SEMI-CLASSICAL ANALYSIS AND BLOCH-FLOQUET THEORY

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ABSTRACT. The aim of these lectures is to discuss different PDEs technics related with a Schrödinger equation describing the dynamics of an electron in a crystal in presence of impurities. Because the size of the cells of the crystal are supposed to be very small comparatively with the macroscopic scale, it is a multi-scale problem with periodic aspects. We shall use semi-classical measures (also called Wigner measures) to take care of the multi-scale features, and Bloch theory to deal with the periodicity. These notions will be explained and used for calculating the density of probability of presence of the electron in the limit where the size of the cells is much smaller than the macroscopic one.

CONTENTS

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1. Introduction

This lecture is devoted to the analysis of the Schrödinger equation

$$
(1.1)\qquad \left\{ \begin{array}{l} i\partial_t \psi^\varepsilon(t,x) + \dfrac{1}{2}\Delta_x \psi^\varepsilon(t,x) - \dfrac{1}{\varepsilon^2} V_{\rm per}\left(\dfrac{x}{\varepsilon}\right)\psi^\varepsilon(t,x) - V(t,x)\psi^\varepsilon(t,x) = 0, \\ \psi^\varepsilon|_{t=0} = \psi^\varepsilon_0. \end{array}\right.
$$

where $(\psi^\varepsilon_0)_{\varepsilon>0}$ is a bounded family in $L^2(\mathbb{R}^d)$ with $\|\psi^\varepsilon_0\|_{L^2(\mathbb{R}^d)} = 1$, $V_{\rm per}$ a $\mathbb{Z}^d$-periodic potential that we will suppose smooth, $V(t,\cdot)$ a time dependent exterior potential that will be supposed to be in $L^\infty(\mathbb{R}, C^1(\mathbb{R}^d))$, in the sense that for all $t\in\mathbb{R}$, $V(t,\cdot)\in C^1(\mathbb{R})$ and has bounded derivatives, uniformly in time. The parameter ε is the so-called semi-classical parameter, $\varepsilon \ll 1$, because of the scaling of the problem that we will discuss in the next section, and we are interested in the description as ε goes to 0 of the density $|\psi^\varepsilon(t,x)|^2dx$ which gives the probability of finding the particule at time t at the position x. We will consider quadratic functions of $\psi^\varepsilon(t)$ involving more general observables.

The first section of this introduction is devoted to the motivations leading to using this equation for describing the dynamics of an electron in a crystal, in presence of an external potential. The second subsection will explain the basic ideas of Effective mass theory, that we will implement in simplified situations, exhibiting some of the main ideas of the lecture. We will finish by presenting the result that we are going to prove and the schedule of the lecture.

This lecture is issued from works with Victor Chabu and Fabricio Macia (see [13, 14, 15]). The presentation of the different notions treated in this text is also highly impacted by collaborations with Caroline Lasser and Fabricio Macia, independently and, more recently, simultaneously. They will recognize their influence. It is an opportunity to thank them for these collaborations that have been, and still are, a source of major mathematical satisfaction.

1.1. **The dynamics of an electron in a crystal.**

The dynamics of an electron in a crystal in the presence of impurities is described by a wave function $\Psi(t',x')$ that solves the Schrödinger equation:

$$
(1.2)\qquad \left\{ \begin{array}{l} i\hbar\partial_{t'}\Psi(t',x') + \dfrac{\hbar^2}{2m}\Delta_{x'}\Psi(t',x') - e\,Q_{\rm per}(x')\,\Psi(t',x') - e\,Q_{\rm ext}(t',x')\Psi(t',x') = 0, \\ \Psi|_{t'=0} = \Psi_0, \qquad (t',x')\in\mathbb{R}\times\mathbb{R}^d. \end{array}\right.
$$

The potential $Q_{\rm per}$ is periodic with respect to some lattice in $\mathbb{R}^d$ and describes the interactions between the electron and the crystal. The external potential $Q_{\rm ext}$ takes into account the effects of impurities on the otherwise perfect crystal. Here $\hbar$ denotes the Planck constant, e is the charge of the electron and m its mass. In many cases of physical interest, the ratio between the mean spacing of the lattice and the characteristic length scale of variation of $Q_{\rm ext}$ is very small. We shall denote that ratio by ε and consider the limit $\varepsilon\to 0$.

Following [42], one observes that there are two scales in the problem:

- the *quantum scale* characterized by the typical length λ of the lattice,
- the *macroscopic scale* of which we shall denote by L its typical length.

With these *length scales* are associated *time scales*: the *quantum time scale* characterized by the typical time τ and and the *macroscopic time scale* characterized by the typical time T which are related to the length scale by

$$
\tau = \frac{m\lambda^2}{\hbar},\ \ T = \frac{mL^2}{\hbar}.
$$

Strictly speaking, we should consider the Planck constant in macroscopic units h and define T as $T = \frac{m\lambda^2}{h}$. We have implicitly assumed that $\hbar/h$ is a constant, that we have set to 1.

Since the periodic potential acts on the quantum scale, we rescale it as

$$e\,Q_{\rm per}(x') = \frac{m\lambda^2}{\tau^2} V_{\rm per}\left(\frac{x'}{\lambda}\right),$$

and we rescale the external potential that acts at macroscopic scale as

$$e\,Q_{\rm ext}(t',x') = \frac{mL^2}{T^2} V_{\rm per}\left(\frac{t'}{T},\frac{x'}{L}\right).$$

The meaning of these new scales consists in saying that a free electron under the influence of $Q_{\rm per}$ will travel a distance of length λ in the time unit τ and, similarly, a free electron under the influence of $Q_{\rm ext}(t')$ will travel a distance of length L in the time unit T.

We shall reformulate our problem in terms of the variables

$$(t,x) = \left(\frac{t'}{T},\frac{x'}{L}\right),$$

that are usually called the *slow variables*. The so-called *fast variables*

$$(s,y) = \left(\frac{t'}{\tau},\frac{x'}{\lambda}\right),$$

will of course play a role in the analysis. They are linked with the slow ones by

$$x = \varepsilon y \text{ and } t = \varepsilon^2 s \text{ with } \varepsilon = \frac{\lambda}{L} = \sqrt{\frac{\tau}{T}} \ll 1.$$

Since the wave function is normalized in $L^2(\mathbb{R}^d)$ ($\|\Psi\|_{L^2(\mathbb{R}^d)} = 1$), we choose the new unknown

$$\psi^\varepsilon(t,x) = L^{-d/2}\Psi(t',x') = L^{-d/2}\Psi(T\,t, L\,x).$$

Lemma 1.1. *Setting $\psi_0^\varepsilon(x) = L^{-d/2}\Psi_0(L\,x)$, the family $\psi^\varepsilon(t,x)$ satisfies* (1.1).

Proof
We just have to perform carefully the computation.

$$\begin{aligned} i\hbar\partial_t\psi^\varepsilon(t,x) &= T\,L^{-d/2} i\hbar\partial_t\Psi(T\,t,L\,x) \\ &= T\,L^{-d/2}\left(-\frac{\hbar^2}{2m}\Delta_{x'}\Psi(T\,t,L\,x) + e\,Q_{\rm per}(x)\Psi(T\,t,L\,x) + e\,Q_{\rm ext}(T\,t,L\,x)\Psi(T\,t,L\,x)\right) \\ &= -\frac{\hbar^2 T}{2mL^2}\Delta_x\psi^\varepsilon(t,x) + \frac{Tm\lambda^2}{\tau^2}V_{\rm per}\left(\frac{L}{\lambda}x\right)\psi^\varepsilon(t,x) + \frac{mL^2}{T}V_{\rm ext}(t,x)\psi^\varepsilon(t,x). \end{aligned}$$

Dividing the equation by $\hbar$, we obtain

$$i\partial_t\psi^\varepsilon(t,x) = -\frac{1}{2}\cdot\frac{\hbar T}{mL^2}\Delta_x\psi^\varepsilon(t,x) + \frac{Tm\lambda^2}{\hbar\tau^2}V_{\rm per}\left(\frac{L}{\lambda}x\right) + \frac{mL^2}{T\hbar}V_{\rm ext}(t,x)\psi^\varepsilon(t,x).$$

Since $\varepsilon = \frac{\lambda}{L}$ and $\frac{m\lambda^2}{\hbar\tau} = \frac{mL^2}{\hbar T} = 1$, we have

$$\frac{Tm\lambda^2}{\hbar\tau^2} = \frac{m\lambda^2}{\hbar\tau}\times\frac{T}{\tau} = \frac{1}{\varepsilon^2}$$

and we obtain

$$i\partial_t\psi^\varepsilon(t,x) = -\frac{1}{2}\Delta_{\widetilde{x}}\psi^\varepsilon(t,x) + \frac{1}{\varepsilon^2}V_{\rm per}\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon(t,x) + V_{\rm ext}(t,x)\psi^\varepsilon(t,x),$$

which concludes the proof of the Lemma.

In the following, we shall consider equation (1.1) with $\|\psi_0^\varepsilon\|_{L^2(\mathbb{R}^d)} = 1$ and we shall assume that the potential $V_{\rm per}$ is periodic with respect to a fixed lattice in $\mathbb{R}^d$, which, for the sake of definiteness will be assumed to be $\mathbb{Z}^d$. We shall focus on the description of the density

$$n^\varepsilon(t,x) = |\psi^\varepsilon(t,x)|^2 dxdt \tag{1.3}$$

which gives the probability of finding the electron at time t in the position x. More precisely, we are interested in the computation of time averages of quadratic functions of $\psi^\varepsilon(t,x)$, that is, in describing the limit as ε goes to 0 of quantities of the form

$$\frac{1}{T}\int_0^T a(x) n^\varepsilon(t,x) dx\, dt, \quad T>0, \quad a \in C_c^\infty(\mathbb{R}^d).$$

1.2. **Effective mass theory.** Effective Mass Theory consists in showing that, under suitable assumptions on the initial data ψ_0^ε, the solutions of (1.1) can be approximated for small values of ε by those of a simpler Schrödinger equation, called the *effective mass equation*, which is for example of the form:

$$i\partial_t \phi(t,x) + \frac{1}{2} B\, \nabla_x \cdot \nabla_x \phi(t,x) - V_{\rm ext}(t,x)\phi(t,x) = 0. \tag{1.4}$$

Above, B is a $d\times d$ matrix called the *effective mass tensor*. It is an experimentally accessible quantity that can be used to study the effect of the impurities on the dynamics of the electrons. Both the question of finding those initial conditions for which the corresponding solutions of (1.1) converge (in a suitable sense) to solutions to the effective mass equation and that of clarifying the dependence of B on the sequence of initial data have been extensively studied in the literature [9, 42, 3, 27, 8].

The equation (1.4) is an approximation of the equation (1.1) in the sense that the limit as a distribution of the density $n^\varepsilon(t,x)$ is $|\phi(t,x)|^2$, at least in time average, or, equivalently, that for all $a \in C_c^\infty(\mathbb{R}^d)$ and $T>0$,

$$\frac{1}{T}\int_0^T \int a(x) n^\varepsilon(t,x) dxdt \underset{\varepsilon\to 0}{\longrightarrow} \frac{1}{T}\int_0^T \int a(x) |\phi(t,x)|^2 dxdt.$$

One has to notice that the effective mass equation is independent of the small parameter and, thus, is easiest to treat, for example numerically. When replacing the original equation by (1.4), one can say that one has solved the question of the oscillations of size $\frac{1}{\varepsilon}$ of the function $\psi^\varepsilon(t,x)$.

Dealing with the limit $\varepsilon \to 0$ expresses in mathematical terms as looking for weak-$\star$ accumulation points of the sequence of densities $|\psi^\varepsilon(t,x)|^2$, that we are going to study in terms of time-dependent Wigner distribution. Therefore, Wigner measure approach is a good way to handle this question. It allows to treat quite general initial data and give a new insight on the status of the function $\phi(t,x)$ satisfying the Effective mass equation.

A typical example of this sort of results has been obtained in [3] for data that we will call *well-prepared initial data*. We describe below a weaker result that is a consequence of the work [3]. For this, we need some notations.

(i) With $\xi \in \mathbb{R}^d$, we associate the operator $P(\xi)$ with domain $H^2(\mathbb{T}^d) \subset L^2(\mathbb{T}^d)$

$$P(x) = -\frac{1}{2}|\xi + D_y|^2 + V_{\rm per}(y), \quad y \in \mathbb{T}^d, \tag{1.5}$$

where $\mathbb{T}^d = \mathbb{R}^d \backslash \mathbb{Z}^d$ is a flat torus.

We will see in Section 3 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*

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

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

$$P(\xi)\varphi_n(\cdot,\xi) = \varrho_n(\xi)\varphi_n(\cdot,\xi), \quad \forall \xi\in\mathbb{R}^d, \quad \forall n\in\mathbb{N}^*. \tag{1.6}$$

(ii) The initial data $(\psi_0^\varepsilon)_{\varepsilon>0}$ is said *well-prepared* if there exist $n\in\mathbb{N}^*$, $\xi_0\in\mathbb{R}^d$ and $v_0\in\mathcal{S}(\mathbb{R}^d)$ such that

$$\psi_0^\varepsilon(x) = \mathrm{e}^{\frac{i}{\varepsilon}\xi_0\cdot x}\varphi_n\left(\xi_0,\frac{x}{\varepsilon}\right)v_0(x). \tag{1.7}$$

Theorem 1.2. [3] *Let $T>0$. Assume $(\psi_0^\varepsilon)_{\varepsilon>0}$ satisfies* (1.7) *with ξ_0 a critical point of $\xi\mapsto\varrho_n(\xi)$. Assume that the eigenvalue $\varrho_n(\xi)$ is separated from the rest of the spectrum of $P(\xi)$ for ξ in a neighborhood of ξ_0. Then the solution of* (1.1) *satisfies*

$$\psi^\varepsilon(t,x) = \mathrm{e}^{\frac{i}{\varepsilon}\xi_0\cdot x-\frac{i}{\varepsilon^2}\varrho_n(\xi_0)t}\varphi_n\left(\xi_0,\frac{x}{\varepsilon}\right)v^\varepsilon(t,x)$$

and $v^\varepsilon(t)$ converges weakly in $L^2((0,T),H^1(\mathbb{R}^d))$ to the solution $v(t)$ of the equation

$$\left\{\begin{array}{l} i\partial_t v = -\frac{1}{2}d^2\varrho_n(\xi_0)\nabla_x\cdot\nabla_x\, v + V(t,x)v,\\ v|_{t=0} = v_0. \end{array}\right. \tag{1.8}$$

The equation (1.8) typically is an effective equation since it is ε-independent. It involves the eigenfunctions and the eigenmodes of the operator $P(\xi)$. In particular, starting from a data proportional to $\varphi_n\left(\xi_0,\frac{x}{\varepsilon}\right)$, the solution is proportional to $\varphi_n\left(\xi_0,\frac{x}{\varepsilon}\right)$ and the coefficient of proportionality evolve in an autonomous manner involving the Bloch mode $\varrho_n(\xi)$.

We point out that the importance of the assumption that ξ_0 is a critical point of ϱ_n will be made clear in the next chapters. Let us now discuss the role of the operator $P(\xi)$. The existence of two scales in the problem suggests to look for $(\psi^\varepsilon(t))_{\varepsilon>0}$ of the form

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

where the function $U^\varepsilon = U^\varepsilon(t,x,y)$ is defined on $\mathbb{R}\times\mathbb{R}^d\times\mathbb{T}^d$. Formally, if $(U^\varepsilon(t))_{\varepsilon>0}$ satisfies

$$\left\{\begin{array}{l} i\varepsilon^2\partial_t U^\varepsilon(t,x,y) = P(\varepsilon D)U^\varepsilon(t,x,y) + \varepsilon^2 V(t,x)U^\varepsilon(t,x,y),\\ U^\varepsilon|_{t=0} = U_0^\varepsilon, \end{array}\right. \tag{1.9}$$

with $U_0^\varepsilon(x,\frac{x}{\varepsilon}) = \psi_0^\varepsilon$, then $(t,x)\mapsto U^\varepsilon\left(t,x,\frac{x}{\varepsilon}\right)$ solves (1.1). Here, the opeartor $P(\varepsilon D)$ acts as a Fourier multiplier in the variable ξ:

$$P(\varepsilon D)U^\varepsilon(t,x,y) = (2\pi)^{-d}\int_{\mathbb{R}^d}\mathrm{e}^{i\xi\cdot(x-x')}P(\varepsilon\xi)U^\varepsilon(t,x',y)dx'd\xi.$$

Of course, there are several choices possible for realizing $U_0^\varepsilon(x,\frac{x}{\varepsilon}) = \psi_0^\varepsilon$. For example, one can take

$$U_{0,1}^\varepsilon(x,y) = \psi_0^\varepsilon(x)\mathbf{1}_{y\in\mathbb{T}^d}, \quad (x,y)\in\mathbb{R}^d\times\mathbb{T}^d.$$

In the case of well-prepared initial data satisfying (1.7), it looks appropriate to choose

$$U_{0,2}^\varepsilon(x,y) = \mathrm{e}^{\frac{i}{\varepsilon}\xi_0\cdot x}\varphi_n(\xi_0,y)v_0(x), \quad (x,y)\in\mathbb{R}^d\times\mathbb{T}^d.$$

These choices will generate two functions $U_j^\varepsilon(t,x,y)$, $j=1,2$, that are different functions of $\mathbb{R}^d\times\mathbb{T}^d$. However, by unicity of the solution of (1.1), they satisfy

$$U_1^\varepsilon\left(t,x,\frac{x}{\varepsilon}\right) = U_2^\varepsilon\left(t,x,\frac{x}{\varepsilon}\right), \quad (t,x)\in\mathbb{R}\times\mathbb{R}^d.$$

Let us now prove Theorem 1.2 in the simple case $V(t,x)=0$. The next chapters will give the elements for proving the general case.

