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HOMOGENIZATION OF THE SCHRÖDINGER EQUATION WITH A TIME OSCILLATING POTENTIAL

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Abstract. We study the homogenization of a Schrödinger equation in a periodic medium with a time dependent potential. This is a model for semiconductors excited by an external electromagnetic wave. We prove that, for a suitable choice of oscillating (both in time and space) potential, one can partially transfer electrons from one Bloch band to another. This justifies the famous "Fermi golden rule" for the transition probability between two such states which is at the basis of various optical properties of semiconductors. Our method is based on a combination of classical homogenization techniques (two-scale convergence and suitable oscillating test functions) and of Bloch waves theory.

1. Introduction.

This work is devoted to the mathematical justification of a problem of mean field approximation in solid state physics. More precisely, we study the homogenization of the following Schrödinger equation

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

where $0 < T < +\infty$ is a final time. The potential $c(y)$ is a real, bounded and periodic function defined for $y \in \mathbb{T}^N$ (the unit torus). Equation (1) is the so-called one-electron model for describing the electrons in a crystal or in a semiconductor, characterized by the periodic potential $c(y)$ [7], [8], [24]. An exterior field is also applied to the sample: in first approximation it is described by another real potential $d_\epsilon(t,x)$ which depends also on the time variable in contrast to c (see Section 4 for the case of an electromagnetic potential). In (1) the size of the background microscopic potential is of order ϵ^{-2} while that of the exterior macroscopic potential is of order ϵ^0, so d_ϵ is just a small perturbation (the relative size of which is the square of the period). It can also be seen as a control acting on the semiconductor and its specific dependence on ϵ will vary with the initial condition and the desired final or target

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state at time T (see (4) below). For example, the exterior potential can be light illuminating the semiconductor: if its energy is high enough, it can excite electrons from the valence band to conduction band. This effect is called optical absorption. Its converse effect (light emitted by electrons going from the conduction band to the valence band) is at the root of many important devices such as lasers, light emitting diodes and photo-detectors [8], [23], [24].

Remark that Planck's constant has been normalized to unity in (1). We emphasize that the ϵ-scaling in (1) is not the usual semi-classical scaling for Schrödinger equation [6], [11], [12], [13], [14], [19] which would involve a ϵ^{-1} coefficient in front of the time derivative. Instead, it is the scaling of homogenization as in [2], [3], [4]. In physical terms it corresponds to an asymptotic study for much longer times than in the semi-classical limit (we refer to [3] for a more complete discussion of the scaling).

Let us describe a typical example of our results. We introduce the so-called Bloch or shifted cell problem,

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

where $\theta \in \mathbb{T}^N$ is a parameter and $(\lambda_n(\theta), \psi_n(y,\theta))$ is the n-th eigencouple. In physical terms, the Bloch frequency θ is the quasi momentum and the range of $\lambda_n(\theta)$, as θ varies, is a Bloch or energy band. We consider an initial data which is a wave packet of the type

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

and we would like to attain a final state at a different momentum θ^m and energy $\lambda_m(\theta^m)$

$$u_\epsilon^T(x) = \psi_m\left(\frac{x}{\epsilon}, \theta^m\right) e^{2i\pi\frac{\theta^m\cdot x}{\epsilon}} v^T(x). \tag{3}$$

For achieving this goal we choose an oscillating potential

$$d_\epsilon(t,x) = \Re\left(e^{i\frac{(\lambda_m(\theta^m)-\lambda_n(\theta^n))t}{\epsilon^2}} e^{2i\pi\frac{(\theta^m-\theta^n)\cdot x}{\epsilon}}\right) d\left(t, x, \frac{x}{\epsilon}\right), \tag{4}$$

where $\Re$ denotes the real part, and $d(t,x,y)$ is a real potential defined on $[0,T]\times \mathbb{R}^N \times \mathbb{T}^N$. Formula (4) for the potential is quite natural: the oscillating phase in time corresponds to the energy difference between the initial and final state (2), (3), while the oscillating phase in space corresponds to the momentum difference. In other words, the potential puts energy and momentum in the system so as to have global conservation of these quantities.

In truth we cannot reach (even approximately) the desired final state (3). Instead we end up with a mixed state, combination of (2) and (3). Under the assumption that θ^n and θ^m are critical points of their non-degenerate energy levels (which implies that the group velocities of the wave packets (2) and (3) vanish) and are non-resonant (which means that no other state are excited by the external potential), see (7) and (8) below, we shall prove in Theorem 1 that the solution of (1) satisfies

$$u_\epsilon(t,x) \approx e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v_n(t,x) + e^{i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{2i\pi\frac{\theta^m\cdot x}{\epsilon}} \psi_m\left(\frac{x}{\epsilon}, \theta^m\right) v_m(t,x),$$

where the macroscopic profile (v_n, v_m) is the unique solution of the following Schrödinger homogenized coupled system

$$\begin{cases} i\dfrac{\partial v_n}{\partial t} - \operatorname{div}(A_n^* \nabla v_n) + d_{nm}^*(t,x)\, v_m = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ i\dfrac{\partial v_m}{\partial t} - \operatorname{div}(A_m^* \nabla v_m) + d_{mn}^*(t,x)\, v_n = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v_n(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N \\ v_m(t=0,x) = 0 & \text{in } \mathbb{R}^N, \end{cases} \tag{5}$$

with homogenized coefficients A_n^*, A_m^* and $d_{nm}^* = \overline{d}_{mn}^*$. The tensors A_n^* and A_m^* are the inverses of the effective masses of the particles corresponding to the initial and desired final state. The coupling coefficient d_{nm}^* is given by a formula (see (20) and Remark 2) known as "Fermi golden rule" [7], [9], [23]. The homogenized system (5) is a model for light absorption in semiconductors. When $\theta^n = \theta^m$ one talks about "direct" absorption, and when $\theta^n \neq \theta^m$ about "indirect" absorption [7], [8], [23], [24]. In truth, one does not find (5), as it stands, in the physical literature where instead a simpler semi-classical picture is used. Specifically, physicists talk about the transition probability between the two states (2) and (3), which is precisely equal to the squared modulus of the coupling coefficient d_{nm}^*.

To obtain the homogenized limit (5) we follow the method introduced in [2], [3]. The main idea is to use Bloch wave theory to build adequate oscillating test functions and pass to the limit using two-scale convergence [1], [18].

The content of this paper is as follows. Section 2 is devoted to recalling basic facts about Bloch waves and two-scale convergence as well as stating our main assumption. Section 3 gives our main result of homogenization. Section 4 focuses on a generalization of the Schrödinger equation (1) which takes into account an electromagnetic field. Finally Section 5 is concerned with a resonant case where more than two states are coupled.

2. **Bloch spectrum and two-scale convergence.**

In this section we recall some results on Bloch waves and two-scale convergence, and we introduce our main assumptions on the initial and target states.

