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Effective Mass Theorems with Bloch Modes Crossings

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Abstract

We study a Schrödinger equation modeling the dynamics of an electron in a crystal in the asymptotic regime of small wave-length comparable to the characteristic scale of the crystal. Using Floquet Bloch decomposition, we obtain a description of the limit of time averaged energy densities. We make a rather general assumption assuming that the initial data are uniformly bounded in a high order Sobolev spaces and that the crossings between Bloch modes are at worst conical. We show that despite the singularity they create, conical crossing do not trap the energy and do not prevent dispersion. We also investigate the interactions between modes that can occurred when there are some degenerate crossings between Bloch bands.

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1. Introduction

1.1. Description of the problem

We consider the dynamics of an electron in a crystal in the regime of small wave-length comparable to the characteristic scale of the crystal. After a suitable rescaling (see for instance [52]), such an analysis leads to an ε-dependent Schrödinger equation where ε is a small parameter $\varepsilon \ll 1$

$$\begin{cases} i\partial_t \psi^\varepsilon(t,x) + \dfrac{1}{2}\Delta_x \psi^\varepsilon(t,x) - \dfrac{1}{\varepsilon^2} V_{\text{per}}\left(\dfrac{x}{\varepsilon}\right)\psi^\varepsilon(t,x) - V_{\text{ext}}(t,x)\psi^\varepsilon(t,x) = 0, \\ \psi^\varepsilon|_{t=0} = \psi_0^\varepsilon. \end{cases} \tag{1.1}$$

The potential V_{per} is supposed to be smooth, real-valued and $\mathbb{Z}^d$-periodic; it models the interactions due to the crystalline structure. The external potential V_{ext}, takes into accounts the impurities; we assume that $t \mapsto V_{\text{ext}}(t,\cdot)$ is a bounded map from $\mathbb{R}$ into the set of smooth, real-valued functions on $\mathbb{R}^d_x$ with bounded derivatives. The times-scales of the equation 1.1 are characteristic of the analysis of the obstructions to the dispersion of the energy. It is the long time scaling studied in [1,2,7,9,37,52,54], by contrast to the short time analysis that allows to analyze transport effects and is performed for example in [8,13,38,51,55] (the Schrödinger equation therein is obtained from (1.1) by changing t into $\tau = \varepsilon t$).

1.1.1. The Wave Function, Observables and Quadratic Quantities We are interested in the asymptotic behavior of the time-averaged position densities $|\psi^\varepsilon(t,x)|^2$ as ε goes to 0. The wave function itself cannot be directly measured, but these densities that allow to compute the probability $P(A)$ of finding the position of the electron in a set A at time t according to

$$P(A) = \int_A |\psi^\varepsilon(t,x)|^2 \mathrm{d}x.$$

We are interested in describing at leading order in ε the value of this probability for bounded sets A. In other words, we would like to characterize, in the set of

time-dependent probability measures, the time-averaged limit as $\varepsilon \to 0^+$ of the position densities $|\psi^\varepsilon(t,x)|^2 dx$, i.e. the limits as $\varepsilon \to 0^+$ of the quantities

$$\int_a^b \int_{\mathbb{R}^d} \phi(x)|\psi^\varepsilon(t,x)|^2 \mathrm{d}x\, \mathrm{d}t, \quad \phi \in \mathcal{C}_0(\mathbb{R}^d), \quad a < b, \tag{1.2}$$

where $\mathcal{C}_0(\mathbb{R}^d)$ stands for the space of continuous compactly supported functions on $\mathbb{R}^d$. Note that these objects do not capture the fraction of the mass of the measure that goes to infinity in x as ε goes to 0.

We will derive representations of these limits in terms of *Effective mass equations*. In its full generality, our result also describes the evolution of the action of observables on the wave functions. Indeed, the wave function itself has no physical meaning and it is the evolution of quadratic quantities such as those of Section 3.1 that carries information like the average momenta or the average energy. In (1.2), the averaging in time takes into account the fact that a physical observation is not instantaneous and, though small, its duration is not negligible. However, we will discuss situations where local in time point-wise information can be derived about the evolution of the energy densities (see Section 1.4.3).

1.1.2. Floquet-Bloch Theory It is classical in this context to use Floquet-Bloch theory in order to diagonalize $-\frac{1}{2}\Delta_x + V_{\mathrm{per}}$. To this end, one introduces, for $\xi \in \mathbb{R}^d$, the operator

$$P(\xi) := \frac{1}{2}|\xi + D_y|^2 + V_{\mathrm{per}}(y), \quad y \in \mathbb{T}^d,$$

where $\mathbb{T}^d = \mathbb{R}^d \backslash \mathbb{Z}^d$ is a flat torus. It is well known that this operator is essentially self-adjoint on $L^2(\mathbb{T}^d)$ with domain $H^2(\mathbb{T}^d)$, and has a compact resolvent, hence a non-decreasing sequence of eigenvalues counted with their multiplicities, which are called *Bloch energies* or *band functions*

$$\varrho_1(\xi) \le \varrho_2(\xi) \le \cdots \le \varrho_n(\xi) \longrightarrow +\infty,$$

and an orthonormal basis of eigenfunctions $(\varphi_n(\cdot,\xi))_{n\in\mathbb{N}^*}$ called *Bloch waves* or *Bloch modes*, satisfying for all $\xi \in \mathbb{R}^d$ and $n \in \mathbb{N}^*$:

$$P(\xi)\varphi_n(\cdot,\xi) = \varrho_n(\xi)\varphi_n(\cdot,\xi). \tag{1.3}$$

Both Bloch waves and Bloch energies are continuous functions of the ξ-variable. Besides, for all $k \in 2\pi\mathbb{Z}^d$, the operator $P(\xi + k)$ is unitarily equivalent to $P(\xi)$ through multiplication by $y \mapsto \mathrm{e}^{ik\cdot y}$, which implies that for all $n \in \mathbb{N}^*$, the maps $\xi \mapsto \varrho_n(\xi)$ are $2\pi\mathbb{Z}^d$-periodic and the map $\xi \mapsto \varphi_n(\cdot,\xi)$ belongs to $\mathcal{C}(\mathbb{R}^d_\xi, L^2(\mathbb{T}^d_y))$. The spectrum of $-\frac{1}{2}\Delta_x + V_{\mathrm{per}}$ is then the union of the *Bloch bands* $B_n := \varrho_n([0,2\pi]^d)$, which are closed intervals:

$$\mathrm{Sp}\left(-\frac{1}{2}\Delta_x + V_{\mathrm{per}}\right) = \bigcup_{n\in\mathbb{N}^*} B_n.$$

The Bloch energies $\xi \mapsto \varrho_n(\xi)$ are Lipschitz functions which are analytic outside a set of zero Lebesgue measure (see [56]). In particular Bloch energies that are of constant multiplicity as ξ varies are always analytic functions of ξ. These energies are then called *isolated*. The opposite situation, that is, when two, otherwise distinct, Bloch energies coincide at some point ξ is referred to as a *crossing*. At those points, the multiplicity is greater than one and the corresponding Bloch bands have non-empty intersection. When the space dimension is one, two Bloch bands can touch at one edge and their crossing set consists on isolated points (see "Appendix A" and the references therein); in higher dimensions more complicated situations can occur: most bands overlap (in fact as soon as $d \geq 2$ only a finite number of gaps exist) and the crossing set may be a higher dimensional manifold (in fact, the union of the graphs of the band functions form a real analytic variety). The survey article [39] provides additional details on these issues.

1.1.3. Effective Mass Theory Sometimes also called *effective Hamiltonian theory*, effective mass theory consists in showing that, under suitable assumptions on the initial data ψ_0^ε, the energy density associated with the solutions of (1.1) can be approximated for ε small by those of a simpler Schrödinger equation, the *Effective mass equation*, which does not depend on ε and involves quantities related to the Bloch energies.

Effective mass equations have then been derived in various contributions [1,2,7,9,37,52,54] under the assumptions that the orthogonal projection of the initial datum ψ_0^ε on spectral subspaces corresponding to the non-simple Bloch energies is negligible, and that critical points of this band functions are non-degenerate.

All these contributions emphasize the important role played by the set of critical points of the Bloch energies. Indeed, the group velocity of the n-th mode is $\varepsilon^{-1}\nabla\varrho_n(\varepsilon\xi)$, which becomes infinite in the limit $\varepsilon \to 0$; this implies that the obstructions to the dispersive effects created by the n-th band, $n \in \mathbb{N}^*$, have to be found above the set Λ_n of critical points of the function ϱ_n:

$$\Lambda_n := \{\xi \in \mathbb{R}^d \,:\, \nabla\varrho_n(\xi) = 0\}. \tag{1.4}$$

Quantifying the loss of mass at infinity due to dispersion can be done for instance as in in [2], where the authors introduce a ε-dependent drift in order to take into account the displacement to infinity of part of the mass.

A second feature that is assumed in the aforementioned references is the simplicity of the band functions, which is an important technical ingredient in the proofs. Simple band functions are smooth, and therefore group velocity is well defined everywhere. This property may fail in the presence of band crossings which produce at worst a loss of regularity at the crossing points. In that case, the group velocity $\varepsilon^{-1}\nabla_\xi\varrho_n(\varepsilon\xi)$ is no longer defined at the crossing points, even though it may have directional limits, the archetype being the conical singularity $\varrho_n(\xi) \sim \xi/|\xi|$ close to $\xi = 0$. Our aim here is to deal with this difficulty: we will not take into account the loss of mass at infinity and focus instead on the limit (1.2); note, however, that our results take into account situations more general than the ones considered in references quoted above, since we allow for band crossings and the singularities they infer.

This motivates the introduction of the crossing set of two distinct Bloch energies:

$$\Sigma_{n,n'} := \{\xi \in \mathbb{R}^d \,:\, \varrho_n(\xi) = \varrho_{n'}(\xi)\}, \quad n, n' \in \mathbb{N}^*, \ \varrho_n \neq \varrho_{n'}. \tag{1.5}$$

The band functions ϱ_n, $n \in \mathbb{N}^*$, are piece-wise real analytic; their non-smoothness points lie in the union of crossing sets $\bigcup_{\varrho_n \neq \varrho_{n'}} \Sigma_{n,n'}$. We will also consider the sets

$$\Sigma_n := \Sigma_{n,n+1}, \quad n \in \mathbb{N}^*. \tag{1.6}$$

The crossing problematic has been addressed since long for equations that are scaled differently in the small parameter, in particular by George Hagedorn in the 90s [36]. Since then, different approaches have been devoted to understand propagation through crossings, from the use of normal forms [16,17], the analysis in terms of Wigner measures [23,26,27] and Wigner functions [29–31], up to, more recently, the analysis in terms of wave packets [55] in the case of non-singular crossings. Indeed, the growing interest in crossings, especially conical ones, is linked with the technological interest of new materials that are topological insulators (see [19,20] and references therein). However, this question has never been addressed in the context of the particular scaling in ε of equation (1.1).

In [14,15], the range of validity of the Effective Mass Theory has been extended to include degenerate critical points, through the introduction of a new class of Effective mass equation which are of von Neumann type. However, the Bloch modes involved in the description of the initial data are still assumed to be of constant multiplicity. Our aim here is to consider situations where different Bloch energies may have non-empty intersections inducing singularities and to treat rather general initial data. Our result gives a a complete description of the weak limits of the densities $|\psi^\varepsilon(t,x)|^2$ as ε goes to 0 when the crossings are conical, in a sense that we shall make precise later. This is done through the analysis of the weak limits of the Wigner function associated with $\psi^\varepsilon(t,x)$. Indeed, the Wigner function introduced in Section 3 below, plays the role of a generalized energy-density in the phase space $T^*\mathbb{R}^d = \mathbb{R}^d_x \times \mathbb{R}^d_\xi$, the density $|\psi^\varepsilon(t,x)|^2$ being its projection in the configuration space $\mathbb{R}^d_x$. Our result covers all possible cases when $d = 1$ and generic situations in higher dimensions. We also complete the description of the picture by providing a characterisation of these limits when crossings are degenerate, exhibiting the persistence of terms due to interactions between the Bloch energies that cross. Our results rely on the use of a two-microlocal analysis in the spirit of [3,4,6,42,45], using two-scale Wigner distributions [22,24,49,50].

1.2. General Assumption on the Initial Data

We denote by $A(\varepsilon D_x)$, for $\varepsilon > 0$, the scaled Fourier multiplier associated with the function $A(\xi)$, *i.e.* the operator satisfying

$$\forall f \in \mathcal{S}(\mathbb{R}^d), \quad A(\widehat{\varepsilon D_x}) f(\xi) = A(\varepsilon\xi)\widehat{f}(\xi),$$

where the following normalization has been used for the Fourier transform

$$\widehat{f}(\xi) = \int_{\mathbb{R}^d} \mathrm{e}^{-i\xi\cdot x} f(x)\mathrm{d}x.$$

Along the paper, we will consider the functions spaces $H^s_\varepsilon(\mathbb{R}^d)$, defined for $s \geq 0$, that are the Sobolev spaces equipped with the norms

$$\|f\|_{H^s_\varepsilon(\mathbb{R}^d)} := \|\langle \varepsilon D_x\rangle^s f\|_{L^2(\mathbb{R}^d)},$$

where $\langle\xi\rangle := (1+|\xi|^2)^{1/2}$.

Any function $U \in L^2(\mathbb{R}^d_x \times \mathbb{T}^d_y)$ can be written in terms of Fourier series as

$$U(x,y) = \sum_{k\in\mathbb{Z}^d} U_k(x)\mathrm{e}^{i2\pi k\cdot y} \quad \text{with} \quad \|U\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} = \sum_{k\in\mathbb{Z}^d} \|U_k\|^2_{L^2(\mathbb{R}^d)}.$$

We denote by $H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$, for $s \geq 0$, the Sobolev space consisting of those functions $U \in L^2(\mathbb{R}^d \times \mathbb{T}^d)$ such that there exists $\varepsilon_0, C > 0$ for which we have

$$\forall \varepsilon \in (0,\varepsilon_0), \quad \|U\|^2_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} := \sum_{k\in\mathbb{Z}^d} \int_{\mathbb{R}^d} (1+|\varepsilon\xi|^2+|k|^2)^s |\widehat{U_k}(\xi)|^2 \mathrm{d}\xi \leq C. \tag{1.7}$$

These functions can be projected on the bands as follows. For every $n \in \mathbb{N}^*$ and $\xi \in \mathbb{R}^d$, we denote by $\Pi_n(\xi)$ the projector from $L^2(\mathbb{T}^d)$ onto the eigenspace corresponding to $\varrho_n(\xi)$. The corresponding Fourier multiplier $\Pi_n(\varepsilon D_x)$ acts on $L^2(\mathbb{R}^d_x \times \mathbb{T}^d_y)$, since band functions are bounded. Finally, we define the operator L^ε acting on functions $F \in H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$, $s > d/2$, by

$$(L^\varepsilon F)(x) := F\left(x, \frac{x}{\varepsilon}\right).$$

Then there exists $C_s > 0$ such that, for every $F \in H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$,

$$\|L^\varepsilon F\|_{L^2(\mathbb{R}^d)} \leq C_s \|F\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)}, \tag{1.8}$$

uniformly in $\varepsilon > 0$. See [15, Lemma 6.2].

We will make the following assumption on the family of initial data in (1.1).

H0 There exists a bounded family (U^ε_0) in $H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$ for some $s > d/2$ such that

$$\psi^\varepsilon_0 = L^\varepsilon U^\varepsilon_0.$$

Note that if $(\psi^\varepsilon_0)_{\varepsilon>0}$ is bounded in $H^s_\varepsilon(\mathbb{R}^d)$ with $s > d/2$, **H0** holds with $U^\varepsilon_0(y,x) = \psi^\varepsilon_0(x) \otimes \mathbf{1}_{\mathbb{T}^d}(y)$.

1.3. The Case of the Dimension One

Let us first state our results in dimension $d = 1$. When $d = 1$, one can prove that Λ_n is contained in $\pi\mathbb{Z}$, and consists only on non-degenerate critical points. In addition, when $|n - n'| > 1$, $\Sigma_{n,n'} = \emptyset$ and $\Sigma_n \cap \Lambda_n = \emptyset$

(see Lemma A.1). In this specific case, we are able to give a complete description of the limit of the energy density of families of solutions to (1.1) with initial data of the form stated in **H0**.

Theorem 1.1. *Assume (ψ_0^ε) satisfies* **H0**. *Then there exists a subsequence $(\psi_0^{\varepsilon_\ell})_{\ell\in\mathbb{N}}$ of the initial data, such that for every $a < b$ and every $\phi \in \mathcal{C}_0(\mathbb{R})$,*

$$\lim_{\ell\to\infty} \int_a^b \int_{\mathbb{R}} \phi(x)|\psi^{\varepsilon_\ell}(t,x)|^2 \mathrm{d}x\mathrm{d}t = \sum_{n\in\mathbb{N}^*} \sum_{\xi\in\Lambda_n} \int_a^b \int_{\mathbb{R}} \phi(x)|\psi_\xi^{(n)}(t,x)|^2 \mathrm{d}x\mathrm{d}t,$$

where, for every $n \in \mathbb{N}^*$ and $\xi \in \Lambda_n$, $\psi_\xi^{(n)}$ solves the effective mass Schrödinger equation

$$i\partial_t \psi_\xi^{(n)}(t,x) = \frac{1}{2}\partial_\xi^2 \varrho_n(\xi)\partial_x^2 \psi_\xi^{(n)}(t,x) + V_{\mathrm{ext}}(t,x)\psi_\xi^{(n)}(t,x) \tag{1.9}$$

with initial datum

$$\psi_\xi^{(n)}|_{t=0} \text{ is the weak limit in } L^2(\mathbb{R}) \text{ of the sequence } \left(\mathrm{e}^{-\frac{i}{\varepsilon_\ell}\xi x} L^{\varepsilon_\ell}\Pi_n(\varepsilon_\ell D_x)U_0^{\varepsilon_\ell}\right).$$

Note some of the accumulation points of $\mathrm{e}^{-\frac{i}{\varepsilon_\ell}\xi x} L^{\varepsilon_\ell}\Pi_n(\varepsilon_\ell D_x)U_0^{\varepsilon_\ell}$ may just be 0. For example if one has $V_{\mathrm{per}} = 0$, only the first Bloch energy ϱ_1 has critical points and they are precisely $\Lambda_1 = 2\pi\mathbb{Z}$. The addition, the associated projector $\Pi_1(\xi)$ coincides with the orthogonal projection onto $\mathbb{C}\mathrm{e}^{iky}$ whenever $\xi \in (k-\pi, k+\pi)$ and $k \in 2\pi\mathbb{Z}$. Therefore, if one takes $U_0^\varepsilon(x,y) = \psi_0^\varepsilon(x) \otimes \mathbf{1}_{y\in\mathbb{T}^d}$, then

$$\Pi_1(\varepsilon\xi)\widehat{U_0^{\varepsilon_\ell}}(\xi,\cdot) = \mathbf{1}_{(-\pi,\pi)}(\varepsilon\xi)\widehat{\psi_0^{\varepsilon_\ell}}(\xi),$$

and $\mathrm{e}^{-\frac{i}{\varepsilon_\ell}2\pi kx}\Pi_1(\varepsilon D_x)(\psi_0^{\varepsilon_\ell} \otimes \mathbf{1}_{y\in\mathbb{T}})$ weakly converges to zero when $k \neq 0$.

Theorem 1.1 is derived as a consequence of a more general analysis that is valid in any dimension under assumptions that are satisfied for all Bloch energies when $d = 1$, and that is presented in the next section.

1.4. The Generic case with $d \geq 1$-Conical Crossings

We now present results that, under a set of assumptions that always hold when $d = 1$, give a description of effective mass equations in higher dimension under the presence of generic crossings for data satisfying **H0**.

1.4.1. Assumptions Our first assumption concern the multiplicity of Bloch bands.

H1 For $n \in \mathbb{N}^*$, the multiplicity of the Bloch energy ϱ_n is one, except at crossing points, where it is two. This implies that a global labeling of the band functions exists such that $\Sigma_{n,n'} \neq \emptyset$ implies $|n - n'| = 1$.

Remark 1.2. Hypothesis **H1** is thought to be generic, as follows from the variational characterization of eigenvalues of Schrödinger operators with Bloch periodicity conditions. We make it in order to avoid having statements that are unnecessarily involved. As we stated it, it prevents from having simultaneous crossings of more than two Bloch energies, and higher multiplicities (both scenarios are non-generic). The proofs we provide can be adapted in order to deal with these situations.

We also consider a generic assumption on the set of critical points Λ_n defined in (1.4).

H2 For $n \in \mathbb{N}^*$, we assume that Hess ϱ_n is of constant rank in a neighborhood of each connected component of Λ_n.

Remark 1.3. Let $X \subseteq \Lambda_n$ be a connected component of Λ_n. By the constant rank level set theorem, this hypothesis implies that each connected component $X \subseteq \Lambda_n$ is a closed submanifold of $\mathbb{R}^d$ of dimension $d - \operatorname{rk} \operatorname{Hess} \varrho_n|_X$.

Finally, our third set of hypothesis concerns the geometry of the crossing sets Σ_n. For stating this assumption, we introduce geometric objects associated with a submanifold X of $(\mathbb{R}^d)^*$: we consider its tangent spaces $T_\xi X$ and define the fibre of the normal bundle NX of X above $\xi \in X$ as the vector space $N_\xi X$ consisting of those $\eta \in (\mathbb{R}^d)^{**} = \mathbb{R}^d$ that annihilate $T_\xi X$

$$NX := \{(\xi, \eta) \in X \times \mathbb{R}^d \,:\, \eta \cdot \zeta = 0, \quad \forall \zeta \in T_\xi X\}. \tag{1.10}$$

With a Bloch mode ϱ_n presenting crossings on a manifold Σ_n, we associate the function g_n defined on $N\Sigma_n$ by

$$(\xi, \eta) \mapsto g_n(\xi, \eta) := \frac{1}{2}\left(\varrho_{n+1}(\xi + \eta) - \varrho_n(\xi + \eta)\right), \quad \xi \in \Sigma_n, \quad \eta \in N_\xi \Sigma_n. \tag{1.11}$$

Note that $g_n(\xi, \eta) \geq 0$ and $g_n(\xi, \eta) = 0$ if and only if $\eta = 0$. Besides, for any $\xi \in \Sigma_n$, $\eta \mapsto g_n(\xi, \eta)$ is differentiable in all $\eta \neq 0$ (see "Appendix B"). We denote by $\nabla_\eta g_n(\xi, \eta)$ this differential, which can be identified with a vector of $N_\xi \Sigma_n \subset T_\xi(\mathbb{R}^d)^*$.

Definition 1.4. We say that the crossings of Σ_n are conic if and only if there exists a neighborhood U of Σ_n such that ϱ_n and ϱ_{n+1} are of multiplicity 1 outside Σ_n in U and there exists $c > 0$ such that

$$\forall (\xi, \eta) \in N\Sigma_n, \quad |g_n(\xi, \eta)| \geq c|\eta|.$$

Note that the critical sets Λ_n contain no conical crossing point. Besides, one can prove (see "Appendix B") that, generically, as soon as the crossing set Σ_n is a closed submanifold of $\mathbb{R}^d$, either ϱ_n has a conical singularity along Σ_n, either ϱ_n is in $\mathcal{C}^{1,1}$. We set, for $n \in \mathbb{N}^*$,

$$\lambda_n(\xi) = \frac{1}{2}\left(\varrho_n(\xi) + \varrho_{n+1}(\xi)\right), \quad \xi \in \mathbb{R}^d, \quad n \in \mathbb{N}^*, \tag{1.12}$$

and we introduce the following last assumption:

H3 For $n \in \mathbb{N}^*$, we assume that the crossing set Σ_n is a smooth closed submanifold of $\mathbb{R}^d$. Moreover, the crossing is of conic type in the sense of Definition 1.4 and for all $\xi \in \Sigma_n$, $\eta \in N_\xi \Sigma_n$ with $\eta \neq 0$,

$$\nabla_\xi \lambda_n(\xi) \pm \nabla_\eta g_n(\xi, \eta) \neq 0.$$

1.4.2. The Result: Dispersion Above Conical Crossings For stating the result, we need to introduce other geometric objects associated with a submanifold X of $(\mathbb{R}^d)^*$. We define its cotangent bundle as the union of all cotangent spaces to X

$$T^*X := \{(\xi, x) \in X \times \mathbb{R}^d \ : \ x \in T^*_\xi X\}, \tag{1.13}$$

each fibre $T^*_\xi X$ is the dual space of the tangent space $T_\xi X$. We shall denote by $\mathcal{M}_+(T^*X)$ the set of non-negative Radon measures on T^*X. We observe that every point $x \in \mathbb{R}^d$ can be uniquely written as

$$x = v + z \quad \text{where} \quad v \in T^*_\xi X \quad \text{and} \quad z \in N_\xi X.$$

Then, given a function $\phi \in L^\infty(\mathbb{R}^d)$ and a point $(\xi, v) \in T^*X$, we denote by $m^X_\phi(\xi, v)$ the operator acting on $L^2(N_\xi X)$ by multiplication by $\phi(v + \cdot)$. We shall denote by $\mathcal{L}(L^2(N_\xi X))$ the set of bounded operators acting on $L^2(N_\xi X)$ and by $\mathcal{L}^1_+(L^2(N_\xi X))$ the set of operators that are non-negative and trace-class. When $X = \Lambda_n$ and assumption **H2** holds, we will consider the operator $\operatorname{Hess} \varrho_n(\xi) D_z \cdot D_z$ acting on $N_\xi \Lambda_n$ for any $\xi \in \Lambda_n$.

Theorem 1.5. *Assume* **H1**, **H2** *and* **H3** *are satisfied for all $n \in \mathbb{N}^*$ and consider $(\psi^\varepsilon)_{\varepsilon>0}$ a family of solutions to equation (1.1) with an initial data $(\psi^\varepsilon_0)_{\varepsilon>0}$ that satisfies* **H0**. *Then, there exist a subsequence $(\psi^{\varepsilon_\ell}_0)_{\ell\in\mathbb{N}}$ of the initial data, a sequence of non negative measures $(\nu_n)_{n\in\mathbb{N}}$ on $T^*\Lambda_n$, and a sequence of measurable non negative trace-class operators $(M_n)_{n\in\mathbb{N}}$*

$$M_n : T^*_\xi \Lambda_n \ni (\xi, v) \mapsto M_n(\xi, v) \in \mathcal{L}^1_+(L^2(N_\xi \Lambda_n)), \quad \operatorname{Tr}_{L^2(N_\xi \Lambda_n)} M_n(\xi, v) = 1,$$

both depending only on $(\psi^{\varepsilon_\ell}_0)_{\ell\in\mathbb{N}}$, such that for every $a < b$ and every $\phi \in \mathcal{C}_0(\mathbb{R}^d)$ one has

$$\begin{aligned} &\lim_{\ell\to+\infty} \int_a^b \int_{\mathbb{R}^d} \phi(x) |\psi^{\varepsilon_\ell}(t, x)|^2 \mathrm{d}x \mathrm{d}t \\ &= \sum_{n\in\mathbb{N}} \int_a^b \int_{T^*\Lambda_n} \operatorname{Tr}_{L^2(N_\xi \Lambda_n)} \left(m^{\Lambda_n}_\phi(\xi, v) M^t_n(\xi, v) \right) \nu_n(d\xi, dv) \mathrm{d}t, \end{aligned} \tag{1.14}$$

where $t \mapsto M_n^t(\xi, v) \in \mathcal{C}(\mathbb{R}, \mathcal{L}^1_+(L^2(N_\xi \Lambda_n))$ *solves the von Neumann equation*

$$\begin{cases} i\partial_t M_n^t(\xi, v) = \left[\frac{1}{2}\mathrm{Hess}\varrho_n(\xi) D_z \cdot D_z + m_{V_{\mathrm{ext}}}^{\Lambda_n}(\xi, v)\ ,\ M_n^t(\xi, v))\right] \\ M_n^0 = M_n. \end{cases} \tag{1.15}$$

(recall that $m_\phi^{\Lambda_n}(\xi, v)$ *(resp.* $m_{V_{\mathrm{ext}}}^{\Lambda_n}(\xi, v)$*) denotes the operator acting on* $L^2(N_\xi \Lambda_n)$ *by multiplication by* $\phi(v + \cdot)$ *(resp.* $V_{\mathrm{ext}}(v + \cdot)$*)).*

Above and throughout this article, when A and B are two operators acting on the same Hilbert space, the notation $[A, B]$ denotes the commutator $AB - BA$. Several remarks are in order. First, note that the n-th term of the sum in (1.14) measures how much the critical points of the n-th Bloch mode trap the energy and prevent the dispersion effects. Theorem 1.5 also tells that conical crossings do not trap energy. This Theorem 1.5 has exactly the same form than Theorem 2.2 in [15] while the assumptions are quite different since crossings between Bloch energies are authorized as long as they are conical. We shall see in the next subsection that crossing points may trap energy when they also are critical points of the Bloch energies (and thus they are no longer conical).

Secondly, we emphasize that Remark 4.2 (1) comments the determination of $(M_n)_{n\in\mathbb{N}^*}$ and $(\nu_n)_{n\in\mathbb{N}^*}$ from the initial data. The special case where Λ_n is a point is discussed in the next subsection.

Thirdly, recall that when $d = 1$, the assumptions **H1**, **H2** and **H3** are automatically satisfied (see "Appendix A"). Therefore, Theorem 1.1 is a consequence of Theorem 1.5 in the case where critical points are isolated.

Finally, we emphasize that Theorem 1.5 extends to situations where the Fourier transform of the initial data is localized on a set of the form $\{\varepsilon\xi \in \Omega + 2\pi\mathbb{Z}^d\}$ for some open subset Ω of a unit cell of $2\pi\mathbb{Z}^d$, provided the assumptions **H2** and **H3** are satisfied for all $n \in \mathbb{N}^*$ above points of $\Omega + 2\pi\mathbb{Z}^d$. We esquiss this approach in Section 7.4 and explain how the arguments of the proofs detailed below can be adapted to this setting by localisation (see Lemma 7.3).