Proof
We first write the equation satisfied by $\widehat{U}^\varepsilon(t,\xi,y)$ where we denote by $\widehat{f}$ the Fourier transform with respect to the variable x:

$$\widehat{f}(\xi) = \int_{\mathbb{R}^d} f(x) \mathrm{e}^{-i\xi\cdot x} dx, \;\; \xi \in \mathbb{R}^d, \;\; f \in \mathcal{S}(\mathbb{R}^d).$$

We have

$$\left\{ \begin{array}{l} i\varepsilon^2 \partial_t \widehat{U}^\varepsilon(t,\xi,y) = P(\varepsilon\xi)\widehat{U}^\varepsilon(t,\xi,y), \\ U^\varepsilon|_{t=0}(\xi,y) = \widehat{v}_0\left(\xi - \frac{\xi_0}{\varepsilon}\right)\varphi_n(\xi_0,y). \end{array} \right.$$

For $\ell \in \mathbb{N}^*$, let us denote by $\Pi_n(\xi)$ the eigenprojector on the n-th mode of $P(\xi)$ and by $\Pi_\perp(\xi)$ the orthogonal projector ($\Pi_\perp = \mathrm{Id} - \Pi_n(\xi)$). We have

$$\widehat{U}^\varepsilon(t,\xi,y) = U^\varepsilon_n(t,\xi,y) + U^\varepsilon_\perp(t,\xi,y), \;\; U^\varepsilon_n(t,\xi,y) = \Pi_n(\varepsilon\xi)U^\varepsilon(t,\xi,y), \;\; (t,x,y) \in \mathbb{R}\times\mathbb{R}^d\times\mathbb{T}^d.$$

Besides, for $\ell \in \{n,\perp\}$, $(\widehat{U}^\varepsilon_\ell(t))_{\varepsilon>0}$ solves

$$i\varepsilon^2\partial_t \widehat{U}^\varepsilon_\ell(t,\xi,y) = (\Pi_\ell P)(\varepsilon\xi)\widehat{U}^\varepsilon_\ell(t,\xi,y)$$

with

$$\begin{aligned} U^\varepsilon_\ell|_{t=0}(\xi,y) &= \widehat{v}_0\left(\xi - \frac{\xi_0}{\varepsilon}\right)\Pi_\ell(\varepsilon\xi)\varphi_n(\xi_0,y) \\ &= \widehat{v}_0\left(\xi - \frac{\xi_0}{\varepsilon}\right)\left(\Pi_\ell(\xi_0) + \varepsilon\int_0^1 \left(\xi - \frac{\xi_0}{\varepsilon}\right)\cdot\nabla_\xi\Pi_\ell\left(\xi_0 + s\varepsilon\left(\xi - \frac{\xi_0}{\varepsilon}\right)\right)ds\right)\varphi_n(\xi_0,y) \end{aligned}$$

where we have used that Π_n is a smooth function (this comes from the assumption on the mode ϱ_n, as we shall see in Section 3). Assuming for example that $\widehat{v}_0$ is compactly supported, we obtain in $L^2(\mathbb{R}^d\times\mathbb{T}^d)$

$$\widehat{U}^\varepsilon_\ell|_{t=0}(\xi,y) = \delta_{\ell,n}\widehat{v}_0\left(\xi - \frac{\xi_0}{\varepsilon}\right)\varphi_n(\xi_0,y) + O(\varepsilon).$$

When $\ell=\perp$, this implies $U^\varepsilon_\perp(t) = O(\varepsilon)$ in $L^2(\mathbb{R}^d\times\mathbb{T}^d)$.

When $\ell = n$, using $\Pi_n(\xi)P(\xi) = \varrho_n(\xi)\Pi_n(\xi)$, we obtain $\widehat{U}^\varepsilon_n(t,\xi,y) = \mathrm{e}^{-\frac{i}{\varepsilon^2}\varrho_n(\varepsilon\xi)t}\widehat{U}^\varepsilon_n(0,\xi,y)$, whence

$$\begin{aligned} U^\varepsilon_n(t,x,y) &= (2\pi)^{-d}\int_{\mathbb{R}^d} \mathrm{e}^{i\xi\cdot x - \frac{i}{\varepsilon^2}\varrho_n(\varepsilon\xi)t}\widehat{U}^\varepsilon_n(0,\xi,y)d\xi \\ &= (2\pi)^{-d}\,\mathrm{e}^{\frac{i}{\varepsilon}\xi_0\cdot x}\varphi_n(\xi_0,y)\int_{\mathbb{R}^{2d}} \mathrm{e}^{i(\xi-\frac{\xi_0}{\varepsilon})\cdot(x-x') - \frac{i}{\varepsilon^2}\varrho_n(\varepsilon\xi)t} v_0(x')d\xi dx' \\ &= (2\pi)^{-d}\,\mathrm{e}^{\frac{i}{\varepsilon}\xi_0\cdot x}\varphi_n(\xi_0,y)\int_{\mathbb{R}^{2d}} \mathrm{e}^{i\xi\cdot(x-x') - \frac{i}{\varepsilon^2}\varrho_n(\xi_0+\varepsilon\xi)t} v_0(x')d\xi dx' \end{aligned}$$

Writing $\varrho_n(\xi_0+\varepsilon\xi) = \varrho_n(\xi_0) + \frac{\varepsilon^2}{2}d^2\varrho_n(\xi_0)\xi\cdot\xi + \varepsilon^3 G^\varepsilon(\xi)[\xi,\xi,\xi]$ for $G^\varepsilon(\xi)$ a smooth bounded 3-tensor, we obtain

$$v^\varepsilon(t) = (2\pi)^{-d}\int_{\mathbb{R}^{2d}} \mathrm{e}^{i\xi\cdot(x-x') - \frac{i}{2}d^2\varrho_n(\xi_0)\xi\cdot\xi\, t + it\varepsilon G^\varepsilon(\xi)[\xi,\xi,\xi]} v_0(x')d\xi dx',$$

whence the result. In the case where $\nabla\varrho_n(\xi_0) \neq 0$, the non-stationary phase theorem gives the convergence to 0 of $(v^\varepsilon(t))_{\varepsilon>0}$.

1.3. **Our aim.** Our aim in this lecture is to provide a similar description for more general initial data, without assumptions on its form, as the well-prepared data of (1.7). However, we will relax our exigence by only asking for a description of the weak limits of quadratic quantities as

$$\int_a^b \int_{\mathbb{R}^d} \phi(x)|\psi^\varepsilon(t,x)|^2 dxdt \quad \text{or} \quad \int_a^b \int_{\mathbb{R}^d} \phi(\varepsilon\xi)|\widehat{\psi^\varepsilon}(t,\xi)|^2 d\xi dt.$$

To unify the position and impulsion (or frequency, or also Fourier) point of view, we shall consider the Wigner transform of the family $(\psi^\varepsilon(t))_{\varepsilon>0}$ and replace the analysis of the densities $|\psi^\varepsilon(t,x)|^2 dxdt$ or $\varepsilon^{-d}|\widehat{\psi^\varepsilon}(t,\xi/\varepsilon)|^2 d\xi dt$ by the one of the distribution on $\mathbb{R}\times\mathbb{R}^{2d}$

$$w^\varepsilon(t,x,\xi) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d} \psi^\varepsilon(t,x+\varepsilon v/2)\overline{\psi}^\varepsilon(t,x-\varepsilon v/2)\mathrm{e}^{iv\cdot\xi}dv.$$

Note that, formally, the marginals of $w^\varepsilon(t,x,\xi)$ give the position and impulsion densities. Things will be made rigorous in Section 2. We are going to prove the following result, in the case $d=1$.

Theorem 1.3. *Consider for each $n\in\mathbb{N}$ the sets of critical values of the Bloch modes*

$$\Lambda_n := \{\xi,\ \nabla\varrho_n(\xi)=0\}. \tag{1.10}$$

Assume (ψ_0^ε) is bounded in $H^s_\varepsilon(\mathbb{R})$ for some $s>1/2$. Assume $V_{\rm per}$ is smooth and that $t\mapsto V(t,x)$ is bounded in $L^\infty(C^1(\mathbb{R}^d))$. Then, there exists a subsequence $(\psi_0^{\varepsilon_\ell})_{\varepsilon_\ell>0}$, such that $\varepsilon_\ell \underset{\ell\to+\infty}{\longrightarrow} 0$ and, for every $a<b$ and every $\phi\in C_c^\infty(\mathbb{R}^2)$ the following holds:

$$\lim_{\ell\to\infty}\int_a^b\int_{\mathbb{R}^2}\phi(x,\xi)w^{\varepsilon_\ell}(t,x,\xi)dxd\xi dt = \sum_{n\in\mathbb{N}^*}\sum_{\xi\in\Lambda_n}\int_a^b\int_{\mathbb{R}^2}\phi(x,\xi)|\psi_\xi^{(n)}(t,x)|^2dxdt \tag{1.11}$$

where, for every $n\in\mathbb{N}^*$ and $\xi\in\Lambda_n$, $\psi^{(n)}_\xi$ solves the Schrödinger equation:

$$i\partial_t\psi_\xi^{(n)}(t,x) = \frac{1}{2}\partial_\xi^2\varrho_n(\xi)\partial_x^2\psi_\xi^{(n)}(t,x) + V_{\rm ext}(t,x)\psi_\xi^{(n)}(t,x), \tag{1.12}$$

with initial datum:

$\psi_\xi^{(n)}|_{t=0}$ *is the weak limit in $L^2(\mathbb{R})$ of the sequence* $\left(\mathrm{e}^{-\frac{i}{\varepsilon_\ell}\xi x}\Pi_n(\varepsilon D_x)(\psi_0^{\varepsilon_\ell}\otimes\mathbf{1}_{y\in\mathbb{T}})\right)$.

Moreover, for all $\phi\in C_c^\infty(\mathbb{R})$,

$$\lim_{\ell\to\infty}\int_a^b\int_{\mathbb{R}}\phi(x)|\psi^{\varepsilon_\ell}(t,x)dxdt = \sum_{n\in\mathbb{N}^*}\sum_{\xi\in\Lambda_n}\int_a^b\int_{\mathbb{R}}\phi(x)|\psi_\xi^{(n)}(t,x)|^2dxdt \tag{1.13}$$

Note that some of the accumulation points of $\mathrm{e}^{-\frac{i}{\varepsilon_\ell}\xi x}\Pi_n(\varepsilon D_x)(\psi_0^{\varepsilon_\ell}\otimes\mathbf{1}_{y\in\mathbb{T}})$ may just be 0. For example, when $V_{\rm per}=0$, only the first Bloch energy ϱ_1 has critical points and they are precisely $\Lambda_1=2\pi\mathbb{Z}$. Besides, 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 $\Pi_1(\varepsilon\xi)(\widehat{\psi_0^{\varepsilon_\ell}}(\xi)\mathbf{1}_{y\in\mathbb{T}}) = \mathbf{1}_{(-\pi,\pi)}(\varepsilon\xi)\widehat{\psi_0^{\varepsilon_\ell}}(\xi)$ 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 $k\neq 0$. As a consequence, in this elementary case $V_{\rm per}=0$, Theorem 1.3 says nothing but that the weak limits of $|\psi^\varepsilon(t,x)|^2$ are equal to $|\psi^0(t,x)|^2$ where $\psi^0(t,x)$ solves (1.1) with initial data ψ_0^0, the weak limit of (ψ_0^ε) in $L^2(\mathbb{R})$.

If the data is well-prepared, one recovers the result of Theorem 1.2.

In higher dimension, the result is more complicated to state. We will discuss it in the last section.

This result relies on a semi-classical analysis of the problem and the use of the Bloch-Floquet theory. The aim of the lecture is to explain these tools (Sections 2 and 3 respectively) and to implement them for analyzing the solutions of equation (1.1) (Section 4). We will see that this requires the introduction of a two-scale analysis, and thus the introduction of a refined notion of two-scale Wigner transform

(Section 5). In the conclusive Section 6, we will be able to prove Theorem 1.3 and we will discuss the higher dimension case.

2. THE SEMI-CLASSICAL APPROACH

In this chapter, we introduce Wigner transforms in Section 2.1. We will use their tight link with semi-classical pseudodifferential operators, of which we shall describe the properties that will be useful for our purpose in Section 2.2. Wigner measures are defined in Section 2.3, together with the analysis of their main properties.

2.1. **Wigner function.**

2.1.1. *Definitions.* The *Wigner function* $W^\varepsilon[f]$ of a function $f \in L^2(\mathbb{R}^d)$ is the function defined on $\mathbb{R}^{2d}$:

$$W^\varepsilon[f](x,\xi) = (2\pi)^{-d} \int_{\mathbb{R}^d} \mathrm{e}^{iv\cdot\xi} f\left(x - \frac{\varepsilon}{2}v\right) \overline{f}\left(x + \frac{\varepsilon}{2}v\right) dv. \tag{2.1}$$

It also writes

$$W^\varepsilon[f](x,\xi) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} \mathrm{e}^{\frac{i}{\varepsilon}v\cdot\xi} f\left(x - \frac{v}{2}\right) \overline{f}\left(x + \frac{v}{2}\right) dv.$$

It has been introduced by Wigner [46] at the beginning of the 20th century. Let us derive a first set of basic properties.

Proposition 2.1 (Wigner distributions)**.** *For $f \in \mathcal{S}(\mathbb{R}^d)$, its Wigner function satisfies the following properties:*

(1) $W^\varepsilon[f] \in \mathcal{S}(\mathbb{R}^d \times \mathbb{R}^d)$ *and for all $N \in \mathbb{N}$, there exists $C_N > 0$*

$$\langle \xi\rangle^N \langle x\rangle^N \ |W^\varepsilon[f](x,\xi)| \le C_N \sup_{|\alpha|,|\beta|\le N} \|x^\alpha(\varepsilon\partial_x)^\beta f\|_{L^2}, \ \ (x,\xi)\in\mathbb{R}^{2d}.$$

(2) $W^\varepsilon[f] \in L^2(\mathbb{R}^d \times \mathbb{R}^d)$ *and* $\|W^\varepsilon[f]\|_{L^2(\mathbb{R}^{2d})} = (2\pi\varepsilon)^{-\frac{d}{2}} \|f\|^2_{L^2(\mathbb{R}^d)}$.

(3) $\langle W^\varepsilon[f], W^\varepsilon[g]\rangle_{L^2(\mathbb{R}^d\times\mathbb{R}^d)} = (2\pi\varepsilon)^{-d} \,|\langle f,g\rangle_{L^2(\mathbb{R}^d)}|^2$.

(4) *The marginals of $W^\varepsilon[f]$ on x or ξ give the position or momentum densities of f respectively :*

$$\int_{\mathbb{R}^d} W^\varepsilon[f](x,\xi)d\xi = |f(x)|^2, \quad \int_{\mathbb{R}^d} W^\varepsilon[f](x,\xi)dx = \frac{1}{(2\pi\varepsilon)^d}\left|\widehat{f}\left(\frac{\xi}{\varepsilon}\right)\right|^2.$$

In particular,

$$\int_{\mathbb{R}^{2d}} W^\varepsilon[f](x,\xi)dxd\xi = \|f\|^2_{L^2(\mathbb{R}^d)}.$$

(5) $W^\varepsilon[f]$ *is real-valued but in general not positive.*

Note that it is proved in [28, 44] that $W^\varepsilon[f]$ is nonnegative if and only if f is Gaussian (the article [28] concerns the dimension 1, while [44] holds in any dimension).

Example 2.2. Consider $z_0 = (x_0,\xi_0) \in \mathbb{R}^{2d}$ and

$$f^\varepsilon_{z_0}(x) = \varepsilon^{-d/4}\, \mathrm{e}^{\frac{i}{\varepsilon}\xi_0\cdot(x-x_0)} f\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right), \quad x\in\mathbb{R}^d.$$

Then,

$$W^\varepsilon[f^\varepsilon_{z_0}](x,\xi) = \varepsilon^{-d}\, W^1[f]\left(\frac{\xi-\xi_0}{\sqrt{\varepsilon}}, \frac{\xi-\xi_0}{\sqrt{\varepsilon}}\right).$$

Proof

1. We observe that the transformation acts on $f\overline{f}$ by the measure preserving change of coordinates $(x,v) \mapsto (x + \frac{1}{2}v, x - \frac{1}{2}v)$ followed by a partial Fourier transform with respect to v. Hence, if f is a

Schwartz function, then the Wigner distribution $W^\varepsilon[f]$, too.
2. Square integrability of $W^\varepsilon[f]$ can be seen as in 1. For calculating the norm, let $(x,\xi)\in\mathbb{R}^{2d}$,

$$|W^\varepsilon[f](x,\xi)|^2 \\ = (2\pi)^{-2d}\int_{\mathbb{R}^{2d}} f\left(x-\frac{\varepsilon v}{2}\right)\overline{f}\left(x+\frac{\varepsilon v}{2}\right) f\left(x+\frac{\varepsilon v'}{2}\right)\overline{f}\left(x-\frac{\varepsilon v'}{2}\right)\mathrm{e}^{i\xi\cdot v}\mathrm{e}^{i\xi\cdot(v-v')}dvdv'.$$

Therefore, after integration in ξ, we obtain

$$\int_{\mathbb{R}^d}|W^\varepsilon[f](x,\xi)|^2 d\xi = (2\pi)^{-d}\int_{\mathbb{R}^d}\left|f\left(x-\varepsilon\frac{v}{2}\right)\right|^2\left|f\left(x+\varepsilon\frac{v}{2}\right)\right|^2 dv.$$

We deduce

$$\begin{aligned}\|W^\varepsilon[f]\|^2_{L^2(\mathbb{R}^{2d})} &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}}|f(x)|^2|f(x+v)|^2 dvdx = (2\pi\varepsilon)^{-d}\|f\|^2_{L^2(\mathbb{R}^d)}\int_{\mathbb{R}^{2d}}|f(x)|^2 dx\\ &= (2\pi\varepsilon)^{-d}\|f\|^4_{L^2(\mathbb{R}^d)}.\end{aligned}$$

One then extends the result by density of Schwartz functions in $L^2(\mathbb{R}^d)$.
3. is essentially the same calculation as in 2.
4. is straightforward.
5. Real-valuedness comes from changing v to $-v$ in the integral. For non-positivity, we take f odd, that is, $f(x)=-f(-x)$, and evaluate in the origin, $W^\varepsilon[f](0,0)=-(\pi\varepsilon)^{-d}\|f\|_{L^2(\mathbb{R}^d)}$.