We assume that the potential $c(y)$ is a real measurable bounded periodic function, i.e. belongs to $L^\infty(\mathbb{T}^N)$, while the potential $d(t,x,y)$, appearing in (4), is real, measurable, uniformly bounded, periodic in y and smooth in (t,x). We recall that, for given θ, the Bloch (or shifted) spectral cell equation

$$-(\operatorname{div}_y + 2i\pi\theta)\Big((\nabla_y + 2i\pi\theta)\psi_n\Big) + c(y)\psi_n = \lambda_n(\theta)\psi_n \quad \text{in } \mathbb{T}^N, \tag{6}$$

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 $\|\psi_n\|_{L^2(\mathbb{T}^N)} = 1$, since its Green operator is a compact self-adjoint complex-valued operator on $L^2(\mathbb{T}^N)$. The dual parameter θ is called the Bloch frequency or quasi momentum and it runs in the dual cell of $\mathbb{T}^N$, which, by our choice of normalization factor 2π in the phase factor, is again the unit torus $\mathbb{T}^N$. In other words, by periodicity it is enough to consider $\theta \in \mathbb{T}^N$. For more details on Bloch waves, see e.g. [10], [22].

In the sequel, we shall consider two energy levels $n, m \geq 1$ and Bloch parameters $\theta^n, \theta^m \in \mathbb{T}^N$ such that the eigenvalues $\lambda_n(\theta^n)$ and $\lambda_m(\theta^m)$ satisfy the following assumption

$$\text{for } p = n, m \quad \begin{cases} (i) & \lambda_p(\theta^p) \text{ is a simple eigenvalue,} \\ (ii) & \theta^p \text{ is a critical point of } \lambda_p(\theta) \text{ i.e., } \nabla_\theta \lambda_p(\theta^p) = 0. \end{cases} \tag{7}$$

Of course, we assume that, either $n \neq m$, or $n = m$ and $\theta^n \neq \theta^m$ (if $n = m$ and $\theta^n = \theta^m$, then $d_\epsilon = d(t, x, x/\epsilon)$ and this case was already treated in [3]). The simplicity assumption, i.e. part (i) of (7), is generic and simplifies considerably the analysis. In particular, it implies that $\lambda_p(\theta)$ is infinitely differentiable in a vicinity of θ^p, and one can introduce the group velocity $\nabla_\theta \lambda_p(\theta)$. The criticality assumption, i.e. part (ii) of (7), is physically relevant when states at the bottom or top of Bloch bands are considered. For a discussion of this type of assumptions, as well as possible weaker ones, we refer to [3].

We also add a non-resonant assumption

$$(iii) \quad \text{for any } p \geq 1, \quad \lambda_p(2\theta^n - \theta^m) \neq 2\lambda_n(\theta^n) - \lambda_m(\theta^m). \tag{8}$$

The interpretation of assumption (8) is the following. The oscillating potential d_ϵ, defined by (4), has been designed to transfer the initial state with (quasi) momentum θ^n and energy $\lambda_n(\theta^n)$ to the target state $\theta^m, \lambda_m(\theta^m)$. The only requirement is that momentum and energy are conserved during this process. Actually there is another possible state that can be reached under the conservative action of d_ϵ, namely the state with momentum $2\theta^n - \theta^m$ and energy $2\lambda_n(\theta^n) - \lambda_m(\theta^m)$. In order to simplify the analysis, assumption (8) forbids this additional state as a standing wave solution of (1) without exterior potential. Section 5 explores the resonant case where (8) is not satisfied.

Under assumption (7) it is well-known [15] that one can make a choice of an eigenvector such that the n-th eigencouple of (6) is smooth in a neighborhood of θ^n. Introducing the operator $\mathbb{A}_n(\theta)$ defined on $L^2(\mathbb{T}^N)$ by

$$\mathbb{A}_n(\theta)\psi = -(\mathrm{div}_y + 2i\pi\theta)\Big((\nabla_y + 2i\pi\theta)\psi\Big) + c(y)\psi - \lambda_n(\theta)\psi, \tag{9}$$

we differentiate (6) with respect to θ. Denoting by $(e_k)_{1\leq k\leq N}$ the canonical basis of $\mathbb{R}^N$ and by $(\theta_k)_{1\leq k\leq N}$ the components of θ, the first derivative satisfies

$$\mathbb{A}_n(\theta)\frac{\partial \psi_n}{\partial \theta_k} = 2i\pi e_k \cdot (\nabla_y + 2i\pi\theta)\psi_n + (\mathrm{div}_y + 2i\pi\theta)\,(2i\pi e_k \psi_n) + \frac{\partial \lambda_n}{\partial \theta_k}(\theta)\psi_n, \tag{10}$$

and the second derivative is

$$\begin{aligned} \mathbb{A}_n(\theta)\frac{\partial^2 \psi_n}{\partial \theta_k \partial \theta_l} \quad &= 2i\pi e_k \cdot (\nabla_y + 2i\pi\theta)\frac{\partial \psi_n}{\partial \theta_l} + (\mathrm{div}_y + 2i\pi\theta)\left(2i\pi e_k \frac{\partial \psi_n}{\partial \theta_l}\right) \\ &+2i\pi e_l \cdot (\nabla_y + 2i\pi\theta)\frac{\partial \psi_n}{\partial \theta_k} + (\mathrm{div}_y + 2i\pi\theta)\left(2i\pi e_l \frac{\partial \psi_n}{\partial \theta_k}\right) \\ &+\frac{\partial \lambda_n}{\partial \theta_k}(\theta)\frac{\partial \psi_n}{\partial \theta_l} + \frac{\partial \lambda_n}{\partial \theta_l}(\theta)\frac{\partial \psi_n}{\partial \theta_k} \\ &-8\pi^2 e_k \cdot e_l \psi_n + \frac{\partial^2 \lambda_n}{\partial \theta_l \partial \theta_k}(\theta)\psi_n \end{aligned} \tag{11}$$

Under assumption (7) we have $\nabla_\theta \lambda_n(\theta^n) = 0$, thus equations (10) and (11) simplify for $\theta = \theta^n$ and we find

$$\frac{\partial \psi_n}{\partial \theta_k}(\theta^n) = 2i\pi\zeta_n^k, \quad \frac{\partial^2 \psi_n}{\partial \theta_k \partial \theta_l}(\theta^n) = -4\pi^2\chi_n^{kl}, \tag{12}$$

where ζ_n^k satisfies

$$\mathbb{A}_n(\theta^n)\zeta_n^k = e_k \cdot (\nabla_y + 2i\pi\theta^n)\psi_n + (\mathrm{div}_y + 2i\pi\theta^n)(e_k\psi_n) \quad \text{in } \mathbb{T}^N, \tag{13}$$

and χ_n^{kl} satisfies

$$\begin{aligned} \mathbb{A}_n(\theta^n)\chi_n^{kl} = \ & e_k \cdot (\nabla_y + 2i\pi\theta^n)\zeta_n^l + (\mathrm{div}_y + 2i\pi\theta^n)\left(e_k\zeta_n^l\right) \\ & + e_l \cdot (\nabla_y + 2i\pi\theta^n)\zeta_n^k + (\mathrm{div}_y + 2i\pi\theta^n)\left(e_l\zeta_n^k\right) \\ & + 2e_k \cdot e_l\psi_n - \frac{1}{4\pi^2}\frac{\partial^2\lambda_n}{\partial\theta_l\partial\theta_k}(\theta^n)\psi_n \quad \text{in } \mathbb{T}^N. \end{aligned} \tag{14}$$

