}\|g(x)\|_{L^2(0,nT_1)}$$
$$\to 0$$

as $k\to\infty$, thus the case $T_1/T_2=m/n$ is proved. Assume now that $T_1/T_2\notin\mathbb{Q}$. By the Fourier expansion, we have that

$$f(x)=\sum_{n=-\infty}^{\infty} a_n\,\mathrm{e}^{2i\pi nx/T_1}$$

in the $L^2(0,T_1)$ sense. Denote $P_n(x)=\sum_{k=-n}^{n} a_k\,\mathrm{e}^{2\mathrm{i}\pi kx/T_1}$, then

$$P_n(x)\to f(x)\quad \text{in } L^2(0,T_1),$$

thus for any $\epsilon>0$, there exists $N\in\mathbb{N}$ such that

$$\|f(x)-P_N(x)\|_{L^2(0,T_1)}\le\epsilon. \tag{B 10}$$

If $a=k_1T_1+r_1=k_2T_2+r_2$ where $k_1,k_2\in\mathbb{N}$ and $0\le r_1<T_1$, $0\le r_2<T_2$, then we have by the Schwartz inequality that for big enough a there holds,

$$\begin{aligned}
&\frac{1}{a}\left|\int_0^a f(x)g(x)\,\mathrm{d}x-\int_0^a P_N(x)g(x)\,\mathrm{d}x\right|\\
&\quad\le\frac{1}{a}\int_0^a|f(x)-P_N(x)||g(x)|\,\mathrm{d}x\\
&\quad\le\frac{1}{a}\|f(x)-P_N(x)\|_{L^2(0,a)}\|g(x)\|_{L^2(0,a)}\\
&\quad\le\frac{1}{a}\sqrt{k_1+1}\|f(x)-P_N(x)\|_{L^2(0,T_1)}\sqrt{k_2+1}\|g(x)\|_{L^2(0,T_2)}\\
&\quad\le\frac{\epsilon\|g(x)\|_{L^2(0,T_2)}}{\sqrt{T_1T_2}}\,\frac{\sqrt{(k_1+1)(k_2+1)}}{\sqrt{k_1k_2}}\\
&\quad\le\frac{2\epsilon\|g(x)\|_{L^2(0,T_2)}}{\sqrt{T_1T_2}},
\end{aligned} \tag{B 11}$$

which implies that it suffices to prove the lemma for $P_N(x)$ instead of $f(x)$. From the condition $\int_0^{T_1} f(x)\,\mathrm{d}x=0$, we get $a_0=0$, thus

$$P_N(x)=\sum_{k=-N}^{-1} a_k\,\mathrm{e}^{2i\pi kx/T_1}+\sum_{k=1}^{N} a_k\,\mathrm{e}^{2i\pi kx/T_1}.$$

Now, an application of lemma B.2 to each of the summands $a_k\,\mathrm{e}^{2i\pi kx/T_1}$ completes the proof. ■

Lemma B.4. *Let $f,g\colon\mathbb{R}\to\mathbb{R}$ and $T_1,T_2>0$ be such that $f(x)$ is T_1-periodic, $g(x)$ is T_2-periodic and $T_1/T_2\notin\mathbb{Q}$. Furthermore, assume that $f(x)\in W^{1,2}(0,T_1)$ and $g(x)\in L^2(0,T_2)$. Then*

$$\lim_{a\to\infty}\frac{1}{a}\int_0^a f'(x)g(x)\,\mathrm{d}x=0. \tag{B 12}$$

Proof. The proof directly follows from lemma B.3 as $\int_0^{T_1} f'(x)\,\mathrm{d}x=0$ by the periodicity of f. ■

Lemma B.5. *Assume the function* $f(\boldsymbol{\xi})\colon \mathbb{R}^d \to \mathbb{R}$ *is cell-periodic and continuous with a cell of periodicity* $R = \prod_{i=1}^{d}[0, T_i]$. *Then for any vector* $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_d) \in \mathbb{R}^d$ *one has*

$$\lim_{Q\to\infty} \frac{1}{|Q|} \int_Q f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi} = 0, \quad \text{if } T_j\lambda_j \neq 2\pi l, \ \in \mathbb{Z} \quad \text{for some } j \in \{1, 2, \ldots, d\},$$

$$\lim_{Q\to\infty} \frac{1}{|Q|} \int_Q f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi} = \frac{1}{|R|} \int_R f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi}, \quad \text{if } T_j\lambda_j = 2\pi l_j, l_j \in \mathbb{Z},\ j = 1, 2, \ldots, d.$$

Proof. The proof is straightforward as this is a consequence of the previous lemma. It has easier to see that

$$\lim_{Q\to\infty} \frac{1}{|Q|} \int_Q f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi} = \lim_{l\to\infty} \frac{1}{l^d|R|} \int_{l\cdot R} f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi},$$

where $l \in \mathbb{N}$. If $T_i\lambda_i = 2\pi l_i, l_i \in \mathbb{Z},\ i = 1, 2, \ldots, d$ then we have

$$\frac{1}{l^d|R|} \int_{l\cdot R} f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi} = \frac{1}{|R|} \int_R f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi},$$

for all $l \in \mathbb{N}$. Assume now the set $I = \{j \,:\, T_j\lambda j \neq 2\pi l, l \in \mathbb{Z}\} \cap \{1, 2, \ldots, d\}$ is not empty. Then we have by the analogy of the proof of lemma B.2 and the Fubini theorem

$$\frac{1}{l^d|R|} \int_{l\cdot R} f(\boldsymbol{\xi})\, \mathrm{e}^{\mathrm{i}\lambda\cdot\boldsymbol{\xi}}\, \mathrm{d}\boldsymbol{\xi} \leq \frac{C}{l^{|I|}} \to 0 \quad \text{as } l \to \infty, \tag{B 13}$$

where C is a constant depending on the value $M = \max_R |f(x)|$. The proof is finished now. ■

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