1.4.3. The Special Case of Isolated Critical Points When **H1**, **H2** and **H3** are satisfied for all $n \in \mathbb{N}^*$ and, moreover, all the sets Λ_n consist in a family of isolated critical points then $T^*\Lambda_n = \Lambda_n \times \{0\}$, $N\Lambda_n = \mathbb{R}^d$ so that the operators M_n^t only depend on the parameter $\xi \in \Lambda_n$ and the operator $m_\phi^{\Lambda_n}(\xi, v)$ simply is the operator of multiplication by ϕ. One can prove a statement very similar to Theorem 1.1 (see also Corollary 1.3 in [15] and Remark 4.2 (2)): the measures ν_n^t are linear combinations of Dirac masses at the points $\xi_n \in \Lambda_n$ and $M_n^t(\xi_n)$ are orthogonal projectors on $\mathbb{C}\psi^{\xi_n}(t)$, the solution to

$$i\partial_t \psi^{\xi_n}(t, x) = \frac{1}{2}\mathrm{Hess}\varrho_n(\xi_n) D_x \cdot D_x \psi^{\xi_n}(t, x) + V_{\mathrm{ext}}\psi^{\xi_n}(t, x) \tag{1.16}$$

with initial data $\psi^{\xi_n}(0)$ that is a weak limit of $\left(\mathrm{e}^{-\frac{i}{\varepsilon_\ell}x\cdot\xi_n} L^{\varepsilon_\ell}\Pi_n(\varepsilon_\ell D_x) U_0^{\varepsilon_\ell}\right)_{\varepsilon_\ell>0}$ in $L^2(\mathbb{R}^d)$.

In order to illustrate this type of result in the multidimensional setting, we state it in the particular case of well-prepared data that satisfy $U_0^\varepsilon(y,x) = \varphi_{n_0}(y,\varepsilon D_x)u_{n_0}^\varepsilon(x)$ for some $n_0 \in \mathbb{N}^*$ (and therefore $\Pi_n(\varepsilon D_x)U_0^\varepsilon = 0$ for $n \neq n_0$). More specifically, the class of well-prepared initial data that we will consider is those of the form

$$\psi_{0,n}^\varepsilon(x) := \varphi_n\left(\frac{x}{\varepsilon}, \varepsilon D_x\right) u_n^\varepsilon(x), \quad u_n^\varepsilon(x) = \mathrm{e}^{\frac{i}{\varepsilon}x\cdot\xi_n} v_n^\varepsilon(x), \quad n \in \mathbb{N}^* \tag{1.17}$$

with $\xi_n \in \Lambda_n$, $(v_n^\varepsilon)_{\varepsilon>0}$ bounded in $H^s(\mathbb{R}^d)$, $s > d/2$ or $s > 1$ when $d = 1$, and such that

$$v_n^\varepsilon \rightharpoonup v_n, \quad \varepsilon \to 0^+, \quad \text{in } L^2(\mathbb{R}^d).$$

These data are closely related with those considered in [1,2] for example (this connection is explained in detail in Lemma E.1). Their main properties are studied in "Appendix E").

Proposition 1.6. *Assume* **H1**, **H2** *and* **H3** *are satisfied for all $n \in \mathbb{N}^*$ and that, for some $n_0 \in \mathbb{N}^*$, the set Λ_{n_0} is discrete. Consider $(\psi^\varepsilon)_{\varepsilon>0}$ a family of solutions to equation* (1.1) *with initial data ψ_0^ε satisfying* (1.17) *for some $\xi_{n_0} \in \Lambda_{n_0}$ and $v_{n_0}^\varepsilon$, v_{n_0} in $L^2(\mathbb{R}^d)$. Then, there exists a subsequence $(\psi_0^{\varepsilon_\ell})_{\ell\in\mathbb{N}}$ of the initial data such that for every $a < b$ and every $\phi \in \mathcal{C}_0(\mathbb{R}^d)$ one has*

$$\lim_{\ell\to+\infty} \int_a^b \int_{\mathbb{R}^d} \phi(x)|\psi^{\varepsilon_\ell}(t,x)|^2 \mathrm{d}x\mathrm{d}t = \int_a^b \int_{\mathbb{R}^d} \phi(x)|\psi^{\xi_{n_0}}(t,x)|^2 \mathrm{d}t,$$

where $\psi^{\xi_{n_0}}(t)$ solves (1.16) *with initial data $\psi^{\xi_{n_0}}(0) = v_{n_0}$*

If $v_0^\varepsilon \to v_{n_0}$ as $\varepsilon \to 0^+$ in $L^2(\mathbb{R}^d)$, then one has for all $t \in \mathbb{R}$, $\|\psi_0^\varepsilon\|_{L^2} \to \|\psi^{\xi_{n_0}}(t)\|_{L^2}$, which implies that no energy is dispersed. As a consequence of Remark 7.2, one obtains that the result of Proposition 1.6 holds locally in time: for all $T > 0$, there exists a subsequence $(\psi_0^{\varepsilon_\ell})$ of the initial data such that for every $\phi \in \mathcal{C}_0(\mathbb{R}^d)$ one has for all $t \in [0, T]$

$$\lim_{\ell\to+\infty} \int_{\mathbb{R}^d} \phi(x)|\psi^{\varepsilon_\ell}(t,x)|^2 \mathrm{d}x\mathrm{d}t = \int_{\mathbb{R}^d} \phi(x)|\psi^{\xi_{n_0}}(t,x)|^2.$$

Proposition 1.6 is an improvement of Theorem 3.2 in [2] since it holds without any simplicity assumption on the Bloch energy ϱ_{n_0}. However, in the case where $\xi_{n_0} \notin \Lambda_{n_0}$ as in Theorem 4.5 of [2] where a drift is taken into account, the application of Theorem 1.1 does not bring any improvement. In particular, if $\xi_{n_0} \in \Sigma_{n_0}$, Theorem 1.1 gives 0 at the limit and Theorem 4.5 of [2] does not apply (the drift $\nabla\varrho_{n_0}(\xi_{n_0})$ is not defined). Studying how the mass goes to infinity in that special case would be an interesting follow-up of the results presented here.

1.5. A Non-generic Case with Interactions of Bloch Bands Above Non-conical Crossing Points

In that section, we consider degenerate crossing points that we define as follows:

Definition 1.7. We say that the crossing set Σ_n is degenerate if some $q \geq 2$ exists such that the function g_n defined in (1.11), satisfies

$$\exists c > 0, \quad \forall (\xi, \eta) \in N\Sigma_n, \ |\eta| < 1, \ g_n(\xi, \eta) \leq c|\eta|^q.$$

If the above inequality fails for any $q' > q$, we say the crossing set has degeneracy of order q.

1.5.1. Assumptions We consider two Bloch energies that cross in a degenerate manner, though isolated from the remainder of the spectrum.

H1' $\varrho_n(\xi)$ and $\varrho_{n+1}(\xi)$ are two Bloch energies that cross on Σ_n and are of multiplicity 1 outside Σ_n.
H2' $\operatorname{Hess} \varrho_n$ (resp. $\operatorname{Hess} \varrho_{n+1}$) is of constant rank in a neighborhood of each connected component of Λ_n (resp. Λ_{n+1}).
H3' The crossing set ξ_n is a smooth closed submanifold of $\mathbb{R}^d$ included in $\Lambda_n \cap \Lambda_{n+1}$ and is degenerated of order q. Besides, $\Sigma_{n-1} = \Sigma_{n+1} = \emptyset$ and

- if $q > 2$, for all $\xi \in \Sigma_n$, the Hessian of λ_n is of rank $d - \operatorname{Rank} \Sigma_n$ in a neighborhood of Σ_n,
- if $q = 2$, for all $(\xi, \eta) \in N\Sigma_n$ with $|\eta| = 1$,

$$\operatorname{Hess} \lambda_n(\xi)\eta \pm \nabla_\eta g_n(\xi, \eta) \neq 0.$$

Note that the latter assumption can be considered as a maximal rank assumption. Indeed, if $q > 2$, the Bloch energies are $\mathcal{C}^2$ and $\operatorname{Hess} \varrho_n(\xi) = \operatorname{Hess} \varrho_{n+1}(\xi) = \operatorname{Hess} \lambda_n(\xi)$ above points $\xi \in \Sigma_n$. Moreover, if $q = 2$ and $(\xi_k, \omega_k)_{k \in \mathbb{N}}$ is a sequence of points satisfying for all $k \in \mathbb{N}$, $\omega_k \in N_{\xi_k}\Sigma_n$ with $|\omega_k| = 1$, we have the following property: if $(\xi_k, \omega_k) \underset{\ell \to +\infty}{\longrightarrow} (\xi, \omega) \in N\Sigma_n$ then

$$\operatorname{Hess} \varrho_n(\xi_k)\omega_k \underset{(\xi_k, \omega_k) \to (\xi, \omega)}{\longrightarrow} \operatorname{Hess} \lambda_n(\xi)\omega \pm \nabla_\eta g_n(\xi, \omega).$$

This property shows the link between $\operatorname{Hess} \lambda_n(\xi)\eta \pm \nabla_\eta g_n(\xi, \eta)$ and $\operatorname{Hess} \varrho_n(\xi)\eta$.

The assumption **H3'** implies that $\nabla\lambda_n = 0$ on Σ_n. We shall see in the proof that if $\nabla\lambda_n$ does not vanish on Σ_n, then these degenerate crossing points do not contribute. The result then is comparable to the one of Theorem 1.5. Notice that one always has

$$\Lambda_n \cap \Lambda_{n+1} = \Sigma_n \cap \Lambda_n = \Sigma_n \cap \Lambda_{n+1} = \Sigma_n \cap \{\nabla\lambda_n(\xi) = 0\}.$$

At the difference with the results of the preceding section that were obtained under the assumption that **H1**, **H2** and **H3** were satisfied for all $n \in \mathbb{N}^*$, we will assume in this section that we have **H1'**, **H2'** and **H3'** for some single $n \in \mathbb{N}^*$ and we will choose well-prepared data concentrating on the bands ϱ_n and ϱ_{n+1} involved in the assumptions.

We assume that

$$\psi_0^\varepsilon(x) = \varphi_n\left(\frac{x}{\varepsilon}, \varepsilon D\right) u_n^\varepsilon(x) + \varphi_{n+1}\left(\frac{x}{\varepsilon}, \varepsilon D\right) u_{n+1}^\varepsilon(x), \tag{1.18}$$

where φ_n (resp. φ_{n+1}) is the Bloch wave associated with ϱ_n (resp. ϱ_{n+1}), and $(u_n^\varepsilon)_{\varepsilon>0}$ and $(u_{n+1}^\varepsilon)_{\varepsilon>0}$ are bounded families in $H_\varepsilon^s(\mathbb{R}^d)$, $s > d/2$. These data are somehow more general than those of (1.17) since no assumption is made on u_n^ε ans u_{n+1}^ε.

1.5.2. The Result: Concentration Above Degenerate Crossings We prove that for data as in (1.18), the way their components interact above the crossing set plays a role in the determination of the weak limits of the time-averaged energy density. We associate with the function g_n defined on $N\Sigma_n$ (see (1.11)) the operator $Q_{g_n}^{\Sigma_n}(\xi)$ acting on $L^2(N_\xi \Sigma_n)$ as a Fourier multiplier.

Theorem 1.8. *Let $(\psi^\varepsilon)_{\varepsilon>0}$ be a family of solutions to equation (1.1) with initial data satisfying (1.18). Assume the Bloch energies ϱ_n and ϱ_{n+1} satisfies* **H1'**, **H2'** *and* **H3'** *with $\Lambda_n = \Lambda_{n+1} = \Sigma_n$. Then, there exists a subsequence $(\psi_0^{\varepsilon_\ell})_{\ell\in\mathbb{N}}$ of the initial data, a non negative measure $\nu^0 \in \mathcal{M}^+(\Sigma_n)$ and a matrix M of measurable trace-class operators*

$$\begin{aligned} &M : T_\xi^*\Sigma_n \ni (\xi, v) \mapsto M(\xi, v) \in \mathcal{L}_+^1(L^2(N_\xi\Sigma_n, \mathbb{C}^2)),\\ &\mathrm{Tr}_{L^2(N_\xi\Sigma_n,\mathbb{C}^2)} M(\xi, v) = 1 \; d\nu^0 \; a.e., \end{aligned}$$

both depending only on $(\psi_0^{\varepsilon_\ell})_{\ell\in\mathbb{N}}$, such that for every $a < b$ and every $\phi \in \mathcal{C}_0(\mathbb{R}^d)$ one has

$$\begin{aligned} &\lim_{\ell\to+\infty} \int_a^b \int_{\mathbb{R}^d} \phi(x)|\psi^{\varepsilon_\ell}(t, x)|^2 \mathrm{d}x\mathrm{d}t\\ &= \int_a^b \int_{T^*\Sigma_n} \mathrm{Tr}_{L^2(N_\xi\Sigma_n,\mathbb{C})}\\ &\qquad [m_\phi^{\Sigma_n}(\xi, v)(m_n^t + m_{n+1}^t + 2\mathrm{Re}(m_{n,n+1}^t))(\xi, v)]\nu^0(d\xi, dv)\mathrm{d}t, \end{aligned}$$

where

$$M^t(\xi, v) = \begin{pmatrix} m_n^t(\xi, v) & m_{n,n+1}^t(\xi, v)\\ m_{n,n+1}^t(\xi, v)^* & m_{n+1}^t(\xi, v) \end{pmatrix}$$

is a non negative trace class operator on $L^2(N_\xi\Sigma_n, \mathbb{C}^2)$. In addition, the map

$$t \mapsto M^t(\xi, v) \in \mathcal{C}(\mathbb{R}, \mathcal{L}_+^1(L^2(N_\xi\Sigma_n, \mathbb{C}^2))$$

solves a von Neumann equation that depends on the value of q:

- *If $q > 2$, it solves*

$$\begin{aligned} &i\partial_t M^t(\xi, v) = \left[\left(\frac{1}{2}\mathrm{Hess}\lambda_n(\xi)D_z \cdot D_z + m_{V_{\mathrm{ext}}}^{\Sigma_n}(\xi, v)\right)\mathrm{Id}_{\mathbb{C}^2}\ ,\ M^t(\xi, v)\right],\\ &M^0 = M. \end{aligned} \tag{1.19}$$

• *If $q = 2$, it solves*

$$i\partial_t M^t(\xi, v) = \left[\left(\frac{1}{2}\mathrm{Hess}\,\lambda_n(\xi)D_z \cdot D_z + m^{\Sigma_n}_{V_{\mathrm{ext}}(t,\cdot)}(\xi, v)\right)\mathrm{Id}_{\mathbb{C}^2} - Q^{\Sigma_n}_{g_n}(\xi)\,J\ ,\ M^t(\xi, v)\right],$$
$$M^0 = M \tag{1.20}$$

with $J = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

(recall that $m^{\Sigma_n}_{\phi}(\xi, v)$ (resp. $m^{\Sigma_n}_{V_{\mathrm{ext}}}(\xi, v)$) denotes the operator acting on $L^2(N_\xi\Sigma_n)$ by multiplication by $\phi(v+\cdot)$ (resp. $V_{\mathrm{ext}}(v+\cdot)$), and $Q^{\Sigma_n}_{g_n}(\xi)$ is the Fourier multiplier on $L^2(N_\xi\Sigma_n)$ associated with the function $g_n(\xi, \cdot)$).

In the latter statement, we have assumed for simplicity that the critical sets of the two Bloch energies ϱ_n and ϱ_{n+1} coincide with the crossing set Σ_n. We indeed prove this result without this assumption; however, the resulting statement is more involved (see Theorem 7.1).

1.5.3. The Special Case of Isolated Degenerate Crossing Points When Σ_n consists in a family of isolated degenerate crossing points, the preceding statement admits a simpler, more transparent formulation. Indeed, as in Section 1.4.3, the operator M^t only depend on the parameter $\xi \in \Sigma_n$ and the operator $m^{\Lambda_n}_{\phi}(\xi, v)$ simply is the operator of multiplication by ϕ and $Q^{\Sigma_n}_{g_n} = g_n(\xi, D_x)$. We now assume that ψ^ε_0 satisfies (1.18) with

$$u^\varepsilon_n(x) = \mathrm{e}^{\frac{i}{\varepsilon}x\cdot\xi_n}v^\varepsilon_n(x) \ \text{ and } \ u^\varepsilon_{n+1}(x) = \mathrm{e}^{\frac{i}{\varepsilon}x\cdot\xi_n}v^\varepsilon_{n+1}(x)$$

with $\xi_n \in \Sigma_n$, and for $j \in \{n, n+1\}$, $(v^\varepsilon_j)_{\varepsilon>0}$ bounded in $H^s(\mathbb{R}^d)$, $s > d/2$ or $s > 1$ when $d = 1$, and such that:

$$v^\varepsilon_j \rightharpoonup v_j, \quad \varepsilon \to 0^+, \quad \text{in } L^2(\mathbb{R}^d).$$

Proposition 1.9. *Let $(\psi^\varepsilon)_{\varepsilon>0}$ be a family of solutions to equation (1.1) with initial data satisfying (1.18). Assume the Bloch energies ϱ_n and ϱ_{n+1} satisfy* **H1'**, **H2'** *and* **H3'**. *Assume moreover $\Lambda_n = \Lambda_{n+1} = \Sigma_n$ consists in a family of isolated critical crossing points. Then, there exists a subsequence $(\psi^{\varepsilon_\ell}_0)_{\ell\in\mathbb{N}}$ of the initial data such that for every $a < b$ and every $\phi \in \mathcal{C}_0(\mathbb{R}^d)$ one has*

$$\lim_{\ell\to+\infty}\int_a^b\int_{\mathbb{R}^d}\phi(x)|\psi^{\varepsilon_\ell}(t, x)|^2\mathrm{d}x\mathrm{d}t = \sum_{\xi\in\Sigma_n}\int_a^b\int_{\mathbb{R}^d}\phi(x)$$
$$|\psi^{\xi_n}_n(t, x) + \psi^{\xi_n}_{n+1}(t, x)|^2\mathrm{d}x\mathrm{d}t,$$

where

• *if $q > 2$, for $j \in \{n, n+1\}$, ψ^ξ_j solves the effective mass Schrödinger equation*

$$i\partial_t\psi^{\xi_n}_j = \frac{1}{2}\mathrm{Hess}\lambda_n(\xi_n)D_x \cdot D_x\psi^{\xi_n}_j + V_{\mathrm{ext}}\psi^{\xi_n}_j \tag{1.21}$$

- *if $q = 2$, for $j \in \{n, n+1\}$, ψ_j^{ξ} solves the effective mass Schrödinger equation*

$$i\partial_t \psi_j^{\xi_n} = \frac{1}{2}\mathrm{Hess}\lambda_n(\xi_n) D_x \cdot D_x \psi_j^{\xi_n} + \eta_j g_n(\xi_n, D_x)\psi_j^{\xi_n} + V_{\mathrm{ext}}\psi_j^{\xi_n}, \quad (1.22)$$

with $\eta_n = 1$ and $\eta_{n+1} = -1$.

Besides, for $j \in \{n, n+1\}$, the initial data $\psi_j^{\xi_n}(0) = v_j$.

We stress the fact that, in contrast to what happened in the presence of a singular crossing, the description of the limiting position density limit involves a term of the form $2\mathrm{Re}(\psi^{\xi_n}\overline{\psi^{\xi_{n+1}}})$ which takes into account the coupling between the modes corresponding to the two Bloch bands.

1.6. Ideas of the Proofs and Organisation of the Paper

We follow the semi-classical approach developed in [14,15] which is based on semi-classical analysis. In these references, the Bloch energies in consideration are smooth, and we have exhibited the role of the critical points of the Bloch energies as principal contributors to the weak limits of the time-averaged energy densities. We have also explained how a second microlocalisation allows to compute quantitatively this contribution. We follow here this scheme of thoughts with additional difficulties that are two-fold.

Firstly, in order to consider general initial data as in Theorem 1.1 and 1.5, and to decompose them on the Bloch energies, we shall need to treat infinite series. The assumption that the data satisfy **H0** is the key point that we use technically for treating this issue. We explain in Section 2 how we perform the decomposition and which properties of the solution we use.

The second difficulty comes from the lack of regularity of the Bloch energies close to the crossing sets, which requires to perform semi-classical calculus with symbols of low regularity, what we do by using and developing ideas from [28]. We explain and construct in Sections 3 and 4 the semi-classical and two-microlocal analysis of our problem.

This led us to the statement of two theorems that are interesting by themselves: in Theorems 4.5 and 4.6, we describe the evolution of two-microlocal semi-classical measures associated to the concentration of the solutions of (1.1) on one of the sets of critical points Λ_n, $n \in \mathbb{N}_0^*$, and in the context given by hypothesis **H1**, **H2** and **H3** for the first one and **H1'**, **H2'** and **H3'** for the second one. These two theorems are proved in Sections 5 and 6 respectively; they are the core of the proofs of Theorems 1.5 and 1.8, which are performed themselves in Section 7, together with the proof of Theorem 1.1, Propositions 1.6 and 1.9.

Finally, some appendices are devoted to technical elements that we use in the proofs of this paper: special features of the Bloch decomposition in dimension 1 ("Appendix A"), properties of the Bloch energies at a crossing ("Appendix B"), elements of matrix-valued pseudo-differential calculus, in particular with low regularity ("Appendix C"), two scale pseudodifferential calculus ("Appendix D") and various remarks above well-prepared data ("Appendix E").

2. Separation of Scales and Control of the Oscillations

Here we present the first steps of the strategy that will lead to the proof of Theorems 1.1, 1.5 and 1.8. Our starting point is the following *Ansatz* that is widely used in this context and consists in separating the slow and fast scales of oscillation. We look for a solution to (1.1) of the form

$$\psi^\varepsilon(t,x) = U^\varepsilon\left(t, x, \frac{x}{\varepsilon}\right), \quad (t,x) \in \mathbb{R}\times\mathbb{R}^d, \tag{2.1}$$

where $U^\varepsilon(t,\cdot,\cdot)$ is a function on $\mathbb{R}^d \times \mathbb{T}^d$. In order to make sense of this, some regularity on the solutions ψ^ε is required, and this partly justifies our assumption **H0**. Uniqueness for solutions to the initial value problem for the Schrödinger equation (1.1) with initial data satisfying **H0** implies that (2.1) holds provided U^ε is a solution to the system

$$\begin{cases} i\varepsilon^2\partial_t U^\varepsilon(t,x,y) = P(\varepsilon D_x)U^\varepsilon(t,x,y) + \varepsilon^2 V_{\text{ext}}(t,x)U^\varepsilon(t,x,y), \\ U^\varepsilon_{|t=0} = U^\varepsilon_0, \end{cases} \tag{2.2}$$

By Lemma 6.5 in [15], this equation is well-posed in $H^s_\varepsilon(\mathbb{T}^d\times\mathbb{R}^d)$: there exists $C_s > 0$ such that for every $t\in\mathbb{R}$ and $U^\varepsilon_0 \in H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)$,

$$\|U^\varepsilon(t,\cdot)\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} \le \|U^\varepsilon_0\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} + C_s\varepsilon|t| \tag{2.3}$$

uniformly in $\varepsilon > 0$.

We shall use a decomposition of the solution U^ε in the basis of Bloch modes. We set, for $j\in\mathbb{N}_0$,

$$P^\varepsilon_{\varphi_j} W(x,y) := \varphi_j(y,\varepsilon D_x)\int_{\mathbb{T}^d}\overline{\varphi_j}(z,\varepsilon D_x)W(x,z)\mathrm{d}z, \quad \forall W\in L^2(\mathbb{T}^d\times\mathbb{R}^d). \tag{2.4}$$

Lemma 2.1. *If $(\psi^\varepsilon_0)_{\varepsilon>0}$ satisfies* **H0**, *then for all $t\in\mathbb{R}$, the solution of* (1.1) *is given by*

$$\psi^\varepsilon(t,\cdot) = \sum_{n\in\mathbb{N}^*}\psi^\varepsilon_n(t,\cdot), \tag{2.5}$$

where the convergence of the series takes place in $L^2(\mathbb{R}^d)$ and

$$\psi^\varepsilon_n(t,x) := L^\varepsilon P^\varepsilon_{\varphi_n}U^\varepsilon(t,x) = \varphi_n\left(\frac{x}{\varepsilon},\varepsilon D_x\right)\int_{\mathbb{T}^d}\overline{\varphi_n}(y,\varepsilon D_x)U^\varepsilon(t,x,y)\mathrm{d}y. \tag{2.6}$$

Moreover, for every $t\in\mathbb{R}$,

$$\limsup_{\varepsilon\to 0^+}\left\|\sum_{n>N}\psi^\varepsilon_n(t,\cdot)\right\|_{L^2(\mathbb{R}^d)} \underset{N\to\infty}{\longrightarrow} 0. \tag{2.7}$$

The proof of this result requires two important technical facts that we gather in the next two remarks.

Remark 2.2. Modulo the addition of a positive constant to equation (1.1), we may assume that $P(\varepsilon D_x)$ is a positive operator (this will modify the solutions only by a constant phase in time). In that case there exists constants $\varepsilon_0, c > 0$ such that

$$\begin{aligned} c^{-1}\|U\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} &\leq \|\langle\varepsilon D_x\rangle^s U\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} + \|P(\varepsilon D_x)^{s/2}U\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} \\ &\leq c\|U\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} \end{aligned}$$

for every $U \in H^s(\mathbb{R}^d \times \mathbb{T}^d)$ and $0 < \varepsilon < \varepsilon_0$.

Remark 2.3. In view of (1.3), and the fact that $P(\xi)$ depends analytically on ξ, follows that $\xi \mapsto \varphi_j(\cdot, \xi)$, $j \in \mathbb{N}^*$, are continuous functions from $\mathbb{R}^d$ to $L^2(\mathbb{T}^d)$ (see also [56]) and that, for every $s > 0$, the family $P(\xi)^s$ depends continuously on ξ (with $P(\xi)$ positive).

These remarks imply the boundedness of the operators P_{φ_j} in $H^s_\varepsilon(\mathbb{T}^d \times \mathbb{R}^d)$ for all $j \in \mathbb{N}_0$. To see this, note that Remark 2.3 implies that formula 2.4 defines a bounded operator on $L^2(\mathbb{T}^d \times \mathbb{R}^d)$. Moreover, we have

$$[P(\varepsilon D_x)^{s/2}, P^\varepsilon_{\varphi_j}] = [\langle\varepsilon D_x\rangle^s, P^\varepsilon_{\varphi_j}] = 0.$$

If follows from Remark 2.2 that there exists $c_1 > 0$ such that, for all $W \in H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$,

$$\|P^\varepsilon_{\varphi_j} W\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} \leq c_1\|W\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)},$$

and, more generally, that every $W \in H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$ can be expressed in the topology of $H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$ as

$$W = \sum_{n\in\mathbb{N}^*} P^\varepsilon_{\varphi_n} W.$$

Proof of Lemma 2.1. The boundedness in $H^s_\varepsilon(\mathbb{T}^d \times \mathbb{R}^d)$ of the operator P_{φ_j} and the boundedness of L^ε from $H^s_\varepsilon(\mathbb{T}^d \times \mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$ for $s > d/2$ imply that that (2.5) holds in $L^2(\mathbb{R}^d)$.

It remains to prove (2.7). In view of (2.3), (1.8), it is enough to show that if $(V^\varepsilon)_{\varepsilon>0}$ is a bounded family in $H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$, $s > d/2$, we have, for $d/2 < r < s$,

$$\limsup_{\varepsilon\to 0^+} \left\| \sum_{n>N} P^\varepsilon_{\varphi_n} V^\varepsilon \right\|_{H^r_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} \underset{N\to\infty}{\longrightarrow} 0.$$

Remark 2.2 implies that we only have to prove

$$\limsup_{\varepsilon\to 0^+} \left\| \sum_{n>N} P(\varepsilon D_x)^{r/2} P^\varepsilon_{\varphi_n} V^\varepsilon \right\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}$$

$$+\limsup_{\varepsilon\to 0^+}\left\|\sum_{n>N}\langle\varepsilon D_x\rangle^r P^\varepsilon_{\varphi_n}V^\varepsilon\right\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}\underset{N\to\infty}{\longrightarrow}0. \tag{2.8}$$

We thus focus on proving (2.8).

Let us consider the series $\sum_{n>N}P(\varepsilon D_x)^{r/2}P^\varepsilon_{\varphi_n}V^\varepsilon$ (the proof for $\sum_{n>N}\langle\varepsilon D_x\rangle^r P^\varepsilon_{\varphi_n}V^\varepsilon$ is similar). In view of (2.4),

$$P(\varepsilon D_x)P^\varepsilon_{\varphi_n}V^\varepsilon(x,y)=\varphi_n(y,\varepsilon D_x)\varrho_n(\varepsilon D_x)\int_{\mathbb{T}^d}\overline{\varphi_n}(z,\varepsilon D_x)V^\varepsilon(x,z)\mathrm{d}z,$$

This implies

$$\left\|\sum_{n>N}P(\varepsilon D_x)^{r/2}P^\varepsilon_{\varphi_n}V^\varepsilon\right\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}=\sum_{n>N}\left\|P(\varepsilon D_x)^{r/2}P^\varepsilon_{\varphi_n}V^\varepsilon\right\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}.$$

We decompose V^ε in Fourier series and write $V^\varepsilon(x,y)=\sum_{j\in\mathbb{Z}^d}V^\varepsilon_j(x)\mathrm{e}^{2i\pi j\cdot y}$, whence

$$\begin{aligned}&P(\varepsilon D_x)P^\varepsilon_{\varphi_n}V^\varepsilon(x,y)\\&\quad=\varphi_n(y,\varepsilon D_x)\sum_{j\in\mathbb{Z}^d}\varrho_n(\varepsilon D_x)\left(\int_{\mathbb{T}^d}\overline{\varphi_n}(z,\varepsilon D_x)\mathrm{e}^{2i\pi j\cdot z}\mathrm{d}z\right)V^\varepsilon_j(x),\end{aligned}$$

and by functional calculus,

$$P(\varepsilon D_x)^{r/2}P^\varepsilon_{\varphi_n}V^\varepsilon(x,y)=\varphi_n(y,\varepsilon D_x)\sum_{j\in\mathbb{Z}^d}d_n(\varepsilon D_x,j)V^\varepsilon_j(x)$$

with

$$d_n(\xi,j)=\varrho_n(\xi)^{r/2}\left(\int_{\mathbb{T}^d}\overline{\varphi_n}(z,\varepsilon D_x)\mathrm{e}^{2i\pi j\cdot z}\mathrm{d}z\right)$$

We use three observations.