We know that ζ_n^k and χ_n^{kl} exist since they are defined by (12) as multiple of the derivatives of ψ_n with respect to θ (and assumption (7) ensures that ψ_n is indeed differentiable). However, if we forget for a moment definition (12), the existence and uniqueness of the solutions to (13) and (14) is not at all obvious. Since the operator $\mathbb{A}_n(\theta^n)$ has a non empty kernel spanned by ψ_n, one should apply the Fredholm alternative: equations (13) and (14) admit a unique solution (up to the addition of a multiple of ψ_n) if and only if their right hand side are orthogonal to ψ_n (i.e. satisfy the Fredholm compatibility condition). This compatibility condition is not immediately satisfied. Actually, it gives new informations which are a consequence of the previously established existence of ζ_n^k and χ_n^{kl}. In particular, the compatibility condition of (14) yields a formula for the Hessian matrix $\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$ in terms of ψ_n and ζ_n^k that we shall use later (see (31)).

Remark 1. All our results can be generalized if we replace the Laplacian in (1) by the more general operator $\mathrm{div}(A(y)\nabla\cdot)$ where $A(y)$ is a symmetric, bounded, periodic and uniformly coercive matrix. In this case, the Bloch spectral cell problem (6) becomes

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

A tensor $A(y) \neq Id$ may be interpreted as a periodic metric. It makes sense for the study of wave propagation in a periodic media (see e.g. [2]).

Finally we recall the notion of two-scale convergence introduced in [1], [18].

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

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

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

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

3. **Main result.** Due to our assumptions on the coefficients, if the initial data u_ϵ^0 belongs to $H^1(\mathbb{R}^N)$, there exists a unique solution of the Schrödinger equation (1) in $C\left([0,T]; H^1(\mathbb{R}^N)\right)$ which satisfies the following a priori estimate.

Lemma 1. *There exists a constant $C > 0$, which depends on T but not on ϵ, such that the solution of (1) satisfies*

$$\begin{array}{lcl} \|u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N))} & = & \|u_\epsilon^0\|_{L^2(\mathbb{R}^N)}, \\ \epsilon\|\nabla u_\epsilon\|_{L^\infty((0,T);L^2(\mathbb{R}^N)^N)} & \leq & C\left(\|u_\epsilon^0\|_{L^2(\mathbb{R}^N)} + \epsilon\|\nabla u_\epsilon^0\|_{L^2(\mathbb{R}^N)^N}\right). \end{array} \tag{15}$$

Proof of Lemma 1. We multiply equation (1) by $\overline{u_\epsilon}$ and we integrate by parts. Since all coefficients are real, taking the imaginary part yields

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

Next we multiply (1) by $\epsilon^2 \frac{\partial \overline{u_\epsilon}}{\partial t}$ and we take the real part to get

$$\frac{d}{dt}\int_{\mathbb{R}^N}\left(\epsilon^2|\nabla u_\epsilon|^2 + \left(c\left(\frac{x}{\epsilon}\right) + \epsilon^2 d_\epsilon(t,x)\right)|u_\epsilon|^2\right)dx = -2\epsilon^2\int_{\mathbb{R}^N}\frac{\partial d_\epsilon}{\partial t}(t,x)|u_\epsilon|^2\,dx,$$

which yields (15) since $\epsilon^2 \frac{\partial d_\epsilon}{\partial t}$ is bounded in view of (4). □

Our main result is the following homogenization theorem.

Theorem 1. *Assume (7) and (8) and that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ is*

$$u_\epsilon^0(x) = \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} v^0(x), \tag{16}$$

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

$$\begin{aligned} u_\epsilon(t,x) = {}& e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v_n(t,x) \\ &+ e^{i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{2i\pi\frac{\theta^m\cdot x}{\epsilon}} \psi_m\left(\frac{x}{\epsilon}, \theta^m\right) v_m(t,x) + r_\epsilon(t,x), \end{aligned} \tag{17}$$

with

$$\lim_{\epsilon\to 0}\int_0^T\int_{\mathbb{R}^N} |r_\epsilon(t,x)|^2\,dx = 0, \tag{18}$$

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

$$\left\{\begin{array}{ll} i\dfrac{\partial v_n}{\partial t} - \operatorname{div}(A_n^*\nabla v_n) + d_{nm}^*(t,x)\,v_m = 0 & \text{in } \mathbb{R}^N\times(0,T) \\ i\dfrac{\partial v_m}{\partial t} - \operatorname{div}(A_m^*\nabla v_m) + d_{mn}^*(t,x)\,v_n = 0 & \text{in } \mathbb{R}^N\times(0,T) \\ v_n(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N \\ v_m(t=0,x) = 0 & \text{in } \mathbb{R}^N, \end{array}\right. \tag{19}$$

with $A_p^* = \frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_p(\theta^p)$, for $p = n, m$, and

$$d_{nm}^*(t,x) = \overline{d}_{mn}^*(t,x) = \frac{1}{2}\int_{\mathbb{T}^N} d(t,x,y)\overline{\psi}_n(y,\theta^n)\psi_m(y,\theta^m)\,dy. \tag{20}$$

Remark 2. Formula (20), giving the coupling coefficient d_{nm}^*, is a version of the famous "Fermi golden rule" in quantum mechanics or solid state physics [7], [9], [23]. More precisely, the squared modulus of d_{nm}^* is called the transition probability per unit time from state n to m and its formula is Fermi golden rule (see e.g. Chapter 6 in [23]). The inverse tensor $(A_n^*)^{-1}$ is called the effective mass of the particle corresponding to the wave function v_n [9], [16], [17]. These effective coefficients not only depend on the chosen periodic crystal (characterized by the potential $c(y)$)

but also on the energy level or Bloch band n, m of the particle, and on the quasi momentum $\theta^{n,m}$. Effective mass theorems were already obtained in [3], chapter 4 of [4], [20], [21]. However, the derivation of the coupled system (19) and the justification of the Fermi golden rule is new to the best of our knowledge.

Since θ^n and θ^m are not necessarily minimum points, the tensors A_n^* and A_m^* can be neither definite nor positive. Nevertheless, the homogenized problem (19) is still well posed in $C([0,T]; L^2(\mathbb{R}^N))^2$ (by using semi-group theory [5]), although its solution may not belong to $L^2((0,T); H^1(\mathbb{R}^N))^2$.