2.1.2. *Wigner transform as a distribution.* The action of the Wigner distribution on smooth compactly supported function simply expresses in terms of pseudodifferential operators. We have

$$\langle W^\varepsilon[f],a\rangle = \int_{\mathbb{R}^{2d}} a(x,\xi)W^\varepsilon[f](x,\xi)dxd\xi = (f,\mathrm{op}_\varepsilon(a)f)_{L^2(\mathbb{R}^d)} \tag{2.2}$$

for $f\in L^2(\mathbb{R}^d)$ and $a\in C_c^\infty(\mathbb{R}^{2d})$, where

$$\forall f\in\mathcal{S}(\mathbb{R}^d),\ \ \mathrm{op}_\varepsilon(a)f(x) = (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^{2d}} a\big(\tfrac12(x+y),\xi\big)\mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)}f(y)dy\,d\xi. \tag{2.3}$$

The properties of the semi-classical pseudodifferential operators then induce properties of the Wigner distribution. The more important ones are the following.

Proposition 2.3 (Wigner distributions)**.** *The Wigner distributions satisfy the following properties:*

(1) *For all $f\in L^2(\mathbb{R}^d)$, the map from $C_c^\infty(\mathbb{R}^d\times\mathbb{R}^d)$ to $\mathbb{C}$,*
$$a\mapsto\langle W^\varepsilon[f],a\rangle$$
is a distribution of finite order.
(2) *If $(f^\varepsilon)_{\varepsilon>0}$ is a bounded sequence in $L^2(\mathbb{R}^d)$ then $(W^\varepsilon[f^\varepsilon])_{\varepsilon>0}$ is a bounded sequence of tempered distributions in $\mathcal{S}'(\mathbb{R}^d\times\mathbb{R}^d,\mathbb{C}^{N\times N})$.*
(3) *If $(f^\varepsilon)_{\varepsilon>0}$ is a bounded sequence in $L^2(\mathbb{R}^d)$, then every limit point of $(W^\varepsilon[f^\varepsilon])_{\varepsilon>0}$ is a positive measure on $\mathbb{R}^d\times\mathbb{R}^d$.*

The distributional interpretation of Wigner transforms in terms of pseudo-differential operators is a powerful tool and in the two last points of Proposition 2.3 lay the fundament for the section about Wigner measures. Proposition 2.3 is proved at the end of Section 2.2.

2.1.3. *Wigner function of a pair of functions.* One sometimes extends the definition of Wigner transform to pairs of functions $f, g \in L^2(\mathbb{R}^d)$ by setting

$$W^\varepsilon[f,g](x,\xi) := (2\pi)^{-d} \int_{\mathbb{R}^d} f\left(x - \frac{\varepsilon v}{2}\right) \overline{g}\left(x + \frac{\varepsilon v}{2}\right) \mathrm{e}^{i\xi\cdot v} dv,$$

with the straightforward properties listed in the next statement.

Proposition 2.4. (1) *For all $f \in L^2(\mathbb{R}^d)$, $W^\varepsilon[f,f] = W^\varepsilon[f]$.*

(2) *For all $f, g \in L^2(\mathbb{R}^d)$, $W^\varepsilon[g,f] = \overline{W^\varepsilon[f,g]}$ and*

$$\int_{\mathbb{R}^{2d}} W^\varepsilon[f,g](x,\xi)\, dx d\xi = (g,f)_{L^2(\mathbb{R}^d)}.$$

(3) *For all $f_1, f_2, g_1, g_2 \in L^2(\mathbb{R}^d)$,*

$$(W^\varepsilon[f_1,g_1], W^\varepsilon[f_2,g_2])_{L^2(\mathbb{R}^{2d})} = (2\pi\varepsilon)^{-d} \left(f_1, f_2\right)_{L^2(\mathbb{R}^d)} \left(g_2, g_1\right)_{L^2(\mathbb{R}^d)}. \tag{2.4}$$

(4) *For all $(f,g) \in (L^2(\mathbb{R}^d))^2$ and $a \in C_c^\infty(\mathbb{R}^{2d})$,*

$$\langle W^\varepsilon[f,g], a\rangle = \left(g, \mathrm{op}_\varepsilon(a) f\right)_{L^2(\mathbb{R}^d)} = \left(\mathrm{op}_\varepsilon(\overline{a}) g, f\right)_{L^2(\mathbb{R}^d)}.$$

Proof

1, 2 and 4 come from the definition.

For 3, one writes

$$\begin{aligned}
&(W^\varepsilon[f_1,g_1], W^\varepsilon[f_2,g_2])_{L^2(\mathbb{R}^{2d})} \\
&= (2\pi\varepsilon)^{-2d} \int_{\mathbb{R}^{4d}} \overline{f}_1(x - \tfrac{v}{2}) g_1(x + \tfrac{v}{2}) f_2(x - \tfrac{v'}{2}) \overline{g}_2(x + \tfrac{v'}{2})\, \mathrm{e}^{i\xi\cdot(v'-v)/\varepsilon}\, dv\, dv'\, dx\, d\xi \\
&= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \overline{f}_1(x - \tfrac{v}{2}) g_1(x + \tfrac{v}{2}) f_2(x - \tfrac{v}{2}) \overline{g}_2(x + \tfrac{v}{2})\, dv\, dx \\
&= (2\pi\varepsilon)^{-d} \left(f_1, f_2\right)_{L^2(\mathbb{R}^d)} \left(g_2, g_1\right)_{L^2(\mathbb{R}^d)}.
\end{aligned}$$

Example 2.5. We consider two functions $f_1, f_2 \in L^2(\mathbb{R}^d)$ and two points in the phase space $z_1 = (x_1, \xi_1)$ and $z_2 = (x_2, \xi_2)$. Denote $Q = \frac{x_1 + x_2}{2}$, $P = \frac{\xi_1 + \xi_2}{2}$. Let

$$f_{z_j}^\varepsilon(x) = \varepsilon^{-\frac{d}{4}}\, \mathrm{e}^{\frac{i}{\varepsilon}\xi_j\cdot(x - x_j)} f_j\left(\frac{x - x_j}{\sqrt{\varepsilon}}\right), \quad x \in \mathbb{R}^d,\ j = 1, 2.$$

Then, the joint Wigner function satisfies for all $(x,\xi) \in \mathbb{R}^{2d}$,

$$\begin{aligned}
&W^\varepsilon[f_{z_1}^\varepsilon, f_{z_2}^\varepsilon](x,\xi) \\
&= W^\varepsilon[\mathrm{e}^{\frac{i}{\sqrt{\varepsilon}}\xi_1\cdot(x - \frac{x_1}{\sqrt{\varepsilon}})} f_1(x - \tfrac{x_1}{\sqrt{\varepsilon}}), \mathrm{e}^{\frac{i}{\sqrt{\varepsilon}}\xi_2\cdot(x - \frac{x_2}{\sqrt{\varepsilon}})} f_2(x - \tfrac{x_2}{\sqrt{\varepsilon}})] \left(\frac{x}{\sqrt{\varepsilon}}, \sqrt{\varepsilon}\xi\right) \\
&= \mathrm{e}^{\frac{i}{\varepsilon}(\xi_1 - \xi_2)\cdot(x - Q)}\, W^\varepsilon[f_1, f_2]\left(\frac{x - Q}{\sqrt{\varepsilon}}, \sqrt{\varepsilon}(\xi - P)\right) \\
&= \varepsilon^{-d}\, \mathrm{e}^{\frac{i}{\varepsilon}(\xi_1 - \xi_2)\cdot(x - Q)}\, W^1[f_1, f_2]\left(\frac{x - Q}{\sqrt{\varepsilon}}, \frac{\xi - P}{\sqrt{\varepsilon}}\right).
\end{aligned}$$

2.2. **Semi-classical calculus.** Let $a \in C_c^\infty(\mathbb{R}^{2d})$ and $\varepsilon \in]0,1]$ a small parameter. The *semi-classical pseudodifferential operator* of symbol a is the operator $\mathrm{op}_\varepsilon(a)$ defined on $\mathcal{S}(\mathbb{R}^d)$ by equation (2.3), namely

$$\mathrm{op}_\varepsilon(a) f(x) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} a\big(\tfrac{1}{2}(x+y), \xi\big) \mathrm{e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)} f(y) dy\, d\xi, \quad f \in \mathcal{S}(\mathbb{R}^d).$$

Note that there exists other choices of quantization.

The integral in (2.3) is convergent because f is rapidly decreasing, also for symbols $a = a(x,\xi)$ that are multi-variate polynomials in x and ξ the integral defining ${\rm op}_\varepsilon(a)f$ exists for $f \in \mathcal{S}(\mathbb{R}^d)$, since $f \in \mathcal{S}(\mathbb{R}^d)$ can compensate the polynomial growth. This property and those of the Fourier transform calls for a generalisation of the notation ${\rm op}_\varepsilon(a)$ to polynomial functions and one talks of ${\rm op}_\varepsilon(x)$ to denote the operator of multiplication with x, and of ${\rm op}_\varepsilon(\xi)$ for the differentiation operator $-i\varepsilon\partial_x$. In particular, one has the following example.

Example 2.6. We have ${\rm op}_\varepsilon(x\cdot\xi) = \frac{1}{2}\left({\rm op}_\varepsilon(x)\cdot {\rm op}_\varepsilon(\xi) + {\rm op}_\varepsilon(\xi)\cdot {\rm op}_\varepsilon(x)\right)$. Indeed, for all $f \in \mathcal{S}(\mathbb{R}^d)$,

$$\begin{aligned}{\rm op}_\varepsilon(x\cdot\xi)f(x) &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d} \tfrac{1}{2}(x+y)\cdot\xi\, {\rm e}^{i\xi\cdot(x-y)/\varepsilon} f(y)\,d\xi dy \\ &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d} \tfrac{1}{2}\left((ix\cdot\partial_y - iy\cdot\partial_x){\rm e}^{i\xi\cdot(x-y)/\varepsilon}\right) f(y)\,d\xi dy \\ &= \tfrac{1}{2}\left(x\cdot(-i\partial_x)f(x) - i\partial_x\cdot(xf(x))\right).\end{aligned}$$

Besides, if $c \in C^\infty(\mathbb{R}^d)$, then for $1 \le j,\ell \le d$,

$$\begin{aligned}&{\rm op}_\varepsilon\left(c(x)\xi_j\right) = \frac{\varepsilon}{i}\,c(x)\partial_{x_j} + \frac{\varepsilon}{2i}\partial_{x_j}c(x)\\ &{\rm op}_\varepsilon(c(x)\xi_j\xi_\ell) = -\varepsilon^2\partial_{x_\ell}\left(c(x)\partial_{x_j}\cdot\right) + \frac{i\varepsilon}{2}{\rm op}_\varepsilon\left(\xi_j\partial_{x_\ell}c(x) - \xi_\ell\partial_{\xi_j}c(x)\right) + \frac{\varepsilon^2}{4}\partial^2_{x_jx_\ell}c(x).\end{aligned}$$

2.2.1. *Action on* $L^2(\mathbb{R}^d)$. Let us now investigate how one can extend the action of ${\rm op}_\varepsilon(a)$ to square integrable functions. The kernel $(x,y)\mapsto k_\varepsilon(x,y)$ of the semi-classical pseudodifferential operator ${\rm op}_\varepsilon(a)$ is given by

$$\begin{aligned}k_\varepsilon(x,y) &= (2\pi\varepsilon)^{-d}\int_{\mathbb{R}^d} {\rm e}^{\frac{i}{\varepsilon}\xi\cdot(x-y)} a\big(\tfrac{1}{2}(x+y),\xi\big)d\xi \\ &= \varepsilon^{-d}\kappa_a\big(\tfrac12(x+y),\tfrac{1}{\varepsilon}(x-y)\big) \qquad (2.5)\end{aligned}$$

where

$$\kappa_a(X,v) = (2\pi)^{-d}\int_{\mathbb{R}^d} {\rm e}^{i\xi\cdot v} a\left(X,\xi\right)d\xi.$$

The function $\kappa_a(x,\cdot)$ is the inverse Fourier transform of $\xi\mapsto a(x,\xi)$, we write

$$\kappa_a(x,v) = \mathcal{F}^{-1}_{\xi\mapsto v}a\left(x,v\right). \tag{2.6}$$

The function $(x,v)\mapsto\kappa_a(x,v)$ is compactly supported in x and Schwartz class in v. Note that the link between a and κ_a also writes

$$a(x,\xi) = \int_{\mathbb{R}^d} {\rm e}^{-i\xi\cdot v}\kappa_a(x,v)dv. \tag{2.7}$$

The precise structure of the kernel of this operator calls for using the next Proposition.

Proposition 2.7. *Let P^ε be an operator of kernel $k_\varepsilon(x,y)$ of the form*

$$k^\varepsilon(x,y) = \varepsilon^{-d}\kappa\big(\tfrac12(x+y),\tfrac{1}{\varepsilon}(x-y)\big)$$

and such that K satisfies $\displaystyle\int \sup_{X\in\mathbb{R}^d}|\kappa(X,v|\,dv < +\infty$. Then, the operator P^ε is bounded in $L^2(\mathbb{R}^d)$ and

$$\|P^\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \le \int \sup_{X\in\mathbb{R}^d}|\kappa(X,v|\,dv.$$

Proof
For $f \in L^2(\mathbb{R}^d)$, we have

$$|P^\varepsilon f(x)| \leq \varepsilon^{-d} \int \sup_{X\in\mathbb{R}^d} \left|k_\varepsilon\big(X, \tfrac{x-y}{\varepsilon}\big)\right| \, |f(y)|dy.$$

Set $g^\varepsilon(x) = \varepsilon^{-d} \sup_{X\in\mathbb{R}^d} \left|k_\varepsilon\big(X, \frac{x}{\varepsilon}\big)\right|$, then $g^\varepsilon \in L^1(\mathbb{R}^d)$ and

$$\|g^\varepsilon\|_{L^1(\mathbb{R}^d)} = \int \sup_{X\in\mathbb{R}^d} |\kappa(X, v| \, dv.$$

We obtain by use of Young's convolution inequality for $p = 1$ and $q = r = 2$,

$$\|P^\varepsilon f\|_{L^2(\mathbb{R}^d)} \leq \|g^\varepsilon * f\|_{L^2(\mathbb{R}^d)} \leq \|g^\varepsilon\|_{L^1(\mathbb{R}^d)} \|f\|_{L^2(\mathbb{R}^d)} \leq \|f\|_{L^2(\mathbb{R}^d)} \left(\int \sup_{X\in\mathbb{R}^d} |\kappa(X, v| \, dv \right).$$

Note that the Young's convolution inequality is straightforward for this choice of indices.

As a consequence of Proposition 2.7, we obtain the boundedness in $\mathcal{L}(L^2(\mathbb{R}^d))$ of pseudodifferential operators. Indeed, for $\kappa = \kappa_a$ as in (2.6), we have

$$\int \sup_{x\in\mathbb{R}^d} |\kappa_a(x, v| \, dv \leq C \sup_{\substack{\beta\in\mathbb{N}^d \\ |\beta|\leq d+1}} \sup_{x\in\mathbb{R}^d} \|\partial_\xi^\beta a(x, \cdot)\|_{L^1(\mathbb{R}^d)}.$$

with $C = \int \langle v \rangle^{-d-1} dv$. In the following, we set

$$N_d(a) := \sup_{\substack{\beta\in\mathbb{N}^d \\ |\beta|\leq d+1}} \sup_{x\in\mathbb{R}^d} \|\partial_\xi^\beta a(x, \cdot)\|_{L^1(\mathbb{R}^d)}. \tag{2.8}$$

We observe that the norm $N_d(a)$ is controlled by Schwartz semi-norms: there exists a constant c_d depending only on d such that

$$N_d(a) \leq c_d \sup_{\substack{\beta\in\mathbb{N}^d \\ |\beta|\leq d+1}} \sup_{x\in\mathbb{R}^d} \left|(1 + |\xi|)^{d+1} \partial_\xi^\beta a(x, \xi)\right|. \tag{2.9}$$

The result is the following.

Theorem 2.8. *There exists a constant* $c > 0$ *which depends only on* d *such that for all* $a \in C_c^\infty(\mathbb{R}^{2d})$*,*

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq c \, N_d(a) \tag{2.10}$$

Let us define the ε-Fourier transform:

$$\forall f \in \mathcal{S}(\mathbb{R}^d), \quad \forall \xi \in \mathbb{R}^d, \quad \mathcal{F}^\varepsilon(f)(\xi) = (\pi\varepsilon)^{-d/2} \int_{\mathbb{R}^d} \mathrm{e}^{-\frac{i}{\varepsilon} x\cdot\xi} f(x) dx. \tag{2.11}$$

Then, if $\underline{a}(x, \xi) = a(-\xi, x)$, one has

$$(f, \mathrm{op}_\varepsilon(a) g)_{L^2(\mathbb{R}^d)} = (2\pi)^{-d} \left(\mathcal{F}^\varepsilon(f), \mathrm{op}_\varepsilon(\underline{a}) \mathcal{F}^\varepsilon(g)\right)_{L^2(\mathbb{R}^d)}, \quad f, g \in L^2(\mathbb{R}^d). \tag{2.12}$$

Therefore, one can get an estimate similar to (2.10) where the roles of x and ξ are exchanged:

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} = \|\mathrm{op}_\varepsilon(\underline{a})\|_{\mathcal{L}(L^2(\mathbb{R}^d))}.$$

which yields the estimate

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq c \sup_{\substack{\beta\in\mathbb{N}^d \\ |\beta|\leq d+1}} \sup_{\xi\in\mathbb{R}^d} \left\|\partial_x^\beta a(\cdot, \xi)\right\|_{L^1(\mathbb{R}^d)}. \tag{2.13}$$

Remark 2.9. Observe that the estimates (2.10) makes possible to define bounded semi-classical pseudo-differential operators with a symbol a which has few regularity in x, as long as a is measurable, compactly supported and that $\partial_\xi^\beta a$ is integrable for all $\beta \in \mathbb{N}^d$ such that $|\beta| \leq d+1$. And similarly exchanging the role of x and ξ, by estimate (2.13) .