(1) First, if $\delta>0$ is fixed, there exists J_0 such that

$$\limsup_{\varepsilon\to 0^+}\sum_{|j|>J_0}\int_{\mathbb{R}^d}(1+|\varepsilon\xi|^2+|j|^2)^r|\widehat{V^\varepsilon_j}(\xi)|^2\mathrm{d}\xi<\delta.$$

To see this note that:

$$\sum_{|j|>J_0}\int_{\mathbb{R}^d}(1+|\varepsilon\xi|^2+|j|^2)^r|\widehat{V^\varepsilon_j}(\xi)|^2\mathrm{d}\xi\le(1+|J_0|^2)^{r-s}\|V^\varepsilon\|^2_{H^s(\mathbb{R}^d\times\mathbb{T}^d)},$$

due to the definition of the H^s_ε-norm (1.7). Since $(V^\varepsilon)_{\varepsilon>0}$ is uniformly bounded in $H^s_\varepsilon(\mathbb{R}^d)$, the claim follows.

(2) Second, given $\delta > 0$ and $J_0 \in \mathbb{N}$, one can find $R = R(\delta, J_0) > 0$ such that

$$\limsup_{\varepsilon \to 0^+} \sum_{|j| < J_0} \int_{|\varepsilon\xi| > R} (1 + |\varepsilon\xi|^2 + |j|^2)^r |\widehat{V_j^\varepsilon}(\xi)|^2 \mathrm{d}\xi < \delta.$$

This follows from the estimate

$$\int_{|\varepsilon\xi| > R} (1 + |\varepsilon\xi|^2 + |j|^2)^r |\widehat{V_j^\varepsilon}(\xi)|^2 \mathrm{d}\xi \leq (1 + R^2)^{r-s} \|V^\varepsilon\|^2_{H^s(\mathbb{R}^d \times \mathbb{T}^d)},$$

and again from the fact that $(V^\varepsilon)_{\varepsilon > 0}$ is uniformly bounded in $H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$.

(3) Third, given $J_0, R > 0$,

$$D_N(R, J_0) := \sup_{|j| \leq J_0} \sup_{|\xi| \leq R} \sum_{n > N} |d_n(\xi, j)|^2 \underset{N \to \infty}{\longrightarrow} 0.$$

To see why this holds, note that, for $j \in \mathbb{Z}^d$,

$$\mathbb{R}^d \ni \xi \longmapsto \sum_{n \in \mathbb{N}^*} |d_n(\xi, j)|^2 = \left\| P(\xi)^{r/2} \mathrm{e}^{2i\pi j \cdot} \right\|^2_{L^2(\mathbb{T}^d)} \in (0, \infty) \tag{2.9}$$

is a non-negative continuous function. The claim then follows from Dini's theorem, which ensures that for every $R > 0$, $j \in \mathbb{Z}^d$ one has

$$\sup_{|\xi| \leq R} \sum_{n > N} |d_n(\xi, j)|^2 \underset{N \to \infty}{\longrightarrow} 0.$$

We now use these observations to treat the series whose terms are

$$\left\| P(\varepsilon D_x)^{r/2} P^\varepsilon_{\varphi_n} V^\varepsilon \right\|^2_{L^2(\mathbb{R}^d \times \mathbb{T}^d))} = \sum_{j \in \mathbb{Z}^d} \int_{\mathbb{R}^d} |d_n(\varepsilon\xi, j)|^2 |\widehat{V}_j^\varepsilon(\xi)|^2 \mathrm{d}\xi.$$

Fix $\delta > 0$, and consider J_0 given by Point (1) and $R = R(\delta, J_0)$ given by Point (2). Decompose the sum of integrals in three terms

$$\sum_{j \in \mathbb{Z}^d} \int_{\mathbb{R}^d} = \sum_{|j| \leq J_0} \int_{|\varepsilon\xi| \leq R} + \sum_{|j| \leq J_0} \int_{|\varepsilon\xi| > R} + \sum_{|j| > J_0} \int_{\mathbb{R}^d}.$$

We start by analyzing the third term. Note that

$$\sum_{n \in \mathbb{N}^*} |d_n(\xi, j)|^2 = \left\| P(\xi)^{r/2} \mathrm{e}^{2i\pi j \cdot} \right\|^2_{L^2(\mathbb{T}^d)} \leq c_r (1 + |\xi|^2 + |j|^2)^r$$

Therefore,

$$\begin{aligned} &\limsup_{\varepsilon \to 0^+} \sum_{n > N} \sum_{|j| > J_0} \int_{\mathbb{R}^d} |d_n(\varepsilon\xi, j)|^2 |\widehat{V}_j^\varepsilon(\xi)|^2 \mathrm{d}\xi \\ &\leq \limsup_{\varepsilon \to 0^+} \sum_{|j| > J_0} \int_{\mathbb{R}^d} \sum_{n \in \mathbb{N}^*} |d_n(\varepsilon\xi, j)|^2 |\widehat{V}_j^\varepsilon(\xi)|^2 d\xi \end{aligned}$$

$$\leq c_r \limsup_{\varepsilon\to 0^+} \sum_{|j|>J_0} \int_{\mathbb{R}^d} (1+|\varepsilon\xi|^2+|j|^2)^r |\widehat{V}_j^\varepsilon(\xi)|^2 \mathrm{d}\xi < c_r\delta,$$

using observation (1).

The second term is analyzed using observation (2):

$$\begin{aligned}\limsup_{\varepsilon\to 0^+} &\sum_{n>N} \sum_{|j|\leq J_0} \int_{|\varepsilon\xi|>R} |d_n(\varepsilon\xi, j)|^2 |\widehat{V}_j^\varepsilon(\xi)|^2 \mathrm{d}\xi \\ &\leq c_r \limsup_{\varepsilon\to 0^+} \sum_{|j|\leq J_0} \int_{|\varepsilon\xi|>R} (1+|\varepsilon\xi|^2+|j|^2)^k |\widehat{V}_j^\varepsilon(\xi)|^2 \mathrm{d}\xi < c_r\delta.\end{aligned}$$

Observation (3) ensures that

$$\sum_{n>N} \sum_{|j|\leq J_0} \int_{|\varepsilon\xi|\leq R} |d_n(\varepsilon\xi, j)|^2 |\widehat{V}_j^\varepsilon(\xi)|^2 \mathrm{d}\xi \leq D_N(R, J_0) \|V^\varepsilon\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}.$$

As a consequence of this analysis,

$$\begin{aligned}\limsup_{N\to+\infty} \limsup_{\varepsilon\to 0^+} &\sum_{n>N} \sum_{j\in\mathbb{Z}^d} \int_{\mathbb{R}^d} \left| \int_{\mathbb{T}^d} \varrho_n(\varepsilon\xi)^{r/2} \overline{\varphi_n}(z, \varepsilon\xi) \mathrm{e}^{2i\pi j\cdot z} \mathrm{d}z \right|^2 |\widehat{V}_j^\varepsilon(\xi)|^2 \mathrm{d}\xi \\ &< 2c_r\delta.\end{aligned}$$

Since δ is arbitrary, the result follows. □

Lemma 2.1 provides an important element of the proof of the Theorems 1.1 and 1.5 of this paper. It allows to reduce the problem to solutions consisting only of finite superposition of Bloch modes, that we are going to study with a semi-classical perspective, as explained in the next section.

3. Semi-classical Approach to the Energy Dynamics

The nature of the propagation of the asymptotic energy density for high-frequency solutions to semi-classical dispersive-type equations is better understood if the usual, physical-space, energy density is lifted to a phase-space energy density. There is no canonical lifting procedure, roughly speaking these choices correspond to different quantization procedures. Here we will work with the lifting procedure that corresponds to the Weyl quantization, from which the Wigner functions are obtained (see the definition in (3.1)).

It should be noted that although the asymptotic limit in equation (1.1) we are interested might not appear to fit in the semi-classical regime one can indeed place it in that context. One can check that any solution ψ^ε of (1.1) becomes, after rescaling in time as $u^\varepsilon(t,\cdot) := \psi^\varepsilon(\varepsilon t, \cdot)$, a solution to a semi-classical Schrödinger equation with highly oscillating potential:

$$i\varepsilon\partial_t u^\varepsilon(t,x) + \frac{\varepsilon^2}{2}\Delta_x u^\varepsilon(t,x) - V_{\mathrm{per}}\left(\frac{x}{\varepsilon}\right) u^\varepsilon(t,x) - \varepsilon^2 V_{\mathrm{ext}}(\varepsilon t, x) u^\varepsilon(t,x) = 0.$$

Hence, the asymptotic limit we are interested in can be viewed as performing simultaneously the semi-classical and long-time limits. This approach was pursued in [14,15] to deal with the case where no crossings between Bloch bands are present, and this point of view is also adopted in references [2,54]. Here the situation is more complicated, as interactions between projections on different Bloch bands may occur. This regime involving performing simultaneously the semi-classical and long time limit has been useful in other contexts, we refer the reader to the survey articles [5,43,44].

In Section 3.1 below, we recall elements of the theory of semi-classical measures that we apply to $(\psi^\varepsilon)_{\varepsilon>0}$ in the next two sections. We first discuss in Section 3.2 the relations between the semi-classical measures of $(\psi^\varepsilon)_{\varepsilon>0}$ and those of the families $(\psi_n^\varepsilon)_{\varepsilon>0}$ that have been introduced in (2.5) and (2.6). Then, we analyze the localisation properties of these semi-classical measures in Section 3.3, which motivates a two-microlocal approach.

3.1. Semi-classical Measures and Energy Densities

Let us recall briefly some basic facts of the theory of semi-classical measures [34,35,40] that will be needed in the sequel. From now on, for every $s \in \mathbb{R}$, $N \in \mathbb{N}^*$, $H^s_\varepsilon(\mathbb{R}^d, \mathbb{C}^N)$ will denote the space $H^s_\varepsilon(\mathbb{R}^d)^N$ equipped with the norm

$$\|\Psi\|_{H^s_\varepsilon(\mathbb{R}^d,\mathbb{C}^N)} = \left(\sum_{j=1}^N \|\Psi_j\|^2_{H^s_\varepsilon(\mathbb{R}^d)}\right)^{1/2}, \quad \Psi = (\Psi_1, \cdots, \Psi_N).$$

We associate to every $\Psi \in L^2(\mathbb{R}^d, \mathbb{C}^N) := H^0_\varepsilon(\mathbb{R}^d, \mathbb{C}^N)$ a microlocal version W^ε_Ψ of the (matrix-valued) energy density

$$\Psi \otimes \overline{\Psi} = (\Psi_i \overline{\Psi}_j)_{1\le i,j\le N} \in \mathbb{C}^{N\times N}.$$

The matrix-valued function $W^\varepsilon_\Psi \in L^2(\mathbb{R}^{2d}, \mathbb{C}^{N\times N})$ is defined by

$$W^\varepsilon_\Psi(x,\xi) = \int_{\mathbb{R}^d} \mathrm{e}^{i\xi\cdot v}\Psi\left(x - \frac{\varepsilon v}{2}\right) \otimes \overline{\Psi}\left(x + \frac{\varepsilon v}{2}\right)\frac{dv}{(2\pi)^d}, \tag{3.1}$$

and its action on symbols $a \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}, \mathbb{C}^{N\times N})$ is related with semi-classical pseudodifferential calculus according to

$$\int_{\mathbb{R}^{2d}} \mathrm{Tr}_{\mathbb{C}^{N\times N}}(a(x,\xi)W^\varepsilon_\Psi(x,\xi))\mathrm{d}x\,\mathrm{d}\xi = \left(\mathrm{op}_\varepsilon(a)\Psi, \Psi\right)_{L^2(\mathbb{R}^d,\mathbb{C}^N)}$$

where $\mathrm{op}_\varepsilon(a)$ denotes the matrix-valued semi-classical pseudodifferential operator of symbol a. The Wigner function satisfies the following bounds for every $a \in \mathcal{C}^\infty_0(\mathbb{R}^{2d}, \mathbb{C}^{N\times N})$ and $\varepsilon > 0$:

$$\left|\left(\mathrm{op}_\varepsilon(a)\Psi, \Psi\right)_{L^2(\mathbb{R}^d,\mathbb{C}^N)}\right| \le C_d\|\Psi\|^2_{L^2(\mathbb{R}^d,\mathbb{C}^N)}\|a\|_{\mathcal{C}^{d+2}(\mathbb{R}^{2d},\mathbb{C}^{N\times N})}; \tag{3.2}$$

for $C_d > 0$ depending only on d. If in addition $a \geq 0$ (meaning that a takes values in the set of non-negative Hermitian matrices),

$$\int_{\mathbb{R}^{2d}} \mathrm{Tr}_{\mathbb{C}^{N\times N}}(a(x,\xi)W^{\varepsilon}_{\Psi}(x,\xi))\mathrm{d}x\,\mathrm{d}\xi \geq -C_a\varepsilon\|\Psi\|^2_{L^2(\mathbb{R}^d,\mathbb{C}^N)}, \tag{3.3}$$

for some $C_a > 0$ that can be computed in terms of a and its derivatives. Estimate (3.2) is a consequence of the Calderón-Vaillancourt theorem (C.1), whereas (3.3) is a reformulation of Gårding's inequality (C.3). A direct computation also shows that W^{ε}_{Ψ} is actually a lift of $\Psi \otimes \overline{\Psi}$:

$$\int_{\mathbb{R}^d} W^{\varepsilon}_{\Psi}(x,\xi)\mathrm{d}\xi = \Psi \otimes \overline{\Psi}(x). \tag{3.4}$$

Suppose now that $(\Psi^{\varepsilon})_{\varepsilon>0}$ is a bounded sequence in $L^2(\mathbb{R}^d,\mathbb{C}^N)$; then (3.2) ensures that $(W^{\varepsilon}_{\Psi^{\varepsilon}})$ is a bounded sequence of distributions. In addition, (3.3) implies that all its accumulation points are non negative Radon matrix-valued measures, that is, measures valued on the set of complex $N \times N$ Hermitian positive-semidefinite matrices. Moreover, any measure μ obtained from $(W^{\varepsilon}_{\Psi^{\varepsilon}})$ along some subsequence (ε_ℓ) satisfies (see (C.4), (C.5))

$$\mu(\mathbb{R}^{2d}) \leq \liminf_{\ell\to\infty} \|\Psi^{\varepsilon_\ell}\|^2_{L^2(\mathbb{R}^d)}.$$

These measures are called *semi-classical* or *Wigner measures* of the family $(\Psi^{\varepsilon})_{\varepsilon>0}$.

Remark 3.1. If $(W^{\varepsilon_\ell}_{\Psi^{\varepsilon_\ell}})$ converges in $\mathcal{S}'(\mathbb{R}^{2d})$ to the semiclassical measure μ then, for every $a \in C_0(\mathbb{R}^d_x \times \mathbb{R}^d_\xi)$ that is $d+2$ times continuously differentiable in x the following holds:

$$\int_{\mathbb{R}^{2d}} \mathrm{Tr}_{\mathbb{C}^{N\times N}}(a(x,\xi)W^{\varepsilon_\ell}_{\Psi^{\varepsilon_\ell}}(x,\xi))dx\,d\xi \underset{\ell\to\infty}{\longrightarrow} \int_{\mathbb{R}^{2d}} \mathrm{Tr}_{\mathbb{C}^{N\times N}}(a(x,\xi)\mu(dx,d\xi)).$$

This follows from Remark C.3 and assertion (1) of Lemma C.4.

Finally, the lift property (3.4) is transferred to an accumulation point μ generated from a subsequence $(\Psi^{\varepsilon_\ell})$,i.e.,

$$\begin{aligned}\forall\phi \in \mathcal{C}_0(\mathbb{R}^d,\mathbb{C}^{N\times N}), \quad \lim_{\ell\to\infty} &\int_{\mathbb{R}^d} \mathrm{Tr}_{\mathbb{C}^{N\times N}}(\phi(x)(\Psi^{\varepsilon_\ell}\otimes\overline{\Psi^{\varepsilon_\ell}})(x))\mathrm{d}x \\ &= \int_{\mathbb{R}^d} \mathrm{Tr}_{\mathbb{C}^{N\times N}}(\phi(x)\mu(dx,d\xi)),\end{aligned}$$

provided that no mass of $(\Psi^{\varepsilon_\ell})$ is lost at infinity in Fourier space:

$$\limsup_{\ell\to\infty} \int_{|\varepsilon_\ell\xi|>R} |\widehat{\Psi^{\varepsilon_\ell}}(\xi)|^2\mathrm{d}\xi \underset{R\to\infty}{\longrightarrow} 0. \tag{3.5}$$

This condition, referred sometimes to as ε-*oscillation*, is fulfilled as soon as the sequence $(\Psi^{\varepsilon})_{\varepsilon>0}$ is bounded in $H^s_{\varepsilon}(\mathbb{R}^d)^N$ for some $s > 0$.

Let us conclude this concise review of semi-classical measures by recalling how the matrix-valued semi-classical measure $\mu = (\mu_{i,j})_{1\le i,j,\le N}$ is related to the semi-classical measures of the families of components (Ψ_j^ε), for $j = 1, \dots, N$. Suppose that the subsequence $(\Psi^{\varepsilon_\ell})$ gives the semi-classical measure μ. Then, for every $1 \le i, j, \le N$,

$$\forall a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}), \quad \lim_{\ell\to\infty} \left(\mathrm{op}_\varepsilon(a)\Psi_i^{\varepsilon_\ell}, \Psi_j^{\varepsilon_\ell}\right)_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} a(x,\xi)\mu_{i,j}(dx, d\xi). \tag{3.6}$$

Moreover, since μ takes values on the set of Hermitian positive-semidefinite matrices, one also has that the $\mu_{i,i}$ are non-negative (scalar) Radon measures and that $\mu_{i,j}$ is absolutely continuous with respect to both $\mu_{i,i}$ and $\mu_{j,j}$. The latter condition implies that $\mu_{i,j} = 0$ as soon as $\mu_{i,i}$ and $\mu_{j,j}$ are mutually singular. In particular,

$$\mu_{i,i} \perp \mu_{j,j} \implies \forall a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}), \quad \lim_{\ell\to\infty} \left(\mathrm{op}_\varepsilon(a)\Psi_i^{\varepsilon_\ell}, \Psi_j^{\varepsilon_\ell}\right)_{L^2(\mathbb{R}^d)} = 0. \tag{3.7}$$

In this article, we are mainly interested in time-dependent versions of these objects. The modifications required in order to adapt the theory to this context are rather straightforward. Suppose now that $(\Psi^\varepsilon)_{\varepsilon>0}$ is bounded in $L^\infty(\mathbb{R}_t; L^2(\mathbb{R}_x^d, \mathbb{C}^N))$. Define $W_{\Psi^\varepsilon}^\varepsilon$ as

$$\begin{aligned} W_{\Psi^\varepsilon}^\varepsilon(t,x,\xi) &:= W_{\Psi^\varepsilon(t,\cdot)}^\varepsilon(x,\xi) \\ &= \int_{\mathbb{R}^d} \mathrm{e}^{i\xi\cdot v}\Psi^\varepsilon\left(t, x - \frac{\varepsilon v}{2}\right) \otimes \overline{\Psi^\varepsilon}\left(t, x + \frac{\varepsilon v}{2}\right) \frac{dv}{(2\pi)^d}. \end{aligned} \tag{3.8}$$

Then (3.2) again implies that, for every $\theta \in L^1(\mathbb{R})$ and every $a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}, \mathbb{C}^{N\times N})$,

$$\begin{aligned} &\left|\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)\,\mathrm{Tr}_{\mathbb{C}^{N\times N}}(a(x,\xi)W_{\Psi^\varepsilon}^\varepsilon(t,x,\xi))\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}t\right| \\ &\quad \le C_d\|\Psi^\varepsilon\|^2_{L^\infty(\mathbb{R}_t;L^2(\mathbb{R}_x^d,\mathbb{C}^N))}\|\theta\|_{L^1(\mathbb{R})}\|a\|_{\mathcal{C}^{d+2}(\mathbb{R}^{2d},\mathbb{C}^{N\times N})}. \end{aligned} \tag{3.9}$$

This ensures that $(W_{\Psi^\varepsilon}^\varepsilon)$ is bounded in $\mathcal{S}'(\mathbb{R}\times\mathbb{R}^{2d})$. Moreover, any accumulation point μ of this family is a non negative Radon measure on $\mathbb{R}\times\mathbb{R}^{2d}$, because of (3.3). It follows from (3.9) that the projection of μ onto the t-variable is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}$. Therefore, we conclude using the disintegration theorem the existence of a measurable map from $t \in \mathbb{R}$ to non negative, finite, matrix-valued Radon measures μ^t on $\mathbb{R}^{2d}$ such that $\mu(dt, dx, d\xi) = \mu^t(dx, d\xi)dt$.

Summing up, for every sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ going to 0 as ℓ goes to $+\infty$ such that $(W_{\Psi^{\varepsilon_\ell}}^{\varepsilon_\ell})$ converges in the sense of distributions the following holds: for all $\theta \in L^1(\mathbb{R})$ and $a \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}, \mathbb{C}^{N\times N})$,

$$\begin{aligned} &\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)\,\mathrm{Tr}_{\mathbb{C}^{N\times N}}(a(x,\xi)W_{\Psi^{\varepsilon_\ell}}^{\varepsilon_\ell}(t,x,\xi))\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}t \underset{\ell\to\infty}{\longrightarrow} \\ &\quad \int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)\,\mathrm{Tr}_{\mathbb{C}^{N\times N}}(a(x,\xi)\mu^t(dx,d\xi))\mathrm{d}t. \end{aligned} \tag{3.10}$$

If the sequence $(\Psi^{\varepsilon_\ell}(t,\cdot))$ is in addition ε-oscillating (3.5) for almost every $t \in \mathbb{R}$, the projections of the measures μ^t on the ξ-variable are the limits of the energy densities: for every $\theta \in L^1(\mathbb{R})$, $\phi \in \mathcal{C}_0(\mathbb{R}^d, \mathbb{C}^{N\times N})$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^d} \theta(t)\,\mathrm{Tr}_{\mathbb{C}^{N\times N}}(\phi(x)(\Psi^{\varepsilon_\ell}\otimes\overline{\Psi^{\varepsilon_\ell}})(t,x))\mathrm{d}x \underset{\ell\to\infty}{\longrightarrow} \int_{\mathbb{R}}\int_{\mathbb{R}^d} \theta(t)\,\mathrm{Tr}_{\mathbb{C}^{N\times N}}(\phi(x)\mu^t(dx,d\xi))\,\mathrm{d}t. \tag{3.11}$$

Remark 3.2. Time-dependent analogues of (3.6), (3.7) also hold after replacing $\mu_{i,j}$ by $\mu^t_{i,j}$ and averaging in the t-variable. So does the analogue of Remark 3.1.

3.2. The Semi-classical Measure of $(\psi^\varepsilon)_{\varepsilon>0}$ in Terms of Those of the Sequences $(\psi^\varepsilon_n)_{\varepsilon>0}$, $n \in \mathbb{N}$

We now focus on the basic properties of semi-classical measures associated to a sequence $(\psi^\varepsilon)_{\varepsilon>0}$ of solutions to (1.1), issued from initial data $(\psi^\varepsilon_0)_{\varepsilon>0}$ that are bounded in $H^s_\varepsilon(\mathbb{R}^d)$ for some $s > d/2$, and onto clarifying how they are related to those of the families of projections $(\psi^\varepsilon_n)_{\varepsilon>0}$ defined in (2.6).

First note that the highly oscillating character of the Schrödinger propagator prevents in general to be able to extract a subsequence along which $W^\varepsilon_{\psi^\varepsilon(t,\cdot)}$ will converge for every $t \in \mathbb{R}$. Following [3,6,41] we consider time averages of the Wigner functions we just described.

Identity (3.10) applied to this context states that whenever $(W^{\varepsilon_\ell}_{\psi^{\varepsilon_\ell}})$ converges in the sense of distributions for some sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ going to 0 as ℓ goes to $+\infty$ the following holds: for all $\theta \in L^1(\mathbb{R})$ and $a \in \mathcal{C}^\infty_0(\mathbb{R}^{2d})$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)a(x,\xi)W^{\varepsilon_\ell}_{\psi^{\varepsilon_\ell}}(t,x,\xi)\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}t \underset{\ell\to\infty}{\longrightarrow} \int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)a(x,\xi)\varsigma^t(dx,d\xi)\mathrm{d}t, \tag{3.12}$$

where, for a.e. $t \in \mathbb{R}$, ς^t is a non negative Radon measure on $\mathbb{R}^{2d}$.

In addition, ς^t can be related to the weak limits of the energy densities since the family $(\psi^\varepsilon)_{\varepsilon>0}$ is ε-oscillating.

Remark 3.3. If $(\psi^\varepsilon_0)_{\varepsilon>0}$ is bounded in $H^s_\varepsilon(\mathbb{R}^d)$ for some $s > d/2$ then $(\psi^\varepsilon(t,\cdot))_{\varepsilon>0}$, the corresponding family of solutions to (1.1), is ε-oscillating for every $t \in \mathbb{R}$. This follows from [15, Lemma 6.2] applied to the family $(U^\varepsilon)_{\varepsilon>0}$ of solutions to (2.2) once one notices that for $r \in (\frac{d}{2}, s)$, $R > 0$ and $t \in \mathbb{R}$,

$$\int_{|\varepsilon\xi|>R} \|\widehat{U^\varepsilon}(t,\xi,\cdot)\|^2_{H^r(\mathbb{T}^d)}\mathrm{d}\xi \le R^{-2(s-r)}(\|\psi^\varepsilon_0\|_{H^s_\varepsilon(\mathbb{R}^d)} + C_s\varepsilon|t|)^2,$$

as follows from estimate (2.3).

As a consequence of this, (3.11) implies one has for the subsequence (ε_ℓ) of (3.12) and for $\theta \in \mathcal{C}^\infty_0(\mathbb{R})$, $\phi \in \mathcal{C}^\infty_0(\mathbb{R}^d)$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^d} \theta(t)\phi(x)|\psi^{\varepsilon_\ell}(t,x)|^2\mathrm{d}x\,\mathrm{d}t \underset{\ell\to+\infty}{\longrightarrow} \int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)\phi(x)\varsigma^t(dx,d\xi)\mathrm{d}t.$$

(3.13)

For $n, n' \in \mathbb{N}^*$, we use the notation $W^{\varepsilon}_{n,n'}$ to refer to the Wigner function of the pair $\psi^{\varepsilon}_n, \psi^{\varepsilon}_{n'}$. In other words, for every $a \in \mathcal{C}^{\infty}_0(\mathbb{R}^{2d})$,

$$\int_{\mathbb{R}^{2d}} a(x,\xi) W^{\varepsilon}_{n,n'}(t,x,\xi)\mathrm{d}x\,\mathrm{d}\xi = \left(\mathrm{op}_{\varepsilon}(a)\psi^{\varepsilon}_n(t,\cdot), \psi^{\varepsilon}_{n'}(t,\cdot)\right)_{L^2(\mathbb{R}^d)}.$$

The same argument presented before shows that for $n, n' \in \mathbb{N}$, there exists a sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ going to 0 as ℓ goes to $+\infty$ such that, for all $\theta \in L^1(\mathbb{R})$, $a \in \mathcal{C}^{\infty}_0(\mathbb{R}^{2d})$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)a(x,\xi)W^{\varepsilon}_{n,n'}(t,x,\xi)\mathrm{d}x\,\mathrm{d}\xi\,\mathrm{d}t \underset{\ell\to\infty}{\longrightarrow} \int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)a(x,\xi)\mu^t_{n,n'}(dx,d\xi))\mathrm{d}t, \tag{3.14}$$

where, for a.e. $t \in \mathbb{R}$, $\mu^t_{n,n'}$ is a (signed) Radon measure on $\mathbb{R}^{2d}$.

Proposition 3.4. *There exist a subsequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ going to 0 as ℓ goes to $+\infty$ such that (3.12) and (3.14) hold simultaneously for all $n, n' \in \mathbb{N}^*$. In addition, for a.e. $t \in \mathbb{R}$,*

$$\varsigma^t = \sum_{n,n'\in\mathbb{N}^*} \mu^t_{n,n'},$$

the convergence of the series being understood in the weak-$*$ topology of the space of Radon measures on $\mathbb{R}^{2d}$.

Proof. We proceed to a first extraction to have (3.12) and we keep denoting by ε the resulting subsequence. We put

$$\Psi^{\varepsilon}_N := (\psi^{\varepsilon}_1, \ldots, \psi^{\varepsilon}_N) \in \mathcal{C}(\mathbb{R}_t; L^2(\mathbb{R}^d_x, \mathbb{C}^N)).$$

We know that $(W^{\varepsilon}_{\Psi^{\varepsilon}_N})$, defined by (3.8), are uniformly bounded in $\mathcal{C}(\mathbb{R}_t; \mathcal{S}'(\mathbb{R}^{2d}, \mathbb{C}^{N\times N}))$, both in $\varepsilon > 0$ and $N \in \mathbb{N}^*$.