In general d_{nm}^* does not vanish, so that there is indeed a coupling between the two modes n and m. Nevertheless, if $d(t,x,y) \equiv d(t,x)$ in (4) and $\theta^n = \theta^m$, then, by orthogonality of the modes, we have $d_{nm}^* = 0$.

Remark 3. As already noticed in [3], the scaling of (1) is not the usual semi-classical scaling for Schrödinger equation [6], [11], [12], [13], [14]. The actual scaling of (1) means that we are interested in much longer times than in the semi-classical limit.

Remark 4. As already said in Remark 1 all our results, including Theorem 1 can be generalized if we replace the Laplacian by the more general operator $\operatorname{div}(A(y)\nabla\cdot)$ with a real symmetric, bounded, periodic and uniformly coercive matrix $A(y)$.

Remark 5. Theorem 1 still holds true if the initial data is given by a combination of the two states

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

instead of (16). Of course, it yields a non-zero initial data for v_m in (19).

Proof of Theorem 1. This proof is in the spirit of our previous works [2], [3]. Define two sequences

$$\begin{aligned} v_\epsilon^n(t,x) &= u_\epsilon(t,x) e^{-i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^n\cdot x}{\epsilon}}, \\ v_\epsilon^m(t,x) &= u_\epsilon(t,x) e^{-i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{-2i\pi\frac{\theta^m\cdot x}{\epsilon}}. \end{aligned} \tag{21}$$

Since $|v_\epsilon^n| = |v_\epsilon^m| = |u_\epsilon|$, by the a priori estimates of Lemma 1 we have, for $p = n, m$,

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

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

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

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

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

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

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

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

$$w_n(t,x,y)=v_n(t,x)\psi_n(y,\theta^n). \tag{22}$$

Replacing n by m in the previous argument, a similar result holds true for $w_m(t,x,y)=v_m(t,x)\psi_m(y,\theta^m)$.

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

$$\Psi_\epsilon=e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}}e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}}\left(\psi_n(\frac{x}{\epsilon},\theta^n)\phi(t,x)+\epsilon\sum_{k=1}^N\frac{\partial\phi}{\partial x_k}(t,x)\zeta^k_n(\frac{x}{\epsilon})\right) \tag{23}$$

where $\phi(t,x)$ is a smooth test function with compact support in $[0,T)\times\mathbb{R}^N$, and $\zeta^k_n(y)$ is the solution of (13). Integrating by parts, the resulting computation was already done in [3] in the absence of the oscillating potential $d_\epsilon(t,x)$. We briefly recall it: after some algebra, and using the summation convention for the repeated index k, we obtain

$$
\begin{aligned}
\int_{\mathbb{R}^N}\nabla u_\epsilon\cdot\nabla\overline{\Psi}_\epsilon dx = \quad &\int_{\mathbb{R}^N}(\nabla+2i\pi\frac{\theta^n}{\epsilon})(\overline{\phi}v^n_\epsilon)\cdot(\nabla-2i\pi\frac{\theta^n}{\epsilon})\overline{\psi}^\epsilon_n\\
&+\epsilon\int_{\mathbb{R}^N}(\nabla+2i\pi\frac{\theta^n}{\epsilon})(\frac{\partial\overline{\phi}}{\partial x_k}v^n_\epsilon)\cdot(\nabla-2i\pi\frac{\theta^n}{\epsilon})\overline{\zeta}^{k,\epsilon}_n\\
&-\int_{\mathbb{R}^N}e_k\frac{\partial\overline{\phi}}{\partial x_k}v^n_\epsilon\cdot(\nabla-2i\pi\frac{\theta^n}{\epsilon})\overline{\psi}^\epsilon_n\\
&+\int_{\mathbb{R}^N}(\nabla+2i\pi\frac{\theta^n}{\epsilon})(\frac{\partial\overline{\phi}}{\partial x_k}v^n_\epsilon)\cdot e_k\overline{\psi}^\epsilon_n\\
&-\int_{\mathbb{R}^N}v^n_\epsilon\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot e_k\overline{\psi}^\epsilon_n\\
&-\int_{\mathbb{R}^N}v^n_\epsilon\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot(\epsilon\nabla-2i\pi\theta^n)\overline{\zeta}^{k,\epsilon}_n\\
&+\int_{\mathbb{R}^N}\overline{\zeta}^{k,\epsilon}_n(\epsilon\nabla+2i\pi\theta^n)v^n_\epsilon\cdot\nabla\frac{\partial\overline{\phi}}{\partial x_k}\,.
\end{aligned} \tag{24}
$$

A first simplification arises from the definition of ψ_n which satisfies, for any smooth compactly supported test function Φ,

$$\int_{\mathbb{R}^N} (\nabla + 2i\pi\frac{\theta^n}{\epsilon})\psi_n^\epsilon \cdot (\nabla - 2i\pi\frac{\theta^n}{\epsilon})\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N}(c^\epsilon - \lambda_n(\theta^n))\psi_n^\epsilon\overline{\Phi} = 0. \tag{25}$$

A second simplification comes from the definition of ζ_n^k

$$\begin{aligned}&\int_{\mathbb{R}^N} (\nabla + 2i\pi\frac{\theta^n}{\epsilon})\zeta_n^{k,\epsilon} \cdot (\nabla - 2i\pi\frac{\theta^n}{\epsilon})\overline{\Phi} + \frac{1}{\epsilon^2}\int_{\mathbb{R}^N}(c^\epsilon - \lambda_n(\theta^n))\zeta_n^{k,\epsilon}\overline{\Phi} = \\ &\quad \epsilon^{-1}\int_{\mathbb{R}^N}(\nabla + 2i\pi\frac{\theta^n}{\epsilon})\psi_n^\epsilon \cdot e_k\overline{\Phi} - \epsilon^{-1}\int_{\mathbb{R}^N} e_k\psi_n^\epsilon\cdot(\nabla - 2i\pi\frac{\theta^n}{\epsilon})\overline{\Phi}.\end{aligned} \tag{26}$$