The estimate the most used in the literature is the one obtained by Calderón and Vaillancourt in [12].

Theorem 2.10 (Calderón-Vaillancourt Theorem). *There exists $N \in \mathbb{N}^*$ and $C > 0$ such that for all $a \in C_c^\infty(\mathbb{R}^{2d})$,*

$$\|\mathrm{op}_\varepsilon(a)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C \sum_{\alpha\in\mathbb{N}^{2d}, |\alpha|\leq d+2} \varepsilon^{\frac{|\alpha|}{2}} \sup_{\mathbb{R}^d\times\mathbb{R}^d} |\partial_{x,\xi}^\alpha a| \tag{2.14}$$

2.2.2. *The adjoint and the composition of semi-classical pseudodifferential operators.* We introduce the notation for the Poisson bracket of two functions. For $f, g \in C^1(\mathbb{R}^d)$, we set

$$\{f, g\} = \nabla_\xi f \cdot \nabla_x g - \nabla_x f \cdot \nabla_\xi f. \tag{2.15}$$

This notation extends to matrix-valued functions, paying attention to the non-commutativity of the product on the set of matrices.

Proposition 2.11. *Let $a, b \in C_c^\infty(\mathbb{R}^{2d})$, then in $\mathcal{L}(L^2(\mathbb{R}^d))$,*

$$\mathrm{op}_\varepsilon(a)^* = \mathrm{op}_\varepsilon(\overline{a}), \tag{2.16}$$

$$\mathrm{op}_\varepsilon(a)\mathrm{op}_\varepsilon(b) = \mathrm{op}_\varepsilon(ab) + \frac{\varepsilon}{2i}\,\mathrm{op}_\varepsilon\left(\{a, b\}\right) + O\left(\varepsilon^2\right), \tag{2.17}$$

$$[\mathrm{op}_\varepsilon(a), \mathrm{op}_\varepsilon(b)] = \frac{\varepsilon}{i}\,\mathrm{op}_\varepsilon(\{a, b\}) + O\left(\varepsilon^3\right) \tag{2.18}$$

We are not going to prove this proposition but another one, with less complicated symbols but low regularity.

2.2.3. *Pseudo-differential calculus with low regularity.* With the observation (2.12) in mind, one can perform some symbolic calculus with low regularity in the ξ-variable. The reader will find applications where this calculus is used in [22] and [20]. We focus on Lipschitz regularity and consider the set $\mathrm{Lip}(\mathbb{R}^d)$ of continuous functions f such that

$$\exists L_f > 0, \ \ \forall x, y \in \mathbb{R}^d, \ \ |f(x) - f(y)| \leq L_f |x - y|.$$

Lemma 2.12. (1) *Suppose $\varrho \in \mathrm{Lip}(\mathbb{R}^d)$, and $a \in C_c^\infty(\mathbb{R}^{2d})$. Then, in $\mathcal{L}(L^2(\mathbb{R}^d))$*

$$\mathrm{op}_\varepsilon(a\,\varrho) = \mathrm{op}_\varepsilon(a)\varrho(x) + O\left(\varepsilon L_\rho N_d((1+\Delta_\xi)a)\right)$$
$$\mathrm{op}_\varepsilon(\varrho\, a) = \varrho(x)\mathrm{op}_\varepsilon(a) + O\left(\varepsilon L_\rho N_d((1+\Delta_\xi)a)\right).$$

(2) *Suppose $\varrho \in C^1(\mathbb{R}^d)$ with $\nabla\varrho \in \mathrm{Lip}(\mathbb{R}^d)$, and $a \in C_c^\infty(\mathbb{R}^{2d})$. Then, in $\mathcal{L}(L^2(\mathbb{R}^d))$*

$$[\mathrm{op}_\varepsilon(a), \varrho(x)] = \frac{\varepsilon}{i}\mathrm{op}_\varepsilon(\nabla_\xi a \cdot \nabla\varrho(x)) + O(\varepsilon^2 L_{\nabla\varrho} N_d(\Delta_\xi a)).$$

Note that the observation of (2.12):

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

induces that properties proved for $\varrho = \varrho(x)$ have their analogue for $\varrho = \varrho(\xi)$.

Proof

Point 1. We consider $R^\varepsilon := \mathrm{op}_\varepsilon(a\,\varrho) - \mathrm{op}_\varepsilon(a)\varrho(x)$. We have

$$R^\epsilon f(x) = \frac{1}{\varepsilon^d} \int_{\mathbb{R}^d} r^\varepsilon\left(\frac{x+y}{2}, \frac{x-y}{\varepsilon}\right) f(y)\, dy, \quad \forall f \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^N),$$

where $r^\varepsilon(x,v) := \mathcal{F}_\xi^{-1}a(x,v)(\varrho(x)-\varrho(x-\varepsilon v))$. By Proposition 2.7,

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

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

$$|\varrho(x)-\varrho(x-\varepsilon v)|_{\mathbb{C}^{N\times N}} \leq L_\varrho \varepsilon |v|, \quad \forall (v,x)\in \mathrm{supp}\mathcal{F}_\xi^{-1}a.$$

Therefore, using $|v||\mathcal{F}_\xi^{-1}a(x,v)| \leq (1+|v|^2)|\mathcal{F}_\xi^{-1}a(x,v)| = |\mathcal{F}_\xi^{-1}a(x,v)| + |\mathcal{F}_\xi^{-1}(-\Delta_\xi a)(x,v)|$, we deduce

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

Point 2. We observe that the kernel of $\tilde{R}^\varepsilon := [\mathrm{op}_\varepsilon(a),\varrho(x)] - \frac{\varepsilon}{i}\mathrm{op}_\varepsilon(\nabla_\xi a\cdot\nabla\varrho)$, is of the form (2.5) with

$$\begin{aligned}\tilde{r}^\varepsilon(x,v) &= \mathcal{F}_\xi^{-1}a(x,v)\,(\varrho(x)-\varrho(x-\varepsilon v)) - \frac{\varepsilon}{i}\mathcal{F}_\xi^{-1}\nabla_\xi a(v,x)\cdot\nabla\varrho(x)\\ &= \mathcal{F}_\xi^{-1}a(x,v)\,(\varrho(x)-\varrho(x-\varepsilon v)-\varepsilon v\cdot\nabla\varrho(x))\\ &= \varepsilon^2\theta(x,v)\mathcal{F}_\xi^{-1}a(x,v)\end{aligned}$$

with $|\theta(x,v)|\leq L_{\nabla\varrho}|v|^2$. Then, we conclude as before using $|v|^2\mathcal{F}_\xi^{-1}a = -\mathcal{F}_\xi^{-1}\Delta_\xi a$.

2.2.4. *Weak Gårding inequality.* Gårding inequality gives an answer to the question of the link between the positivity of the symbol a and the positivity of the operator $\mathrm{op}_\varepsilon(a)$. We prove here a weak version of the Gårding inequality.

Proposition 2.13 (Weak Gårding inequality)**.** *Let $a\in C_c^\infty(\mathbb{R}^{2d})$ such that $a\geq 0$. Then, for all $\delta>0$, there exists $C_\delta>0$ such that for all $f\in L^2(\mathbb{R}^d)$,*

$$(f,\mathrm{op}_\varepsilon(a)f)_{L^2(\mathbb{R}^d)} \geq -(\delta+C_\delta\varepsilon^2)\|f\|^2_{L^2(\mathbb{R}^d)}, \quad \forall f\in L^2(\mathbb{R}^d). \tag{2.19}$$

Remark 2.14. This estimate can be ameliorated into: if $a\geq 0$, there exists a constant $C_a>0$ such that

$$(f,\mathrm{op}_\varepsilon(a)f)\geq C_a\varepsilon\|f\|_{L^2},\ \ \forall f\in L^2(\mathbb{R}^d)$$

Besides, with the assumptions of Proposition 2.13, one can prove the Fefferman-Phong inequality (cf. [48] for a detailed proof):

$$\exists C>0,\quad \forall f\in L^2(\mathbb{R}^d),\quad (f,\mathrm{op}_\varepsilon(a)f)_{L^2(\mathbb{R}^d)}\geq -C\varepsilon^2\|f\|^2_{L^2(\mathbb{R}^d)}.$$

However, the easiest version of Proposition 2.13 is enough for our purpose.

Proof
We associate with a a function $\chi\in C_c^\infty(\mathbb{R}^{2d})$ such that $\chi=1$ on the support of a and we set for some $\lambda>0$ to be fixed later

$$b_\delta(x,\xi)=\chi(x,\xi)\big(a(x,\xi)+\lambda\,\delta\big)^{1/2}.$$

The function b_δ is in $C_c^\infty(\mathbb{R}^{2d})$ and satisfies

$$b_\delta(x,\xi)^2 = a(x,\xi)+\lambda\,\delta\,\chi^2(x,\xi).$$

Therefore, using $\{b_\delta,b_\delta\}=0$, the symbolic calculus gives in $\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\mathrm{op}_\varepsilon(b_\delta)^*\mathrm{op}_\varepsilon(b_\delta) = \mathrm{op}_\varepsilon(a)+\lambda\,\delta\,\mathrm{op}_\varepsilon(\chi^2(x,\xi))+O(\varepsilon^2).$$

Let us now choose λ so that we have

$$\lambda\,\|\mathrm{op}_\varepsilon(\chi^2(x,\xi))\|_{\mathcal{L}(L^2(\mathbb{R}^d))}\leq 1,$$

then, for all $f \in L^2(\mathbb{R}^d)$,

$$\begin{aligned} 0 \leq \|\mathrm{op}_\varepsilon(b_\delta) f\|^2 &= (f, \mathrm{op}_\varepsilon(b_\delta)^* \mathrm{op}_\varepsilon(b_\delta) f)_{L^2(\mathbb{R}^d)} \\ &= (f, \mathrm{op}_\varepsilon(a) f)_{L^2(\mathbb{R}^d)} + \lambda\delta \left(f, \mathrm{op}_\varepsilon(\chi^2(x,\xi)) f\right)_{L^2(\mathbb{R}^d)} + O\left(\varepsilon^2 \|f\|^2_{L^2(\mathbb{R}^d)}\right) \\ &\leq (f, \mathrm{op}_\varepsilon(a) f)_{L^2(\mathbb{R}^d)} + \delta \|f\|^2_{L^2(\mathbb{R}^d)} + O\left(\varepsilon^2 \|f\|^2_{L^2(\mathbb{R}^d)}\right), \end{aligned}$$

whence the result.

2.2.5. *Proof of Proposition 2.3.* Points 1. and 2. are a consequence of (2.10) and (2.2).
For Point 3, we observe that Gårding inequality of Proposition 2.13 implies that every accumulation point of $(W^\varepsilon[f^\varepsilon])$ in $\mathcal{S}'(\mathbb{R}^d \times \mathbb{R}^d)$ is a positive distribution and therefore, a positive measure on $\mathbb{R}^d \times \mathbb{R}^d$, as detailed in the proof of the next Theorem 2.15.

2.3. **Wigner measures.**

2.3.1. *Definition.* In this section, we continue with the observation of Point 3 in Proposition 2.3 and analyze the properties of the weak limits of the Wigner transform.

Theorem 2.15. *Let $(f^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$. There exists a sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ which tends to 0 when n goes to $+\infty$ and a positive measure μ on $\mathbb{R}^{2d}$ such that*

$$\forall a \in C_c^\infty(\mathbb{R}^{2d}),\ \left(f^{\varepsilon_n}, \mathrm{op}_{\varepsilon_n}(a) f^{\varepsilon_n}\right)_{L^2(\mathbb{R}^d)} \underset{n\to+\infty}{\longrightarrow} \int_{\mathbb{R}^{2d}} a(x,\xi)\mu(dx,d\xi). \tag{2.20}$$

Moreover $\mu(\mathbb{R}^{2d}) < +\infty$.

Any measure $\mu \in \mathcal{M}_+(\mathbb{R}^{2d})$ satisfying (2.20) for some sequence $(\varepsilon_n)_{n\in\mathbb{N}}$ is called *Wigner measure* or *semi-classical measure* of the family $(f^\varepsilon)_{\varepsilon>0}$. A given family $(f^\varepsilon)_{\varepsilon>0}$ may have several Wigner measures.

The use of Wigner measures developed in the 90s, in particular with the articles [34] by Pierre-Louis Lions, Thierry Paul and [24] by Patrick Gérard, Éric Leichtnam (see also [22] and [25]). They first appear in [26] in the frame of the analysis of sequences of eigenfunctions of a Laplace Beltrami operator on a compact manifold (see also [6] and [7] for similar problematic on the torus).

Proof
Since the quantity $I_\varepsilon(a) = (f^\varepsilon, \mathrm{op}_\varepsilon(a) f^\varepsilon)_{L^2(\mathbb{R}^d)}$ is uniformly bounded in ε, for a given function $a \in C_c^\infty(\mathbb{R}^{2d})$, one can find an extracted convergent subsequence $I_{\varepsilon_{n,a}}(a)$. Considering a dense countable subset of $C_c^\infty(\mathbb{R}^{2d})$ and using a diagonal extraction process, one builds a sequence ε_n for which $I_{\varepsilon_n}(a)$ has a limit for all $a \in C_c^\infty(\mathbb{R}^{2d})$. The map which sends a on the limit $I(a)$ of the sequence $I_{\varepsilon_n}(a)$ is a linear form on $C_c^\infty(\mathbb{R}^{2d})$. It defines a distribution and Gårding inequality shows that this distribution is positive.

It remains to prove that I satisfies a measure estimate. We consider a nonincreasing function $\chi \in C_c^\infty([0,+\infty))$ such that $0 \leq \chi \leq 1$, $\chi(u) = 0$ for $u \geq 2$ and $\chi(u) = 1$ for $0 \leq u \leq 1$. We set $\chi_R = \chi\left(\frac{\cdot}{R}\right)$. Then, we deduce from

$$\left(f^\varepsilon, \mathrm{op}_\varepsilon(\chi_R(x^2+\xi^2)) f^\varepsilon\right)_{L^2(\mathbb{R}^d)} \leq C$$

that $I(\chi_R(x^2+\xi^2)) < +\infty$ and is uniformly bounded in R. Moreover, the function $R \mapsto I(\chi_R(x^2+\xi^2))$ is nondecreasing and we can set

$$I(1) := \lim_{R\to+\infty} I(\chi_R(x^2+\xi^2)).$$

Then, the positivity of I yields

$$\forall a \in C_c^\infty(\mathbb{R}^{2d}), \quad I\big(\|a\|_{L^\infty(\mathbb{R}^{2d})} - a\big) \geq 0,$$

which implies the measure's type control that we were seeking:

$$\forall a \in C_c^\infty(\mathbb{R}^{2d}), \quad I(a) \leq C\,\|a\|_{L^\infty(\mathbb{R}^{2d})}.$$

Therefore, the linear form I defines a positive finite measure μ on $\mathbb{R}^{2d}$.

2.3.2. *Examples.* Let us compute the Wigner measures associated with some exemplary families.

Example 2.16. Let $x_0, \xi_0 \in \mathbb{R}^d$ and $\varphi \in L^2(\mathbb{R}^d)$.

(1) *Concentration.* Let $u^\varepsilon(x) = \varepsilon^{-d/2}\varphi\left(\frac{\xi-\xi_0}{\varepsilon}\right)$, then $(u^\varepsilon)_{\varepsilon>0}$ has a unique Wigner measure

$$\mu_u(dx, d\xi) = (2\pi)^{-d}\,\delta_{x_0}(x) \otimes |\widehat{\varphi}(\xi)|^2 d\xi.$$

(2) *Oscillation.* Let $v^\varepsilon(x) = \varphi(x)\mathrm{e}^{ix\cdot\xi_0/\varepsilon}$, then $(v^\varepsilon)_{\varepsilon>0}$ has a unique Wigner measure

$$\mu_v(dx, d\xi) = |\varphi(x)|^2 dx \otimes \delta_{\xi_0}(\xi).$$

Note that the ε-Fourier transform transforms an oscillation in position into a concentration in impulsion, and conversely

$$\mathcal{F}^\varepsilon u^\varepsilon(\xi) = \mathrm{e}^{-\frac{i}{\varepsilon}x_0\cdot\xi}\mathcal{F}^1\varphi(\xi) \;\text{ and }\; \mathcal{F}^\varepsilon v^\varepsilon = \varepsilon^{-\frac{d}{2}}\mathcal{F}^1\varphi\left(\frac{\xi-\xi_0}{\varepsilon}\right).$$

The Wigner measure of a family $(f^\varepsilon)_{\varepsilon>0}$ provides information about the strong convergence of this family. In example (1) above, it is the point x_0 of the configuration space that is the obstruction to the strong convergence of u^ε to 0 in the sense that if x_0 is not on the support of $\phi \in C_c^\infty(\mathbb{R}^d)$, then $(\phi, u^\varepsilon)_{L^2(\mathbb{R}^d)}$ goes to 0 as ε goes to 0. Similarly, for the oscillation family $(v^\varepsilon)_{\varepsilon>0}$ of example (2), it is the point ξ_0 of the momentum space that is the obstruction and $(\phi, u^\varepsilon)_{L^2(\mathbb{R}^d)}$ will go to 0 if ξ_0 is not in the support of the $\widehat{\phi}$.