By (3.10), any accumulation point of $(W^{\varepsilon}_{\Psi^{\varepsilon}_N})$ obtained along some subsequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ is a time-dependent family of non negative matrix-valued Radon measures μ^t_N. By diagonal extraction, we can find a sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ such that $(W^{\varepsilon_\ell}_{\Psi^{\varepsilon_\ell}_N})_{\varepsilon>0}$ converge for every $N \in \mathbb{N}^*$. We denote by $(\mu^t_N)_{N\in\mathbb{N}^*}$ their respective limits. By (3.6) we know that, for every $n, n' \le N \le N'$ one has

$$(\mu^t_N)_{n,n'} = (\mu^t_{N'})_{n,n'} = \mu^t_{n,n'},$$

where $\mu^t_{n,n'}$ is obtained through (3.14). This shows that we can find a sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ as claimed.

Define now $\psi^{N,\varepsilon} := \sum_{n=1}^N \psi^{\varepsilon}_n$. One has that for $a \in \mathcal{C}^{\infty}_0(\mathbb{R}^{2d})$ and $t \in \mathbb{R}$,

$$\int_{\mathbb{R}^{2d}} a(x,\xi) W^{\varepsilon_\ell}_{\psi^{N,\varepsilon_\ell}}(t,x,\xi)\mathrm{d}x\,\mathrm{d}\xi = \int_{\mathbb{R}^{2d}} a(x,\xi)\,\mathrm{Tr}_{\mathbb{C}^{N\times N}}\left(Q\,W^{\varepsilon_\ell}_{\Psi^{\varepsilon_\ell}_N}(t,x,\xi)\right)\mathrm{d}x\,\mathrm{d}\xi,$$

where Q is the $N \times N$ matrix whose all entries are equal to one. Therefore, $(W^{\varepsilon_\ell}_{\psi^{N,\varepsilon_\ell}})_{\ell\in\mathbb{N}}$ converges to the semi-classical measure given, for a.e. $t \in \mathbb{R}$, by

$$\varsigma^t_N = \sum_{1\le n,n'\le N} \mu^t_{n,n'}.$$

Finally, (2.5) and Lemma 2.1 imply that for every $\theta \in L^1(\mathbb{R})$,

$$\limsup_{\ell\to\infty} \int_{\mathbb{R}} \theta(t)\|\psi^{\varepsilon_\ell}(t,\cdot) - \psi^{N,\varepsilon_\ell}(t,\cdot)\|^2_{L^2(\mathbb{R}^d)}\mathrm{d}t \underset{N\to\infty}{\longrightarrow} 0;$$

which in turn guarantees that, for every $\theta \in L^1(\mathbb{R})$, $a \in \mathcal{C}^\infty_0(\mathbb{R}^{2d})$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)a(x,\xi)\varsigma^t_N(dx,d\xi)dt \underset{N\to\infty}{\longrightarrow} \int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)a(x,\xi)\varsigma^t(dx,d\xi)\mathrm{d}t.$$

□

The rest of this article is devoted to computing the measures $\mu^t_{n,n'}$.

3.3. Localization of Semi-classical Measures

If the operator $L^\varepsilon P^\varepsilon_{\varphi_n}$ is applied to problem (2.2), one deduces that ψ^ε_n (which is defined by (2.6)) satisfies the pseudo-differential equation

$$\begin{cases} i\varepsilon^2\partial_t\psi^\varepsilon_n(t,x)) = \varrho_n(\varepsilon D_x)\psi^\varepsilon_n(t,x) + \varepsilon^2 f^\varepsilon_n(t,x), & (t,x)\in\mathbb{R}\times\mathbb{R}^d, \\ \psi^\varepsilon_n(0,x) = \varphi_n\left(\frac{x}{\varepsilon},\varepsilon D_x\right)\int_{\mathbb{T}^d}\overline{\varphi_n}(y,\varepsilon D_x)\psi^\varepsilon_0(x)\mathrm{d}y, \end{cases} \tag{3.15}$$

with

$$f^\varepsilon_n(t,x) := \varphi_n\left(\frac{x}{\varepsilon},\varepsilon D_x\right)\int_{\mathbb{T}^d}\overline{\varphi_n}(y,\varepsilon D_x)(V_{\mathrm{ext}}(t,x)U^\varepsilon(t,x,y))\mathrm{d}y.$$

This fact will be used to obtain all the information on the measures $\mu^t_{n,n'}$ defined in (3.14) that is relevant to our purposes. In this section we gather some basic facts; in following sections we will introduce a more precise machinery that will allow us to obtain a complete picture.

Proposition 3.5. *Let (ψ^ε_0) be bounded in $H^s_\varepsilon(\mathbb{R}^d)$ for some $s > d/2$. For any $n, n' \in \mathbb{N}^*$, let $(\psi^\varepsilon_n)_{\varepsilon>0}$ and $(\psi^\varepsilon_{n'})$ be defined by (2.6) and let $\mu^t_{n,n'}$ be given by (3.14). Let $\Omega \subseteq \mathbb{R}^d$ be open and invariant by translations by $2\pi\mathbb{Z}^d$. Then the following hold:*

(1) *If $\nabla_\xi\varrho_n \in \mathrm{Lip}(\mathbb{R}^d)$ on Ω and $\nabla_\xi\varrho_n|_\Omega \neq 0$, then*

$$\mu^t_{n,n}(\mathbb{R}^d\times\Omega) = 0, \quad \textit{for a.e. } t\in\mathbb{R}.$$

(2) *Let $\delta > 0$ and suppose that*

$$\Omega \subset \{\xi\in\mathbb{R}^d : |\varrho_n(\xi) - \varrho_{n'}(\xi)| \ge \delta\}.$$

Then $|\mu^t_{n,n'}|(\mathbb{R}^d\times\Omega) = 0$, for a.e. $t\in\mathbb{R}$.

Proof. Point 1 is proved in an analogous manner than Proposition 3.4 in [15]. Using the calculus of semi-classical pseudo-differential operators with low regularity of Lemma C.4 it is possible to prove that for every $\theta \in \mathcal{C}_0^\infty(\mathbb{R})$ and $a \in \mathcal{C}_0^\infty(\mathbb{R}^d \times \Omega)$,

$$\int_{\mathbb{R}} \theta(t)(\mathrm{op}_\varepsilon(\nabla_\xi \varrho_n \cdot \nabla_x a)\psi_n^\varepsilon(t,\cdot), \psi_n^\varepsilon(t,\cdot))_{L^2(\mathbb{R}^d)}\mathrm{d}t \underset{\varepsilon\to 0}{\longrightarrow} 0.$$

By (3.14), this implies that, for almost every $t \in \mathbb{R}$,

$$\int_{\mathbb{R}^d\times\Omega} \nabla_\xi \varrho_n(\xi) \cdot \nabla_x a(x,\xi)\mu_{n,n}^t(dx, d\xi) = 0.$$

This implies that the measure $\mu_{n,n}^t \mathbf{1}_{\mathbb{R}^d\times\Omega}$ is invariant by the flow $(x,\xi) \mapsto (x + s\nabla\varrho_n(\xi), \xi)$. Since $\mu_{n,n}^t$ is non negative and finite, necessarily it is identically 0.

For proving Point 2, it is enough to obtain, for every $\theta \in \mathcal{C}_0^\infty(\mathbb{R})$ and $a \in \mathcal{C}_0^\infty(\mathbb{R}^d \times \Omega)$:

$$\int_{\mathbb{R}} \theta(t)\left(\mathrm{op}_\varepsilon(a)\psi_n^\varepsilon(t,\cdot), \psi_{n'}^\varepsilon(t,\cdot)\right)_{L^2(\mathbb{R}^d)}\mathrm{d}t \underset{\varepsilon\to 0}{\longrightarrow} 0.$$

We have

$$\begin{aligned} i\varepsilon^2 \frac{d}{dt}&\left(\mathrm{op}_\varepsilon(a)\psi_n^\varepsilon(t,\cdot), \psi_{n'}^\varepsilon(t,\cdot)\right)_{L^2(\mathbb{R}^d)} \\ &= \left(\left(\varrho_{n'}(\varepsilon D_x)\mathrm{op}_\varepsilon(a) - \mathrm{op}_\varepsilon(a)\varrho_n(\varepsilon D_x)\right)\psi_n^\varepsilon(t,\cdot), \psi_{n'}^\varepsilon(t,\cdot)\right)_{L^2(\mathbb{R}^d)} + \varepsilon^2 R^\varepsilon(t), \end{aligned} \tag{3.16}$$

where $|R^\varepsilon(t)| \le C\|f_n^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)}^2$ is locally uniformly bounded in $t \in \mathbb{R}$ for every $\varepsilon > 0$.

By Lemma C.4 (2), the following holds with respect to the $\mathcal{L}(L^2(\mathbb{R}^d))$ norm:

$$\varrho_{n'}(\varepsilon D_x)\mathrm{op}_\varepsilon(a) - \mathrm{op}_\varepsilon(a)\varrho_n(\varepsilon D_x) = \mathrm{op}_\varepsilon\left((\varrho_{n'} - \varrho_n)a\right) + O(\varepsilon).$$

This identity together with integration by parts transforms (3.16) into

$$\begin{aligned} &\int_{\mathbb{R}} \theta(t)\left(\mathrm{op}_\varepsilon\left((\varrho_{n'} - \varrho_n)a\right)\psi_n^\varepsilon(t,\cdot), \psi_{n'}^\varepsilon(t,\cdot)\right)_{L^2(\mathbb{R}^d)}\mathrm{d}t \\ &\quad = \frac{\varepsilon^2}{i}\int_{\mathbb{R}} \theta'(t)\left(\mathrm{op}_\varepsilon(a)\psi_n^\varepsilon(t,\cdot), \psi_{n'}^\varepsilon(t,\cdot)\right)_{L^2(\mathbb{R}^d)}\mathrm{d}t + O(\varepsilon). \end{aligned}$$

Taking limits $\varepsilon \to 0$, which is possible by Remarks 3.1 and 3.2, we obtain

$$\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)(\varrho_{n'}(\xi) - \varrho_n(\xi))a(x,\xi)\mu_{n,n'}^t(dx, d\xi)\mathrm{d}t = 0.$$

By density, this relation holds for all $a \in \mathcal{C}_0(\mathbb{R}^d \times \Omega)$, in particular for $\tilde{a} = (\varrho_n - \varrho_{n'})^{-1}a$. This shows that, as we wanted to prove

$$\forall\theta \in \mathcal{C}_0^\infty(\mathbb{R}),\ \forall a \in \mathcal{C}_0(\mathbb{R}^d \times \Omega), \quad \int_{\mathbb{R}}\int_{\mathbb{R}^{2d}} \theta(t)a(x,\xi)\mu_{n,n'}^t(dx, d\xi)\mathrm{d}t = 0.$$

□

Proposition 3.5 shows that $\mu^t_{n,n}$ can only charge the sets Λ_n of critical points of ϱ_n or the set where ϱ_n has a conical crossing with another Bloch energy (*i.e.* where ϱ_n ceases to be $\mathcal{C}^{1,1}(\mathbb{R}^d)$). It also shows that $\Sigma_{n,n'}$ is the only region where the measures $\mu^t_{n,n'}$ can be non-zero. Since, assuming **H1**, the crossing sets reduce to $\cup_{n\in\mathbb{N}_0}\Sigma_n$, the analysis of the measures $\mu^t_{n,n'}$ will be performed in the following sections by means of a second microlocalisation above the sets Λ_n and Σ_n, under the assumption **H1**, **H2** and **H3**.

4. Two Microlocal Analysis

The analysis of the concentration of a family on a submanifold of the phase space turned out to be an important element of the analysis of its behavior. Two-microlocal semi-classical measures gives a quantitative overview on these concentration phenomena. They were first introduced simultaneously and independently in [50] and by one of the author in her thesis (see the articles [21,22,24]), and they have found applications in different fields, as for example [26,42] and articles connected to these ones. We recall in Section 4.1 the definition of two-microlocal semi-classical measures that is useful in our context and apply the theory to families $(\psi^\varepsilon)_{\varepsilon>0}$ of solution to (1.1) in Section 4.1 in the frameworks of Theorem 1.5 and of Theorem 1.8. This leads to the statement of two results (Theorems 4.5 and 4.6) that will be proved in the next Sections 5 and 6.

4.1. Two-Scale Semi-classical Measures

We study here the concentration of a bounded family $(\Psi^\varepsilon)_{\varepsilon>0}$ of $L^\infty(\mathbb{R}, L^2(\mathbb{R}^d, \mathbb{C}^N))$ on a set $\mathbb{R}^d \times X$ where X is assumed to be a connected, closed embedded submanifold of $(\mathbb{R}^d)^*$ of codimension p. Following [15], we achieve a second microlocalization above $\mathbb{R}^d \times X$ and we crucially use that the geometric properties of X imply that there exists a tubular neighbourhood U of $\{(\sigma, 0) : \sigma \in X\} \subseteq NX$ such that the tubular coordinate map

$$U \ni (\sigma, v) \longmapsto \sigma + v \in (\mathbb{R}^d)^*$$

is a diffeomorphism onto its image V. In that case, there exists a smooth map $\sigma_X : V \longrightarrow X$ such that, for every $\xi \in V$,

$$\xi = \sigma + v, \quad (\sigma, v) = (\sigma_X(\xi), \xi - \sigma_X(\xi)) \in U. \tag{4.1}$$

We extend the phase space $T^*\mathbb{R}^d := \mathbb{R}^d_x \times (\mathbb{R}^d)^*_\xi$ with a new variable $\eta \in \overline{\mathbb{R}^d}$, where $\overline{\mathbb{R}^d}$ is the compactification of $(\mathbb{R}^d)^*$ obtained by adding a sphere $\mathbf{S}^{d-1}$ at infinity. The space $\mathcal{A}^{(2)}$ of test functions associated with this extended phase space is formed by those functions

$$a \in \mathcal{C}^\infty(T^*\mathbb{R}^d_{x,\xi} \times \mathbb{R}^d_\eta, \mathbb{C}^{N\times N})$$

which satisfy the two following properties:

(1) there exists a compact $K \subset T^*\mathbb{R}^d$ such that, for all $\eta \in \mathbb{R}^d$, the map $(x, \xi) \longmapsto a(x, \xi, \eta)$ is a smooth matrix-valued function compactly supported in K;
(2) there exists a smooth matrix-valued function a_∞ defined on $T^*\mathbb{R}^d \times \mathbf{S}^{d-1}$ and $R_0 > 0$ such that, if $|\eta| > R_0$, then $a(x, \xi, \eta) = a_\infty(x, \xi, \eta/|\eta|)$.

For $a \in \mathcal{A}^{(2)}$ supported in $\mathbb{R}^d \times V \times \mathbb{R}^d$, we write

$$a_\varepsilon(x, \xi) := a\left(x, \xi, \frac{\xi - \sigma_X(\xi)}{\varepsilon}\right).$$

We associate to $\Psi^\varepsilon(t)$ a two-microlocal Wigner distribution

$$W^{X,\varepsilon}(t) \in \mathcal{D}'(\mathbb{R}^d \times V \times \overline{\mathbb{R}^d}), \quad W^{X,\varepsilon}_{\Psi^\varepsilon}(t) = (W^{X,\varepsilon}_{j,k})_{1 \le j,k \le N};$$

its action on test functions $a \in \mathcal{A}^{(2)}$ supported in $\mathbb{R}^d \times V \times \mathbb{R}^d$ is defined by

$$\left\langle W^{X,\varepsilon}_{\Psi^\varepsilon}(t), a \right\rangle := \left(\mathrm{op}_\varepsilon(a_\varepsilon)\Psi^\varepsilon(t),\ \Psi^\varepsilon(t)\right)_{L^2(\mathbb{R}^d, \mathbb{C}^N)}. \tag{4.2}$$

Since the family of operators $(\mathrm{op}_\varepsilon(a_\varepsilon))_{\varepsilon>0}$ is uniformly bounded in $L^2(\mathbb{R}^d, \mathbb{C}^{N\times N})$ (as a consequence of the Calderón-Vaillancourt theorem, see "Appendix C"), it follows that $(W^{X,\varepsilon}_{\Psi^\varepsilon}(t))$ is a bounded sequence of distributions. In addition, any smooth, compactly supported test function $a \in \mathcal{C}^\infty_0(\mathbb{R}^d \times V, \mathbb{C}^{N\times N})$ can be naturally identified to an element of $\mathcal{A}^{(2)}$ which does not depend on the last variable. For such a, one clearly has

$$\left\langle W^{X,\varepsilon}_{\Psi^\varepsilon}(t), a \right\rangle = \left\langle W^{\varepsilon}_{\Psi^\varepsilon}(t), a \right\rangle;$$

hence $W^{X,\varepsilon}_{\Psi^\varepsilon}(t)$ is a lift of $W^{\varepsilon}_{\psi^\varepsilon}(t)$ to the extended phase-space. We thus focus on the asymptotic description of the quantities

$$\int_{\mathbb{R}} \theta(t)\langle W^{X,\varepsilon}_{\Psi^\varepsilon}(t), a\rangle \mathrm{d}t, \quad \theta \in L^1(\mathbb{R}), \quad a \in \mathcal{A}^{(2)}. \tag{4.3}$$

In order to describe the limits of these quantities, we must introduce some notations. We consider an open subset W of V where there exists $\varphi : W \longrightarrow \mathbb{R}^p$ a smooth function such that the $\xi \in W$ for which $\varphi(\xi) = 0$ are precisely those which are in $W \cap X$. We also assume that $d\varphi(\sigma)$ for $\sigma \in W \cap X$ is of maximal rank. These coordinates functions give parametrization of the manifolds under consideration and for every $\sigma \in W \cap X$, we can write

$$N_\sigma X = \{{}^t d\varphi(\sigma) z \ :\ z \in \mathbb{R}^p\}.$$

This parametrization allows to define a measure on $N_\sigma X$ and the space $L^2(N_\sigma X, \mathbb{C}^2)$. Different φ will give equivalent norms. The function φ also induces a smooth map B from the neighbourhood W of σ into the set of $d \times p$ matrices such that

$$\xi - \sigma_X(\xi) = B(\xi)\varphi(\xi), \quad \xi \in W. \tag{4.4}$$

Therefore, given a function $a \in \mathcal{C}_0^\infty(\mathbb{R}^d \times W \times \mathbb{R}^d, \mathbb{C}^{N\times N})$ and a point $(\sigma, v) \in T_\sigma^* X$, we can use φ to define an operator acting on $f \in L^2(N_\sigma X, \mathbb{C}^N)$ by

$$Q_a^\varphi(\sigma, v) f(z) = \int_{\mathbb{R}^p\times\mathbb{R}^p} a\left(v + {}^t d\varphi(\sigma)\frac{z+y}{2}, \sigma, B(\sigma)\eta\right) f(y) \mathrm{e}^{i\eta\cdot(z-y)} \frac{d\eta\, dy}{(2\pi)^p}.$$

In other words, $Q_a^\varphi(\sigma, v)$ is obtained from a by applying the non-semi-classical Weyl quantization to the symbol $a\left(v + {}^t d\varphi(\sigma)\cdot, \sigma, B(\sigma)\cdot\right) \in \mathcal{C}_0^\infty(\mathbb{R}^p \times \mathbb{R}^p, \mathbb{C}^{N\times N})$,

$$Q_a^\varphi(\sigma, v) = a^W\left(v + {}^t d\varphi(\sigma) z, \sigma, B(\sigma) D_z\right). \tag{4.5}$$

Using invariance properties with respect to changes of coordinate systems that are precisely described in [15], Section 4, one can conclude that a induces an operator Q_a^X on $L^2(N_\sigma X, \mathbb{C}^N)$. Clearly, $Q_a^X(\sigma, v)$ is smooth and compactly supported in (σ, v); moreover, $Q_a^X(\sigma, v)$ is a compact operator on $L^2(N_\sigma X, \mathbb{C}^N)$ for every $(\sigma, v) \in T^* X$.

Proposition 4.1. *(Proposition 4.2 and 4.4 of [15]) There exist a sequence (ε_ℓ), a measurable map $t \mapsto \gamma^t$ valued in the set of non negative (matrix-valued) measures on $T^*\mathbb{R}^d \times \mathbf{S}^{d-1}$, a measurable family of (scalar) non negative measures ν^t on T^*X and a measurable map $t \mapsto M^t$, where*

$$\begin{aligned} &M^t : T^*X \ni (\sigma, v) \longmapsto M^t(\sigma, v) \in \mathcal{L}^1(L^2(N_\sigma X, \mathbb{C}^N)) \\ &\quad \textit{and} \qquad \mathrm{Tr}_{L^2(N_\sigma X, \mathbb{C}^N)} M^t(\sigma, v) = 1, \quad \nu^t\text{-a.e. } (\sigma, v) \in T^*X \end{aligned}$$

such that, for every $\theta \in \mathcal{C}_0^\infty(\mathbb{R})$ and $a \in \mathcal{A}^{(2)}$ supported in $\mathbb{R}^d \times V \times \mathbb{R}^d$, one has:

$$\begin{aligned} &\int_{\mathbb{R}} \theta(t) \left\langle W^{X,\varepsilon_\ell}(t), a\right\rangle \mathrm{d}t \underset{\varepsilon_\ell\to 0}{\longrightarrow} \\ &\quad \int_{\mathbb{R}} \theta(t) \int_{T^*X} \mathrm{Tr}_{L^2(N_\sigma X, \mathbb{C}^N)}(Q_a^X(\sigma, v) M^t(\sigma, v)) \nu^t(d\sigma, dv) \mathrm{d}t \\ &\quad + \int_{\mathbb{R}} \theta(t) \int_{T^*\mathbb{R}^d\times\mathbf{S}^{d-1}} \mathrm{Tr}_{\mathbb{C}^{N\times N}}\left(a_\infty(x, \sigma, \omega)\gamma^t(dx, d\sigma, d\omega)\right) \mathrm{d}t. \end{aligned} \tag{4.6}$$

The family of operators $M^t(\sigma, v)$ describes the part of the concentration that comes from finite distance while the measure $\gamma^t(dx, d\sigma, d\omega)$ is often called the part at infinity of the two-scale semi-classical measure. In particular

$$\gamma^t(x, \xi, \omega)\mathbf{1}_{\xi\notin X} = \mu^t(x, \xi) \otimes \delta\left(\omega - \frac{\xi - \sigma_X(\xi)}{|\xi - \sigma_X(\xi)|}\right),$$

where μ^t is a semi-classical measure of $(\Psi^\varepsilon(t))_{\varepsilon>0}$.

Remark 4.2. (1) In a stationary setting, similar objects can be associated with (non time dependent) bounded families in $L^2(\mathbb{R}^d)$. More precisely, if $(f^\varepsilon)_{\varepsilon>0}$ is a bounded family in $L^2(\mathbb{R}^d, \mathbb{C}^N)$, one can associate with $(f^\varepsilon)_{\varepsilon>0}$ a pair $M_0 d\nu_0$

defined by the existence of a subsequence (ε_ℓ) such that for all $a \in \mathcal{C}_0^\infty(\mathbb{R}^{3d}, \mathbb{C}^{N\times N})$,

$$\left(\mathrm{op}_{\varepsilon_\ell}(a_{\varepsilon_\ell})f^{\varepsilon_\ell}, f^{\varepsilon_\ell}\right) \underset{\varepsilon_\ell\to 0}{\longrightarrow} \int_{T^*X} \mathrm{Tr}_{L^2(N_\sigma X,\mathbb{C}^N)}(Q_a^X(\sigma,v)M_0(\sigma,v))\nu_0(d\sigma,dv).$$

The initial data in the the von Neumann Equation (1.15) (Theorem 1.5) and in the von Neumann Equations (1.19) and (1.20) (Theorems 1.8) are constructed in that manner, with $N = 1$, $X = \Lambda_n$ and $f^\varepsilon = \psi_n^\varepsilon(0)$ for Equation (1.15) and with $N = 2$, $X = \Sigma_n$ and $f^\varepsilon = {}^t(\psi_n^\varepsilon(0), \psi_{n+1}^\varepsilon(0)) \in \mathbb{C}^2$ for Equations (1.19) and (1.20).

(2) When $X = \{\xi_0\}$, then $\sigma_X(\xi) = \xi - \xi_0$ and one has for $a \in \mathcal{C}_0^\infty(\mathbb{R}^{3d})$

$$\left(\mathrm{op}_\varepsilon(a_\varepsilon)f^\varepsilon, f^\varepsilon\right) = \left(\mathrm{op}_1(a(x,\xi_0+\varepsilon\xi,\xi)\mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi_0}f^\varepsilon, \mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi_0}f^\varepsilon\right)$$

and the operator $\mathrm{op}_1(a(x,\xi_0,\xi)$ is compact As a consequence, the part at finite distance of any two-microlocal measure associated with the concentration of (f^ε) on X is a projector $|f^{\xi_0}\rangle\langle f^{\xi_0}|$ where f^{ξ_0} is a weak limit in L^2 of the family $(\mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi_0}f^\varepsilon)$.

(3) Note that for determining the part of the concentration that comes from finite distance, it is enough to consider symbols a that are compactly supported in all the variables.

4.2. Two Microlocal Semi-classical Measures for the Families $(\psi_n^\varepsilon(t))_{n\in N}$

These objects allow to determine the semi-classical measure ς^t. Indeed, in [15], we have proved that they allow to describe ς^t above critical points of ϱ_n for which the hessian of ϱ_n is of maximal rank on the set of critical points Λ_n (see assumption **H2** and **H2'**). We will use them to prove that $\varsigma^t = 0$ above all crossing sets satisfying **H3** and to show that ς^t can be non zero because of modes interactions above degenerate crossing points satisfying **H3'**.

4.2.1. Critical Points We recall here results from [14,15], mainly Theorem 2.2 in [15] which gives a precise description of the measures $\mu_{n,n}^t$ above the set Λ_n of critical points of ϱ_n (see (1.4)). Let Ω be an open set of $\mathbb{R}^d$ such that $\Lambda_n \cap \Omega$ is a submanifold.

Theorem 4.3. [15] *Let $(M_n^t dv_n^t, \gamma_n^t)$ be a pair of two-microlocal semi-classical measures associated with the concentration of $(\psi_n^\varepsilon(t))$ above $\Lambda_n \cap \Omega$. Then, there exists $M_n dv_n$, a two-microlocal measure associated to the concentration at finite distance of $(\psi_n^\varepsilon(0))$ on $\Lambda_n \cap \Omega$ such that $\nu_n^t = \nu_n^0 = \nu_n$, $t \mapsto M_n^t(\xi, v)$ belongs to the space $\mathcal{C}(\mathbb{R}; \mathcal{L}_+^1(L^2(N_\xi\Lambda_n))$ and solves the von Neumann equation (1.15) with initial data $M_n^0 = M_n$. Moreover, if the Hessian of ϱ_n is of maximal rank on $\Lambda_n \cap \Omega$, then $\gamma_n^t = 0$.*

Remark 4.4. (1) The maximal rank assumption consists in saying that

$$\mathrm{Rank\,Hess}\,\varrho_n(\sigma) = \mathrm{codim}\,\Lambda_n, \quad \sigma \in \Lambda_n,$$

or equivalently: $\mathrm{Ker\,Hess}\,\varrho_n(\sigma) = T_\sigma\Lambda_n, \quad \sigma \in \Lambda_n$.

(2) It is important to notice that the families (M_n^t) are completely determined by the initial data: up to a subsequence for which one has

$$\left(\mathrm{op}_{\varepsilon_\ell}(a)\psi_n^{\varepsilon_\ell}(0), \psi_n^{\varepsilon_\ell}(0)\right) \underset{\varepsilon_\ell\to 0}{\longrightarrow} \int_{T^*\Lambda_n} \mathrm{Tr}_{L^2(N_\xi\Lambda)}\left[Q_a^{\Lambda_n}(\xi, v)M_n^0(\xi, v)\right]\nu_n^0(d\xi, dv).$$

4.2.2. Conical Crossing Points When **H1**, **H2** and **H3** for all $n \in \mathbb{N}^*$, the crossing sets Σ_n are manifolds. Besides, because of the periodicity of the Bloch energies, Σ_n thus is the union of connected, closed embedded submanifold of $(\mathbb{R}^d)^*$ and we can focus on each of these connected components by considering the two-microlocal setting of Section 4.1 with $N = 1$ and the family $(\psi_n^\varepsilon)_{\varepsilon>0}$ for this submanifold.

Theorem 4.5. *Assume* **H1**, **H2** *and* **H3** *holds for some* $n \in \mathbb{N}^*$. *Let* Σ *be a connected component of* Σ_n. *Then any pair* $(M_n^t d\nu_n^t, d\gamma_n^t)$ *of two-microlocal semi-classical measures associated with the concentration of* $(\psi_n^\varepsilon(t))$ *on* Σ *satisfy* $\nu_n^t = 0$ *and* $\gamma_n^t = 0$. *Therefore* $\mu_{n,n}^t \mathbf{1}_\Sigma = 0$.

The proof of this result is performed in Section 5.