Combining (24) with the other terms of the variational formulation of (1), we easily check that the first line of its right hand side cancels out because of (25) with $\Phi = \overline{\phi}v_\epsilon^n$, and the next three lines cancel out because of (26) with $\Phi = \frac{\partial\overline{\phi}}{\partial x_k}v_\epsilon^n$. We keep the three last terms of (24) which are bounded. Finally, (1) multiplied by $\overline{\Psi}_\epsilon$ yields after simplification

$$\begin{aligned}&-i\int_{\mathbb{R}^N} u_\epsilon^0\overline{\Psi}_\epsilon(t=0)dx - i\int_0^T\int_{\mathbb{R}^N} v_\epsilon^n\left(\overline{\psi}_n^\epsilon\frac{\partial\overline{\phi}}{\partial t} + \epsilon\frac{\partial^2\overline{\phi}}{\partial x_k\partial t}\overline{\zeta}_n^{k,\epsilon}\right)dt\,dx \\ &-\int_0^T\int_{\mathbb{R}^N} v_\epsilon^n\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot e_k\overline{\psi}_n^\epsilon dt\,dx \\ &-\int_0^T\int_{\mathbb{R}^N} v_\epsilon^n\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot(\epsilon\nabla - 2i\pi\theta^n)\overline{\zeta}_n^{k,\epsilon}dt\,dx \\ &+\int_0^T\int_{\mathbb{R}^N}\overline{\zeta}_n^{k,\epsilon}(\epsilon\nabla + 2i\pi\theta^n)v_\epsilon^n\cdot\nabla\frac{\partial\overline{\phi}}{\partial x_k}dt\,dx \\ &+\int_0^T\int_{\mathbb{R}^N} d^\epsilon u_\epsilon\overline{\Psi}_\epsilon\,dt\,dx \qquad\qquad = 0.\end{aligned} \tag{27}$$

We can pass to the two-scale limit in each term of (27) as was done in [3], except for the last one which is the only new and different term. The last line of (27) is equal to

$$\begin{aligned}&\int_0^T\int_{\mathbb{R}^N} d\left(t,x,\frac{x}{\epsilon}\right)\frac{1}{2}\left(e^{i\frac{(\lambda_m(\theta^m)-2\lambda_n(\theta^n))t}{\epsilon^2}}e^{2i\pi\frac{(\theta^m-2\theta^n)\cdot x}{\epsilon}} + e^{-i\frac{\lambda_m(\theta^m)t}{\epsilon^2}}e^{-2i\pi\frac{\theta^m\cdot x}{\epsilon}}\right) \\ &\qquad u_\epsilon\left(\overline{\psi}_n(\frac{x}{\epsilon},\theta^n)\overline{\phi}(t,x) + \mathrm{O}(\epsilon)\right)dt\,dx \\ &= \int_0^T\int_{\mathbb{R}^N} d\left(t,x,\frac{x}{\epsilon}\right)\frac{1}{2}\left(v_\epsilon^{2n-m} + v_\epsilon^m\right)\left(\overline{\psi}_n(\frac{x}{\epsilon},\theta^n)\overline{\phi}(t,x) + \mathrm{O}(\epsilon)\right)dt\,dx\end{aligned}$$

where we introduced a new sequence v_ϵ^{2n-m} defined, similarly to (21), by

$$v_\epsilon^{2n-m}(t,x) = u_\epsilon(t,x)e^{-i\frac{(2\lambda_n(\theta^n)-\lambda_m(\theta^m))t}{\epsilon^2}}e^{-2i\pi\frac{(2\theta^n-\theta^m)\cdot x}{\epsilon}}. \tag{28}$$

Applying the same arguments as in the first step, this sequence v_ϵ^{2n-m} is easily shown to two-scale converge to $w_{2n-m}(t,x,y)$ which satisfies

$$\begin{aligned}&-(\mathrm{div}_y + 2i\pi(2\theta^n - \theta^m))\Big((\nabla_y + 2i\pi(2\theta^n - \theta^m))w_{2n-m}\Big) \\ &+c(y)w_{2n-m} = (2\lambda_n(\theta^n) - \lambda_m(\theta^m))w_{2n-m} \quad \text{ in } \mathbb{T}^N.\end{aligned} \tag{29}$$

Because of the non-resonance assumption (8), namely that $2\lambda_n(\theta^n) - \lambda_m(\theta^m)$ is not equal to any eigenvalue $\lambda_p(2\theta^n - \theta^m)$, the spectral problem (29) has no solution other than 0, which implies that $w_{2n-m}(t,x,y) \equiv 0$. The two-scale limit of (27) is thus

$$
\begin{aligned}
&-i\int_{\mathbb{R}^N}\int_{\mathbb{T}^N}|\psi_n|^2 v^0\overline{\phi}(t=0)\,dx\,dy - i\int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N}|\psi_n|^2 v_n\frac{\partial\overline{\phi}}{\partial t}dt\,dx\,dy\\
&-\int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N}\psi_n v_n\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot e_k\overline{\psi}_n dt\,dx\,dy\\
&-\int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N}\psi_n v_n\nabla\frac{\partial\overline{\phi}}{\partial x_k}\cdot(\nabla_y-2i\pi\theta^n)\overline{\zeta}_n^k dt\,dx\,dy\\
&+\int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N}\overline{\zeta}_n^k(\nabla_y+2i\pi\theta^n)\psi_n v_n\cdot\nabla\frac{\partial\overline{\phi}}{\partial x_k}dt\,dx\,dy\\
&+\frac{1}{2}\int_0^T\int_{\mathbb{R}^N}\int_{\mathbb{T}^N}d(t,x,y)\psi_m v_m\overline{\psi}_n\overline{\phi}\,dt\,dx\,dy \qquad = 0.
\end{aligned}
\tag{30}
$$

To simplify (30) we recall that $\int_{\mathbb{T}^N}|\psi_n|^2dy = 1$, that $d^*_{nm}(t,x)$ is defined by (20), and we introduce

$$
\begin{aligned}
2\,(A_n^*)_{jk} = \quad &\int_{\mathbb{T}^N}\Big(\psi_n e_j\cdot e_k\overline{\psi}_n + \psi_n e_k\cdot e_j\overline{\psi}_n\\
&+\psi_n e_j\cdot(\nabla_y-2i\pi\theta^n)\overline{\zeta}_n^k + \psi_n e_k\cdot(\nabla_y-2i\pi\theta^n)\overline{\zeta}_n^j\\
&-\overline{\zeta}_n^k(\nabla_y+2i\pi\theta^n)\psi_n\cdot e_j - \overline{\zeta}_n^j(\nabla_y+2i\pi\theta^n)\psi_n\cdot e_k\Big)dy.
\end{aligned}
\tag{31}
$$

Because of the Fredholm compatibility condition of equation (14) for the second derivative of ψ_n, the matrix A_n^*, defined by (31), is actually equal to $\frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_n(\theta^n)$. Finally (30) is equivalent to

$$
\begin{aligned}
-i\int_{\mathbb{R}^N}v^0\overline{\phi}(t=0)\,dx - i\int_0^T\int_{\mathbb{R}^N}v_n\frac{\partial\overline{\phi}}{\partial t}dt\,dx - \int_0^T\int_{\mathbb{R}^N}A_n^*v_n\cdot\nabla\nabla\overline{\phi}dt\,dx\\
+\int_0^T\int_{\mathbb{R}^N}d^*_{nm}(t,x)v_m\overline{\phi}\,dt\,dx = 0.
\end{aligned}
\tag{32}
$$