Another important class consists in *Coherent states.*

Example 2.17. Let $\alpha \in (0,1)$, $\beta > 0$ and

$$u^\varepsilon_{\alpha,\beta} = \varepsilon^{-d\alpha/2}\varphi\left(\frac{\xi-\xi_0}{\varepsilon^\alpha}\right)\mathrm{e}^{ix\cdot\xi_0/\varepsilon^\beta},$$

then $(u_\varepsilon^{\alpha,\beta})_{\varepsilon>0}$ has a unique Wigner measure

$$\mu_{\alpha,\beta}(x,\xi) = \begin{cases} \delta_{x_0}(x) \otimes \delta_{\xi_0}(\xi) & \text{if } \beta = 1 \\ \delta_{x_0}(x) \otimes \delta_0(\xi) & \text{if } \beta < 1 \\ 0 & \text{if } \beta > 1 \end{cases}.$$

Notice that when $\beta > 1$, the family $(u^\varepsilon_{\alpha,\beta})_{\varepsilon>0}$ is not ε-oscillating and its Wigner measures at the scale ε do not capture its mass. The coherent states for which $\alpha = \frac{1}{2}$ and $\beta = 1$ are called *wave packets.*

The *WKB states* are often used in semi-classical analysis (see [11]).

Example 2.18. Let $S \in C^2(\mathbb{R}^d)$ and $g^\varepsilon(x) = \mathrm{e}^{\frac{i}{\varepsilon}S(x)}\varphi(x)$, then $(g^\varepsilon)_{\varepsilon>0}$ has a unique Wigner measure

$$\mu_S(x,\xi) = |\varphi(x)|^2 dx \otimes \delta_{\nabla S(x)}(\xi).$$

Proof
We have for $a \in \mathcal{S}(\mathbb{R}^{2d})$,

$$(g^\varepsilon, \mathrm{op}_\varepsilon(a)g^\varepsilon)_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^{2d}} \mathcal{F}_\xi^{-1}(X,v)\mathrm{e}^{\frac{i}{\varepsilon}(S(X+\varepsilon\frac{v}{2})-S(X-\varepsilon\frac{v}{2}))}\overline{\varphi}\left(X+\varepsilon\frac{v}{2}\right)\varphi\left(X-\varepsilon\frac{v}{2}\right)dX\,dv$$

and the result follows from Lebesgue dominated convergence Theorem.

Actually, the proof shows that the result extends to functions S for which there exists a function $\nabla S \in L^\infty(\mathbb{R}^d)$ such that

$$\forall x, v \in \mathbb{R}^d, \;\; \frac{1}{t}(S(x) - S(x+tv)) \underset{t\to 0}{\longrightarrow} \nabla S(x)\cdot v.$$

When $\nabla S \neq 0$ almost everywhere, one deduces from the result on the measure that WKB states with phase of low regularity goes weakly to 0 in L^2.

2.3.3. *Wigner measures and ε-oscillation.* One can wonder how using Wigner measures may help to calculate the weak limits of energy densities, since the measures are obtained by testing against smooth, compactly supported functions a. In particular, the symbols a are compactly supported in the Fourier variable ξ, while the limits that we wanted to compute do not present cut-off in frequencies. This question is solved via the notion of *ε-oscillation* which allows to link the Wigner measures with the accumulation points of the energy density, provided that the family of functions under investigation is ε-oscillating.

Definition 2.19. A family $(f^\varepsilon)_{\varepsilon>0}$ in $L^2(\mathbb{R}^d)$ is ε-oscillating if

$$\limsup_{\varepsilon\to 0} \int_{|\xi|>R/\varepsilon} \left|\widehat{f}^\varepsilon(\xi)\right|^2 d\xi \underset{R\to+\infty}{\longrightarrow} 0, \tag{2.21}$$

Remark 2.20. If a family $(f^\varepsilon)_{\varepsilon>0}$ in $L^2(\mathbb{R}^d)$ has a H^s_ε norm uniformly bounded for some $s>0$:

$$\exists C>0, \;\; \|\langle\varepsilon D\rangle^s f^\varepsilon\|_{L^2(\mathbb{R}^d)} \leq C,$$

then, using that $\mathbf{1}_{|\varepsilon D|\geq R} \leq R^{-2s}\langle\varepsilon D\rangle^{2s}$, one obtains that this family is ε-oscillating. Indeed,

$$\begin{aligned}\int_{|\xi|>R/\varepsilon} \left|\widehat{f}^\varepsilon(\xi)\right|^2 d\xi &= \left(\mathbf{1}_{|\varepsilon D|\geq R} f^\varepsilon, f^\varepsilon\right)_{L^2(\mathbb{R}^d)} \\ &\leq R^{-2s}\left(\langle\varepsilon D\rangle^{2s} f^\varepsilon, f^\varepsilon\right)_{L^2(\mathbb{R}^d)} \leq C^2 R^{-2s} \underset{R\to+\infty}{\longrightarrow} 0.\end{aligned}$$

The families of Example 2.16 are ε-oscillating. We exemplarily verify this claim for the concentration family $(u^\varepsilon)_{\varepsilon>0}$. Indeed, for any $R>0$,

$$\begin{aligned}\int_{|\xi|>R/\varepsilon} |\widehat{u}^\varepsilon(\xi)|^2 d\xi &= \varepsilon^{-d}\int_{|\xi|>R/\varepsilon}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \overline{\varphi}(\tfrac{\xi-\xi_0}{\varepsilon})\varphi(\tfrac{y-x_0}{\varepsilon})\mathrm{e}^{i\xi\cdot(x-y)}d(x,y,\xi) \\ &= \int_{|\xi|>R}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}\overline{\varphi}(x)\varphi(y)\mathrm{e}^{i\xi\cdot(x-y)}d(x,y,\xi) \\ &= \int_{|\xi|>R}|\varphi(\xi)|^2 d\xi \underset{R\to+\infty}{\longrightarrow} 0.\end{aligned}$$

Proposition 2.21 ([22, 24, 25])**.** *If $\mu \in \mathcal{M}_+(\mathbb{R}^d\times\mathbb{R}^d)$ is an accumulation point of $(W^\varepsilon[f^\varepsilon])_{\varepsilon>0}$ along some subsequence $(\varepsilon_n)_{n\in\mathbb{N}}$, and if the measure $|f^{\varepsilon_n}(x)|^2dx$ converges weakly towards a measure $\nu \in \mathcal{M}_+(\mathbb{R}^d)$ then*

$$\int_{\mathbb{R}^d}\mu(\cdot, d\xi) \leq \nu. \tag{2.22}$$

Equality holds in (2.22) *if and only if $(f^\varepsilon)_{\varepsilon>0}$ is ε-oscillating.*

Proof

We use the function $\chi_R = \chi\left\{\frac{\cdot}{R}\right)$ where $\chi \in C^\infty_C(\mathbb{R}, [0,1])$ is compactly supported in $\{|\xi] \leq 2\}$. For $R>0$ and $\varphi \in C^\infty_c(\mathbb{R}^d)$, $\varphi \geq 0$, we have

$$\int_{\mathbb{R}^d}\varphi(x)|f^{\varepsilon_n}(x)|^2dx = \left(f^{\varepsilon_n}, \varphi(1-\chi_R)\left(\varepsilon_n D\right)f^{\varepsilon_n}\right) + \left(f^{\varepsilon_n}, \varphi\chi_R\left(\varepsilon_n D\right)f^{\varepsilon_n}\right).$$

Besides,

$$\lim_{n\to+\infty}\left(f^{\varepsilon_n},\varphi\chi_R\left(\varepsilon_n D\right)f^{\varepsilon_n}\right)=\int_{\mathbb{R}^{2d}}\varphi(x)\chi(\xi/R)\mu(dx,d\xi)$$

and, in view of

$$\begin{aligned}\left(f^{\varepsilon_n},\varphi(1-\chi_R)\left(\varepsilon_n D\right)f^{\varepsilon_n}\right) &= \int_{\mathbb{R}^d}\varphi(x)|(1-\chi_R)(\varepsilon_n D)f^{\varepsilon_n}(x)|^2dx\\ &\quad+\left(\chi_R\left(\varepsilon_n D\right)f^{\varepsilon_n},\varphi(1-\chi_R)\left(\varepsilon_n D\right)f^{\varepsilon_n}\right)\\ &\geq \left(\chi_R\left(\varepsilon_n D/R\right)f^{\varepsilon_n},\varphi(1-\chi_R)\left(\varepsilon_n D\right)f^{\varepsilon_n}\right),\end{aligned}$$

we have

$$\lim_{n\to+\infty}\left(f^{\varepsilon_n},\varphi(1-\chi_R)\left(\varepsilon_n D\right)f^{\varepsilon_n}\right)\geq\int_{\mathbb{R}^{2d}}\varphi(x)\chi_R(\xi)(1-\chi_R(\xi))\mu(dx,d\xi).$$

We deduce that for all $R>0$,

$$\liminf_{n\to+\infty}\int_{\mathbb{R}^d}\varphi(x)|f^{\varepsilon_n}(x)|^2dx\geq\int_{\mathbb{R}^{2d}}\varphi(x)\chi_R(\xi)\mu(dx,d\xi)+\int_{\mathbb{R}^{2d}}\varphi(x)\chi_R(\xi)(1-\chi_R(\xi))\mu(dx,d\xi).$$

Using Fatou lemma, we have

$$\liminf_{R\to+\infty}\int_{\mathbb{R}^{2d}}\varphi(x)\chi_R(\xi)\mu(dx,d\xi)\geq\int_{\mathbb{R}^{2d}}\varphi(x)\liminf_{R\to+\infty}\chi_R(\xi)\mu(dx,d\xi)=\int_{\mathbb{R}^{2d}}\varphi(x)\mu(dx,d\xi).$$

Moreover

$$\liminf_{R\to+\infty}\int_{\mathbb{R}^{2d}}\varphi(x)\chi_R(\xi)(1-\chi_R(\xi))\mu(dx,d\xi)\geq 0.$$

Therefore,

$$\liminf_{n\to+\infty}\int_{\mathbb{R}^d}\varphi(x)|f^{\varepsilon_n}(x)|^2dx\geq\int_{\mathbb{R}^{2d}}\varphi(x)\mu(dx,d\xi).$$

One notices that the ε-oscillation property implies that for χ as before,

$$\limsup_{n\to+\infty}\left(\varphi\left(1-\chi_R\left(\varepsilon_n D\right)\right)f^{\varepsilon_n},f^{\varepsilon_n}\right)\underset{R\to+\infty}{\longrightarrow}0.$$

We then get the result by letting n and then R go to $+\infty$ in the equality

$$\begin{aligned}\int_{\mathbb{R}^d}\varphi(x)|f^{\varepsilon_n}(x)|^2dx &= \left(f^{\varepsilon_n},\varphi\chi_R\left(\varepsilon_n D\right)f^{\varepsilon_n}\right)+\left(f^{\varepsilon_n},\varphi\left(1-\chi_R\left(\varepsilon_n D\right)\right)f^{\varepsilon_n}\right)\\ &= \left(f^{\varepsilon_n},\mathrm{op}_{\varepsilon_n}\left(\varphi(x)\chi_R\left(\xi\right)\right)f^{\varepsilon_n},\right)+\left(f^{\varepsilon_n},\varphi(x)\left(1-\chi_R\left(\varepsilon_n D\right)\right)f^{\varepsilon_n}\right)\\ &\quad+O(\varepsilon_n).\end{aligned}$$

2.3.4. *Wigner measures of vector-valued families and orthogonality.* Suppose now that $(f^\varepsilon)_{\varepsilon>0}$ is a bounded sequence in $L^2(\mathbb{R}^d,\mathbb{C}^N)$; then one can consider the N by N matrix

$$W^\varepsilon[f^\varepsilon](x,\xi)=(W^\varepsilon[f_i^\varepsilon,f_j^\varepsilon](x,\xi))_{1\leq i,j\leq N},\ \ x,\xi\in\mathbb{R}^d.$$

The family $W^\varepsilon[f^\varepsilon])_{\varepsilon>0}$ is a distribution acting on matrix-valued Schwartz functions via

$$\langle a,W^\varepsilon[f^\varepsilon]\rangle=\int_{\mathbb{R}^{2d}}\mathrm{Tr}_{\mathbb{C}^N}(a(x,\xi)W^\varepsilon[f^\varepsilon](x,\xi))dxd\xi,\ \ a\in\mathcal{S}(\mathbb{R}^{2d},\mathbb{C}^{N,N}).$$

Its accumulation points are called *semi-classical* or *Wigner measures* of the sequence $(f^\varepsilon)_{\varepsilon>0}$. The coefficients $(\mu_{i,j})_{1\leq i,j\leq N}$ of this matrix-valued distribution are measures. Indeed, the diagonal ones are positive measures, as Wigner measures of the sequences $(f_i^\varepsilon)_{\varepsilon>0}$, the coordinates functions of $(f^\varepsilon)_{\varepsilon>0}$. Moreover, denoting by ε_ℓ the subsequence $(f^{\varepsilon_\ell})_{\ell\in\mathbb{N}}$ giving the semi-classical measure μ, one has

$$\forall a\in C_c^\infty(\mathbb{R}^{2d}),\quad\lim_{\ell\to\infty}\left(\mathrm{op}_\varepsilon(a)f_i^{\varepsilon_\ell},f_j^{\varepsilon_\ell}\right)_{L^2(\mathbb{R}^d)}=\int_{\mathbb{R}^{2d}}a(x,\xi)\mu_{i,j}(dx,d\xi),\tag{2.23}$$

Therefore, the distributions $\mu_{i,j}$ are express as linear combination of Wigner measures of linear combination of the $(f_j^\varepsilon)_{1\leq j\leq N}$, and thus are Radon measures.

In other words, μ takes values in the set of Hermitian positive semi-definite matrices: the elements $\mu_{i,i}$ are positive (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:

$$\mu_{i,i}\perp\mu_{j,j} \implies \forall a\in C_c^\infty(\mathbb{R}^{2d}),\quad \lim_{\ell\to\infty}\left(\mathrm{op}_\varepsilon(a)f_i^{\varepsilon_\ell},f_j^{\varepsilon_\ell}\right)_{L^2(\mathbb{R}^d)}=0. \tag{2.24}$$

Remark 2.22. One can generalize the above study to a more general setting by considering L^2 families from $\mathbb{R}^d$ into some Hilbert space $\mathcal{H}$. One then defines pseudodifferential operators with symbol $a(x,\xi)$ which are compact operators on $\mathcal{H}$ and semi-classical measures are positive elements of the dual to $C_c^\infty(\mathbb{R}^{2d},\mathcal{K}(\mathcal{H}))$, that is elements of $C_c^\infty(\mathbb{R}^{2d},\mathcal{L}^1_+(\mathcal{H}))$, where $\mathcal{K}(\mathcal{H})$ denotes the set of compact operators on $\mathcal{H}$, $\mathcal{L}^1(\mathcal{H})$ the set of trace class operators on $\mathcal{H}$ and $\mathcal{L}^1_+(\mathcal{H})$ the subset of its positive elements.

The above description has important consequences when passing to the limit in bilinear quantities depending on two families.

Lemma 2.23 (Orthogonality lemma)**.** *Let $(f^\varepsilon)_{\varepsilon>0}$ and $(g^\varepsilon)_{\varepsilon>0}$ be two bounded families in $L^2(\mathbb{R}^d)$. We assume that each of them has only one Wigner measure that we denote by μ_f and μ_g respectively. Assume $\mu_f\perp\mu_g$, then for all $a\in C_c^\infty(\mathbb{R}^{2d})$, $(f^\varepsilon,\mathrm{op}_\varepsilon(a)g^\varepsilon)\underset{\varepsilon\to0}{\longrightarrow}0$.*

Moreover, if the families are ε-oscillating, then for all $\varphi\in C_c^\infty(\mathbb{R}^d)$, $\displaystyle\int_{\mathbb{R}^d}\varphi(x)g^\varepsilon(x)\overline{f^\varepsilon(x)}dx\underset{\varepsilon\to0}{\longrightarrow}0$.

In that situation, one says that the families $(f^\varepsilon)_{\varepsilon>0}$ and $(g^\varepsilon)_{\varepsilon>0}$ are *orthogonal families*.

This sort of result is at the origine of the emergence of the concept of microlocal defect measures, also called H-measures, which are the non semi-classical version of Wigner measures. They were introduced independently and simultaneously in [23] and [45] and allow generalizations of div-curl Lemma in the context of homogeneization.

Proof

One considers the vector valued family $\Psi^\varepsilon=(f^\varepsilon,g^\varepsilon)$ and one of its Wigner measures μ, which is a 2×2 matrix with diagonal elements μ_f and μ_g. The off-diagonal elements of μ are absolutely continuous with respect to μ_f and μ_g and thus are 0 if $\mu_f\perp\mu_g$. This implies the first statement of the Lemma. The second one comes by combining the previous result with ε-oscillation.