4.2.3. Degenerate Crossing Points We now suppose that n is fixed and we consider the concentration of $\psi_n^\varepsilon(t)$ and $\psi_{n+1}^\varepsilon(t)$ when the crossing set Σ_n involving the two Bloch energies ϱ_n and ϱ_{n+1} satisfies **H3'**. We consider a connected component Y of Σ_n which is assumed to be included into Λ_n and Λ_{n+1}, the sets of critical points of ϱ_n and ϱ_{n+1} respectively. We consider the two-microlocal setting of Section 4.1 for $N = 2$, the submanifold Y and the family

$$\Psi^\varepsilon(t) = (\psi_n^\varepsilon(t), \psi_{n+1}^\varepsilon(t)) \in \mathbb{C}^2.$$

In view of Lemma B.1, the equation satisfied by Ψ^ε is

$$i\varepsilon^2\partial_t\Psi^\varepsilon = \Theta(\varepsilon D)\Psi^\varepsilon + \varepsilon^2 V_{\mathrm{ext}}(t, x)\Psi^\varepsilon + \varepsilon^3 F^\varepsilon(t, x) \tag{4.7}$$

with $(F^\varepsilon(t))$ uniformly bounded in $L^2(\mathbb{R}^d)$ and

$$\begin{aligned}\Theta(\xi) &= \mathrm{Diag}(\varrho_n(\xi), \varrho_{n+1}(\xi)) = \lambda_n(\xi)\mathrm{Id} - g_n(\xi, \xi - \sigma_Y(\xi))\, J,\\ J &= \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\end{aligned} \tag{4.8}$$

where $g_n \in \mathcal{C}^\infty\left(\sqcup_{\xi\in\Omega}\left(\{\xi\} \times N_{\sigma_{\Sigma_n}(\xi)}\Sigma_n\right)\right)$ (see also (1.11) where the restriction of g_n to points of Σ_n is introduced), and the function λ_n is defined in (1.12). Note that by assumption **H3'**, there exists $c > 0$ such that we have $g_n(\sigma, \eta) \le c|\eta|^q$ for all $\sigma \in \Sigma_n$ and $\eta \in N_\sigma\Sigma_n$, and $g_n(\xi, \eta) = |\eta|^2\theta_n(\xi)$ by (2) of Lemma B.1.

Theorem 4.6. *We suppose that* **H1'**, **H2'** *and* **H3'** *hold. Consider a connected component* Y *of* Σ_n *that is included in* $\Lambda_n \cap \Lambda_{n+1}$. *Let* $(M^t d\nu^t, d\gamma^t)$ *be a pair associated with the concentration of the family* $(\Psi^\varepsilon(t))_{\varepsilon>0}$ *on* Y. *Then,* $\gamma^t = 0$ *and there exists* $M d\nu^0$ *associated with the concentration at finite distance of* $(\Psi^\varepsilon(0))_{\varepsilon>0}$ *on* Y *such that* $\nu^t = \nu^0$ *and the following holds:*

(1) *If* $q = 2$, M^t *satisfies* (1.20) *with initial data* M.

(2) *If* $q > 2$, M^t *satisfies* (1.19) *with initial data* M.

Remark 4.7. Note that, even in Case (2), it can happen that the modes interact above the crossing, if they were doing so at time $t = 0$. Corollary E.3 provides examples of such initial data.

The proof of Theorem 4.6 is the subject of Section 6.

5. Proof of Theorem 4.5

We prove Theorem 4.5 in two steps: first we focus on the part of the two-scale semi-classical measure that comes from infinity in Section 5.1, then we concentrate on the part at finite distance in Section 5.2. We use the characterization of Lemma B.1 and write

$$\varrho_n(\xi) = \lambda_n(\xi) - g_n(\xi, \xi - \sigma_\Sigma(\xi)), \quad \varrho_{n+1}(\xi) = \lambda_n(\xi) + g_n(\xi, \xi - \sigma_\Sigma(\xi)) \tag{5.1}$$

with λ_n smooth and $g_n \in \mathcal{C}^\infty\left(\sqcup_{\xi\in\Omega}\left(\{\xi\} \times N_{\sigma_{\Sigma_n}(\xi)}\Sigma_n\right)\right)$ and $\eta \mapsto g_n(\xi, \eta)$ homogeneous of order 1 in η (see (1) in Lemma B.1). Note that the function introduced in the introduction in (1.11) is the restriction of g_n to $N\Sigma_n$ (and thus have been denoted similarly).

5.1. The Two-Scale Semiclassical Measures at Infinity

Let $a \in \mathcal{A}^{(2)}$ supported in $\mathbb{R}^d \times W \times \mathbb{R}^d$ where W is an open subset of $\mathbb{R}^d$ where we have tubular coordinates for Σ. Let $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ such that $\chi = 1$ on $B(0, 1)$ and $\chi = 0$ on $B(0, 2)^c$ with $0 \le \chi \le 1$. We set, for $R, \delta > 0$

$$a^{R,\delta}(x, \xi, \eta) = a(x, \xi, \eta)((1 - \chi(\eta/R))\chi((\xi - \sigma_\Sigma(\xi))/\delta).$$

Then, in view of equation (3.15),

$$i\varepsilon\frac{d}{dt}(\mathrm{op}_\varepsilon(a_\varepsilon^{R,\delta})\psi_n^\varepsilon(t), \psi_n^\varepsilon(t)) = \varepsilon^{-1}\left([\mathrm{op}_\varepsilon(a_\varepsilon^{R,\delta}), \varrho_n(\varepsilon D)]\psi_n^\varepsilon(t), \psi_n^\varepsilon(t)\right) + O(\varepsilon). \tag{5.2}$$

Using (5.1), the homogeneity of g_n, and the notation introduced in (D.1), we write

$$\varrho_n(\varepsilon D) = \lambda_n(\varepsilon D) - \varepsilon g_n(\varepsilon D, D - \varepsilon^{-1}\sigma_\Sigma(\varepsilon D)) = \lambda_n(\varepsilon D) - \varepsilon(g_n)_\varepsilon(\varepsilon D).$$

Therefore, we have

$$\varepsilon^{-1}\left[\mathrm{op}_\varepsilon(a_\varepsilon^{R,\delta}), \varrho_n(\varepsilon D)\right] = \mathrm{op}_\varepsilon(\nabla_x a_\varepsilon^{R,\delta} \cdot \nabla\lambda_n) - \left[\mathrm{op}_\varepsilon(a_\varepsilon^{R,\delta}), (g_n)_\varepsilon(\varepsilon D)\right] + O(\varepsilon).$$

We can now apply Lemma D.1 with $k = 0$, and we obtain

$$\varepsilon^{-1}\left[\mathrm{op}_\varepsilon(a_\varepsilon^{R,\delta}), \varrho_n(\varepsilon D)\right] = \mathrm{op}_\varepsilon(b_\varepsilon) + O(\varepsilon) + O(R^{-1}) + O(\delta)$$

with $b = \nabla_x a^{R,\delta} \cdot \nabla\lambda_n - \nabla_x a^{R,\delta} \cdot \nabla_\eta g_n$. Passing to the limits $\varepsilon \to 0$, then $R \to +\infty$ after time integration against $\theta \in \mathcal{C}_0^\infty(\mathbb{R})$, we obtain by (5.2),

$$\int_{\mathbb{R}} \theta(t) \left(\mathrm{op}_\varepsilon(b_\varepsilon)\psi_n^\varepsilon(t), \psi_n^\varepsilon(t)\right) \mathrm{d}t = O(\varepsilon) + O(R^{-1}) + O(\delta).$$

We deduce that

$$\int_{\mathbb{R}\times\mathbb{R}^d\times\Sigma\times\mathbf{S}^{d-1}} \theta(t)(\nabla\lambda_n(\sigma) - \nabla_\eta g_n(\sigma,\omega)) \cdot \nabla_x a_\infty(x,\sigma,\omega) d\gamma_n^t(x,\sigma,\omega) = 0.$$

This implies that the measure $\gamma_n^t(x,\sigma,\omega)$ is invariant by the flow

$$(x,\sigma,\omega) \mapsto (x + s(\nabla\lambda_n(\sigma) - \nabla_\eta g_n(\sigma,\omega), \sigma, \omega), \quad s \in \mathbb{R}.$$

As a consequence, γ_n^t is supported on $\{\nabla\lambda_n(\sigma) - \nabla_\eta g_n(\sigma,\omega) = 0\}$, and by **H3**, $\gamma_n^t = 0$.

5.2. The Two-Scaled Semiclassical Measures Coming from Finite Distance

In view of Remark 4.2 (3), we now choose $a \in \mathcal{C}_0^\infty(\mathbb{R}^d \times W \times \mathbb{R}^d)$ where W is as above. Let $\theta \in L^1(\mathbb{R})$. Arguing as in (5.2), we observe

$$\int_{\mathbb{R}} \theta(t) \left([\mathrm{op}_\varepsilon(a_\varepsilon), \varepsilon^{-1}\varrho_n(\varepsilon D_x)]\psi_n^\varepsilon(t), \psi_n^\varepsilon(t)\right) = O(\varepsilon).$$

Using that a is compactly supported in the variable η and the homogeneity of g, we obtain in $\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\frac{1}{\varepsilon}[\mathrm{op}_\varepsilon(a_\varepsilon), \varrho_n(\varepsilon D_x)] = i\,\mathrm{op}_\varepsilon(\nabla\lambda_n(\xi) \cdot \nabla_x a_\varepsilon) - [\mathrm{op}_\varepsilon(a_\varepsilon), (g_n)_\varepsilon(\varepsilon D)] + O(\varepsilon).$$

Passing to the limit $\varepsilon \to 0$ thanks to Lemma D.2, we obtain

$$\int_{\mathbb{R}} \theta(t)\mathrm{Tr}_{L^2(N_\sigma\Sigma)}(i\,Q^\Sigma_{\nabla\lambda_n\cdot\nabla_x a} - [Q^\Sigma_a(\sigma,v), Q^\Sigma_g(\sigma)]M_n^t(\sigma,v))\nu_n^t(\sigma,v)\mathrm{d}t = 0. \tag{5.3}$$

This relation has important consequences on the structure of $M_{n,n}^t$ and ν_n^t. For stating them, we write

$$\nabla\lambda_n(\sigma) = \nabla^\perp\lambda_n(\sigma) + \nabla^\sharp\lambda_n(\sigma), \quad \nabla^\perp\lambda_n(\sigma) \in N_\sigma\Sigma \quad \text{and} \quad \nabla^\sharp\lambda_n(\sigma) \in T_\sigma\Sigma.$$

Lemma 5.1. *Equation* (5.3) *implies*

$$\mathrm{supp}(\nu_n^t) \subset \{(\sigma,v) \in T\Sigma, \quad \nabla^\sharp\lambda_n(\sigma) = 0\}$$

and

$$[Q^\Sigma_F(\sigma), M_n^t(\sigma,v)] = 0 \;\; d\nu_n^t\, a.e.\, (\sigma,v) \in N\Sigma,$$

where $F(\sigma,\eta) = \nabla^\perp\lambda_n(\sigma) \cdot \eta + g_n(\sigma,\eta)$.

Proof of Lemma 5.1. We use a system of equations $\varphi(\xi) = 0$ of Σ and the matrix B defined in (4.4). For $\sigma \in X$ and $\zeta \in T_\sigma \mathbb{R}^d$, we have

$$(\mathrm{Id} - d\sigma_\Sigma(\sigma))\zeta = B(\sigma)d\varphi(\sigma)\zeta,$$

which allows to decompose ζ as

$$\zeta = d\sigma_\Sigma(\sigma)\zeta + B(\sigma)d\varphi(\sigma)\zeta, \quad d\sigma_\Sigma(\sigma)\zeta \in T_\sigma\Sigma \ \text{ and } \ B(\sigma)d\varphi(\sigma)\zeta \in N_\sigma\Sigma.$$

In particular, $B(\sigma)d\varphi(\sigma) = \mathrm{Id}$ on $N_\sigma\Sigma$. In view of this observation, we write for $(\sigma, v) \in T\Sigma$, and $(z, \zeta) \in (N_\sigma\Sigma)^*$

$$\begin{aligned}
&\nabla\lambda_n(\sigma) \cdot \nabla_x a(v + {}^t d\varphi(\sigma)z, \sigma, B(\sigma)\zeta) \\
&= \nabla^\sharp\lambda_n(\sigma) \cdot \nabla_v a(v + {}^t d\varphi(\sigma)z, \sigma, B(\sigma)\zeta) + \nabla^\perp\lambda_n(\sigma) \cdot (B(\sigma)\nabla_z) \\
&\quad \cdot \big(a(v + {}^t d\varphi(\sigma)z, \sigma, B(\sigma)\zeta)\big)
\end{aligned}$$

We obtain

$$Q^\varphi_{\nabla\lambda_n(\xi)\cdot\nabla_x a}(\sigma, v) = \nabla^\sharp\lambda_n(\sigma) \cdot \nabla_v Q^\varphi_a(\sigma, v) - i[Q^\varphi_F(\sigma), Q^\varphi_a(\sigma, v)],$$

with $Q^\varphi_F(\sigma) = F(\sigma, B(\sigma)D_z)$. Therefore, equation (5.3) can be written as

$$\begin{aligned}
\int_{\mathbb{R}} \theta(t)\mathrm{Tr}_{L^2(N_\sigma\Sigma)}(&i\nabla^\sharp\lambda_n(\sigma) \cdot \nabla_v Q^\Sigma_a(\sigma, v) \\
&+ [Q^\Sigma_a(\sigma, v), Q^\Sigma_F(\sigma)]M^t_n(\sigma, v))\nu^t_n(\sigma, v)\mathrm{d}t = 0,
\end{aligned}$$

We deduce that

$$i\nabla^\sharp\lambda_n(\sigma) \cdot \nabla_v(M^t_n d\nu^t_n) + [Q^\Sigma_F(\sigma), M^t_n d\nu^t_n] = 0.$$

Taking the trace gives

$$\nabla^\sharp\lambda_n(\sigma) \cdot \nabla_v \nu^t_n = 0,$$

whence the invariance of ν^t_n by the flow defined on $T\Sigma$ by

$$(\sigma, v) \mapsto (\sigma, v + s\nabla^\sharp\lambda_n(\sigma)), \quad s \in \mathbb{R},$$

which implies the results. □

We conclude the analysis of the two-scaled Wigner measures at finite distance M^t by using Lemma 5.2 below. For this, we need to check that its assumptions are satisfied. Hypothesis **H3** implies that if $\nabla^\sharp\lambda_n(\sigma) = 0$, then for all $\eta \in N_\sigma\Sigma \setminus \{0\}$,

$$\nabla^\perp\lambda_n(\sigma) - \nabla_\eta g_n(\sigma, \eta) \neq 0.$$

Considering $\nabla_\zeta(F(\sigma, B(\sigma)\zeta))$, we have

$$\nabla_\zeta(F(\sigma, B(\sigma)\zeta)) = {}^t B(\sigma)\Big(\nabla^\perp\lambda_n(\sigma) - \partial_\eta g_n(\sigma, \eta)\Big) \neq 0,$$

because $B(\sigma)$ is invertible on $N_\sigma\Sigma$, and the assumptions of the next lemma are satisfied.

Lemma 5.2. *Let $p \in \mathbb{N}$ and M be a non negative trace-class operator on $L^2(\mathbb{R}^p)$, and $F \in \mathcal{C}^\infty(\mathbb{R}^p \setminus \{0\})$ such that $\nabla_\zeta F(\zeta) \neq 0$ for all $\zeta \in \mathbb{R}^p \setminus \{0\}$. Assume $\left[F(D_z), M\right] = 0$. Then $M = 0$.*

Proof. Let $\phi \in L^2(\mathbb{R}^p)$ be an eigenvector of M for an eigenvalue $\ell \neq 0$. Then, for all $j \in \mathbb{N}$,

$$\phi_j := (F(D_z))^j \phi$$

is also an eigenvector for ℓ. Since ℓ is of finite multiplicity because M is trace-class, we deduce that the set $\{\phi_j, j \in \mathbb{N}\}$ is of finite dimension. Let $k \in \mathbb{N}^*$ the first index such that the family $(\phi_j)_{0 \leq j \leq k}$ is not a family of independent vectors. Then, there exist $\alpha_0, \cdots \alpha_k \in \mathbb{R}$ non all equal to 0, and such that $\sum_{j=0}^{k} \alpha_j \phi_j = 0$. In Fourier variables, we obtain $\left(\sum_{j=0}^{k} \alpha_j F(\zeta)^j\right) \widehat{\phi}(\zeta) = 0$. The set $\mathcal{C} = \left\{\zeta \in \mathbb{R}^p, \ \sum_{j=0}^{k} \alpha_j F(\zeta)^j = 0\right\}$ is the union of a finite number of sets $\mathcal{C}_\beta$,

$$\mathcal{C}_\beta = \{F(\zeta) = \beta\}$$

for β a real-valued root of the polynomial $\sum_{0 \leq j \leq k} \alpha_j X^j$. Since $\nabla_\zeta F(\zeta) \neq 0$ for all $\zeta \neq 0$, these sets $\mathcal{C}_\beta$ are hypersurfaces of $\mathbb{R}^p$ and thus of Lebesgues measure 0. So it is for $\mathcal{C}$ and we deduce that $\phi = 0$. $\square$

6. Proof of Theorem 4.6

Theorem 4.6 contains two statements. First, it states that the two-scale semi-classical measures at infinity is 0, what we prove in Section 6.1 below, by showing invariance properties of its diagonal elements. Secondly, it gives transport equations that allow to compute the two-scale semi-classical measures coming from finite distance from the knowledge of the initial data. We focus on this latter point in Section 6.2.

6.1. Analysis at Infinity

We perform the proof for $q = 2$, the proof for $q > 2$ is similar. Let Ψ^ε be a family of solutions to equation (4.7). Let $a \in \mathcal{A}^{(2)}$ supported in $\mathbb{R}^d \times W \times \mathbb{R}^d$ where W is an open subset of $\mathbb{R}^d$ where we have tubular coordinates for the manifold Y. Let $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ such that $\chi = 1$ on $B(0, 1)$ and $\chi = 0$ on $B(0, 2)^c$ with $0 \leq \chi \leq 1$. We set for $R, \delta > 0$

$$a^{R,\delta}(x, \xi, \eta) = a(x, \xi, \eta)((1 - \chi(\eta/R))\chi((\xi - \sigma_Y(\xi))/\delta)$$

and we consider the symbol

$$\tilde{a}^{R,\delta}(x, \xi, \eta) = |\xi - \sigma_Y(\xi)|^{-1} a^{R,\delta}(x, \xi, \eta).$$

By Lemma C.4 (1) (see also "Appendix D"), there exists a constant $C > 0$ such that

$$\|\mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta})\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C(\varepsilon R)^{-1}.$$

In view of (4.8) and of (2) in Lemma B.1, we write with the notations introduced in (D.1)

$$\Theta(\varepsilon D) = \lambda_n(\varepsilon D)\mathrm{Id} - \varepsilon^2 (g_n)_\varepsilon(\varepsilon D).$$

Therefore, if E is a constant diagonal matrix of $\mathbb{C}^{2\times 2}$, we obtain

$$\begin{aligned}\left[\mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta} E)\ ,\ \Theta(\varepsilon D)\right] &= \left[\mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta})\ ,\ \lambda_n(\varepsilon D)\right] E \\ &\quad -\varepsilon^2 \left[\mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta})\ ,\ (g_n)_\varepsilon(\varepsilon D)\right] EJ,\end{aligned}$$

where we have used that $EJ = JE$. We observe that setting

$$b(x,\xi,\eta) = |\eta|^{-1} a^{R,\delta}(x,\xi,\eta),$$

we have

$$\varepsilon\, \mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta}) = \mathrm{op}_\varepsilon(b_\varepsilon)$$

and we can apply Lemma D.1 because $b \in \mathcal{A}_{-1}^{(2)}$ and $g_n \in \mathcal{H}_2$. We deduce that

$$\varepsilon \left[\mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta})\ ,\ (g_n)_\varepsilon(\varepsilon D)\right] = \left[\mathrm{op}_\varepsilon(b_\varepsilon)\ ,\ (g_n)_\varepsilon(\varepsilon D)\right] = \mathrm{op}_\varepsilon((\nabla_x b \cdot \nabla_\eta g)_\varepsilon)$$

with $\nabla_x b(x,\xi,\eta) = |\eta|^{-1}\nabla_x a^{R,\delta}(x,\xi,\eta)$. Therefore, we are left with

$$\begin{aligned}\frac{1}{\varepsilon}\left[\mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta} E)\ ,\ \Theta(\varepsilon D)\right] &= \mathrm{op}_\varepsilon(\nabla_x \tilde{a}_\varepsilon^{R,\delta} \cdot \nabla_\xi \lambda_n(\xi))E - \mathrm{op}_\varepsilon((\nabla_x b \cdot \nabla_\eta g_n)_\varepsilon) EJ \\ &\quad + O(\varepsilon) + O(R^{-1}) + O(\delta).\end{aligned}$$

We use $\nabla\lambda_n(\xi) = \mathrm{Hess}\,\lambda_n(\sigma_Y(\xi))(\xi - \sigma_Y(\xi)) + O((\xi - \sigma_Y(\xi))^2)$ and we set

$$\begin{aligned}c(x,\xi,\eta) &:= \nabla_x a^{R,\delta}(x,\xi,\eta) \cdot \mathrm{Hess}\,\lambda_n(\sigma_Y(\xi))\frac{\eta}{|\eta|} E \\ &\quad - \nabla_x a^{R,\delta}(x,\xi,\eta) \cdot \frac{1}{|\eta|}\nabla_\eta g_n\,(\xi,\eta)\, EJ.\end{aligned}$$

Note that $c \in \mathcal{A}^{(2)}$ and

$$\frac{1}{\varepsilon}\left[\mathrm{op}_\varepsilon(\tilde{a}_\varepsilon^{R,\delta} E)\ ,\ \Theta(\varepsilon D)\right] = \mathrm{op}_\varepsilon(c_\varepsilon) + O(\varepsilon) + O(R^{-1}) + O(\delta).$$

Therefore, passing to the limit ε to 0, then R to $+\infty$ and finally δ to 0, we obtain for all $\theta \in \mathcal{C}_0^\infty(\mathbb{R})$,

$$\begin{aligned}&\int_{\mathbb{R}} \theta(t) \int_{\mathbb{R}^d \times Y \times \mathbf{S}^{d-1}} \mathrm{Tr}_{\mathbb{C}^{2\times 2}}\left(\nabla_x a_\infty(x,\sigma,\omega) \cdot (\mathrm{Hess}\,\lambda_n(\sigma)\omega\, E - \nabla_\eta g_n(\sigma,\omega) EJ)\right) \\ &\quad \gamma^t(dx, d\sigma, d\omega)\mathrm{d}t = 0.\end{aligned}$$

Let us denote by $\gamma^t_{n,n}$ and $\gamma^t_{n+1,n+1}$ the diagonal coefficients of the matrix-valued measure γ^t. Choosing the 2×2 diagonal matrix E such that $EJ = E$, we deduce that the measure $\gamma^t_{n,n}$ is invariant by the flow

$$(x,\sigma,\omega)\mapsto (x+s(\mathrm{Hess}\,\lambda_n(\sigma)\omega-\nabla_\eta g_n(\sigma,\omega)),\sigma,\omega),\quad s\in\mathbb{R}.$$

Then, choosing E such that $EJ = -E$, we obtain that the measure $\gamma^t_{n+1,n+1}$ is invariant by the flow

$$(x,\sigma,\omega)\mapsto \left(x+s(\mathrm{Hess}\,\lambda_n(\sigma)\omega+\nabla_\eta g_n(\sigma,\omega)),\sigma,\omega\right),\quad s\in\mathbb{R}.$$

From assumption **H3'**, we deduce $\gamma^t_{n,n}=0$ and $\gamma^t_{n+1,n+1}=0$, and the positivity of γ^t implies that $\gamma^t=0$. One argues similarly when $q>2$, and proves that the term in g_n does not contribute to the limit.

6.2. The Two-Scale Semiclassical Measures Coming from Finite Distance

Here again, we write the proof for $q=2$. We choose $\theta\in L^1(\mathbb{R}^d)$, $a\in\mathcal{C}^\infty_0(\mathbb{R}^d\times W\times\mathbb{R}^d,\mathbb{C}^{2\times 2})$ where W is a tubular neighborhood of Y where the function σ_Y is defined. Using the homogeneity of the function $g(\xi,\eta)$, we have

$$i\frac{d}{dt}\left(\mathrm{op}_\varepsilon(a_\varepsilon)\Psi^\varepsilon(t),\Psi^\varepsilon(t)\right)=I_1^\varepsilon(t)+I_2^\varepsilon(t) \tag{6.1}$$

with

$$\begin{aligned}
I_1^\varepsilon(t)&=\left([\mathrm{op}_\varepsilon(a_\varepsilon),\varepsilon^{-2}\lambda_n(\varepsilon D_x)+V_{\mathrm{ext}}(t,x)]\Psi^\varepsilon(t),\Psi^\varepsilon(t)\right)\\
I_2^\varepsilon(t)&=-\left(\left(\mathrm{op}_\varepsilon(a_\varepsilon)J(g_n)_\varepsilon(\varepsilon D)-(g_n)_\varepsilon(\varepsilon D)J\,\mathrm{op}_\varepsilon(a_\varepsilon)\right)\Psi^\varepsilon(t),\Psi^\varepsilon(t)\right).
\end{aligned}$$

Note that if $q>2$, the homogeneity implies $I_2^\varepsilon(t)=O(\varepsilon^{q-2})$. Section 5.1 in [15] gives the uniform boundedness of the family of time dependent functions $t\mapsto I_1^\varepsilon(t)$ and Lemma D.2 yields the uniform boundedness of the family of time dependent functions $t\mapsto I_2^\varepsilon(t)$. Therefore, the left-hand side of (6.1) is uniformly bounded with respect to ε. Therefore, the maps $t\mapsto M^t(\sigma,v)d\nu^t(\sigma,v)$ defined on TY will be continuous in time.

Remark 6.1. At that level of the proof, one sees that by Ascoli theorem, one can find for each $T>0$ a sequence ε_ℓ for which the limit of $\left(\mathrm{op}_{\varepsilon_\ell}(a_{\varepsilon_\ell})\Psi^{\varepsilon_\ell}(t),\Psi^{\varepsilon_\ell}(t)\right)$ exists for all $t\in\mathbb{R}$. One then deduces the convergence t by t of these quantities.

We now integrate equation (6.1) against a function θ and pass to the limit $\varepsilon\to 0$. By Section 5.1 in [15], we have for $\theta\in\mathcal{C}^\infty_0(\mathbb{R})$, up to the subsequence defining $M^t d\nu^t$

$$\begin{aligned}
&\int\theta(t)I_1^\varepsilon(t)\mathrm{d}t\underset{\varepsilon\to 0}{\longrightarrow}\\
&\int_{\mathbb{R}}\theta(t)\int_{TY}\mathrm{Tr}_{L^2(N_\sigma Y,\mathbb{C}^2)}\left(\left[Q_a^Y(\sigma,v),\frac{1}{2}\mathrm{Hess}\lambda_n(\sigma)\,D_z\cdot D_z\;+m_{V_{\mathrm{ext}}(t,\cdot)}(x,v)\right]M^t(\sigma,v)\right)\\
&\nu^t(\sigma,v)\mathrm{d}t.
\end{aligned}$$

By Lemma D.2 for studying the term I_2^ε,

$$\int \theta(t) I_2^\varepsilon(t) dt \underset{\varepsilon\to 0}{\longrightarrow}$$
$$\int_{\mathbb{R}} \theta(t) \int_{TY} \mathrm{Tr}_{L^2(N_\sigma Y,\mathbb{C}^2)} \left(Q_a^Y(\sigma,v) J Q_{g_n}^Y(\sigma) - Q_{g_n}^Y(\sigma) J Q_a^Y(\sigma,v) \right) M^t(\sigma,v) \Big) \nu^t(\sigma,v) \mathrm{d}t.$$
$$= \int_{\mathbb{R}} \theta(t) \int_{TY} \mathrm{Tr}_{L^2(N_\sigma Y,\mathbb{C}^2)} \left(\left[Q_a^Y(\sigma,v)\ ,\ J Q_{g_n}^Y(\sigma) \right] M^t(\sigma,v) \right) \nu^t(\sigma,v) \mathrm{d}t$$

Reporting the result in (6.1), we obtain

$$-i \int_{\mathbb{R}} \theta'(t) \int_{TY} \mathrm{Tr}_{L^2(N_\sigma Y,\mathbb{C}^2)} (Q_a^Y(\sigma,v) M^t(\sigma,v)) \mathrm{d}\nu^t(\sigma,v) \mathrm{d}t$$
$$= \int_{\mathbb{R}} \theta(t) \int_{TY} \mathrm{Tr}_{L^2(N_\sigma Y,\mathbb{C}^2)} \Bigg(\Bigg[Q_a^Y(\sigma,v), \left(\frac{1}{2} \mathrm{Hess}\lambda_n(\sigma)\, D_z \cdot D_z + m_{V_{\mathrm{ext}}(t,\cdot)}(x,v) \right) \mathrm{Id}$$
$$+ J Q_{g_n}^Y(\sigma) \Bigg] M^t(\sigma,v) \Bigg) \nu^t(\sigma,v) \mathrm{d}t.$$

We deduce that

$$\partial_t (M^t d\nu^t) = \left[\left(\frac{1}{2} \mathrm{Hess}\lambda_n(\sigma)\, D_z \cdot D_z + m_{V_{\mathrm{ext}}(t,\cdot)}(x,v) \right) \mathrm{Id} + Q_{g_n}^Y(\sigma) J\ ,\ M^t d\nu^t \right] d\nu^t.$$

Taking the trace of this expression gives $\partial_t \nu^t = 0$, whence $\nu^t = \nu^0$ (because of the continuity of $t \mapsto \nu^t$), and the equation satisfied by M^t.

7. Proof of the Main Theorems

7.1. Proofs of Theorem 1.5 and Proposition 1.6

We prove here the results obtained under **H1**, **H2** and **H3**, which corresponds to a general setting without too much assumptions on the initial data and with generic hypothesis on the Bloch energies.