A symmetric argument works for v_m (changing n in m in the test function Ψ_ϵ). However, the initial condition is zero in the homogenized equation for v_m. Indeed, either $\theta^m \neq \theta^n$ and we already know that $v_\epsilon^m(0)$ two-scale converges to 0, or $\theta^m = \theta^n$ and the orthogonality property

$$\int_{\mathbb{T}^N}\psi_n\overline{\psi}_m\,dy = 0 \quad \text{for} \quad m \neq n$$

implies that the coefficient in front of the test function $\phi(0)$ vanishes, which in the variational formulation implies that $v_m(0) = 0$. Therefore, (32) and its counterpart for m instead of n yield a very weak form of the homogenized system (19). Since A_n^*, A_m^* are real symmetric matrices and $d^*_{nm} = \overline{d}^*_{mn}$, (19) admits a unique solution in $C\left([0,T];L^2(\mathbb{R}^N)\right)^2$. By uniqueness of this solution, the entire sequence v_ϵ^p two-scale converges weakly to $\psi_p\left(y,\theta^p\right)v_p(t,x)$ for $p = n, m$.

It remains to prove the strong convergence (18). We compute

$$\begin{aligned}\|r_\epsilon(t)\|^2_{L^2(\mathbb{R}^N)} = \|u_\epsilon(t)\|^2_{L^2(\mathbb{R}^N)} + \|\psi^\epsilon_n v_n(t)\|^2_{L^2(\mathbb{R}^N)} + \|\psi^\epsilon_m v_m(t)\|^2_{L^2(\mathbb{R}^N)} \\ - 2\Re \int_{\mathbb{R}^N} v^n_\epsilon(t)\overline{\psi}^\epsilon_n \overline{v}_n(t)\, dx - 2\Re \int_{\mathbb{R}^N} v^m_\epsilon(t)\overline{\psi}^\epsilon_m \overline{v}_m(t)\, dx \\ + 2\Re \int_{\mathbb{R}^N} e^{i\frac{(\lambda_n(\theta^n)-\lambda_m(\theta^m))t}{\epsilon^2}} e^{2i\pi\frac{(\theta^n-\theta^m)\cdot x}{\epsilon}} \psi^\epsilon_n v_n(t)\overline{\psi}^\epsilon_m \overline{v}_m(t)\, dx.\end{aligned} \tag{33}$$

By the orthogonality property of the Bloch waves, the last integral in (33) converges to 0. By applying two-scale convergence, we can pass to the limit in the second line and in the last two terms of the first line of (33). For the remaining term we use Lemma 1 which implies

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

by the normalization condition of ψ_n. Thus we deduce

$$\lim_{\epsilon\to 0} \|r_\epsilon(t)\|^2_{L^2(\mathbb{R}^N)} = \|v^0\|^2_{L^2(\mathbb{R}^N)} - \|v_n(t)\|^2_{L^2(\mathbb{R}^N)} - \|v_m(t)\|^2_{L^2(\mathbb{R}^N)}$$

which is precisely 0 because of the conservation of energy of the homogenized system (19), i.e.

$$\|v_n(t)\|^2_{L^2(\mathbb{R}^N)} + \|v_m(t)\|^2_{L^2(\mathbb{R}^N)} = \|v^0\|^2_{L^2(\mathbb{R}^N)}.$$

Since $\lim_{\epsilon\to 0} \|r_\epsilon(t)\|^2_{L^2(\mathbb{R}^N)} = 0$, the Lebesgue dominated convergence theorem yields (18). □

Remark 6. Recall that the function $\zeta_k(y)$ is the solution of (13), unique up to the addition of a multiple of ψ_n. This multiple may depend on (t,x) and therefore the test function Ψ_ϵ, as well as the homogenized system could depend on the choice of this additive term. Actually the homogenized system depends on ζ_k only through the homogenized tensor A^*_n, defined by (31). If we replace $\zeta_k(y)$ by $\zeta_k(y)+c_k(t,x)\psi_n(y)$, an easy calculation shows that all terms c_k cancel out because of the Fredholm alternative for ζ_k, i.e. the right-hand side of (13) is orthogonal to ψ_n. Thus, the homogenized system is uniquely defined whatever the choice of the additive constant in $\zeta_k(y)$.

Remark 7. A formal two-scale asymptotic expansion (in the spirit of [4]) of the solution u_ϵ of (1) would give

$$\begin{aligned}u_\epsilon(t,x) \approx e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \left(\psi_n\left(\frac{x}{\epsilon},\theta^n\right) v_n(t,x) + \epsilon\sum_{k=1}^N \frac{\partial v_n}{\partial x_k}(t,x)\zeta^k_n(\frac{x}{\epsilon})\right) \\ + e^{i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{2i\pi\frac{\theta^m\cdot x}{\epsilon}} \left(\psi_m\left(\frac{x}{\epsilon},\theta^m\right) v_m(t,x) + \epsilon\sum_{k=1}^N \frac{\partial v_m}{\partial x_k}(t,x)\zeta^k_m(\frac{x}{\epsilon})\right).\end{aligned}$$

As usual in periodic homogenization, this expansion suggests the choice of the test function Ψ_ϵ, in the proof of Theorem 1. Another possible interpretation of Ψ_ϵ is as follows. The large ϵ^{-2} terms in the variational formulation of (1) cancel out because of the equation satisfied by ψ_n. However, new terms of order ϵ^{-1} appear because of the first order derivatives of ψ_n. They are compensated in turn by the second order derivatives of the corrector ζ^k_n.

Remark 8. Part (i) of assumption (7) states that the eigenvalues $\lambda_n(\theta^n)$ and $\lambda_m(\theta^m)$ are simple. This hypothesis is crucial in order to be able to differentiate the spectral cell problem with respect to θ. If one of these eigenvalues is not simple then, as is well known, it is not anymore differentiable, but merely directionally differentiable (which is not enough for our purpose). So, we do not know how to generalize Theorem 1 in the case of multiple eigenvalues. There is one notable exception when one eigenvalue is of multiplicity, say $p > 1$, and there exists locally a labelling of the eigenvalues and eigenvectors in p smooth branches. Note that it is a very strong assumption, which is rarely meet in practice. Then, using an argument of [3], one can generalize Theorem 1 and obtain a limit system similar to (19), with as many equations as the repeated multiplicities of the eigenvalues $\lambda_n(\theta^n)$ and $\lambda_m(\theta^m)$, and coupled only by zero-order terms.