2.4. **Wigner measures and time-dependent families.** We are now interested in time-dependent families, such as the family $(\psi^\varepsilon(t))_{\varepsilon>0}$ of solutions to the Schrödinger equation (1.1). 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 $L^\infty(\mathbb{R}_t;L^2(\mathbb{R}^d_x))$ and define the *time-dependent Wigner transform* $W^\varepsilon_{\psi^\varepsilon}(t)$ as

$$W^\varepsilon_{\psi^\varepsilon}(x,\xi):=W^\varepsilon[\psi^\varepsilon(t,\cdot)](x,\xi)=\int_{\mathbb{R}^d}\mathrm{e}^{i\xi\cdot v}\psi^\varepsilon\left(t,x-\frac{\varepsilon v}{2}\right)\overline{\psi^\varepsilon}\left(t,x+\frac{\varepsilon v}{2}\right)\frac{dv}{(2\pi)^d}. \tag{2.25}$$

Proposition 2.24. *Any accumulation point μ of the family $(W^\varepsilon_{\psi^\varepsilon})_{\varepsilon>0}$ in $\mathcal{S}'(\mathbb{R}\times\mathbb{R}^{2d})$ is a positive Radon measure μ on $\mathbb{R}\times\mathbb{R}^{2d}$ of the form $\mu(dt,dx,d\xi)=\mu^t(dx,d\xi)dt$.*

Such a measure $\mu^t dt$ is called *Wigner measure* or *semi-classical measure* of the time-dependent family $(\psi^\varepsilon)_{\varepsilon>0}$.

Proof

Estimates (2.10) (or (2.14)) implies that for every $\theta\in L^1(\mathbb{R})$ and every $a\in C_c^\infty(\mathbb{R}^{2d})$,

$$\left|\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}}\theta(t)a(x,\xi)W^\varepsilon_{\psi^\varepsilon}(t,x,\xi)dx\,d\xi\,dt\right|\leq C_d\|\psi^\varepsilon\|^2_{L^\infty(\mathbb{R}_t;L^2(\mathbb{R}^d_x))}\|\theta\|_{L^1(\mathbb{R})}N_d(a). \tag{2.26}$$

This ensures that $(W^\varepsilon_{\psi^\varepsilon})$ is bounded in $\mathcal{S}'(\mathbb{R}\times\mathbb{R}^{2d})$. Moreover, any accumulation point μ of this sequence is a positive Radon measure on $\mathbb{R}\times\mathbb{R}^{2d}$. It follows from (2.26) 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 (see Theorem 9.1 in [1] or Section 2.5 of [2]) the existence of a measurable map from $t\in\mathbb{R}$ to positive, 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 $(W^{\varepsilon_\ell}_{\psi^{\varepsilon_\ell}})$ converges in the sense of distributions the following holds: for all $\theta\in L^1(\mathbb{R})$ and $a\in C^\infty_c(\mathbb{R}^{2d})$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}}\theta(t)a(x,\xi)W^{\varepsilon_\ell}_{\psi^{\varepsilon_\ell}}(t,x,\xi)dx\,d\xi\,dt\underset{\ell\to\infty}{\longrightarrow}\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}}\theta(t)a(x,\xi)\mu^t(dx,d\xi)dt. \tag{2.27}$$

If the sequence $(\psi^{\varepsilon_\ell}(t,\cdot))$ is in addition ε-oscillating 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 $\theta\in L^1(\mathbb{R})$, $\phi\in C_0(\mathbb{R}^d)$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^d}\theta(t)\phi(x)|\psi^{\varepsilon_\ell}(t,x)|^2dx\underset{\ell\to\infty}{\longrightarrow}\int_{\mathbb{R}}\int_{\mathbb{R}^d}\theta(t)\phi(x)\mu^t(dx,d\xi)\,dt. \tag{2.28}$$

Remark 2.25. Time-dependent analogues of (2.23), (2.24) also hold after replacing $\mu_{i,j}$ by $\mu^t_{i,j}$ and averaging in the t-variable.

3. Floquet-Bloch theory

.
In this section, we consider the operator on $L^2(\mathbb{T}^d)$ defined by

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

In the next sections, we focus on the spectral analysis of the operator $P(\xi)$ for $\xi \in \mathbb{R}^d$ (Section 3.1). It turns out that much more can be said in dimension 1 (see Section 3.2) than in higher dimension. We discuss regularity issues in Section 3.3.

3.1. Spectral analysis of the operator $P(\xi)$.

One associates with the lattice $\mathbb{Z}^d$ its *dual lattice* $2\pi\mathbb{Z}^d$. The *centered fundamental domain* of $2\pi\mathbb{Z}^d$ is called the *Brillouin zone*:

$$\mathcal{B} = [-\pi, \pi[^d\,.$$

Note that if $\xi \in \mathbb{R}^d$, there exists a unique decomposition

$$\xi = \eta + 2\pi k, \ \ k \in \mathbb{Z}^d \ \text{ and } \ \eta \in \mathcal{B}.$$

The operator $P(\xi)$ has the important property that, for $k \in \mathbb{Z}^d$ and $\xi \in \mathbb{R}^d$, the operator $P(\xi + 2\pi k)$ is unitarily equivalent to $P(\xi)$. More precisely, one has

$$P(\xi + 2\pi k) = {\rm e}^{-i2\pi\langle k,\cdot\rangle} P(\xi) {\rm e}^{i2\pi\langle k,\cdot\rangle}, \ \ \forall \xi \in \mathbb{R}^d, \ \ \forall k \in \mathbb{Z}^d. \tag{3.1}$$

Therefore, we can restrict our analysis to $\xi \in \mathcal{B}$.

For $\xi \in \mathbb{R}^d$, we shall denote by $P_0(\xi)$ the operator $P_0(\xi) = |D_y + \xi|^2$ acting on the space $L^2(\mathbb{T}^d)$

$$L^2(\mathbb{T}^d) = \left\{ f(y) = \sum_{k\in\mathbb{Z}^d} c_k {\rm e}^{2i\pi k\cdot y}, \ \ \sum_{k\in\mathbb{Z}^d} |c_k|^2 < +\infty \right\}.$$

Both $P(\xi)$ and $P_0(\xi)$ have ξ-independent domain $H^2(\mathbb{T}^d) \subset L^2(\mathbb{T}^d)$ where for $s > 0$ the spaces $H^s(\mathbb{T}^d)$ are defined by

$$H^s(\mathbb{T}^d) = \left\{ f(y) = \sum_{k\in\mathbb{Z}^d} c_k {\rm e}^{2i\pi k\cdot y}, \ \ \sum_{k\in\mathbb{Z}^d} \langle k\rangle^s |c_k|^2 < +\infty \right\}.$$

It is also interesting to link the operator $P_0(\xi)$ with the operator $-\Delta^{(\xi)}$, which consists in the Laplace operator on the cube $\bar{C} = [0,1]^d$ with boundary conditions

$$f(y+\ell) = {\rm e}^{i\xi\cdot\ell} f(y), \ \ \partial_n f(y+\ell) = -\partial_n f(y) {\rm e}^{i\xi\ell}, \ \ \forall (y,\ell) \in \partial C \times \mathbb{Z}^d \text{ such that } y+\ell \in \partial C.$$

This operator is unitarily equivalent to $P_0(\xi)$ by the map which associates to any function $f \in L^2(\mathbb{T}^d)$ the function f_ξ of $L^2(C)$ defined by

$$\forall y \in [0,1]^d, \ \ f_\xi(y) = f(y) {\rm e}^{i\xi\cdot y}. \tag{3.2}$$

One has $\|f_\xi\|_{L^2([0,1]^d)} = \|f\|_{L^2(\mathbb{T}^d)}$ and $\|\Delta f_\xi\|_{L^2([0,1]^d)} = \|P_0(\xi) f\|_{L^2(\mathbb{T}^d)}$.

Theorem 3.1. *Assume that the operator $V_{\rm per}$ is smooth. Then, for all $\xi \in \mathcal{B}$, the operator $P(\xi)$ is self-adjoint and its spectrum is bounded from below. Besides it has a compact resolvent, thus a non-decreasing sequence of eigenvalues*

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

and there exists an orthonormal basis of $L^2(\mathbb{T}^d)$ consisting of eigenfunctions $(\varphi_n(\xi,\cdot))_{n\in\mathbb{N}}$ of $P(\xi)$:

$$\varphi_n(\xi) \in H^2(\mathbb{T}^d), \ \ P(\xi)\varphi_n(y,\xi) = \varrho_n(\xi)\varphi_n(y,\xi), \quad \text{for } y \in \mathbb{T}^d.$$

Remark 3.2. If the potential $V_{\rm per}$ is in $L^p(\mathbb{T}^d)$ with

$$p = 2 \text{ if } \ d = 1, 2, 3, \ \ p > 2 \ \text{ if } \ d = 4 \ \textit{ or } \ p = \frac{d}{2} \ \text{ if } \ d \geq 5,$$

then Theorem 3.1 holds (see [32] and Appendix A). This includes 3d potentials developing Coulombian singularity in a point, $V_{\rm per}(y) \sim \frac{a_0}{|y-y_0|}$ close to some $y = y_0$, $a_0 > 0$ and $y_0 \in \mathbb{T}^d$.

Definition 3.3. The functions defined on $\mathbb{R}^d$, $\xi \mapsto \varrho_n(\xi)$ are called *Bloch energies* or *Bloch modes* and the functions on $\mathbb{T}^d \times \mathbb{R}^d$ defined by $(y, \xi) \mapsto \varphi_n(\xi)$ are called *Bloch waves*.

Remark 3.4. The property (3.1) yields that the Bloch energies $\varrho_n(\xi)$ are $2\pi\mathbb{Z}^d$-periodic functions whereas the Bloch waves satisfy

$$\varphi_n(y, \xi + 2\pi k) = e^{-i2\pi k\cdot y}\varphi_n(y, \xi), \qquad \text{for every } k \in \mathbb{Z}^d.$$

The Bloch modes have a MinMax characterization (see Appendix C)

$$\varrho_1(\xi) = \min_{\|f\|=1} \left(\frac{1}{2} \|(D_y + \xi)f\|^2_{L^2(\mathbb{T}^d)} + (V_{\rm per} f, f)_{L^2(\mathbb{T}^d)} \right) \tag{3.3}$$

and, for $n \in \mathbb{N} \setminus \{1\}$,

$$\varrho_n(\xi) = \min_{\dim M = n,\ M \subset H^1(\mathbb{T}^d)} \ \max_{f \in M,\ \|f\|=1} \left(\frac{1}{2} \|(D_y + \xi)f\|^2_{L^2(\mathbb{T}^d)} + (V_{\rm per} f, f)_{L^2(\mathbb{T}^d)} \right) \tag{3.4}$$

One defines the crossing sets of two distinct Bloch energies as the sets;

$$\Sigma_{n,n'} := \{\xi \in \mathbb{R}^d \ : \ \varrho_n(\xi) = \varrho_{n'}(\xi)\}, \quad n, n' \in \mathbb{N}^*, \ \varrho_n \neq \varrho_{n'}. \tag{3.5}$$

It is proved in [47] that the Bloch energies ϱ_n are continuous and piecewise analytic functions of $\xi \in \mathbb{R}^d$, and that the Bloch waves φ_n can be chosen in such a way there exists a subset $\mathcal{Z}$ of the Brillouin zone $\mathcal{B}$ of zero Lebesgue measure such that each φ_n is analytic in $\xi \in \mathcal{B} \setminus \mathcal{Z}$. However, in the following, we shall only use the Lipschitz regularity of the Bloch modes, together with the smoothness of the Bloch modes and of their associated eigenprojectors outside the crossing sets. These properties are proved in Sections 3.2 (for $d = 1$) and Section 3.3 (in general);

Let us prove Theorem 3.1.

Proof

We first observe that $P_0(\xi)$ is self-adjoint with domain $H^2(\mathbb{T}^d)$, spectrum $\{\frac{1}{2}|\xi + 2k\pi|^2, \ \ k \in \mathbb{Z}^d\}$ and eigenvectors $y \mapsto \mathrm{e}^{2i\pi k\cdot y}$. Moreover, $V_{\rm per}$ being bounded, the Kato-Rellich criterium is satisfied (see [33] and Appendix A): there exists a constant $C = \|V\|_{L^\infty(\mathbb{T}^d)}$, such that for all $\alpha \in (0, 1)$ and all $\xi \in \mathbb{R}^d$,

$$\forall f \in H^2(\mathbb{T}^d), \ \ \|V_{\rm per} f\|_{L^2(\mathbb{T}^d)} \leq C\|f\|_{L^2(\mathbb{T}^d)} + \alpha\|P_0(\xi)f\|_{L^2(\mathbb{T}^d)}.$$

Therefore $P(\xi) = P_0(\xi) + VB_{\rm per}$ is self-adjoint with domain $H^2(\mathbb{T}^d)$.

The second step consists in observing that the operator $(P_0(\xi) - i)^{-1}$ is compact as the limit of finite rank operators in the strong topology.

To close the proof, we choose μ large enough so that the operator $V_{\rm per}(P_0(\xi) + i\mu)^{-1}$ has a norm strictly smaller than 1. As a consequence, the operator $\left(1 + V_{\rm per}(P_0(\xi) + i\mu)^{-1}\right)$ is invertible and we can write

$$(P(\xi) + i\mu)^{-1} = (P_0(\xi) + i\mu)^{-1} \left(1 + V_{\rm per}(P_0(\xi) + i\mu)^{-1}\right)^{-1}.$$

We conclude by observing that the $(P_0(\xi) + i\mu)^{-1}$ is compact and $\left(1 + V_{\rm per}(P_0(\xi) + i\mu)^{-1}\right)^{-1}$ is bounded, thus their composition is compact. In view of Appendix B, the spectral properties of the operator $P(\xi)$ follow.

3.2. **One dimensional Bloch modes and Bloch waves.** When $d = 1$, the equation satisfied by the eigenfunctions of the operator $P(\xi)$ are second order differential equations, which simplifies the analysis. The material of this section mainly comes from the books [37, 43] or the articles [31, 38, 21] among others for additional details. Let us consider $\phi \in L^2(\mathbb{T})$, ϕ 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 the ODE

$$-\frac{1}{2}\partial_y^2 f(y,\lambda) + V_{\rm per}(y) f(y,\lambda) = \lambda f(y,\lambda), \quad y \in \mathbb{R}, \tag{3.6}$$

satisfying the conditions derived from (3.2)

$$f(1,\lambda) = \mathrm{e}^{i\xi} f(0,\lambda) \text{ and } \partial_y f(1,\lambda) = \mathrm{e}^{i\xi}\partial_y f(0,\lambda). \tag{3.7}$$

Given $\lambda \in \mathbb{R}$, the solutions of (3.6) 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 the matrix

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

then the existence of a solution to (3.6) satisfying (3.7) 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 $\mathrm{e}^{i\xi} \in \mathrm{SpM}_\lambda(1)$ if and only if:

$$\Delta(\lambda) = 2\cos\xi. \tag{3.8}$$

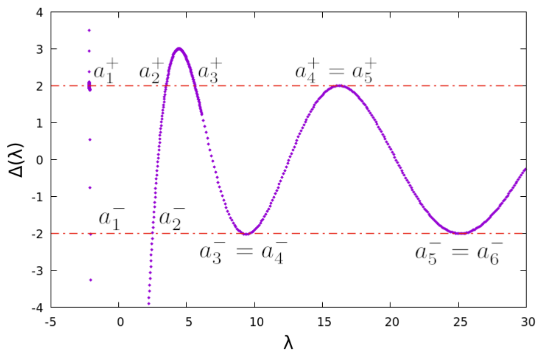
It can be shown that solutions to (3.6) depend analytically on λ, and that moreover, Δ extends to an entire function of order $1/2$. The real solutions to equations $\Delta(\lambda) = \pm 2$ form infinite increasing sequences $(a_i^\pm)$ that tend to infinity.

The following facts hold (the reader may find helpful to consult [38, Figure 1, p. 145] or [43, Section XIII.16]) (note also that complete study of $\Delta(\lambda)$ in one dimension is found in [36] and some figures in [15]):

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

$$a_1^+ < a_1^- \leq a_2^- < a_2^+ \leq a_3^+ < a_3^- \cdots, \tag{3.9}$$

- 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 $\Delta_{|\, I_i}$ 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.

(1) The $n^{\rm th}$ Bloch energy is the solution to $\Delta_{|\, I_n}(\varrho_n(\xi)) = 2\cos\xi$.

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

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

(3) $\varrho_{n|\,[0,\pi]}$ 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.

(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

$$\Delta'(\varrho_n(\xi)) = 0, \quad \forall \xi \in \Sigma_n. \tag{3.10}$$

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

Lemma 3.5. *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 modes 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 (3.8) and evaluating at a critical point $\xi = k\pi$, $k \in \mathbb{Z}$ to get:

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

This relation also shows that $\Delta'(\lambda)$ cannot vanish at $\lambda = \varrho_n(k\pi)$. Together with (3.10) this shows that a critical point cannot be a crossing point.

Remark 3.6. In the free case ($V_{\rm per} = 0$) 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 $V_{\rm per}$ being constant.

3.3. **Regularity of Bloch modes and waves.**

3.3.1. *Lipchitz properties of the Bloch modes.* Using MinMax formula (3.3) and (3.4), we prove the Lipschitz regularity of the Bloch modes $(\varrho_n(\xi))_{n\in\mathbb{N}}$.

Proposition 3.7. *For all $n \in \mathbb{N}$, there exists a constant C_n such that*

$$\forall \xi, \xi' \in \mathcal{B}, \;\; |\varrho_n(\xi) - \varrho_n(\xi')| \leq C_n|\xi - \xi'|.$$

Therefore, the functions $\xi \mapsto \varrho_n(\xi)$ are Lipschitz continuous.

Remark 3.8. Recall that it is proved in [47] that the Bloch energies ϱ_n are continuous and piecewise analytic functions of $\xi \in \mathbb{R}^d$.