Proof of Theorem 1.5. Let (ε_ℓ) be a sequence given by Proposition 3.4 and ς^t and $\mu_{n,n'}^t$ the corresponding semi-classical measures along that sequence. Because of the assumption **H1** and Part (2) of Proposition 3.5, $\mu_{n,n'}^t = 0$ for a.e. $t \in \mathbb{R}$ as soon as $|n - n'| > 1$. Besides, by **H2**, we can use Theorem 4.3 to determine $\mu_{n,n}^t \mathbf{1}_{\Lambda_n}$. Finally, by **H3** and Theorem 4.5, $\mu_{n,n}^t = \mu_{n,n}^t \mathbf{1}_{\Lambda_n}$ and the result follows. We obtain that for a subsequence ε_ℓ for $a, b \in \mathbb{R}$ and $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

$$\int_a^b \int_{\mathbb{R}^d} \phi(x) |\psi^{\varepsilon_\ell}(t,x)|^2 dx \mathrm{d}t \underset{\varepsilon_\ell\to 0}{\longrightarrow}$$
$$\sum_{n\in\mathbb{N}_0} \int_a^b \int_{T^*X} \mathrm{Tr}_{L^2(N_\sigma \Lambda_n}(m_\phi^{\Lambda_n}(\sigma) M_n^t(\sigma,v)) \nu_n(d\sigma, dv) \mathrm{d}t,$$

once if; observed that, for $a(x,\xi) := \phi(x)$, the operator $Q_a(\sigma,v)$ coincides with $m_\phi^{\Lambda_n}(\sigma)$. $\square$

Proof of Proposition 1.6. For the data considered in that statement, one has $U_0^\varepsilon = \varphi_{n_0}(y, \varepsilon D_x)u_{n_0}^\varepsilon$. Therefore, $M_n = 0$ for $n \neq n_0$ and M_n^t too. We then focus on calculating M_{n_0} above any $\xi \in \Lambda_{n_0}$. By Corollary E.3 (1), since ξ is an isolated point of Λ_{n_0}, the measure ν_{n_0} is given by

$$\nu_{n_0}(d\xi) = \|v_{n_0}\|_{L^2}^2 \sum_{j\in 2\pi\mathbb{Z}^d} |c_{n_0}(\xi_{n_0}+j)|^2 \delta(\xi - \xi_{n_0} - j),$$

and, for $j \in 2\pi\mathbb{Z}^d$, the operator $M_{n_0}(\xi_{n_0}+j)$ is the projector on $\mathbb{C}v_{n_0}$. As a consequence, the solution $M^t(\xi_{n_0}+j)$ of (1.15) is the orthogonal projection on $\mathbb{C}\psi^{\xi_{n_0}}(t)$ where $\psi^{\xi_{n_0}}$ satisfies (1.16). We obtain that for any $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

$$\begin{aligned}\int_{\Lambda_{n_0}} \mathrm{Tr}_{L^2(\mathbb{R}^d)} m_\phi^{\Lambda_{n_0}}(M_{n_0}^t(\xi))\nu_{n_0}(d\xi) &= \left(\int_{\mathbb{R}^d} \phi(x)|\psi^{\xi_{n_0}}(t,x)|^2 dx\right) \sum_{j\in\mathbb{Z}^d} |c_{n_0}(\xi_{n_0}+j)|^2 \\ &= \int_{\mathbb{R}^d} \phi(x)|\psi^{\xi_{n_0}}(t,x)|^2 dx,\end{aligned}$$

where we have used that $N\Lambda_{n_0} = \mathbb{R}^d$, $m_\phi^{\Lambda_{n_0}}$ is the operator of multiplication by ϕ, and the conservation of L^2 norms for the equation (1.16) ($\|v_{n_0}\|_{L^2} = \|\psi^{\xi_{n_0}}(t)\|_{L^2}$ for all $t \in \mathbb{R}$). □

7.2. *Proof of Theorem 1.8 and Proposition 1.9*

We focus here on degenerate crossings involving two energies isolated from the remainder of the spectrum and well-prepared data that concentrate on these modes. We will indeed prove a more general result than Theorem 1.8, assuming that Σ_n is included in $\Lambda_n \cup \Lambda_{n+1}$ but not necessarily equal to Λ_n and Λ_{n+1} (the latter being non necessarily equal). Thus, one has to take into account the additional contributions to the energy densities generated by the points of $(\Lambda_n \cup \Lambda_{n+1}) \setminus \Sigma_n$ and Theorem 1.8 is a straightforward corollary of the next result.

Theorem 7.1. *Then, there exists a subsequence $\varepsilon_\ell \underset{\ell\to+\infty}{\longrightarrow} 0$, three non negative measures $\nu_n \in \mathcal{M}^+(T^*\Lambda_n)$, $\nu_{n+1} \in \mathcal{M}^+(T^*\Lambda_{n+1})$ and $\nu^0 \in \mathcal{M}^+(\Sigma_n)$ depending on $(\psi_0^{\varepsilon_\ell})$, three measurable trace-class operators M_n, M_{n+1} and M*

$$\begin{aligned}
&M_n : T_\xi^*\Lambda_n \ni (\xi, v) \mapsto M_n(\xi, v) \in \mathcal{L}_+^1(L^2(N_\xi\Lambda_n)),\\
&\quad \mathrm{Tr}_{L^2(N_\xi\Lambda_n)} M_n(\xi, v) = 1 \ d\nu_n \ a.e.\\
&M_{n+1} : T_\xi^*\Lambda_{n+1} \ni (\xi, v) \mapsto M_{n+1}(\xi, v) \in \mathcal{L}_+^1(L^2(N_\xi\Lambda_{n+1})),\\
&\quad \mathrm{Tr}_{L^2(N_\xi\Lambda_{n+1})} M_{n+1}(\xi, v) = 1 \ d\nu_{n+1} \ a.e.\\
&M : T_\xi^*\Sigma_n \ni (\xi, v) \mapsto M(\xi, v) \in \mathcal{L}_+^1(L^2(N_\xi\Sigma_n, \mathbb{C}^2)),\\
&\quad \mathrm{Tr}_{L^2(N_\xi\Sigma_n, \mathbb{C}^2)} M(\xi, v) = 1 \ d\nu^0 \ a.e.
\end{aligned}$$

such that for every $a < b$ and every $\phi \in \mathcal{C}_0(\mathbb{R}^d)$ one has

$$\lim_{\ell\to+\infty} \int_a^b \int_{\mathbb{R}^d} \phi(x)|\psi^{\varepsilon_\ell}(t,x)|^2 dx\mathrm{d}t$$

$$= \sum_{j=n,n+1} \int_a^b \int_{T^*(\Lambda_j \setminus \Sigma_n)} \mathrm{Tr}_{L^2(N_\xi \Lambda_j)}[m_\phi^{\Sigma_n}(\xi, v) M_j^t(\xi, v)] \nu_j(d\xi, dv) \mathrm{d}t$$
$$+ \int_a^b \int_{T^*\Sigma_n} \mathrm{Tr}_{L^2(N_\xi \Sigma_n, \mathbb{C})}[m_\phi^{\Sigma_n}(\xi, v)(m_n^t + m_{n+1}^t$$
$$+ 2\mathrm{Re}(m_{n,n+1}^t))(\xi, v)] \nu^0(d\xi, dv) \mathrm{d}t,$$

where

$$M^t(\xi, v) = \begin{pmatrix} m_n^t(\xi, v) & m_{n,n+1}^t(\xi, v) \\ m_{n,n+1}^t(\xi, v)^* & m_{n+1}^t(\xi, v) \end{pmatrix}$$

is a non negative trace class operators on $L^2(N_\xi \Sigma_n, \mathbb{C}^2)$.

Besides, the map $t \mapsto M_n^t(x, \xi) \in \mathcal{C}(\mathbb{R}, \mathcal{L}_+^1(L^2(N_\xi \Lambda_n))$ *solves the von Neumann equation* (1.15) *and similarly for* M_{n+1}^t *and* ϱ_{n+1}, *and the map* $t \mapsto M^t(\xi, v) \in \mathcal{C}(\mathbb{R}, \mathcal{L}_+^1(L^2(N_\xi \Sigma_n, \mathbb{C}^2))$ *solves* (1.19) *if* $q > 2$ *and* (1.20) *if* $q = 2$. *All the initial data depend on* $(\psi_0^{\varepsilon_\ell})$ *as in Remark* 4.2.

Proof. We have

$$U_0^\varepsilon(x, y) = \varphi_n(y, \varepsilon D_x) u_n^\varepsilon(x) + \varphi_{n+1}(y, \varepsilon D_x) u_{n+1}^\varepsilon(x)$$

and we are going to take advantage of the fact that $U_0^\varepsilon \in \mathrm{Ran}\, \Pi(\xi)$, the spectral projector on

$$\mathrm{Ker}(P(\xi) - \varrho_n(\xi)) \oplus \mathrm{Ker}(P(\xi) - \varrho_{n+1}(\xi)).$$

By assumption **H1'**, the band of the spectrum of $P(\xi)$ consisting of the pair $\{\varrho_n(\xi), \varrho_{n+1}(\xi)\}$ is separated from the remainder of the spectrum by a gap, which implies that $\xi \mapsto \Pi(\xi)$ is analytic. We claim that a consequence of this is that if (ε_ℓ) is a sequence given by Proposition 3.4, then

$$\varsigma^t = \mu_{n,n}^t + \mu_{n+1,n+1}^t + \mu_{n,n+1}^t + \mu_{n+1,n}^t. \tag{7.1}$$

By Proposition 3.5, ς^t has only support above Λ_n (because of $\mu_{n,n}^t$), Λ_{n+1} (because of $\mu_{n,n+1}^t$) and Σ_n (because of the crossed terms). Then, the result of Theorem 1.8 comes from two observations:

(1) assumption **H2'** allows to use Theorem 4.3 to determine $\mu_{n,n}^t$ above $\Lambda_n \setminus \Sigma_n$ and $\mu_{n+1,n+1}^t$ above $\Lambda_{n+1} \setminus \Sigma_{n+1}$,
(2) assumption **H3'** allows to use Theorem 4.6 to compute $\mu_{n,n}^t$, $\mu_{n+1,n+1}^t$, $\mu_{n,n+1}^t$ and $\mu_{n+1,n}^t$ above Σ_n in terms of the coefficients of the matrix-valued measure $M^t d\nu^0$. In view of (7.1), we obtain that for all $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d \times \Sigma_n} \phi(x) \varsigma^t(dx, d\xi) = \int_{T^*\Sigma_n} \mathrm{Tr}\left[m_\phi^{\Sigma_n}(\xi, v) E M^t(\xi, v)\right] \nu^0(d\xi, dv),$$
$$E = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{7.2}$$

It remains to discuss Equation (7.1), which comes from (1.8) and the estimate

$$\left\|(1-\Pi(\varepsilon D_x))U^\varepsilon(t)\right\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} \leq \varepsilon\, C_s(1+|t|)$$

for $s > d/2$. We observe that the family

$$W^\varepsilon(t,x) = (1-\Pi)(\varepsilon D_x)U^\varepsilon(t,x).$$

satisfies the system

$$i\varepsilon^2\partial_t W^\varepsilon = P(\varepsilon D_x)W^\varepsilon + \varepsilon^2 V_{\text{ext}} W^\varepsilon + \varepsilon^3 G^\varepsilon, \quad W^\varepsilon(0) = 0$$

with $G^\varepsilon(t) = -\varepsilon^{-1}\left[\Pi(\varepsilon D_x), V_{\text{ext}}(t)\right] U^\varepsilon(t)$ uniformly bounded in $L^2(\mathbb{R}^d\times\mathbb{T}^d)$. Therefore, when $s = 0$, the estimate comes from an energy argument. We then proceed as in Lemma 6.7 in [15] by induction in $s \in \mathbb{N}$ and interpolation between s and $s+1$, observing that, in view of Remark 2.2, it is enough to prove that $P(\varepsilon D_x)^{s/2}W^\varepsilon$ and $\langle\varepsilon D_x\rangle^s W^\varepsilon$ go to 0 in $L^2(\mathbb{R}^d\times\mathbb{T}^d)$. $\square$

As a by-product of the proofs, we have the following remark:

Remark 7.2. In view of Remark 6.1, for all $T > 0$, there exists a sequence ε_ℓ for which one has for any $\phi \in \mathcal{C}^\infty(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d}\phi(x)|\psi^\varepsilon(t,x)|^2dx \geq \int_{T^*\Sigma_n}\mathrm{Tr}_{L^2(N_\xi\Sigma_n)}\Big(m_\phi^{\Sigma_n}(\xi,v)(m_n^t+m_{n+1}^t \\ +2\mathrm{Re}\, m_{n,n+1}^t)(\sigma,v)\Big)\,\nu^0(d\xi,dv). \tag{7.3}$$

Let us assume

$$\int_{T^*\Sigma_n}\mathrm{Tr}_{L^2(N_\xi\Sigma_n)}\left(m_n^0+m_{n+1}^0+2\mathrm{Re}\, m_{n,n+1}^0\right)d\nu^0 = \|\psi_0^\varepsilon\|_{L^2}.$$

Then $\int_{T^*\Sigma_n}\mathrm{Tr}_{L^2(N_\xi\Sigma_n)}\left(m_n^t+m_{n+1}^t+2\mathrm{Re}\, m_{n,n+1}^t\right)d\nu = |\psi^\varepsilon(t,x)|^2dx$, and the inequality (7.3) becomes an equality. One has obtained a t by t description of the limit of the energy density. The same observation holds in the frame of Theorem 4.3.

It remains to prove Proposition 1.9.

Proof of Proposition 1.9. According to the assumptions, we have $\Lambda_n = \Lambda_{n+1} = \Sigma_n$. Therefore, we only have to compute $M d\nu^0$ and solve the von Neumann equations defining M^t in both studied cases. For the data considered in that statement, one has $\psi_0^\varepsilon = \psi_{0,n}^\varepsilon + \psi_{0,n+1}^\varepsilon$ (where the latter families are defined in (1.16)) with $\xi_n = \xi_{n+1}$. Therefore, by Corollary E.3, ν^0 is given by

$$\nu^0(d\xi) = (\|v_n\|_{L^2}^2 + v_{n+1}\|_{L^2}^2)\sum_{j\in 2\pi\mathbb{Z}^d}|c_n(\xi_n+j)|^2\delta(\xi-\xi_n-j)$$

and, for $j \in 2\pi\mathbb{Z}^d$, the operator $M^0(\xi_n+j)$ is the projector on $\mathbb{C}^t(v_n, v_{n+1})$. The solution of the Heisenberg equations (1.19) and (1.20) then are orthogonal

projectors on $\mathbb{C}^t(\psi_n^{\xi_n}, \psi_{n+1}^{\xi_n})$ as defined in the statement of Proposition 1.9. In view of (7.2) and of $m_\phi^{\Sigma_n} = \phi(x)$, we conclude for $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

$$\begin{aligned}
&\int_{\Sigma_n} \mathrm{Tr}_{L^2(\mathbb{R}^d,\mathbb{C}^2)}(m_\phi^{\Sigma_n} E M^t(\xi))\nu^0(d\xi) \\
&= \left(\int_{\mathbb{R}^d} \phi(x)|\psi_n^{\xi_n}(t,x) + \psi_{n+1}^{\xi_n}(t,x)|^2 dx\right) \sum_{j\in\mathbb{Z}^d} |c_{n_0}(\xi_{n_0}+j)|^2 \\
&= \int_{\mathbb{R}^d} \phi(x)|\psi_n^{\xi_n}(t,x) + \psi_{n+1}^{\xi_n}(t,x)|^2 dx
\end{aligned}$$

□

7.3. The 1-d Case: Proof of Theorem 1.1 and Discussion of Proposition 1.6

We now focus on the results devoted to the 1-dimensional case. By Lemma A.1, the Bloch energies ϱ_n have only non-degenerate critical points and $\Lambda_n \subset \pi\mathbb{Z}$. Besides, they are smooth outside the set of crossing points $\Sigma_n = \pi\mathbb{Z} \setminus \Lambda_n$, that are all conical. Therefore, the assumptions of Theorem 1.5 are satisfied and

$$\varsigma^t = \sum_{n\in I_n} \mu_{n,n}^t.$$

with $\mu_{n,n}^t$ determined by the pairs $M_n^t)\nu_n^t$. It remains to characterize the pairs (M_n^t, ν_n) that are associated with the discrete sets Λ_n. For this reason, $T^*\Lambda_n = \Lambda_n \times \{0\}$ and $N\Lambda_n = \mathbb{R}^d$, the measure ν_n^t is a sum of Dirac masses and the operator M_n^t is constant and an orthogonal projector on a function $\psi_\xi^{(n)}$ that has to satisfy (1.9) since M_n^t satisfies (1.15) (see also Corollary 1.4 in [15]).

It can be illuminating to see how Proposition 1.6 can be deduced from Theorem 1.1 when $d = 1$. The assumptions of Proposition 1.6 correspond to the choice of

$$\psi_0^\varepsilon(x) = \varphi_{n_0}\left(\frac{x}{\varepsilon}, \varepsilon D_x\right) \mathrm{e}^{\frac{i}{\varepsilon}x\xi_{n_0}} v_{n_0}^\varepsilon(x)$$

with $\xi_{n_0} \in \Lambda_{n_0}$ and $(v_{n_0}^\varepsilon)_{\varepsilon>0}$ bounded in $H^s(\mathbb{R})$ with $s > 1$. This in turn, corresponds to setting

$$U_{n_0}^\varepsilon(x,y) = \varphi_{n_0}(y, \varepsilon D_x)\, \mathrm{e}^{\frac{i}{\varepsilon}x\xi_{n_0}} v_{n_0}^\varepsilon(x).$$

As a consequence, we have $\Pi_n(\varepsilon D_x)U_0^\varepsilon = 0$ for $n \neq n_0$ and $\Pi_{n_0}(\varepsilon D_x)U_0^\varepsilon = U_0^\varepsilon$, whence

$$L^\varepsilon \Pi_n(\varepsilon D_x)U_0^\varepsilon = \begin{cases} 0 \text{ for } n \neq n_0, \\ \psi_0^\varepsilon \text{ for } n = n_0. \end{cases}$$

We deduce that the weak limits $\psi_\xi^{(n)}$ ($n \in \mathbb{N}^*$ and $\xi \in \Lambda_n$) that we have to consider in Theorem 1.1 satisfy

$$\psi_\xi^{(n)}(0) = \begin{cases} 0 & \text{for } n \neq n_0, \\ \mathrm{w}-\lim\limits_{\varepsilon\to 0} \mathrm{e}^{-\frac{i}{\varepsilon}x\xi}\psi_0^\varepsilon & \text{for } n = n_0. \end{cases}$$

Lemma E.2 yields

$$\psi_\xi^{(n_0)}(0) = \mathrm{w}-\lim_{\varepsilon\to 0} \mathrm{e}^{-\frac{i}{\varepsilon}x\xi}\psi_0^\varepsilon = \begin{cases} 0 & \text{if } \xi \notin \xi_{n_0} + 2\pi\mathbb{Z}, \\ c_{n_0}(\xi_{n_0}+j)v_{n_0} & \text{if } \xi = \xi_{n_0}+j,\ \ j \in 2\pi\mathbb{Z}. \end{cases}$$

We recall that the sequence $(c_n(\xi + j))_{j\in\mathbb{Z}}$ are the Fourier coefficients of $y \mapsto \varphi_n(y,\xi)$. As a consequence, for $t \in \mathbb{R}$, we have

$$\psi_\xi^{(n_0)}(t) = \begin{cases} 0 & \text{if } \xi \notin \xi_{n_0} + 2\pi\mathbb{Z}, \\ c_{n_0}(\xi_{n_0}+j)\psi^{\xi_{n_0}}(t) & \text{if } \xi = \xi_{n_0}+j,\ \ j \in 2\pi\mathbb{Z} \end{cases}$$

where $\psi^{\xi_{n_0}}(t)$ solves (1.9) with $n = n_0$ and initial data $\psi^{\xi_{n_0}} = v_{n_0}$. Applying Theorem 1.1, we obtain

$$\begin{aligned}\lim_{\varepsilon\to 0}\int_a^b\int_{\mathbb{R}} \phi(x)|\psi^\varepsilon(t,x)|^2 dxdt &= \sum_{j\in 2\pi\mathbb{Z}}\int_a^b\int_{\mathbb{R}} \phi(x)|c_{n_0}(\xi_{n_0}+j)|^2|\psi^{\xi_{n_0}}(t,x)|^2 dxdt \\ &= \int_a^b\int_{\mathbb{R}} \phi(x)|\psi^{\xi_{n_0}}(t,x)|^2 \mathrm{d}x\mathrm{d}t,\end{aligned}$$

where we have used that

$$\sum_{j\in 2\imath\mathbb{Z}} |c_{n_0}(\xi_{n_0}+j)|^2 = \|\varphi(\cdot,\xi_{n_0}\|^2_{L^2(\mathbb{T})} = 1.$$

7.4. Extension of the Setting to More General Situations

Our results could be formulated differently by assuming that the initial data is localised in Fourier variables on a set Ω in which the assumptions **H1**, **H2** and **H3** of Theorem 1.5 are satisfied. More precisely, we assume that Ω is a $\mathbb{Z}^d$-periodic open subset of $\mathbb{R}^d$ such that there exists a unit cell $\mathcal{B}$ of $\mathbb{Z}^d$ for which $\Omega\cap\mathcal{B}$ is strictly included in $\mathcal{B}$. We prove here that the analysis of the semi-classical measure ς^t of $(\psi^\varepsilon)_{\varepsilon>0}$ in $\mathbb{R}\times\mathbb{R}^d\times\Omega$ can be performed by localizing the initial data ψ_0^ε, which allows to extend the results of Theorem 1.5 to data with less strict assumptions on the Bloch energies.

Lemma 7.3. *Let Ω as above and $\chi \in \mathcal{C}^\infty(\mathbb{R}^d)$ be $2\pi\mathbb{Z}^d$-periodic, supported in the interior of $\mathcal{B}+2\pi\mathbb{Z}^d$ and equal to 1 on Ω. Let $U_\chi^\varepsilon(t)$ be the solution of equation (2.2) with initial data $\chi(\varepsilon D)U_0^\varepsilon$. Then, for every $s \geq 0$ there exists a constant $C_s > 0$ such that, for all $t \in \mathbb{R}$,*

$$\left\| U_\chi^\varepsilon(t) - \chi(\varepsilon D_x)U^\varepsilon(t)\right\|_{H_\varepsilon^s(\mathbb{R}^d\times\mathbb{T}^d)} \leq \varepsilon\, C_s(1+|t|).$$

Moreover, if $\psi_0^\varepsilon = L^\varepsilon U_0^\varepsilon$, then there exist $C > 0$ such that

$$\left\| L^\varepsilon U_\chi^\varepsilon(t) - \chi(\varepsilon D_x)\psi^\varepsilon(t)\right\|_{L^2(\mathbb{R}^d)} \leq \varepsilon\, C(1+|t|).$$

Proof of Lemma 7.3. Note that we have $U_\chi^\varepsilon(0) = \chi(\varepsilon D_x)U_0^\varepsilon$. We observe that $\widetilde{U}^\varepsilon = \chi(\varepsilon D_x)U^\varepsilon$ satisfies the system

$$i\varepsilon^2\partial_t\widetilde{U}^\varepsilon = P(\varepsilon D_x)\widetilde{U}^\varepsilon + \varepsilon^2 V_{\text{ext}}\widetilde{U}^\varepsilon + \varepsilon^3 F^\varepsilon,$$

with $F^\varepsilon(t) = \varepsilon^{-1}[\chi(\varepsilon D_x), V_{\text{ext}}(t)]U^\varepsilon(t)$ is uniformly bounded in $L^2(\mathbb{R}^d \times \mathbb{T}^d)$. A standard energy estimate then gives the result for $s = 0$. Then, in view of Remark 2.2, it is enough to prove that $P(\varepsilon D_x)^{s/2}(\widetilde{U}^\varepsilon - U_\chi^\varepsilon)$ and $\langle\varepsilon D_x\rangle^s(\widetilde{U}^\varepsilon - U_\chi^\varepsilon)$ go to 0 in $L^2(\mathbb{R}^d \times \mathbb{T}^d)$. We proceed by induction in $s \in \mathbb{N}$ and interpolation between s and $s+1$, following the arguments of the proof of Lemma 6.7 in [15]. This proves the first estimate of the lemma.

To prove the second estimate, note that whenever χ is $2\pi\mathbb{Z}^d$-periodic, we have

$$\chi(\varepsilon D)\left(\mathrm{e}^{\frac{i}{\varepsilon}k\cdot x}\cdot\right) = \mathrm{e}^{\frac{i}{\varepsilon}k\cdot x}\chi(\varepsilon D + k) = \mathrm{e}^{\frac{i}{\varepsilon}k\cdot x}\chi(\varepsilon D)$$

for $k \in 2\pi\mathbb{Z}^d$. Thus $[\chi(\varepsilon D), L^\varepsilon] = 0$ where L^ε is the operator defined in (1.8). We deduce that

$$\chi(\varepsilon D)\psi^\varepsilon(t) = \chi(\varepsilon D)L^\varepsilon U^\varepsilon(t) = L^\varepsilon\chi(\varepsilon D)U^\varepsilon(t).$$

Therefore, combining (1.8) and the previous estimate, finishes the proof of the lemma. □

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Appendix A. One Dimensional Bloch Modes

We review the main aspects of the theory that are needed here; the reader can refer to the books [48,53] or the articles [32,39,47] among others for additional details.
First of all, note that $\phi \in L^2(\mathbb{T})$ solves $P(\xi)\phi = \lambda\phi$ for some $\xi, \lambda \in \mathbb{R}$ if and only if $f(y,\lambda) := \mathrm{e}^{i\xi y}\phi(y)$ is a solution to:

$$-\frac{1}{2}\partial_y^2 f(y,\lambda) + V_{\mathrm{per}}(y) f(y,\lambda) = \lambda f(y,\lambda), \quad y \in \mathbb{R}, \tag{A.1}$$

satisfying the periodicity condition

$$f(1,\lambda) = \mathrm{e}^{i\xi} f(0,\lambda). \tag{A.2}$$

Given $\lambda \in \mathbb{R}$, the solutions of (A.1) are linear combinations of two solutions $f_1(y,\lambda)$ and $f_2(y,\lambda)$ satisfying

$$f_1(0,\lambda) = \partial_y f_2(0,\lambda) = 1, \quad f_2(0,\lambda) = \partial_y f_1(0,\lambda) = 0.$$

Define:

$$M_\lambda(y) := \begin{pmatrix} f_1(y,\lambda) & f_2(y,\lambda) \\ \partial_y f_1(y,\lambda) & \partial_y f_2(y,\lambda) \end{pmatrix};$$

then the existence of a solution to (A.1) satisfying (A.2) is equivalent to the fact that $\mathrm{e}^{i\xi}$ is an eigenvalue of $M_\lambda(1)$. One can check that $\det M_\lambda(y) = 1$ for every $y, \lambda \in \mathbb{R}$; therefore, letting $\Delta(\lambda) := \mathrm{Tr}\, M_\lambda(1)$, we find that $\mathrm{e}^{i\xi} \in \mathrm{Sp}\, M_\lambda(1)$ if and only if:

$$\Delta(\lambda) = 2\cos\xi. \tag{A.3}$$

It can be shown that solutions to (A.1) depend analytically on λ, and that moreover, Δ extends to an entire function of order $1/2$. The real solutions to equations $\Delta(\lambda) = \pm 2$ form infinite increasing sequences $(a_i^\pm)$ that tend to infinity.
The following facts (the reader may find helpful to consult [47, Figure 1, p. 145] or [53, Section XIII.16]) are illustrated in Fig. 1:

- The sequences $(a_i^\pm)$ are intertwined. More precisely, one has:

$$a_1^+ < a_1^- \le a_2^- < a_2^+ \le a_3^+ < a_3^- \cdots, \tag{A.4}$$

- Let be $I_{2i-1} = (a_{2i-1}^+, a_{2i-1}^-)$ and $I_{2i} = (a_{2i}^-, a_{2i}^+)$. Then I_i has non-empty interior and $\Delta\big|_{I_i}$ is strictly decreasing for i odd and strictly increasing for i even.
- If $a_i^\sigma = a_{i+1}^\sigma$ for some $i \in \mathbb{N}$, $\sigma \in \{+,-\}$ then $\Delta'(a_i^\sigma) = 0$.

These properties have important implications on the behavior of Bloch energies. For every $n \in \mathbb{N}$ the following hold.

Fact 1 The nth Bloch energy is the solution to $\Delta\big|_{I_n}(\varrho_n(\xi)) = 2\cos\xi$.

Fact 2 ϱ_n is $2\pi\mathbb{Z}$-periodic (we knew this already), and moreover

$$\varrho_n(\xi) = \varrho_n(2\pi - \xi), \quad \forall \xi \in \mathbb{R}.$$

Fact 3 $\varrho_n\big|_{[0,\pi]}$ is strictly increasing if n is odd (resp. strictly decreasing if n is even) and analytic in the interior of the interval. If it is differentiable at $\xi = 0, \pi$ then necessarily $\varrho_n'(\xi) = 0$ and ϱ_n is analytic around that point.