Remark 9. Part (ii) of assumption (7) states that the group velocities vanish, $\nabla_\theta\lambda_n(\theta^n) = \nabla_\theta\lambda_m(\theta^m) = 0$. If it is not the case, then it induces a large drift of order ϵ^{-1} and the homogenized system (19) can be obtained only in a moving frame of reference, following this large drift (see [3] for more details). Therefore, if $\nabla_\theta\lambda_n(\theta^n) \neq \nabla_\theta\lambda_m(\theta^m)$, one can not generalize Theorem 1 since both initial and target states move with large different speeds, so no coupling is possible in the limit as ϵ goes to zero. In the case $\nabla_\theta\lambda_n(\theta^n) = \nabla_\theta\lambda_m(\theta^m) \neq 0$ it is technically possible to generalize Theorem 1, following the argument of [3], but this result would not make much sense since it would assume that the exterior potential $d_\epsilon(t,x)$ move with the same velocity, or at least is macroscopically constant, which is usually not the case in physical applications.

4. **Electromagnetic potential.** Instead of (1) we now consider a Schrödinger equation with an exterior electromagnetic field

$$\begin{cases} i\dfrac{\partial u_\epsilon}{\partial t} - (\mathrm{div} + i\epsilon\mathbf{A}_\epsilon)(\nabla + i\epsilon\mathbf{A}_\epsilon) u_\epsilon + \epsilon^{-2} c\left(\dfrac{x}{\epsilon}\right) u_\epsilon = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ u_\epsilon(t=0,x) = u_\epsilon^0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{34}$$

where $\mathbf{A}_\epsilon(t,x)$ is the electromagnetic vector potential, i.e. a function from $\mathbb{R}^+ \times \mathbb{R}^N$ into $\mathbb{R}^N$ [7], [9], [23]. The electric field E and magnetic field B are recovered by

$$E(t,x) = -\frac{\partial \mathbf{A}_\epsilon}{\partial t}(t,x) \quad \text{and} \quad B(t,x) = \mathrm{curl}\mathbf{A}_\epsilon(t,x).$$

For an electromagnetic wave, the vector potential is assumed to be given by

$$\mathbf{A}_\epsilon(t,x) = \Re\left(e^{i\frac{(\lambda_m(\theta^m)-\lambda_n(\theta^n))t}{\epsilon^2}} e^{2i\pi\frac{(\theta^m-\theta^n)\cdot x}{\epsilon}}\right) a\left(t,x,\frac{x}{\epsilon}\right), \tag{35}$$

where $\Re$ denotes the real part and $a(t,x,y)$ is a bounded smooth function from $\mathbb{R}^+ \times \mathbb{R}^N \times \mathbb{T}^N$ into $\mathbb{R}^N$. As before, $c(y)$ is a bounded function from $\mathbb{T}^N$ into $\mathbb{R}$, the initial data u_ϵ^0 belongs to $H^1(\mathbb{R}^N)$, and the conclusion of Lemma 1 still holds true: there exists a unique solution of (34) in $C\left([0,T]; H^1(\mathbb{R}^N)\right)$ which is uniformly bounded in $L^2\left((0,T)\times\mathbb{R}^N\right)$, independently of ϵ. Theorem 1 can be generalized as follows.

Theorem 2. *Assume (7) and (8) and that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ is*

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

with $v^0 \in H^1(\mathbb{R}^N)$. The solution of (34) can be written as

$$\begin{aligned} u_\epsilon(t,x) = {} & e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon},\theta^n\right) v_n(t,x) \\ & + e^{i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{2i\pi\frac{\theta^m\cdot x}{\epsilon}} \psi_m\left(\frac{x}{\epsilon},\theta^m\right) v_m(t,x) + r_\epsilon(t,x), \end{aligned}$$

with

$$\lim_{\epsilon\to 0}\int_0^T \int_{\mathbb{R}^N} |r_\epsilon(t,x)|^2\, dx = 0,$$

and $(v_n, v_m) \in C\left([0,T]; L^2(\mathbb{R}^N)\right)^2$ *is the unique solution of the homogenized Schrödinger system*

$$\begin{cases} i\dfrac{\partial v_n}{\partial t} - \operatorname{div}\left(A_n^* \nabla v_n\right) + d_{nm}^*(t,x)\, v_m = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ i\dfrac{\partial v_m}{\partial t} - \operatorname{div}\left(A_m^* \nabla v_m\right) + d_{mn}^*(t,x)\, v_n = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v_n(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N \\ v_m(t=0,x) = 0 & \text{in } \mathbb{R}^N, \end{cases} \tag{36}$$

with $A_p^* = \frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_p(\theta^p)$*, for* $p = n, m$*, and*

$$\begin{aligned} d_{nm}^*(t,x) = \overline{d}_{mn}^*(t,x) \quad &= \frac{i}{2}\int_{\mathbb{T}^N} \psi_m(y,\theta^m) a(t,x,y)\cdot\left(\nabla - 2i\pi\theta^n\right)\overline{\psi}_n(y,\theta^n)\, dy \\ &-\frac{i}{2}\int_{\mathbb{T}^N} \overline{\psi}_n(y,\theta^n) a(t,x,y)\cdot\left(\nabla + 2i\pi\theta^m\right)\psi_m(y,\theta^m)\, dy. \end{aligned} \tag{37}$$

Remark 10. In general d_{nm}^* does not vanish, even if $a(t,x,y)$ is a constant vector and $\theta^n = \theta^m$, so that there is indeed a coupling between the two modes n and m.

Proof of Theorem 2. The proof is very similar to that of Theorem 1. The first step is identical, and in the second step we choose the same test function Ψ_ϵ, defined by (23). The higher order term in the variational formulation is

$$\begin{aligned} \int_{\mathbb{R}^N} \left(\nabla + i\epsilon\mathbf{A}_\epsilon\right) u_\epsilon \cdot \left(\nabla - i\epsilon\mathbf{A}_\epsilon\right)\overline{\Psi}_\epsilon dx \quad &= \int_{\mathbb{R}^N} \nabla u_\epsilon \cdot \nabla\overline{\Psi}_\epsilon \\ &+ i\epsilon\int_{\mathbb{R}^N} \left(u_\epsilon\mathbf{A}_\epsilon\cdot\nabla\overline{\Psi}_\epsilon - \overline{\Psi}_\epsilon\mathbf{A}_\epsilon\cdot\nabla u_\epsilon\right) dx \\ &+ \epsilon^2\int_{\mathbb{R}^N} |\mathbf{A}_\epsilon|^2 u_\epsilon\overline{\Psi}_\epsilon\, dx. \end{aligned} \tag{38}$$