Proof
We associate with $P(\xi)$ the positive quadratic form

$$Q_\xi(f) = \frac{1}{2}\|(D_y + \xi)f\|^2_{L^2(\mathbb{T}^d)} + (V_{\rm per}f, f)_{L^2(\mathbb{T}^d)} + K\|f\|^2_{L^2(\mathbb{T}^d)}.$$

where K is chosen such that for all $\xi \in \mathcal{B}$, the spectrum of $P(\xi)$ is included in $]-K+1, +\infty[$. Note that the Proposition is equivalent to proving the Lipschitz property of the functions

$$\lambda_n(\xi) = \varrho_n(\xi) + K + 1.$$

which we are going to do now. We observe first that for $\xi, \xi' \in \mathcal{B}$ and $f \in L^2('\mathbb{T}^d)$, we have

$$\begin{aligned} Q_{\xi'}(f) - Q_\xi(f) &= \frac{1}{2}\int_{\mathbb{T}^d} \left(|D_y f(y) + \xi f(y)|^2 - |Df(y) + \xi' f(y)|^2\right) dy \\ &= 2\sum_{j=1}^d \mathrm{Re}\left((\xi_j - \xi'_j)\left(f\ ,\ D_{y_j} f - \frac{\xi_j + \xi'_j}{2} f\right)_{L^2(\mathbb{T}^d)}\right). \end{aligned}$$

Therefore, there exists a constant $C > 0$ such that for all $\xi, \xi' \in \mathcal{B}$ and for all $f \in L^2(\mathbb{T}^d)$,

$$|Q_\xi(f) - Q_{\xi'}(f)| \leq C|\xi - \xi'| \left(\|f\|^2_{L^2(\mathbb{T}^d)} + \frac{1}{2}(Q_\xi(f) + Q_{\xi'}(f))\right). \tag{3.11}$$

We are going to use the Min-Max characterization of the eigenvalues (see (3.3) and (3.4)). Let M be a subset of $H^1(\mathbb{T}^d)$ of dimension n. We deduce from (3.11), that for any $f \in M$, $\|f\|_{L^2(\mathbb{T}^d)} = 1$ and $f \in H^1(\mathbb{T}^d)$,

$$Q_{\xi'}(f) \leq Q_\xi(f) + C|\xi - \xi'|(1 + \frac{1}{2}(Q_\xi(f) + Q_{\xi'}(f))).$$

We deduce

$$\min_{\mathrm{dim}M=n,\ M\subset H^1(\mathbb{T}^d)} \ \max_{f\in M,\ \|f\|=1} Q_{\xi'}(f) \leq (1 + C|\xi - \xi'|) \max_{f\in M,\ \|f\|=1} Q_\xi(f) + C|\xi - \xi'|,$$

and

$$\begin{aligned} &\min_{\mathrm{dim}M=n,\ M\subset H^1(\mathbb{T}^d)} \ \max_{f\in M,\ \|f\|=1} Q_{\xi'}(f) \\ &\quad \leq (1 + C|\xi - \xi'|) \min_{\mathrm{dim}M=n,\ M\subset H^1(\mathbb{T}^d)} \ \max_{f\in M,\ \|f\|=1} Q_\xi(f) + C|\xi - \xi'|. \end{aligned}$$

Therefore, we obtain the first relation:

$$\lambda_n(\xi') - \lambda_n(\xi) \leq C|\xi - \xi'|(1 + \lambda_n(\xi)). \tag{3.12}$$

We now fix $\alpha > 0$ and we assume $|\xi - \xi'| < \alpha$, then

$$\lambda_n(\xi') - (1 + C\alpha)\lambda_n(\xi) \leq C|\xi - \xi'|$$

which writes

$$(1 + C\alpha)(\lambda_n(\xi') - \lambda_n(\xi)) \leq C|\xi - \xi'| + C\alpha\lambda_n(\xi').$$

We deduce the second relation

$$\lambda_n(\xi') - \lambda_n(\xi) \leq \frac{C}{1 + C\alpha}|\xi - \xi'| + \frac{C\alpha}{1 + C\alpha}\lambda_n(\xi') \leq C|\xi - \xi'| + C\alpha\lambda_n(\xi').$$

Exchanging the roles of ξ and ξ', we obtain

$$\lambda_n(\xi) - \lambda_n(\xi') \leq C|\xi - \xi'| + C\alpha\lambda_n(\xi). \tag{3.13}$$

Combining (3.12) and (3.13), we obtain

$$|\lambda_n(\xi) - \lambda_n(\xi')| \leq C|\xi - \xi'| + C\alpha\lambda_n(\xi).$$

Let us now fix $\xi \in \mathcal{B}$ and consider $\eta > 0$, we choose α such that $C\alpha(1+\lambda_n(\xi)) < \eta$. Then if $|\xi-\xi'| < \alpha$, we have $|\lambda_n(\xi)-\lambda_n(\xi')| < \eta$. We deduce that the function λ_n is continuous in any point ξ of the compact $\mathcal{B}$. Thus, this function is bounded on $\mathcal{B}$. Let $\Lambda_n = \sup_{\xi\in\mathcal{B}} \lambda_n(\xi)$, equation (3.12) implies that for all $\xi, \xi' \in \mathcal{B}$,

$$\lambda_n(\xi) - \lambda_n(\xi') \leq C(1 + \Lambda_n)|\xi - \xi'|,$$

which yields

$$|\lambda_n(\xi) - \lambda_n(\xi')| \leq C(1 + \Lambda_n)|\xi - \xi'|,$$

by exchanging the roles of ξ and ξ'. As a conclusion, $\xi \mapsto \lambda_n(\xi)$ is Lipschitz.

3.3.2. *Smoothness of the Bloch modes and associated eigenprojectors outside the crossing sets.* We consider here the eigenprojector on a Bloch mode isolated from the remainder of the spectrum. Denote by $\mathrm{Sp}\, P(\xi)$ the spectrum of $P(\xi)$, we suppose that there exists $n_0 \in \mathbb{N}$, an open subset $U \subset \mathcal{B}$ and $\delta_0 > 0$ such that

$$d\left(\varrho_{n_0}(\xi), \mathrm{Sp}\, P(\xi) \setminus \{\varrho_{n_0}(\xi)\}\right) \geq \delta_0, \quad \forall \xi \in U. \tag{3.14}$$

Then, since the map ϱ_n is continuous on the compact $\overline{U}$, there exists a contour C of the complex plane which delimitates an open set $\Omega \subset \mathbb{C}$ such that

$$\overline{\{\varrho_{n_0}(\xi),\ \xi \in U\}} \subset \Omega \text{ and } \Omega \cap \mathrm{Sp}\, P(\xi) = \{\varrho_{n_0}(\xi),\ \xi \in U\}, \quad \forall \xi \in \mathbb{R}^d.$$

Then, applying the residue formula applied to the resolvent written as

$$R(z,\xi) = (z - P(\xi))^{-1} = \sum_{n \in \mathbb{N}} (z - \varrho_n(\xi))^{-1} |\varphi_n(\cdot,\xi)\rangle\langle\varphi_n(\cdot,\xi)|,$$

one gets

$$\Pi_{n_0}(\xi) = \frac{1}{2\pi i} \oint_C R(z,\xi) dz, \quad \forall \xi \in U. \tag{3.15}$$

Besides, we have

$$\forall z \in C, \quad \|(z - P(\xi))^{-1}\|_{\mathcal{L}(L^2(\mathbb{T}^d)} \leq \delta_0^{-1}. \tag{3.16}$$

One deduces the following proposition.

Proposition 3.9. *Let $n_0 \in \mathbb{N}$, U an open subset of $\mathcal{B}$ and δ_0 such that* (3.14) *holds. Then, the function $\xi \mapsto \Pi_{n_0}(\xi)$ is smooth in U, and therefore is of constant rank.*

Corollary 3.10. *Assume that the eigenmodes $\varrho_{n_0}(\xi)$ is isolated from the remainder of the spectrum, then the function $\varrho_{n_0}(\xi) = (\mathrm{Rk}\Pi_{n_0}(\xi))^{-1}\, \mathrm{tr}\,(\Pi_{n_0}(\xi)P(\xi))$ is smooth.*

Proposition 3.11. *If they exist, the derivatives of Π_{n_0} satisfy the following properties :*

(1) *They are off-diagonal operators with respect to $P(\xi)$:*

$$\forall \xi \in \mathbb{R}^d, \ \forall k \in \{1, \cdots d\}, \ \partial_{\xi_k} \Pi_{n_0}(\xi) = \sum_{n \in \mathbb{N}} \left(\Pi_n(\xi) \partial_{\xi_k} \Pi_{n_0}(\xi)\, \Pi_{n_0}(\xi) + \Pi_{n_0}(\xi)\, \partial_{\xi_k} \Pi_{n_0}(\xi)\, \Pi_n(\xi)\right).$$

(2) *They are bounded operators:*

$$\exists C_0 > 0, \ \forall \xi \in \mathbb{R}^d, \ \forall j \in \{1, \cdots, d\}, \ \left\|\partial_{\xi_j} \Pi_{n_0}(\xi)\right\|_{\mathcal{L}(L^2(\mathbb{T}^d), H^2(\mathbb{T}^d))} \leq C_0. \tag{3.17}$$

Proof
Point 1 comes from the derivation of $\Pi_{n_0}(\xi)^2 = \Pi_{n_0}(\xi)$. Indeed, the later relation yields

$$\Pi_{n_0}(\xi) \partial_{\xi_k} \Pi_{n_0}(\xi) + \partial_{\xi_k} \Pi_{n_0}(\xi)\, \Pi_{n_0}(\xi) = \partial_{\xi_k} \Pi_{n_0}(\xi).$$

Multiplying the left hand side of the above equality by $\Pi_n(\xi)$ with $n \neq n_0$ and the right hand-side by $\Pi_{n'}(\xi)$ with $n' \neq n_0$ gives

$$\Pi_n(\xi) \partial_{\xi_k} \Pi_{n_0}(\xi) \Pi_{n'}(\xi) = 0,$$

whence the above decomposition.

The second relation comes from equation (3.15). Taking $f \in L^2(\mathbb{T}^d)$, we write

$$\partial_{\xi_j} \Pi_n(\xi) = \frac{1}{2\pi i} \oint_C (z - P(\xi))^{-1} \partial_{\xi_j} P(\xi) (z - P(\xi))^{-1} dz.$$

In view of (3.16), it is enough to prove that the operator $\partial_{\xi_j}P(\xi)(z-P(\xi))^{-1}$ is uniformly bounded in $\mathcal{L}(L^2(\mathbb{T}^d))$ with respect to z for $z\in C$. Let $f\in L^2(\mathbb{T}^d)$ and set $u_z=(z-P(\xi))^{-1}f$, then for $z\in C$, we have

$$\|u_z\|_{L^2(\mathbb{T}^d)}\leq \delta_0^{-1}\|f\|_{L^2(\mathbb{T}^d)}.$$

Besides, by (3.16), and with $C=\|V_{\rm per}\|_{L^\infty(\mathbb{T}^d)}$,

$$\begin{aligned}\left\|\partial_{\xi_j}P(\xi)(z-P(\xi)^{-1})f\right\|^2_{L^2(\mathbb{T}^d)} &= \left\|\partial_{\xi_j}P(\xi)u_z\right\|^2_{L^2(\mathbb{T}^d)}\leq \|(\xi+D_\xi)u_z\|^2_{L^2(\mathbb{T}^d)}\\ &\leq (P(\xi)u_z,u_z)_{L^2(\mathbb{T}^d)}+C\|u_z\|^2_{L^2(\mathbb{T}^d)}\\ &\leq |(f-zu_z,u_z)_{L^2(\mathbb{T}^d)}|+C\|u_z\|^2_{L^2(\mathbb{T}^d)}\\ &\leq \delta_0^{-1}(1+|z|\delta_0^{-1}+C\delta_0^{-1})\,\|f\|^2_{L^2(\mathbb{T}^d)}.\end{aligned}$$

3.3.3. *Singularities of the Bloch modes at crossing points.* We are interested here in the properties of the Bloch modes close to the sets $\Sigma_{n,n'}$ (see (3.5)). We assume that these sets are union of closed connected submanifolds of $\mathbb{R}^d$.

We will use the geometric notion of the normal bundle to a manifold. If $\Sigma_{n,n'}$ is a manifold, its tangent bundle $T\Sigma_{n,n'}$ is defined by its fiber above $\sigma\in\Sigma_{n,n'}$ which is the tangent space $T_\sigma\Sigma_{n,n'}$ at σ to $\Sigma_{n,n'}$. The normal bundle $N\Sigma_{n,n'}$ to $\Sigma_{n,n'}$ has fiber $N_\sigma\Sigma_{n,n'}=T_\sigma\mathbb{R}^d/T_\sigma\Sigma_{n,n'}$. If moreover $\Sigma_{n,n'}$ is a closed connected manifold, the geodesic coordinates give a mapping from a tubular neighborhood U of $\Sigma_{n,n'}$ into $\Sigma_{n,n'}$

$$\sigma_{\Sigma_{n,n'}}:\xi\in U\mapsto \sigma_{\Sigma_{n,n'}}(\xi)\in\Sigma_{n,n'}$$

such that for all $\xi\in U$, $\xi-\sigma_{\Sigma_{n,n'}}(\xi)\in N_{\sigma(\xi)}\Sigma_{n,n'}$.

We consider crossings between two successive Bloch modes ϱ_n and ϱ_{n+1}.

Definition 3.12. Let $n\in\mathbb{N}^*$. We say that the crossings of the set $\Sigma_{n,n+1}$ are conic if and only if there exists a neighborhood U of $\Sigma_{n,n+1}$ such that ϱ_n and ϱ_{n+1} are of multiplicity 1 outside $\Sigma_{n,n+1}$ in U and there exists $c>0$ such that for all $(\sigma,\eta)\in N\Sigma_{n,n+1}$,

$$|\varrho_{n+1}(\sigma+r\eta)-\varrho_n(\sigma+r\eta)|\geq c|\eta|.$$

Conical crossings are in some sense generic in view of the next Lemma which gives a normal form for the expression of two Bloch modes $\varrho_n(\xi)$ and $\varrho_{n+1}(\xi)$ close to the crossing set $\Sigma_{n,n+1}$.

Lemma 3.13. *Let σ_0 be a point in the crossing set $\Sigma_{n,n+1}$ of two consecutive Bloch energies ϱ_n and ϱ_{n+1} having neighborhood U with the following properties:*

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

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

Then, there exist $\Omega\subseteq U$, a neighborhood of σ_0 that is $2\pi\mathbb{Z}^d$-invariant, two functions $\lambda_n\in C^\infty(\Omega)$ and $g_n\in C^\infty\left(\sqcup_{\xi\in\Omega}\left(\{\xi\}\times N_{\sigma_{\Sigma_{n,n+1}}(\xi)}\Sigma_{n,n+1}\right)\right)$, and a function $m\in L^\infty(U)$ which is constant on each connected component of U such that for all $\xi\in\Omega\setminus\Sigma_{n,n+1}$,

$$\begin{aligned}\varrho_n(\xi)&=\lambda_n(\xi)-g_n(\xi,\xi-\sigma_{\Sigma_{n,n+1}}(\xi)),\\ \varrho_{n+1}(\xi)&=\lambda_n(\xi)+m(\xi)g_n(\xi,\xi-\sigma_{\Sigma_{n,n+1}}(\xi)).\end{aligned}$$

Moreover,

(1) *If the crossing set $\Sigma_{n,n+1}$ is conical in U, then for all $\xi\in U$, the map $N_{\sigma(\xi)}\sigma\eta\mapsto g_n(\xi,\eta)$ 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* $\Sigma_{n,n+1}$ *are conical crossings in* U*, then there exists* $\theta_n \in C^\infty(\mathbb{R}^d)$ *such that* $g_n(\xi,\eta) = |\eta|^2\theta_n(\xi)$*, which implies that* ϱ_n*,* $\varrho_{n+1} \in C^{1,1}(\mathbb{R}^d)$*,*
(3) *If the multiplicities of* ϱ_n*,* ϱ_{n+1} *are equal on* $U \setminus \Sigma_{n,n+1}$ *then* $m = 1$*.*
(4) *If* $d = 1$ *and* $\sigma \in \pi\mathbb{Z} \setminus 2\mathbb{Z}$*, then* $\nabla\lambda_n(\sigma) \mp g'(\omega) \neq 0$ *or* $\omega = \pm 1$*.*

Remark 3.14. Note that in case (2), the function θ_n can be zero on $\Sigma_{n,n+1}$.

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

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

By the assumption (iii) 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 $U\xi \mapsto \Pi(\xi) \in \mathcal{L}(L^2(\mathbb{T}^d))$ 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 $\xi \in U \setminus \Sigma_{n,n+1}$. 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 $\xi \in \Omega \setminus \Sigma_{n,n+1}$, $m(\xi)$ 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 component of $U \setminus \Sigma_{n,n+1}$.