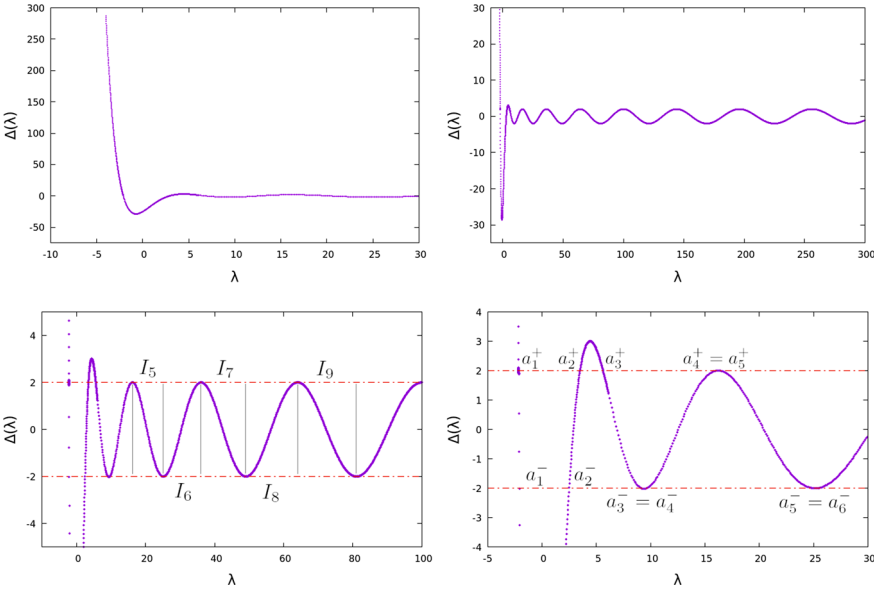

Fig. 1. Hill's discriminant for $V_{\text{per}}(y) = 5\cos(2y)$ numerically calculated. All graphics show the same set of data plotted with different ranges. In the first two it is possible to observe both divergence of $\Delta(\lambda)$ in the region $\lambda \approx \inf_y V_{\text{per}}(y)$ and non-decaying oscillations of period $\sim \sqrt{\lambda}$ for $\lambda \longrightarrow \infty$. The third one illustrates how the intervals I_i, wherein solutions to (A.1) are stable, are never empty, and why their borders $a_i^{\pm}$ must satisfy (A.4). Roots a_i^+ admit π-periodic solutions, and a_i^- 2π-periodic solutions; in each case, there are two linearly independent such solutions if and only if $a_i^{\pm}$ coincides with $a_{i+1}^{\pm}$ or $a_{i-1}^{\pm}$. If this is not the case, as for roots $a_1^{\pm}, a_2^{\pm}$ and a_3^+ seen in the last image, then the equation also admits a unstable solution. A complete study of $\Delta(\lambda)$ in one dimension is found in [46]

Fact 4 A crossing can happen only at two consecutive Bloch energies. Let $n \in \mathbb{N}$ be such that

$$\Sigma_n := \{\xi \in \mathbb{R} : \varrho_n(\xi) = \varrho_{n+1}(\xi)\} \neq \emptyset;$$

then $\Sigma_n = \pi\mathbb{Z} \setminus 2\pi\mathbb{Z}$ if n is odd, $\Sigma_n = 2\pi\mathbb{Z}$ if n is even. Moreover

$$\Delta'(\varrho_n(\xi)) = 0, \quad \forall \xi \in \Sigma_n. \tag{A.5}$$

In addition, critical points of Bloch energies in the one dimensional case are never degenerate nor can occur at a crossing point.

Lemma A.1. *The set of critical points of any Bloch energy ϱ_n is contained in $\pi\mathbb{Z}$ and all the critical points are non-degenerate. Moreover, the crossing set Σ_n associated with two consecutive Bloch energies ϱ_n and ϱ_{n+1} does not contain any critical points of the Bloch energies ϱ_n and ϱ_{n+1}.*

Proof. The first assertion on the critical points is property (3) above, whereas the second follows from differentiating twice equation (A.3) and evaluating at a critical point $\xi = k\pi$, $k \in \mathbb{Z}$ to get:

$$\Delta'(\varrho_n(k\pi))\varrho_n''(k\pi) = (-1)^{k+1}2.$$

This relation also shows that $\Delta'(\lambda)$ cannot vanish at $\lambda = \varrho_n(k\pi)$. Together with (A.5) this shows that a critical point cannot be a crossing point. $\square$

Remark A.1. In the free case ($V_{\text{per}} = 0$) there is only a Bloch band of infinite multiplicity. More generally, it has been proved in [10] that the absence of spectral gap is equivalent to the periodic potential V_{per} being constant.

Appendix B. The Properties of the Bloch Energies at Crossing Points

Here we present a normal form for the expression of two Bloch energies $\varrho_n(\xi)$ and $\varrho_{n+1}(\xi)$ close to the crossing set Σ_n (defined as $\Sigma_n = \Sigma_{n,n+1}$ in (1.5)).

Lemma B.1. *Let σ_0 be a point in the crossing set Σ_n of two consecutive Bloch energies ϱ_n and ϱ_{n+1} having neighborhood U with the following properties:*

(i) *$\Sigma_n \cap U$ is a smooth manifold.*
(ii) *The multiplicities of $\varrho_n(\xi), \varrho_{n+1}(\xi)$ are constant on each connected component of $U \setminus \Sigma_n$.*
(iii) *There exists $\delta_0 > 0$ such that for all $\xi \in U$,*

$$d\left(\{\varrho_n(\xi), \varrho_{n+1}(\xi)\}, \operatorname{Sp} P(\xi) \setminus \{\varrho_j(\xi), \quad \varrho_j(\xi) = \varrho_n(\xi) \text{ or } \varrho_j(\xi) = \varrho_{n+1}(\xi)\}\right) \geq \delta_0.$$

Then, there exist $\Omega \subseteq U$, a neighborhood of σ_0 that is $2\pi\mathbb{Z}^d$-invariant, two functions $\lambda_n \in \mathcal{C}^\infty(\Omega)$, $g_n \in \mathcal{C}^\infty\left(\sqcup_{\xi\in\Omega}\left(\{\xi\} \times N_{\sigma_{\Sigma_n}(\xi)}\Sigma_n\right)\right)$, and a function $m \in L^\infty(U)$ which is constant on each connected component of U such that

$$\forall \xi \in \Omega \setminus \Sigma_n, \quad \varrho_n(\xi) = \lambda_n(\xi) - g_n(\xi, \xi - \sigma_{\Sigma_n}(\xi)),$$
$$\varrho_{n+1}(\xi) = \lambda_n(\xi) + m(\xi) g_n(\xi, \xi - \sigma_{\Sigma_n}(\xi)).$$

Moreover,

(1) *If the crossing set Σ_n is conical in U, then for all $\xi \in U$, the map $N_{\sigma(\xi)}\Sigma \ni \eta \mapsto g_n(\xi, \eta)$ is homogeneous of degree 1 and $g_n(\sigma, \eta) \neq 0$ when $(\sigma, \eta) \in N\Sigma_n$ with $\eta \neq 0$,*
(2) *If none of the points of Σ_n are conical crossings in U, then there exists $\theta_n \in \mathcal{C}^\infty(\mathbb{R}^d)$ such that $g_n(\xi, \eta) = |\eta|^2\theta_n(\xi)$, which implies that $\varrho_n, \varrho_{n+1} \in \mathcal{C}^{1,1}(\mathbb{R}^d)$,*
(3) *If the multiplicities of ϱ_n, ϱ_{n+1} are equal on $U \setminus \Sigma_n$ then $m = 1$.*

Remark B.2. Note that in case (2), the function θ_n can be zero on Σ_n.

Proof. We denote by $j_-(\xi), j_+(\xi)$ the functions valued in $\mathbb{N}$ and constant on connected component of $U \setminus \Sigma_n$ such that for all $\xi \in U \setminus \Sigma_n$ $\varrho_{n-j+1}(\xi) = \varrho_n(\xi)$ for $1 \leq j \leq j_-(\xi)$ and $\varrho_{n+j}(\xi) = \varrho_{n+1}(\xi)$ for $1 \leq j \leq j_+(\xi)$. We denote by $\Pi(\xi)$ the projector on

$$F_\xi = \operatorname{Ker}(P(\xi) - \varrho_n(\xi)) \oplus \operatorname{Ker}(P(\xi) - \varrho_{n+1}(\xi)).$$

By the assumptions on U, the pair $\{\varrho_n(\xi), \varrho_{n+1}(\xi)\}$ is isolated from the remainder of the spectrum of $P(\xi)$ when $\xi \in U$, this implies that the map $U \ni \xi \mapsto \Pi(\xi) \in \mathcal{L}(L^2(\mathbb{T}^d))$ is analytic and the function $\dim F_\xi$ is constant for $\xi \in U$. We denote by ℓ_0 this constant and we have $\ell_0 = j_-(\xi) + j_+(\xi)$ for all $\xi \in U \setminus \Sigma_n$. Moreover, $\varrho_n(\xi)$ and $\varrho_{n+1}(\xi)$ are the two only eigenvalues of the operator $\Pi(\xi)P(\xi)\Pi(\xi)$ which maps F_ξ onto F_ξ for any $\xi \in \mathbb{R}^d$. Let us first show that it is possible to find $\Omega \subseteq U$, with $\sigma_0 \in \Omega$ and construct, for every $\xi \in \Omega$, an orthonormal basis $(\phi_j(\xi, \cdot))_{1\leq j\leq \ell_0}$ of F_ξ such that the maps $\xi \mapsto \phi_j(\xi, \cdot)$ are analytic for all $j \in \{1, \cdots \ell_0\}$. To see this, consider $(\varphi_i(\sigma_0, \cdot))_{1\leq i\leq \ell_0}$, a basis of F_{σ_0}. Chose a neighborhood Ω of σ_0 small enough to ensure that the vectors

$$\Pi(\xi)\varphi_j(\sigma_0, \cdot), \quad j \in \{1, \ldots, \ell_0\}$$

form a rank ℓ_0 family. Then apply the standard Schmidt orthonormalization process to this family.
Let $A(\xi)$, $\xi \in \Omega$, be the matrix of the operator $\Pi(\xi)P(\xi)\Pi(\xi)$ in the basis we just constructed. This is a $\ell_0 \times \ell_0$ analytic matrix that we can write

$$A(\xi) = \lambda_n(\xi)\mathrm{Id} + A_0(\xi)$$

with $\lambda_n(\xi) := \frac{1}{\ell_0}\mathrm{Tr}_{\mathbb{C}^{\ell_0}} A(\xi)$ and $A_0(\xi)$ analytic and trace-free. Moreover, $A(\xi)$ is diagonalizable and has only two eigenvalues $\varrho_n(\xi)$ and $\varrho_{n+1}(\xi)$ that we write

$$\varrho_n(\xi) = \lambda_n(\xi) - g(\xi), \quad \varrho_{n+1}(\xi) = \lambda_n(\xi) + m(\xi)g(\xi),$$

with $g(\xi) > 0$ and where, for $\xi \in \Omega \setminus \Sigma_n$, $m(\xi)$ is the ratio between the multiplicities of $\varrho_n(\xi)$ and $\varrho_{n+1}(\xi)$,

$$m(\xi) = \frac{j_-(\xi)}{j_+(\xi)}$$

and m is constant in the connected componnent of $U \setminus \Sigma_n$.
The functions $-g(\xi)$ and $m(\xi)g(\xi)$ are the two eigenvalues of $A_0(\xi)$. Therefore, they are homogeneous function of degree 1 of the coefficients of $A_0(\xi) = (a_{i,j}(\xi))_{1\leq i,j\leq \ell_0}$: we write $g(\xi) = G(A_0(\xi))$ where G is a homogeneous function on $\mathbb{R}^{\frac{\ell_0^2-1}{2}}$. Here, we have considered that a $\ell_0 \times \ell_0$ trace-free Hermitian matrix is a function of $\ell_0 - 1$ real-valued diagonal coefficients and of $\frac{\ell_0(\ell_0-1)}{2}$ complex-valued coefficients (those under the diagonal being the conjugate of those above the diagonal), and we have observed that $(\ell_0 - 1) + \frac{\ell_0(\ell_0-1)}{2} = \frac{\ell_0^2-1}{2}$.
By the definition of the crossing set, $A_0(\xi) = 0$ if and only if $\xi \in \Sigma_n$. Since the map $\xi \mapsto A_0(\xi)$ is analytic, it vanishes on Σ_n at finite order $q \in \mathbb{N}$ and the crossing set is conical if and only if $q = 1$ for all points of Σ_n. Therefore, in case (1), there exists a smooth tensor $T^{\ell_0,1}(\xi)$ such that

$$A_0(\xi) = T^{\ell_0,1}(\xi)[\xi - \sigma_{\Sigma_n}(\xi)],$$

with

$$\forall \sigma \in \Sigma_n \cap \Omega, \quad \forall \eta \in N_\sigma \Sigma_n \setminus \{0\}, \quad T^{\ell_0,1}(\sigma)\eta \neq 0_{\mathbb{C}^{\ell_0\times\ell_0}}.$$

We deduce that

$$g(\xi) = g_n(\xi, \xi - \sigma_{\Sigma_n}(\xi)), \quad \text{with} \quad g_n(\xi,\eta) := G\left(T^{\ell_0,1}(\xi)\,[\eta]^q\right)$$

where g_n is homogeneous of degree 1 in the variable η. Besides, if none of the crossing points are conical, we write $A_0(\xi) = T^{\ell_0,2}(\xi)[\xi - \sigma_{\Sigma_n}(\xi)]^2$ with $T^{\ell_0,2}(\xi)$ a smooth tensor, which allows to prove Point (2) with

$$\theta_n(\xi) = |\xi - \sigma_{\Sigma_n}(\xi)|^{-2} G(T^{\ell_0,2}(\xi)[\xi - \sigma_{\Sigma_n}(\xi)]^2).$$

That concludes the proof since Point (3) is obvious. □

Appendix C. Semi-classical Pseudo-differential Calculus

We recall here results about matrix-valued semi-classical pseudo-differential operators. We denote by $S_{N\times N}$ the set of functions $a = (a_{i,j}) \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^{N\times N})$ which are bounded together with their derivatives in matrix-norm. Then, for $a \in S_{N\times N}$, one defines the Weyl semi-classical pseudo-differential operator of symbol a as

$$\mathrm{op}_\varepsilon(a)f(x) = \int_{\mathbb{R}^{2d}} \mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)} a\left(\frac{x+y}{2}, \xi\right) f(y)\mathrm{d}y \, \frac{d\xi}{(2\pi\varepsilon)^d}, \quad \forall f \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^N).$$

Properties of these matrix-valued pseudo-differential operators follow from the well-understood scalar theory, once the definition of the product of matrices and its non-commutativity is taken into account. Unless stated otherwise, the reader may found proofs of the scalar versions of the results presented here in [18,25,57], for instance.
The Calderón-Vaillancourt theorem [11,12] extends to the matrix-valued case and ensures the existence of a constant $C_d > 0$ such that for every $a \in S_{N\times N}$ one has

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} \leq C_d \, N_d^\varepsilon(a), \tag{C.1}$$

where

$$N_d^\varepsilon(a) := \sum_{\alpha\in\mathbb{N}^{2d}, |\alpha|\leq d+2} \varepsilon^{|\alpha|/2} \sup_{\mathbb{R}^d\times\mathbb{R}^d} |\partial_{x,\xi}^\alpha a|_{\mathbb{C}^{N\times N}}.$$

This estimate shows that semi-classical pseudo-differential operators are uniformly bounded in $L^2(\mathbb{R}^d, \mathbb{C}^N)$ for $\varepsilon \in (0, 1]$. Moreover, for every $a \in S_{N\times N}$,

$$\mathrm{op}_\varepsilon(a)^* = \mathrm{op}_\varepsilon(a^*). \tag{C.2}$$

In particular, semi-classical pseudo-differential operators whose symbols take values in the space of Hermitian matrices are self-adjoint on $L^2(\mathbb{R}^d, \mathbb{C}^N)$.
In addition, the symbolic calculus for matrix-valued pseudodifferential operators goes as follows:

Proposition C.1. *Let $a, b \in S_{N\times N}$, then*

$$\mathrm{op}_\varepsilon(a)\mathrm{op}_\varepsilon(b) = \mathrm{op}_\varepsilon(ab) + \frac{\varepsilon}{2i}\mathrm{op}_\varepsilon(\{a, b\}) + \varepsilon^2 R_\varepsilon^{(1)},$$

with $\{a, b\} = \sum_{j=1}^d \partial_{\xi_j} a \, \partial_{x_j} b - \partial_{x_j} a \, \partial_{\xi_j} b$ and

$$\big[\mathrm{op}_\varepsilon(a), \mathrm{op}_\varepsilon(b)\big] = \mathrm{op}_\varepsilon([a, b]) + \frac{\varepsilon}{2i}(\mathrm{op}_\varepsilon(\{a, b\}) - \mathrm{op}_\varepsilon(\{b, a\})) + \varepsilon^2 R_\varepsilon^{(2)},$$

$$\|R_\varepsilon^{(j)}\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} \leq C \sup_{|\alpha|+|\beta|=2} N_d^\varepsilon(\partial_\xi^\alpha \partial_x^\beta a) N_d^\varepsilon(\partial_\xi^\beta \partial_x^\alpha b), \quad j \in \{1, 2\},$$

for some constant $C > 0$ independent of a, b and ε.

Remark C.2. The term of order ε^2 above has a particularly simple expression when $b \in S_{N\times N}$ does not depend on x. The following hold in $\mathcal{L}(L^2(\mathbb{R}^d, \mathbb{C}^N))$:

$$\mathrm{op}_\varepsilon(b)\mathrm{op}_\varepsilon(a) = \mathrm{op}_\varepsilon(ba) + \frac{\varepsilon}{2i}\sum_{j=1}^d \mathrm{op}_\varepsilon(\partial_{\xi_j} b \, \partial_{x_j} a)$$
$$+\frac{\varepsilon^2}{8}\sum_{1\leq \ell, p\leq d} \mathrm{op}_\varepsilon(\partial^2_{\xi_\ell \xi_p} b \, \partial^2_{x_\ell x_p} a) + O(\varepsilon^3),$$

$$\mathrm{op}_\varepsilon(a)\mathrm{op}_\varepsilon(b) = \mathrm{op}_\varepsilon(ab) - \frac{\varepsilon}{2i}\sum_{j=1}^{d}\mathrm{op}_\varepsilon(\partial_{x_j} a\, \partial_{\xi_j} b)$$
$$+\frac{\varepsilon^2}{8}\sum_{1\le \ell, p\le d}\mathrm{op}_\varepsilon(\partial^2_{x_\ell x_p} a\, \partial^2_{\xi_\ell \xi_p} b) + O(\varepsilon^3).$$

There are also analogues of Gårding's inequality for elliptic differential operators [33] in this context. If $a \in S_{N\times N}$ takes values in the set of non-negative Hermitian matrices then there exist $C_a > 0$, which depends on a finite number of derivatives of a such that

$$\mathrm{op}_\varepsilon(a) + C_a\varepsilon\,\mathrm{Id} \ge 0. \tag{C.3}$$

This follows by considering $a * \rho_\varepsilon$, with $\rho_\varepsilon(x,\xi) := (\pi\varepsilon)^{-d} e^{-\frac{|x|^2+|\xi|^2}{\varepsilon}}$. A direct computation shows that $\mathrm{op}_\varepsilon(a*\rho_\varepsilon)$ is a non-negative operator (see for instance [35]). One concludes by noticing that, due to (C.1),

$$\mathrm{op}_\varepsilon(a) - \mathrm{op}_\varepsilon(a*\rho_\varepsilon) = O(\varepsilon), \tag{C.4}$$

in $\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))$. The operator $\mathrm{op}_\varepsilon(a*\rho_\varepsilon)$ is called the anti-Wick quantization of the symbol $a \in S_{N\times N}$, besides the fact that non-negative symbols correspond to non-negative operators, the operator norm satisfies a simpler bound than that satisfied by their Weyl counterparts, namely:

$$\|\mathrm{op}_\varepsilon(a*\rho_\varepsilon)\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} \le \|a\|_{L^\infty(\mathbb{R}^{2d},\mathbb{C}^{N\times N})}. \tag{C.5}$$

Through the article, it is necessary to understand the boundedness and symbolic calculus properties of operators with symbols of limited regularity. Denote by $\mathcal{A}$ the completion of $\mathcal{C}_0^\infty(\mathbb{R}^{2d},\mathbb{C}^{N\times N})$ with respect to the norm:

$$\|a\|_{\mathcal{A}} := \sup_{\xi\in\mathbb{R}^d}\sup_{|\alpha|\le d+2}\int_{\mathbb{R}^d}|\partial_x^\alpha a(x,\xi)|_{\mathbb{C}^{N\times N}}\,\mathrm{d}x. \tag{C.6}$$

Remark C.3. By a mollification argument, one can show that $\mathcal{A}$ contains all the functions $a \in \mathcal{C}_0(\mathbb{R}^d_x \times \mathbb{R}^d_\xi, \mathbb{C}^{N\times N})$ that are $d+2$ times continuously differentiable with respect to the first variable.

This regularity assumption is sufficient for our purposes (see [34, Lemma 3.7] and [28, Section 3] for related results).

Lemma C.4. *The space $\mathcal{A}$ enjoys the following properties:*

(1) *There exists a universal constant $C_d > 0$ only depending on d such that, for every $a \in \mathcal{A}$,*

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} \le C_d\|a\|_{\mathcal{A}}.$$

(2) *Suppose $\varrho \in Lip(\mathbb{R}^d_\xi, \mathbb{C}^{N\times N})$ and $a \in \mathcal{A}$. The following hold in $\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))$:*

$$\mathrm{op}_\varepsilon(a\,\varrho) = \mathrm{op}_\varepsilon(a)\varrho(\varepsilon D_x) + O(\varepsilon),$$
$$\mathrm{op}_\varepsilon(\varrho\, a) = \varrho(\varepsilon D_x)\mathrm{op}_\varepsilon(a) + O(\varepsilon).$$

(3) *Suppose $\varrho \in \mathcal{C}^{1,1}(\mathbb{R}^d_\xi,\mathbb{R})$ (that is $\nabla\varrho \in Lip(\mathbb{R}^d,\mathbb{R}^d)$) and $a \in \mathcal{A}$. The following hold in $\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))$:*

$$\frac{i}{\varepsilon}[\mathrm{op}_\varepsilon(a), \varrho(\varepsilon D_x)\mathrm{Id}] = \mathrm{op}_\varepsilon(\nabla_x a\cdot\nabla\varrho(\xi)) + O(\varepsilon).$$

Proof. Suppose that $A \in \mathcal{L}(L^2(\mathbb{R}^d, \mathbb{C}^N))$ is of the form

$$Af(x) = \frac{1}{\varepsilon^d} \int_{\mathbb{R}^d} k\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right) f(y)\mathrm{d}y, \quad \forall f \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^N); \tag{C.7}$$

then one deduces, after change of variables and using Hölder's inequality, that

$$|(A\,f, g)_{L^2(\mathbb{R}^d,\mathbb{C}^N)}| \leq \|f\|_{L^2(\mathbb{R}^d,\mathbb{C}^N)} \|g\|_{L^2(\mathbb{R}^d,\mathbb{C}^N)} \int_{\mathbb{R}^d} \sup_{x\in\mathbb{R}^d} |k(x,v)|_{\mathbb{C}^{N\times N}} \mathrm{d}v.$$
$$\forall f, g \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^N). \tag{C.8}$$

In order to prove item (1), notice that the following identity holds,

$$\mathrm{op}_\varepsilon(a) = (\mathcal{F}^\varepsilon)^* \mathrm{op}_\varepsilon(\underline{a})\mathcal{F}^\varepsilon, \quad \underline{a}(x,\xi) := a(-\xi, x), \tag{C.9}$$

where $\mathcal{F}^\varepsilon$ stands for the semi-classical Fourier transform:

$$\mathcal{F}^\varepsilon(f)(\xi) = \int_{\mathbb{R}^d} \mathrm{e}^{-i\frac{\xi}{\varepsilon}\cdot x} f(x) \frac{dx}{(2\pi\varepsilon)^{d/2}}.$$

The operator $\mathrm{op}_\varepsilon(\underline{a})$ is of the form (C.7) with $k = (2\pi)^{-d}\widehat{a}$, where $\widehat{a}$ denotes the Fourier transform of a with respect to the first variable. Using (C.8), (C.9) and Plancherel's formula we conclude

$$\begin{aligned}
&|(\mathrm{op}_\varepsilon(a) f, g)_{L^2(\mathbb{R}^d,\mathbb{C}^N)}| \\
&\quad \leq \|f\|_{L^2(\mathbb{R}^d,\mathbb{C}^N)} \|g\|_{L^2(\mathbb{R}^d,\mathbb{C}^N)} \int_{\mathbb{R}^d} \sup_{\xi\in\mathbb{R}^d} |\widehat{a}(v,\xi)|_{\mathbb{C}^{N\times N}} \frac{dv}{(2\pi)^d} \\
&\forall f, g \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^N).
\end{aligned}$$

The constant $C_d > 0$ is then chosen such that:

$$\int_{\mathbb{R}^d} \sup_{\xi\in\mathbb{R}^d} |\widehat{a}(v,\xi)|_{\mathbb{C}^{N\times N}} \frac{dv}{(2\pi)^d} \leq C_d \|a\|_{\mathcal{A}}.$$

This concludes the proof of the first assertion.
In order to prove the second assertion, we show that

$$R^\varepsilon := (\mathcal{F}^\varepsilon)^* (\mathrm{op}_\varepsilon(a\,\varrho) - \mathrm{op}_\varepsilon(a)\varrho(\varepsilon D_x))\mathcal{F}^\varepsilon,$$

satisfies $\|R^\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} = O(\varepsilon)$; the proof of the other identity is analogous. From (C.9), we deduce that

$$R^\epsilon f(x) = \int_{\mathbb{R}^d} r^\varepsilon\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right) f(y) \frac{dy}{(2\pi\varepsilon)^d}, \quad \forall f \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^N),$$

where $r^\varepsilon(x,v) := \widehat{a}(v,x)(\varrho(x) - \varrho(x-\varepsilon v))$. By (C.8) we can estimate:

$$\|R^\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} \leq \int_{\mathbb{R}^d} \sup_{x\in\mathbb{R}^d} |r^\varepsilon(x,v)|_{\mathbb{C}^{N\times N}} \frac{dv}{(2\pi)^d}.$$

By hypothesis, we can find $L_\varrho > 0$ such that

$$|\varrho(x) - \varrho(x-\varepsilon v)|_{\mathbb{C}^{N\times N}} \leq L_\varrho \varepsilon |v|, \quad \forall (v,x) \in \operatorname{supp}\widehat{a}.$$

Therefore, using

$$|v||\widehat{a}(v,x)| \leq (1+|v|^2)|\widehat{a}(x,v)| = |\widehat{a}(x,v)| + |(\widehat{-\Delta a})(x,v)|,$$

we deduce

$$\|R^\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} \leq \varepsilon\, C_d L_\varrho(\|a\|_{\mathcal{A}} + \|\Delta a\|_{\mathcal{A}}).$$

For the third assertion, we show that

$$\tilde{R}^\varepsilon := (\mathcal{F}^\varepsilon)^*(\frac{1}{\varepsilon}[\mathrm{op}_\varepsilon(a), \varrho(\varepsilon D)] - \mathrm{op}_\varepsilon(\nabla_x \cdot \nabla\varrho))\mathcal{F}^\varepsilon,$$

satisfies $\|\tilde{R}^\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} = O(\varepsilon)$. Indeed, the kernel of $\tilde{R}^\varepsilon$ is of the form (C.7) with

$$\begin{aligned}\tilde{r}^\varepsilon(x,v) &= \frac{i}{\varepsilon}\widehat{a}(v,x)\,(\varrho(x) - \varrho(x-\varepsilon v)) - \widehat{\nabla_x a}(v,x)\cdot\nabla\varrho(x)\\ &= i\widehat{a}(v,x)v\cdot\nabla\varrho(x) - \widehat{\nabla_x a}(v,x)\cdot\nabla\varrho(x) + \varepsilon\theta(x,v)\widehat{a}(x,v)\end{aligned}$$

and there exists $L_{\nabla\varrho} > 0$ such that

$$|\theta(x,v)| \leq L_{\nabla\varrho}|v|^2.$$

Using $iv\widehat{a}(v,x) = \widehat{\nabla_x a}(x,v)$ and $|v|^2|\widehat{a}(x,v)| = |(\widehat{-\Delta a})(x,v)|$, we deduce

$$\|\tilde{R}^\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathbb{C}^N))} \leq \varepsilon C_d L_{\nabla\varrho}\|\Delta a\|_{\mathcal{A}}.$$

□

Appendix D. Two-Scale Pseudodifferential Operators

We prove here technical lemma concerning the pseudodifferential operators considered in Section 4.1, the formalism of which we follow. Due to the properties of Bloch energies, we are going to consider more general classes of symbols than those of $\mathcal{A}^{(2)}$ (as defined in Section 4.1). For $k \in \mathbb{Z}$, we introduce the class $\mathcal{A}_k^{(2)}$ of smooths functions on $\mathbb{R}^{3d}$ that are compactly supported in the variables (x,ξ) uniformly with respect to η and coincide with an homogeneous function of degree k in η as soon as $|\eta| > R_0$ for some $R_0 > 0$. With these notations, $\mathcal{A}^{(2)} = \mathcal{A}_0^{(2)}$.

Of particular interest for us are functions $g(\xi,\eta)$, independent of the variable x, that are smooth in ξ, and satisfy a symbol estimate of order k in η. We denote by $\mathcal{H}_k$ the set of these functions. For X a connected, closed embedded submanifold of $(\mathbb{R}^d)^*$ and $g \in \mathcal{H}_k$, the operator

$$g_\varepsilon(\varepsilon D) = g(\varepsilon D, D - \varepsilon^{-1}\sigma_X(\varepsilon D)) \tag{D.1}$$

is then well defined as an operator mapping $H^s(\mathbb{R}^d)$ into $H^{s-k}(\mathbb{R}^d)$ uniformly in ε when $s \in \mathbb{R}$. We are interested in the pseudodifferential calculus involving two-scale pseudodifferential operator of the form $\mathrm{op}_\varepsilon(a)$ for a in $\mathcal{A}_k^{(2)}$ for some $k \in \mathbb{Z}$ and Fourier multipliers $g_\varepsilon(\varepsilon D)$ with $g \in \mathcal{H}_p$ for some $p \in \mathbb{Z}$.