The first term in the right hand side of (38) is exactly the previous term (24). The last one goes to zero, while the second one is the only new term which yields a non-zero limit. Indeed, integrating by parts in this term gives

$$\begin{aligned} & i\epsilon\int_{\mathbb{R}^N} \left(u_\epsilon\mathbf{A}_\epsilon\cdot\nabla\overline{\Psi}_\epsilon - \overline{\Psi}_\epsilon\mathbf{A}_\epsilon\cdot\nabla u_\epsilon\right) dx = i\epsilon\int_{\mathbb{R}^N} u_\epsilon\left(2\mathbf{A}_\epsilon\cdot\nabla\overline{\Psi}_\epsilon + \overline{\Psi}_\epsilon \operatorname{div}\mathbf{A}_\epsilon\right) dx \\ & = i/2\int_{\mathbb{R}^N} (v_\epsilon^{2n-m} + v_\epsilon^m)\overline{\phi}\left(2a^\epsilon\cdot(\nabla_y - 2i\pi\theta^n)\overline{\psi}_n^\epsilon + \overline{\psi}_n^\epsilon \operatorname{div}_y a^\epsilon\right) dx \\ & + i/2\int_{\mathbb{R}^N} 2i\pi\left(v_\epsilon^{2n-m}(\theta^m - \theta^n)\cdot a^\epsilon + v_\epsilon^m(\theta^n - \theta^m)\cdot a^\epsilon\right)\overline{\phi\psi}_n^\epsilon dx + \mathrm{O}(\epsilon). \end{aligned} \tag{39}$$

Recalling that the two-scale limit of v_ϵ^{2n-m} is 0, the limit of (39) is

$$i/2\int_{\mathbb{R}^N}\int_{\mathbb{T}^N} v_m\overline{\phi}\psi_m\left(2a\cdot(\nabla_y - 2i\pi\theta^n)\overline{\psi}_n + \overline{\psi}_n \operatorname{div}_y a + 2i\pi\overline{\psi}_n(\theta^n - \theta^m)\cdot a\right) dx\, dy$$

which yields formula (37) for the coupling coefficient d_{nm}^*. The rest of the proof is identical to that of Theorem 1. $\square$

5. **The resonant case.** In this section we come back to the original Schrödinger equation (1) but we change assumption (8) by assuming that there is a single resonance between the initial data and the target state, namely

$$\begin{cases} (iii) & \text{there exists } l \geq 1 \text{ such that } \lambda_l(2\theta^n - \theta^m) = 2\lambda_n(\theta^n) - \lambda_m(\theta^m), \\ (iv) & \text{for any } p \geq 1, \quad \lambda_p(3\theta^n - 2\theta^m) \neq 3\lambda_n(\theta^n) - 2\lambda_m(\theta^m). \end{cases} \tag{40}$$

We keep assumption (7) that we extend to the new eigenvalue λ_l for the Bloch parameter $\theta^l = 2\theta^n - \theta^m$, i.e.

$$\text{for } p = n, m, l \begin{cases} (i) & \lambda_p(\theta^p) \text{ is a simple eigenvalue,} \\ (ii) & \theta^p \text{ is a critical point of } \lambda_p(\theta) \text{ i.e., } \nabla_\theta \lambda_p(\theta^p) = 0. \end{cases} \tag{41}$$

With these new assumptions we generalize Theorem 1 by obtaining a limit system coupling three possible states instead of just two.

Theorem 3. *Assume (41) and (40) and that the initial data $u_\epsilon^0 \in H^1(\mathbb{R}^N)$ is*

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

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

$$\begin{aligned} u_\epsilon(t,x) &= e^{i\frac{\lambda_n(\theta^n)t}{\epsilon^2}} e^{2i\pi\frac{\theta^n\cdot x}{\epsilon}} \psi_n\left(\frac{x}{\epsilon}, \theta^n\right) v_n(t,x) \\ &+ e^{i\frac{\lambda_m(\theta^m)t}{\epsilon^2}} e^{2i\pi\frac{\theta^m\cdot x}{\epsilon}} \psi_m\left(\frac{x}{\epsilon}, \theta^m\right) v_m(t,x) \\ &+ e^{i\frac{\lambda_l(\theta^l)t}{\epsilon^2}} e^{2i\pi\frac{\theta^l\cdot x}{\epsilon}} \psi_l\left(\frac{x}{\epsilon}, \theta^l\right) v_l(t,x) + r_\epsilon(t,x), \end{aligned}$$

with

$$\lim_{\epsilon\to 0} \int_0^T \int_{\mathbb{R}^N} |r_\epsilon(t,x)|^2\, dx = 0,$$

and $(v_n, v_m, v_l) \in C\left([0,T]; L^2(\mathbb{R}^N)\right)^3$ is the unique solution of the homogenized Schrödinger system

$$\begin{cases} i\dfrac{\partial v_n}{\partial t} - \operatorname{div}(A_n^*\nabla v_n) + d_{nm}^*(t,x)\, v_m + d_{nl}^*(t,x)\, v_l = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ i\dfrac{\partial v_m}{\partial t} - \operatorname{div}(A_m^*\nabla v_m) + d_{mn}^*(t,x)\, v_n = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ i\dfrac{\partial v_l}{\partial t} - \operatorname{div}(A_l^*\nabla v_l) + d_{ln}^*(t,x)\, v_n = 0 & \text{in } \mathbb{R}^N \times (0,T) \\ v_n(t=0,x) = v^0(x) & \text{in } \mathbb{R}^N \\ v_m(t=0,x) = 0 & \text{in } \mathbb{R}^N \\ v_l(t=0,x) = 0 & \text{in } \mathbb{R}^N, \end{cases}$$

with $A_p^* = \frac{1}{8\pi^2}\nabla_\theta\nabla_\theta\lambda_p(\theta^p)$, for $p = n, m, l$, and

$$d_{np}^*(t,x) = \overline{d}_{pn}^*(t,x) = \frac{1}{2}\int_{\mathbb{T}^N} d(t,x,y)\overline{\psi}_n(y,\theta^n)\psi_p(y,\theta^p)\, dy \tag{42}$$

for $p = m, l$.

Remark 11. More generally, there could be multiple resonances between the initial and target state. Let $k_0 \geq 1$ be the order of the resonance. Under a suitable generalization of assumption (40), all modes of momentum $(k+1)\theta^n - k\theta^m$ and energy $(k+1)\lambda_n(\theta^n) - k\lambda_m(\theta^m)$ are coupled for $-1 \leq k \leq k_0$. Theorem 3 can be generalized to obtain an homogenized system for $(v_m, v_n, v_{2n-m}, ..., v_{(k_0+1)n-k_0m})$

in which the coupling matrix d^* is hermitian of size k_0+2 with the following sparse structure

$$d^* = \begin{pmatrix} 0 & \times & 0 & & & & \\ \times & 0 & \times & 0 & & & \\ 0 & \times & 0 & \times & 0 & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & 0 & \times & 0 & \times & 0 \\ & & & 0 & \times & 0 & \times \\ & & & & 0 & \times & 0 \end{pmatrix}$$

Proof of Theorem 3. The only modification with respect to the proof of Theorem 1 is the fact that the sequence v_ϵ^{2n-m}, defined by (28), now admits a non-zero two-scale limit $\psi_l(y,\theta^l)v_l(t,x)$ because the spectral cell problem (29) has a non-trivial solution ψ_l, as a consequence of part (iii) of assumption (40). No other states appear because of part (iv) in (40). The rest of the proof is similar to that of Theorem 1 and we safely leave it to the reader. □

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