The first type of pseudodifferential calculus results that we shall use concerns the large values of η. We consider $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ such that $\chi = 1$ on $B(0,1)$ and $\chi = 0$ on $B(0,2)^c$ with $0 \leq \chi \leq 1$. We set for $R, \delta > 0$

$$a^{R,\delta}(x,\xi,\eta) = a(x,\xi,\eta)((1-\chi(\eta/R))\chi((\xi - \sigma_\Sigma(\xi))/\delta).$$

On the support of $a^{R,\delta}$, $\varepsilon R \leq |\xi - \sigma_\Sigma(\xi)| \leq 2\delta$. Note that if $k > 0$ and $a \in \mathcal{A}_{-k}^{(2)}$, the estimate (C.6) yields that in $\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\mathrm{op}_\varepsilon(a_\varepsilon^{R,\delta}) = O((\varepsilon R)^{-k}).$$

Lemma D.1. *Let $k \in \mathbb{N}$, $a \in \mathcal{A}^{(2)}_{-k}$, $g = g(\xi, \eta)$ in $\mathcal{H}_{k+1}$ and δ, $R > 0$. Then, in $\mathcal{L}(L^2(\mathbb{R}^d))$,*

$$\left[\mathrm{op}_\varepsilon(a^{R,\delta}_\varepsilon), g_\varepsilon(\varepsilon D)\right] = i\,\mathrm{op}_\varepsilon\left((\nabla_x a^{R,\delta} \cdot \nabla_\eta g)_\varepsilon\right) + O(\varepsilon) + O(\delta) + O(1/R).$$

Proof. We want to take advantage from the fact that we have $|\xi - \sigma_\Sigma(\xi)| > R\varepsilon$ on the support of $a^{R,\delta}_\varepsilon$ to avoid the singularity of the function g. Indeed, $a^{R,\delta}_\varepsilon$ is supported outside the singularity of the function g. Let $\kappa \in \mathcal{C}^\infty(\mathbb{R}^d)$ supported outside 0 and such that $(1-\chi)\kappa = (1-\chi)$ and denote by κ^R the function defined by $\kappa^R(\eta) = \kappa(\eta/R)$ so that

$$\kappa^R_\varepsilon(\xi) = \kappa\left(\frac{\xi - \sigma_X(\xi)}{R\varepsilon}\right).$$

Standard symbolic calculus gives that for all $N \in \mathbb{N}$, we have

$$\begin{aligned}\mathrm{op}_\varepsilon(a^{R,\delta}_\varepsilon) &= \mathrm{op}_\varepsilon(a^{R,\delta}_\varepsilon)\kappa^R_\varepsilon(\varepsilon D) + R^{-N}\mathrm{op}_\varepsilon(r^{1,N}_\varepsilon(x,\xi))\\ &= \kappa^R_\varepsilon(\varepsilon D)\mathrm{op}_\varepsilon(a^{R,\delta}_\varepsilon) + R^{-N}\mathrm{op}_\varepsilon(r^{2,N}_\varepsilon(x,\xi))\end{aligned}$$

where the symbols $r^{j,N}_\varepsilon$ have symbol norms that are uniformly bounded and are supported in the set $\{c_0\varepsilon R < \xi - \sigma_X(\xi) < C_0\varepsilon R\}$ for some $0 < c_0 < C_0$. In particular, by Proposition C.1 and because $g \in \mathcal{H}_{k+1}$, $a \in \mathcal{A}^{(2)}_{-k}$,

$$\mathrm{op}_\varepsilon(r^{1,N}_\varepsilon)g_\varepsilon(\varepsilon D) = \mathrm{op}_\varepsilon(r^{1,N}_\varepsilon g_\varepsilon) + O(R^{k+1-k}) = \mathrm{op}_\varepsilon(r^{1,N}_\varepsilon g_\varepsilon) + O(R),$$

whence

$$\mathrm{op}_\varepsilon(r^{1,N}_\varepsilon)g_\varepsilon(\varepsilon D) = O(R).$$

Similarly, we have

$$g_\varepsilon(\varepsilon D)\mathrm{op}_\varepsilon(r^{2,N}_\varepsilon) = O(R).$$

We deduce that

$$\left[\mathrm{op}_\varepsilon(a^{R,\delta}_\varepsilon), g_\varepsilon(\varepsilon D)\right] = \left[\mathrm{op}_\varepsilon(a^{R,\delta}_\varepsilon), (\kappa^R g)_\varepsilon(\varepsilon D)\right] + O(R^{-N+1}).$$

The function $\xi \mapsto \kappa^R g$ is now smooth, which allows to use standard results of symbolic calculus, what we shall do in local coordinates.
We consider a system of local coordinates $\varphi(\xi) = 0$ of X and the $d \times p$ smooth matrix $B(\xi)$ such that

$$\xi - \sigma_X(\xi) = B(\xi)\varphi(\xi)$$

where $\varphi(\xi) \in \mathbb{C}^{p\times 1}$ is a column. We associate with φ the diffeomorphism

$$\Phi : ({}^t\varphi(\xi), \xi'') \mapsto \xi$$

and, according to Lemma 4.3 in [15], there exists an isometry $\mathcal{U}_\varepsilon$ of $L^2(\mathbb{R}^d)$ such that for all $b \in \mathcal{A}^{(2)}$ and $f \in L^2(\mathbb{R}^d)$

$$(\mathrm{op}_\varepsilon(b_\varepsilon)f, f) = \left(\mathrm{op}_\varepsilon\left(b\left({}^t d\Phi(\xi)^{-1}x, \Phi(\xi), B(\Phi(\xi))\frac{\xi'}{\varepsilon}\right)\right)\mathcal{U}_\varepsilon f, \mathcal{U}_\varepsilon f\right) + O(\varepsilon).$$

Note that if $\xi, \zeta, x \in \mathbb{R}^d$,

$$d\Phi(\xi)^{-1}\zeta = (d\varphi(\Phi(\xi))\zeta, \zeta''), \quad {}^t d\Phi(\xi)^{-1}x = {}^t d\varphi(\Phi(\xi))x' + (0, x''),$$

where $d\varphi(\xi)$ is the $p \times d$ matrix with lines the gradient of each of the component of φ. Therefore, focusing on the commutator

$$L^\varepsilon = \left[\mathrm{op}_\varepsilon \left(a^{R,\delta} \left({}^t d\Phi(\xi)^{-1} x, \Phi(\xi), B(\Phi(\xi)) \frac{\xi'}{\varepsilon} \right) \right), (\kappa^R g)\,(\Phi(\varepsilon D), B(\Phi(\varepsilon D)) D_{x'}) \right],$$

we obtain, in $\mathcal{L}(L^2(\mathbb{R}^d))$, that

$$L^\varepsilon = \mathrm{op}_\varepsilon \left(d\varphi(\Phi(\xi)) \nabla_x a^{R,\delta} \left({}^t d\Phi(\xi)^{-1} x, \Phi(\xi), B(\Phi(\xi)) \frac{\xi'}{\varepsilon} \right) \cdot {}^t B(\Phi(\xi)) \nabla_\eta (\kappa^R g) \right.$$
$$\left. \left(\Phi(\xi), B(\Phi(\xi)) \frac{\xi'}{\varepsilon} \right) \right) + O(R^{-1}) + O(\varepsilon).$$

We observe that if $\sigma \in X$, $B(\sigma) d\varphi(\sigma) = \mathrm{Id} - d\sigma_X(\sigma)$ and $d\sigma_X(\sigma) \nabla_\eta g(\sigma, \eta) = 0$ because $\nabla_\eta g(\sigma, \eta) \in N_\sigma X$ and $d\sigma_X(\sigma)\zeta = 0$ if $\zeta \in N_\sigma X$. We deduce

$$[\mathrm{op}_\varepsilon(a_\varepsilon^{R,\delta}), g_\varepsilon(\varepsilon D)] = i\,\mathrm{op}_\varepsilon(b_\varepsilon) + O(\varepsilon) + O(R^{-1}) + O(\delta),$$

with

$$b(x, \xi, \eta) = \kappa^R(\eta) \nabla_x a^R(x, \xi, \eta) \cdot \nabla_\eta g\,(\xi, \eta) \in \mathcal{A}_0^{(2)}.$$

Using $\kappa(1 - \chi) = 1 - \chi$, we obtain

$$b(x, \xi, \eta) = \nabla_x a^R(x, \xi, \eta) \cdot \nabla_\eta g\,(\xi, \eta)\,.$$

□

We shall also need properties of two-scale symbolic calculus at finite distance, i.e. for symbols that are compactly supported in all the variables, including the variable η. Here again, the use of local coordinates and Lemma 4.3 in [15] are a crucial argument.

Lemma D.2. *Let $a \in \mathcal{C}_0^\infty(\mathbb{R}^{3d})$ and $g \in \mathcal{H}_k$ for $k \in \mathbb{N}$. Let $(f^\varepsilon)_{\varepsilon>0}$ a bounded family in $L^2(\mathbb{R}^d)$ and $M dv$ the two-scale Wigner measure at finite distance associated with its concentration on X. Then, there exists a constant $C > 0$ such that for all $\varepsilon > 0$,*

$$\left(\mathrm{op}_\varepsilon(a) g_\varepsilon(\varepsilon D) f^\varepsilon, f^\varepsilon\right) \leq C \| f^\varepsilon \|_{L^2(\mathbb{R}^d)}.$$

In addition, up to the subsequence defining $M dv$,

$$\left(\mathrm{op}_\varepsilon(a) g_\varepsilon(\varepsilon D) f^\varepsilon, f^\varepsilon\right) \underset{\varepsilon \to 0}{\longrightarrow} \int_{TX^*} \mathrm{Tr}_{L^2(N_\sigma X)} (Q_a^X(v, \sigma) Q_g^X(\sigma) M(\sigma, v)) dv(\sigma, v).$$

We recall that the notations of this section have been introduced in Section 4.1. Of course, this lemma has standard generalizations to vector-valued families and to time dependent families which are bounded in $L^\infty(\mathbb{R}, L^2(\mathbb{R}^d, \mathbb{C}^N)$.

Proof. Here again, we work in local coordinates $\varphi(\xi) = 0$ of X and we consider the $d \times p$ smooth matrix $B(\xi)$ such that

$$\xi - \sigma_X(\xi) = B(\xi)\varphi(\xi)$$

where $\varphi(\xi) \in \mathbb{C}^{p \times 1}$ is a column. We associate with φ the diffeomorphism

$$\Phi : ({}^t\varphi(\xi), \xi'') \mapsto \xi$$

and, we consider the isometry $\mathcal{U}_\varepsilon$ of $L^2(\mathbb{R}^d)$ given by Lemma 4.3 in [15] such that for all $b \in \mathcal{A}^{(2)}$ and $f \in L^2(\mathbb{R}^d)$

$$(\mathrm{op}_\varepsilon(b_\varepsilon)f, f) = \left(\mathrm{op}_\varepsilon\left(b\left({}^t d\Phi(\xi)^{-1}x, \Phi(\xi), B(\Phi(\xi))\frac{\xi'}{\varepsilon}\right)\right)\mathcal{U}_\varepsilon f, \mathcal{U}_\varepsilon f\right) + O(\varepsilon).$$

We then concentrate on the operator

$$\mathrm{op}_\varepsilon\left(a\left({}^t d\Phi(\xi)^{-1}x, \Phi(\xi), B(\Phi(\xi))\frac{\xi'}{\varepsilon}\right)\right)\mathrm{op}_\varepsilon\left(g\left(\Phi(\xi), B(\Phi(\xi))\frac{\xi'}{\varepsilon}\right)\right).$$

Since a is compactly supported in all variables, we obtain, in $\mathcal{L}(L^2(\mathbb{R}^d))$, that

$$\begin{aligned}
&\mathrm{op}_\varepsilon\left(a\left({}^t d\Phi(\xi)^{-1}x, \Phi(\xi), B(\Phi(\xi))\frac{\xi'}{\varepsilon}\right)\right)\\
&\quad = \mathrm{op}_\varepsilon\left(a\left({}^t d\Phi(0,\xi'')^{-1}x, \Phi(0,\xi''), B(\Phi(0,\xi''))\frac{\xi'}{\varepsilon}\right)\right) + O(\varepsilon)\\
&\quad = \mathrm{op}_\varepsilon\left(a^W\left({}^t d\Phi(0,\xi'')^{-1}x, \Phi(0,\xi''), B(\Phi(0,\xi''))D_{x'}\right)\right) + O(\varepsilon).
\end{aligned}$$

One can then interpret this operator as an operator acting on $L^2(\mathbb{R}^d_{x''}, L^2(\mathbb{R}^d_{x'}))$ where, as explained in Section 4.1 of [15], for any $(\sigma, v) = ((0,\xi''), (0,x'')) \in TX^*$, the map

$$(z,\zeta) \mapsto a\left({}^t d\Phi(0,\xi'')^{-1}(z,x''), \Phi(0,\xi''), B(\Phi(0,\xi''))\zeta\right)$$

defines a function on $T^*(N_\sigma X)$, which implies that the operator

$$a^W\left({}^t d\Phi(0,\xi'')^{-1}x, \Phi(0,\xi''), B(\Phi(0,\xi''))D_{x'}\right)$$

acts on $L^2(N_\sigma X)$. It is the expression of the operator $Q_a(\sigma, v)$ in the local coordinates induced by the choice of equations $\varphi(\xi) = 0$ of X.
The difficulty with $g_\varepsilon(\varepsilon D)$ is that the map $(\sigma,\eta) \mapsto g(\sigma,\eta)$ is not bounded in η. Therefore, we decompose $g(\sigma,\eta)$ into two parts thanks to a function $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ such that $\chi = 1$ on $B(0,1)$ and $\chi = 0$ on $B(0,2)^c$ with $0 \le \chi \le 1$. Writing like before $\chi^R(\eta) = \chi(\eta/R)$ for $R > 0$, we set

$$g = g\chi^R + g(1-\chi^R)$$

and we first focus on $\mathrm{op}_\varepsilon(a_\varepsilon)(g(1-\chi^R))_\varepsilon(\varepsilon D)$. Since now $g(1-\chi_R)$ is smooth, we can use standard symbolic calculus, and we have

$$\mathrm{op}_\varepsilon(a_\varepsilon)(g(1-\chi^R))_\varepsilon(\varepsilon D) = \mathrm{op}_\varepsilon((ag(1-\chi^R))_\varepsilon) + O(R^{-1})$$

because $\nabla_\xi((g(1-\chi^R))_\varepsilon) = O(R^{-1})$. Moreover, as soon as R is large enough, we have $ag(1-\chi^R) = 0$. We conclude

$$g_\varepsilon(\varepsilon D) = (g\chi^R)_\varepsilon(\varepsilon D) + O(R^{-1})$$

and

$$\begin{aligned}
\mathrm{op}_\varepsilon\left(g\left(\Phi(\xi), B(\Phi(\xi))\frac{\xi'}{\varepsilon}\right)\right) &= \mathrm{op}_\varepsilon\left((g\chi^R)(\Phi(0,\xi''), B(\Phi(0,\xi''))D_{x'})\right)\\
&\quad + O_R(\varepsilon) + O(R^{-1})
\end{aligned}$$

in $\mathcal{L}(L^2(\mathbb{R}^d))$. Note that in the following we will let first ε go to 0, and then R to $+\infty$, so that $O_R(\varepsilon)$ is negligible. Besides, when R goes to $+\infty$, we are left with the operator $g(\Phi(0,\xi''), B(\Phi(0,\xi'')D_{x'})$ (with strong convergence), which is the expression in local coordinates of the operator $Q_g(\sigma)$.
At this stage of the proof, we are left with the quantity

$$\Big(\mathrm{op}_\varepsilon\left(a^W\left({}^t d\Phi(0,\xi'')^{-1}x, \Phi(0,\xi''), B(\Phi(0,\xi''))D_{x'}\right)\right)\mathrm{op}_\varepsilon(g(\Phi(0,\xi''),$$
$$B(\Phi(0,\xi''))D_{x'}))\mathcal{U}_\varepsilon f, \mathcal{U}_\varepsilon f\Big).$$

It turns out that the pair $M d\nu$ has been defined in [15] (see Proposition 4.2) as a semi-classical measure of the family $(\mathcal{U}_\varepsilon f)$, which is a bounded family in $L^2(\mathbb{R}^{d-p}_{x''}, L^2(\mathbb{R}^p_{x'}))$. Therefore, in coordinates

$$\Big(\mathrm{op}_\varepsilon\left(a^W\left({}^t d\Phi(0,\xi'')^{-1}x, \Phi(0,\xi''), B(\Phi(0,\xi''))D_{x'}\right)\right)$$
$$\mathrm{op}_\varepsilon(g(\Phi(0,\xi''), B(\Phi(0,\xi''))D_{x'}))\mathcal{U}_\varepsilon f, \mathcal{U}_\varepsilon f\Big)$$
$$\underset{\varepsilon\to 0}{\longrightarrow}\int_{\mathbb{R}^{2(d-p)}}\mathrm{Tr}_{L^2(\mathbb{R}^p)}$$
$$\Big(\mathrm{op}_\varepsilon\left(a^W\left({}^t d\Phi(0,\xi'')^{-1}x, \Phi(0,\xi''), B(\Phi(0,\xi''))D_{x'}\right)\right)M(\xi'',x'')\Big)\,\mathrm{d}\nu(\xi'',x'')$$
$$=\int_{TX^*}\mathrm{Tr}_{L^2(N_\sigma X)}(Q_a^X(v,\sigma)Q_g^X(\sigma)M(\sigma,v))\mathrm{d}\nu(\sigma,v).$$

□

Appendix E. Well-Prepared Data

We prove here properties of well-prepared initial (1.17). We shall use the Fourier coefficients of the Bloch waves $\varphi_n(y,\xi)$ for $n\in\mathbb{N}^*$. Recall that they satisfy the Bloch periodicity condition:

$$\varphi_n(y,\xi+j)=\mathrm{e}^{-ij\cdot y}\varphi_n(y,\xi),\quad \forall j\in 2\pi\mathbb{Z}^d. \tag{E.1}$$

Integrating (E.1) with respect to y on $\mathbb{T}^d$ gives an expression for the Fourier coefficients of $\varphi_n(\cdot,\xi)$: for all $y\in\mathbb{T}^d$ and $\xi\in\mathbb{R}^d$

$$\varphi_n(y,\xi)=\sum_{j\in 2\pi\mathbb{Z}^d}c_n(\xi+j)\mathrm{e}^{ij\cdot y},\quad c_n(\xi)=\int_{\mathbb{T}^d}\varphi_n(y,\xi)dy. \tag{E.2}$$

For $s>0$, there exists $C_{n,s}>0$ such that

$$\sum_{j\in 2\pi\mathbb{Z}^d}\langle j\rangle^{2s}|c_n(\xi+j)|^2\le C_{n,s}\langle\xi\rangle^{2s} \tag{E.3}$$

It turns out that these class of data are closely related to those studied in [1,2].

Lemma E.1. *Let $(\psi^\varepsilon_{0,n})_{\varepsilon>0}$ as in (1.17) with $u^\varepsilon_n=\mathrm{e}^{\frac{i}{\varepsilon}\xi_n\cdot x}v^\varepsilon_n(x)$, v^ε_n uniformly bounded in $H^s(\mathbb{R}^d)$, $s>d/2$ (or $s>1$ when $d=1$). Assume that $\xi\mapsto\varphi_n(\cdot,\xi)$ is Lipschitz. Then, we have, in $L^2(\mathbb{R}^d)$,*

$$\psi^\varepsilon_{0,n}=\mathrm{e}^{\frac{i}{\varepsilon}x\cdot\xi_n}\varphi_n\left(\frac{x}{\varepsilon},\xi_n\right)v^\varepsilon_n+O(\varepsilon).$$

Besides, if $v^\varepsilon_n\to v_n$ in L^2, then $\|\psi^\varepsilon_{0,n}\|_{L^2}=\|v_n\|_{L^2}+o(1)$ as ε goes to 0.

Proof. We set $\widetilde{\psi}^{\varepsilon}_{0,n} = \mathrm{e}^{\frac{i}{\varepsilon}x\cdot\xi_n}\varphi_n\left(\frac{x}{\varepsilon},\xi_n\right)v^{\varepsilon}_n$. We write for $x\in\mathbb{R}^d$

$$\psi^{\varepsilon}_{0,n}(x) = \sum_{j\in 2\pi\mathbb{Z}^d} \mathrm{e}^{\frac{i}{\varepsilon}j\cdot x}c_n(j+\varepsilon D_x)u^{\varepsilon}_n(x).$$

Let $\theta\in L^2(\mathbb{R}^d)$, we write $(\theta,\psi^{\varepsilon}_{0,n})_{L^2(\mathbb{R}^d)} = \sum_{j\in 2\pi\mathbb{Z}^d}\alpha^{\varepsilon}_j$ with

$$\alpha^{\varepsilon}_j = \left(\theta, \mathrm{e}^{\frac{i}{\varepsilon}j\cdot x}c_n(j+\varepsilon D_x)u^{\varepsilon}_n\right)_{L^2} = \left(\theta, \mathrm{e}^{\frac{i}{\varepsilon}(j+\xi_n)\cdot x}c_n(j+\xi_n+\varepsilon D_x)v^{\varepsilon}_n\right)_{L^2}.$$

By (E.3), there exists $C>0$ such that

$$|\alpha^{\varepsilon}_j| \le C\langle j\rangle^{-s}\|\langle\varepsilon D_x\rangle^s u^{\varepsilon}_n\|_{L^2}\|\theta\|_{L^2}.$$

Therefore, the sum enters into the frame of Lebesgue dominated convergence. The same holds for the series

$$(\theta,\widetilde{\psi}^{\varepsilon}_{0,n})_{L^2(\mathbb{R}^d)} = \sum_{j\in 2\pi\mathbb{Z}^d}\widetilde{\alpha}^{\varepsilon}_j,\quad \widetilde{\alpha}^{\varepsilon}_j = \left(\theta, \mathrm{e}^{\frac{i}{\varepsilon}(j+\xi_n)\cdot x}c_n(j+\xi_n)v^{\varepsilon}_n\right)_{L^2}.$$

Besides

$$\alpha^{\varepsilon}_j - \widetilde{\alpha}^{\varepsilon}_j = \left(\theta, \mathrm{e}^{\frac{i}{\varepsilon}(j+\xi_n)\cdot x}(c_n(j+\xi_n+\varepsilon D_x)-c_n(j+\xi_n))v^{\varepsilon}_n\right)_{L^2}.$$

The conclusion then comes from the observation that $\xi\mapsto c_n(\xi)$ is uniformly Lipschitz and thus, one has

$$\left|\alpha^{\varepsilon}_j - \widetilde{\alpha}^{\varepsilon}_j\right| \le \|\theta\|_{L^2}\|(c_n(j+\xi_n+\varepsilon D_x)-c_n(j+\xi_n))v^{\varepsilon}_n\|_{L^2} \le C\varepsilon\|\theta\|_{L^2}\|D_x v^{\varepsilon}_n\|_{L^2}$$

which gives the result by the boundedness of the family $(v^{\varepsilon}_n)_{\varepsilon>0}$ in $H^s(\mathbb{R}^d)$ with $s\ge 1$. Let us now compute the norm of $\psi^{\varepsilon}_{0,n}$. One has $\|\psi^{\varepsilon}_{0,n}\|^2_{L^2} = \sum_{j,j'\in 2\pi\mathbb{Z}^d}\beta^{\varepsilon}_{j,j'}$ with

$$\beta^{\varepsilon}_{j,j'} = \left(\mathrm{e}^{\frac{i}{\varepsilon}\cdot x(j-j')}c_n(j+\xi_n+\varepsilon D_x)v^{\varepsilon}_n(x), c_n(j'+\xi_n+\varepsilon D_x)v^{\varepsilon}_n(x)\right)_{L^2}.$$

Additionally, by (E.3), there exists $C>0$ such that

$$|\beta^{\varepsilon}_{j,j'}| \le C\langle j\rangle^{-s}\langle j'\rangle^{-s}\|\langle\varepsilon D_x\rangle^s v^{\varepsilon}_n\|^2_{L^2}.$$

Therefore, the sum enters into the frame of Lebesgue dominated convergence. If $|j-j'|\ge 1$ with $j_\ell - j'_\ell \ne 0$, $0\le\ell\le d$, an integration by parts give

$$\begin{aligned}\beta^{\varepsilon}_{j,j'} = i\varepsilon(j_\ell - j'_\ell)^{-1}\int_{\mathbb{R}^d}&\mathrm{e}^{\frac{i}{\varepsilon}\cdot x(j-j')}\\ &\partial_{x_\ell}\left(c_n(j+\xi_n+\varepsilon D_x)v^{\varepsilon}_n(x)\overline{c_n(j'+\xi_n+\varepsilon D_x)v^{\varepsilon}_n(x)}\right)\mathrm{d}x,\end{aligned}$$

whence $\beta^{\varepsilon}_{j,j'}\to 0$ as $\varepsilon\to 0$ since $(v^{\varepsilon}_n)_{\varepsilon>0}$ is uniformly bounded in $H^1(\mathbb{R}^d)$. Moreover

$$\sum_{j\in 2\pi\mathbb{Z}^d}\beta^{\varepsilon}_{j,j} = \sum_{j\in 2\pi\mathbb{Z}^d}(2\pi)^{-d}\int_{\mathbb{R}^d}|c_n(j+\xi_n+\varepsilon\xi)|^2|\widehat{v}^{\varepsilon}_n(\xi)|^2\mathrm{d}\xi.$$

Using $\sum_{j\in 2\pi\mathbb{Z}^d}|c_n(\xi)|^2 = \|\varphi_n(\cdot,\xi)\|^2_{L^2(\mathbb{T}^d)} = 1$, we deduce

$$\sum_{j\in 2\pi\mathbb{Z}^d}\beta^{\varepsilon}_{j,j} = (2\pi)^{-d}\int_{\mathbb{R}^d}|v^{\varepsilon}_n(\xi)|^2\mathrm{d}\xi = \|v^{\varepsilon}_n\|^2_{L^2}\underset{\varepsilon\to 0}{\longrightarrow}\|v_n\|^2$$

and the conclusion follows. □

Let us now examine weak limits of such families.

Lemma E.2. *Let* $(\psi^\varepsilon_{0,n})_{\varepsilon>0}$ *as in* (1.17) *with* $u^\varepsilon_n = \mathrm{e}^{\frac{i}{\varepsilon}\xi_n\cdot x} v_n(x)$, $(v^\varepsilon_n)_{\varepsilon>0}$ *bounded in* $H^s(\mathbb{R}^d)$ *with* $s > d/2$ *(or* $s > 1$ *when* $d = 1$*). Assume one has as* ε *goes to* 0

$$v^\varepsilon_n \rightharpoonup v_n \ \text{ in } \ L^2.$$

Then, the weak limits of $\left(\mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi}\psi^\varepsilon_{0,n}\right)_{\varepsilon>0}$ *are non zero if and only if* $\xi \in \xi_n + 2\pi\mathbb{Z}^d$. *Besides, for any* $j \in 2\pi\mathbb{Z}^d$, *one has as* ε *goes to* 0

$$\mathrm{e}^{-\frac{i}{\varepsilon}x\cdot(\xi_n+j)}\psi^\varepsilon_{0,n} \rightharpoonup c_n(\xi_n + j)v_n \ \text{ in } \ L^2.$$

Proof. One writes

$$\begin{aligned}\mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi}\psi^\varepsilon_{0,n} &= \mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi}\sum_{j\in 2\pi\mathbb{Z}^d}\mathrm{e}^{-\frac{i}{\varepsilon}x\cdot j}c_n(\varepsilon D_x + j)\mathrm{e}^{\frac{i}{\varepsilon}x\cdot\xi_n}v^\varepsilon_n\\ &= \sum_{j\in 2\pi\mathbb{Z}^d}\mathrm{e}^{-\frac{i}{\varepsilon}x\cdot(j+\xi-\xi_n)}c_n(\xi_n + j + \varepsilon D_x)v^\varepsilon_n\end{aligned}$$

and the result follows. □

As a corollary, we obtain a description of the concentration of these families on subsets of interest.

Corollary E.3. *Let* X *be a* $2\pi\mathbb{Z}^d$ *periodic subset* X *of* $\mathbb{R}^d$ *consisting of isolated points and containing* ξ_n.

(1) *Let* $M^X d\nu^X$ *be the two-microlocal measures at finite distance associated with the concentration of* $(\psi^\varepsilon_{0,n})_{\varepsilon>0}$ *on* X. *Then,*

$$\nu^X = \|v_n\|^2_{L^2}\sum_{j\in 2\pi\mathbb{Z}^d}|c_n(\xi_n + j)|^2\delta(\xi - \xi_n - j)$$

and, for $j \in 2\pi\mathbb{Z}^d$, *the operator* $M^X(\xi_n + j)$ *is the projector of* $L^2(\mathbb{R}^d)$ *on* $\mathbb{C}v_n$.

(2) *Consider the family of* $L^2(\mathbb{R}^d, \mathbb{C}^2)$, $\Psi^\varepsilon_{n,n'} = {}^t\left(\psi^\varepsilon_{0,n}, \psi^\varepsilon_{0,n'}\right)$ *with* $n \neq n'$ *and* $\xi_{n'} = \xi_n$. *Let* $M^X d\nu^X$ *be the two-microlocal measures at finite distance associated with the concentration of* $\Psi^\varepsilon_{n,n'}$ *on* X. *Then*

$$\nu^X = \left(\|v_n\|^2_{L^2} + \|v_{n+1}\|^2_{L^2}\right)\sum_{j\in 2\pi\mathbb{Z}^d}|c_n(\xi_n + j)|^2\delta(\xi - \xi_n - j)$$

and, for $j \in 2\pi\mathbb{Z}^d$, *the operator* $M^X(\xi_n + j)$ *is the projector of* $L^2(\mathbb{R}^d, \mathbb{C}^2)$ *on* $\mathbb{C}\,{}^t(v_n, v_{n+1})$.

Proof. Since ξ_n is an isolated point of X, by Remark 4.2, M^X is the orthogonal projector on a weak limit in L^2 of

$$x \mapsto \mathrm{e}^{-\frac{i}{\varepsilon}x\cdot\xi}\varphi_n\left(\frac{x}{\varepsilon}, \varepsilon D_x\right)u^\varepsilon_n.$$

By Lemma E.2, any of this weak limit is 0 if $\xi \notin \xi_n + 2\pi\mathbb{Z}^d$ and if $\xi = \xi_n + j$ with $j \in 2\pi\mathbb{Z}^d$, then the limit is $c_{n_0}(\xi_{n_0} + j)v_{n_0}$ whence we get the Part 1 of the result. The proof of Part 2 follows the same lines. □

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