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 $\Sigma_{n,n+1}$ 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

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

with
$$\forall \sigma \in \Sigma_{n,n+1} \cap \Omega, \;\; \forall \eta \in N_\sigma \Sigma_{n,n+1} \setminus \{0\}, \;\; T^{\ell_0,1}(\sigma)\eta \neq 0_{\mathbb{C}^{\ell_0 \times \ell_0}}.$$
We deduce that
$$g(\xi) = g_n(\xi, \xi - \sigma_{\Sigma_{n,n+1}}(\xi)), \;\; \text{with} \;\; g_n(\xi, \eta) := G\left(T^{\ell_0,1}(\xi)\,[\eta]^q\right)$$
where g_n is homogeneous of degree 1 in the variable η. Besides, if none of the crossing points are conical, we write $A_0(\xi) = T^{\ell_0,2}(\xi)[\xi - \sigma_{\Sigma_{n,n+1}}(\xi)]^2$ with $T^{\ell_0,2}(\xi)$ a smooth tensor, which allows to prove Point (2) with
$$\theta_n(\xi) = |\xi - \sigma_{\Sigma_{n,n+1}}(\xi)|^{-2} G(T^{\ell_0,2}(\xi)[\xi - \sigma_{\sigma_n}(\xi)]^2).$$
Since Point (3) is obvious, it remains to examine the case $d = 1$. At a crossing point $\sigma = k\pi$, $k \in \mathbb{Z}$, we have $m(\sigma) = 1$. Moreover, the function g_n can be written in a simple manner: there exists $\alpha_-, \alpha_+ \in \mathbb{R}$ such that
$$g_n(\eta) = \alpha_- \,\eta \mathbf{1}_{\eta<0} + \alpha_+ \,\eta \mathbf{1}_{\eta>0}, \;\; \alpha_\pm = g'(\eta)\mathbf{1}_{\pm\eta>0}.$$
Let $\eta < 0$, then $\varrho_n'(\sigma+\eta) = \lambda_n'(\sigma+\eta) - \alpha_-$. and $\varrho_n''(\sigma+\eta)$ has a limit when η go to 0^-. Differentiating twice (3.8), we obtain
$$\Delta'(\varrho_n(\sigma+\eta))\varrho_n''(\sigma+\eta) + \Delta''(\varrho_n(\sigma+\eta))\varrho_n'(\sigma+\eta) = 2(-1)^{k+1}.$$
Letting η go to O^-, we obtain
$$\Delta''(\varrho_n(\sigma))(\lambda_n'(\sigma) - \alpha_-) \neq 0.$$
Arguing similarly with $\varrho_n(\sigma + \eta$ with $\eta > 0$, we deduce $\lambda_n'(\sigma) - \alpha_+ \neq 0$. Therefore, $\lambda_n'(\sigma) - g'(\omega) \neq 0$ for $\omega \in \{-1, +1\}$. Considering now the Bloch mode ϱ_{n+1}, we obtain in the same manner $\lambda_n'(\sigma) + g'(\omega) \neq 0$ for $\omega \in \{-1, +1\}$, which finishes the proof.

4. Wigner measures and Bloch modes

We resume with the family $(\psi^\varepsilon(t))_{\varepsilon>0}$ solution to (1.1). We look for the solution as

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

with $(U^\varepsilon(t))_{\varepsilon>0}$ solution to equation (1.9) in $L^2(\mathbb{R}^d\times\mathbb{T}^d)$ and

$$U_0^\varepsilon\left(x,\frac{x}{\varepsilon}\right) = \psi_0^\varepsilon(x).$$

Using the spectral resolution of the operator $P(\xi)$ we write

$$U^\varepsilon(t,x,y) = \sum_{n\in\mathbb{N}} \varphi_n(y,\varepsilon D_x) U_n^\varepsilon(t,x),$$

with

$$U_n^\varepsilon(t,x) := \int_{\mathbb{T}^d} \overline{\varphi_n}(y,\varepsilon D_x)U^\varepsilon(t,x,y)dy = \int_{\mathbb{T}^d}\int_{\mathbb{R}^d\times\mathbb{R}^d} \overline{\varphi_n}(y,\varepsilon\xi)U^\varepsilon(t,w,y)\mathrm{e}^{i\xi\cdot(x-w)}\frac{dwd\xi}{(2\pi)^d}dy.$$

We deduce a (formal) representation formula for the solution of the equation (1.1):

$$\psi^\varepsilon(t,x) = \sum_{n\in\mathbb{N}} \psi_n^\varepsilon(t,x),\ \ \psi_n^\varepsilon(t,x) = \varphi_n\left(\frac{x}{\varepsilon},\varepsilon D_x\right)U_n^\varepsilon(t,x). \tag{4.1}$$

We work under the assumption that $(\psi_0^\varepsilon)_{\varepsilon>0}$ is uniformly bounded in $H^s_\varepsilon(\mathbb{R}^d)$ for some $s>\frac{d}{2}$ and we choose

$$U_0^\varepsilon(x,y) = \psi_0^\varepsilon(x)\mathbf{1}_{\mathbb{T}^d}(y),\ \ (x,y)\in\mathbb{R}^d\times\mathbb{T}^d. \tag{4.2}$$

The formula (4.1) implies that the solutions of (1.1) can be decomposed as a countable superposition of waves whose dependence on the fast variable is given by a Bloch wave, whereas the profile U_n^ε describing the dependence on the slow variable is given by a time-evolution whose dispersion relation involves Bloch energies. Several questions then are in order:

(i) Are the families $(\psi_n^\varepsilon)_{\varepsilon>0}$ bounded in $L^2(\mathbb{R}^d)$?
(ii) Is the series converging and in which space ?
(iii) Is the function $(\psi^\varepsilon)_{\varepsilon>0}$ ε-oscillating so that a semi-classical analysis is adapted ?

Answering those questions is the subject of that chapter. A key point is the understanding of the restriction operator L^ε defined on functions F on $\mathbb{R}^d\times\mathbb{T}^d$ by

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

Of course, to define $L^\varepsilon F$, the function F needs to enjoy enough Sobolev regularity, which motivates the introduction of adapted functional spaces on $\mathbb{R}^d\times\mathbb{T}^d$.

4.1. **The functional framework and the restriction operator.** Recall that via the decomposition in Fourier series in the second variable, any function $U\in L^2(\mathbb{R}^d_x\times\mathbb{T}^d_y)$ can be written as:

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

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

$$\forall\varepsilon\in(0,\varepsilon_0),\ \ \|U\|^2_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} := \sum_{k\in\mathbb{Z}^d}\int_{\mathbb{R}^d}(1+|\varepsilon\xi|^2+|k|^2)^s|\widehat{U_k}(\xi)|^2d\xi\leq C, \tag{4.3}$$

where $\widehat{U_k}(\xi) = \displaystyle\int_{\mathbb{R}^d}\mathrm{e}^{-ix\cdot\xi}U_k(x)dx.$

Note that the data $(U_0^\varepsilon)_{\varepsilon>0}$ defined in (4.2) with $(\psi_0^\varepsilon)_{\varepsilon>0}$ uniformly bounded in $H^s_\varepsilon(\mathbb{R}^d)$, then is uniformly bounded in $H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)$.

It turns out that L^ε acts continuously from $H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)$ to $L^2(\mathbb{R}^d)$ provided $s>\frac{d}{2}$ and that the equation (1.9) satisfied by $(U^\varepsilon(t))_{\varepsilon>0}$ can be solved in these spaces. The following results are proved in [14] (Sections 6.1 and 6.2) and in [15] (Section 2).

Proposition 4.1. (1) *There exists $C>0$ such that, for every $F\in L^2(\mathbb{R}^d,H^s(\mathbb{T}^d))$, uniformly in $\varepsilon>0$,*

$$\|L^\varepsilon F\|_{L^2(\mathbb{R}^d)}\leq C\|F\|_{L^2(\mathbb{R}^d,H^s(\mathbb{T}^d))}. \tag{4.4}$$

Moreover if $\xi\mapsto\varrho(\xi)$ is $2\pi\mathbb{Z}^d$-periodic, then L^ε commutes with $\varrho(\varepsilon D_x)$.

(2) *If $(U^\varepsilon)_{\varepsilon>0}$ is a bounded family in $L^2(\mathbb{R}^d_x;H^s(\mathbb{T}^d_y))$ and satisfies the estimate:*

$$\limsup_{\varepsilon\to 0^+}\|\mathbf{1}_{|\varepsilon D_x|>R}U^\varepsilon\|_{L^2(\mathbb{R}^d;H^s(\mathbb{T}^d))}\underset{R\to\infty}{\longrightarrow}0, \tag{4.5}$$

then the sequence $(L^\varepsilon U^\varepsilon)_{\varepsilon>0}$ is bounded in $L^2(\mathbb{R}^d)$ and ε-oscillating (see Definition 2.19).

(3) *Assume $V_{\rm ext}\in L^\infty(\mathbb{R},C^1(\mathbb{R}^d))$ with $\nabla_xV_{\rm ext}\in L^\infty(\mathbb{R}\times\mathbb{R}^d)$ and suppose that the potential $V_{\rm per}$ is such that the operator $P(\varepsilon D)$ with domain $H^2(\mathbb{T}^d)$ is self-adjoint. Then, there exists $C_s>0$ such that for every $t\in\mathbb{R}$, $\varepsilon>0$ and $U_0^\varepsilon\in H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)$, the solution $U^\varepsilon(t)$ of* (1.9) *satisfies*

$$\|U^\varepsilon(t,\cdot)\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)}\leq\|U_0^\varepsilon\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)}+C_s\varepsilon|t|, \tag{4.6}$$

Note that in Point 3, it is enough to assume that the operator $P(\xi)$, with domain $H^2(\mathbb{T}^d)$, is self-adjoint for all $\xi\in\mathcal{B}$, which is possible with less restrictive assumptions on $V_{\rm per}$ than smoothness (see Remark 3.2).

Proof
Point 1 comes from the Sobolev embedding $H^s(\mathbb{T}^d)\subset L^\infty(\mathbb{T}^d)$: we use the Fourier resolution of F and write for $x\in\mathbb{R}^d$ and $y\in\mathbb{T}^d$,

$$F(x,y)=\sum_{k\in\mathbb{Z}^d}F_k(x)\mathrm{e}^{2i\pi k\cdot y}.$$

Then, by Cauchy-Schwartz inequality

$$|F(x,y)|\leq\left(\sum_{k\in\mathbb{Z}^d}|F_k(x)|^2\langle k\rangle^{2s}\right)^{\frac12}\left(\sum_{k\in\mathbb{Z}^d}\langle k\rangle^{-2s}\right)^{\frac12}$$

Since $s>\frac{d}{2}$, we have $\sum_{k\in\mathbb{Z}^d}\langle k\rangle^{-2s}<c_0<+\infty$ and we deduce

$$\|L^\varepsilon F\|^2_{L^2(\mathbb{R}^d)}=\int_{\mathbb{R}^d}|F(x,\frac{x}{\varepsilon})|^2dx\leq c_0\int_{\mathbb{R}^{2d}}\sum_{k\in\mathbb{Z}^d}|F_k(x)|^2\langle k\rangle^{2s}dx=c_0\|F\|^2_{L^2(\mathbb{R}^d;H^s(\mathbb{T}^d))},$$

whence the result. Moreover,

$$\begin{aligned}\varrho(\varepsilon D_x)(L^\varepsilon F)(x)&=\sum_{k\in\mathbb{Z}^d}\varrho(\varepsilon D_x)\left(\mathrm{e}^{\frac{2i\pi}{\varepsilon}k\cdot x}F_k\right)(x)\\&=\sum_{k\in\mathbb{Z}^d}\mathrm{e}^{\frac{2i\pi}{\varepsilon}k\cdot x}\varrho(\varepsilon D_x-2k\pi)F_k(x)\\&=\sum_{k\in\mathbb{Z}^d}\mathrm{e}^{\frac{2i\pi}{\varepsilon}k\cdot x}\varrho(\varepsilon D_x)F_k(x)\\&=L^\varepsilon\left(\varrho_\varepsilon D_x)F\right)(x).\end{aligned}$$

For Point 2, we take $\delta > 0$, since $s > d/2$, there exists $N_\delta > 0$ such that
$$\sum_{|k|>N_\delta} |k|^{-2s} < \delta^2.$$
Define
$$v_\delta^\varepsilon(x) = \sum_{|k|\leq N_\delta} U_k^\varepsilon(x) \mathrm{e}^{i2\pi k\cdot\frac{x}{\varepsilon}}.$$
Then,
$$\|L^\varepsilon U^\varepsilon - v_\delta^\varepsilon\|_{L^2(\mathbb{R}^d)} \leq \delta \|U^\varepsilon\|_{L^2(\mathbb{R}^d;H^s(\mathbb{T}^d))}.$$
Therefore, it suffices to show that for any $\delta > 0$ the sequence (v_δ^ε) is ε-oscillating. The Fourier transform of v_δ^ε is:
$$\widehat{v_\delta^\varepsilon}(\xi) = \sum_{|k|\leq N_\delta} \widehat{U_k^\varepsilon}\left(\xi - \frac{2\pi k}{\varepsilon}\right).$$
Therefore,
$$\|\mathbf{1}_{|\varepsilon D_x|>R} v_\delta^\varepsilon\|_{L^2(\mathbb{R}^d)} \leq \sum_{|k|\leq N_\delta} \|\mathbf{1}_{|\varepsilon D_x + 2\pi k|>R} U_k^\varepsilon\|_{L^2(\mathbb{R}^d)}.$$
If $R > R_0$ for $R_0 > 0$ large enough, one has $\mathbb{1}_R(\cdot + 2\pi k) \leq \mathbb{1}_{R/2}$ for every $|k| \leq N_\delta$. This allows us to conclude that for $R > R_0$:
$$\|\mathbf{1}_{|\varepsilon D_x|>R} v_\delta^\varepsilon\|_{L^2(\mathbb{R}^d)} \leq \sum_{|k|\leq N_\delta} \|\mathbf{1}_{|\varepsilon D_x|>R/2} U_k^\varepsilon\|_{L^2(\mathbb{R}^d)} \leq C_{d,s} \|\mathbf{1}_{|\varepsilon D_x|>R/2} U^\varepsilon\|_{L^2(\mathbb{R}^d;H^s(\mathbb{T}^d))}$$
and the conclusion follows.

The proof of Point 3 uses that modulo the addition of a positive constant to equation (1.1), we may assume that $P(\varepsilon D_x)$ is a non-negative 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:

$$c^{-1}\|U\|_{H_\varepsilon^s(\mathbb{R}^d\times\mathbb{T}^d)} \leq \| \langle \varepsilon D_x\rangle^s U\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} + \|P(\varepsilon D_x)^{s/2} U\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} \leq c\|U\|_{H_\varepsilon^s(\mathbb{R}^d\times\mathbb{T}^d)}, \tag{4.7}$$

for every $U \in L^2(\mathbb{R}^d \times \mathbb{T}^d)$ and $0 < \varepsilon < \varepsilon_0$. Moreover, $P(\varepsilon D_x)^k$ and $\langle\varepsilon D_x\rangle^s$ commutes with $P(\varepsilon)$ while
$$\|[P(\varepsilon D_x)^{s/2}, V(t,x)]U^\varepsilon\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} \leq \varepsilon C \sup_{0\leq r\leq s-1} \|P(\varepsilon D_x)^{\frac{r}{2}} U^\varepsilon\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}$$
and a similar estimate holds for $[\langle\varepsilon D_x\rangle^s, V(t,x)]U^\varepsilon$. We then conclude by a recursive argument and energy estimate.

4.2. **Decomposition of the Wigner transform on Bloch modes.** We focus on the families $(\psi_n^\varepsilon(t))_{\varepsilon>0}$. They satisfy

$$\psi_n^\varepsilon(t,x) := L^\varepsilon P_{\varphi_n}^\varepsilon U^\varepsilon(t,x) = \varphi_n\left(\frac{x}{\varepsilon}, \varepsilon D_x\right) \int_{\mathbb{T}^d} \overline{\varphi_n}(y, \varepsilon D_x) U^\varepsilon(t,x,y)dy, \tag{4.8}$$

where we define for $j \in \mathbb{N}^*$ the operator

$$P_{\varphi_j}^\varepsilon W(x,y) := \varphi_j\left(y, \varepsilon D_x\right) \int_{\mathbb{T}^d} \overline{\varphi_j}(z, \varepsilon D_x) W(x,z)dz, \quad \forall W \in L^2(\mathbb{T}^d \times \mathbb{R}^d). \tag{4.9}$$

Since $[P(\varepsilon D_x)^{s/2}, P_{\varphi_j}^\varepsilon] = [\langle\varepsilon D_x\rangle^s, P_{\varphi_j}^\varepsilon] = 0$, if follows from (4.7) that there exists $c_1 > 0$ such that for all $W \in H_\varepsilon^s(\mathbb{R}^d \times \mathbb{T}^d)$,
$$\|P_{\varphi_j}^\varepsilon W\|_{H_\varepsilon^s(\mathbb{R}^d\times\mathbb{T}^d)} \leq c_1 \|W\|_{H_\varepsilon^s(\mathbb{R}^d\times\mathbb{T}^d)},$$
and, more generally, that every $W \in H_\varepsilon^s(\mathbb{R}^d \times \mathbb{T}^d)$ can be expressed in the topology of $H_\varepsilon^s(\mathbb{R}^d \times \mathbb{T}^d)$ as:
$$W = \sum_{n\in\mathbb{N}^*} P_{\varphi_n}^\varepsilon W.$$

As a corollary of Proposition 4.1, we have the following result.

Corollary 4.2. *Assume* $V_{\rm ext} \in L^\infty(\mathbb{R}, C^1(\mathbb{R}^d))$ *with* $\nabla_x V_{\rm ext} \in L^\infty(\mathbb{R}\times\mathbb{R}^d)$ *and suppose that the potential* $V_{\rm per}$ *is such that the operator* $P(\varepsilon D)$ *with domain* $H^2(\mathbb{T}^d)$ *is self-adjoint. Assume* (ψ_0^ε) *is uniformly bounded in* $H^s_\varepsilon(\mathbb{R}^d)$ *for some* $s > d/2$*. Then, for every* $t\in\mathbb{R}$*, we have the following properties*

(i) *The series* (4.1) *is uniformly convergent*

$$\limsup_{\varepsilon\to 0^+} \left\| \sum_{n>N} \psi_n^\varepsilon(t,\cdot)\right\|_{L^2(\mathbb{R}^d)} \underset{N\to\infty}{\longrightarrow} 0. \tag{4.10}$$

(ii) *The family* $(\psi^\varepsilon(t))_{\varepsilon>0}$ *is* ε*-oscillating, locally uniformly in time, i.e. for all* $T\in\mathbb{R}$*,*

$$\limsup_{\varepsilon\to 0^+} \sup_{t\in[0,T]} \|\mathbf{1}_{|\varepsilon D|>R}\psi^\varepsilon(t)\|_{L^2(\mathbb{R}^d)} \underset{R\to\infty}{\longrightarrow} 0.$$

(iii) *Any Wigner measure* ς^t *of* $(\psi^\varepsilon(t))_{\varepsilon>0}$ *writes*

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

where the signed measures $\mu^t_{n,n'}$ *are joint Wigner measures of the pair* $(\psi_n^\varepsilon(t),\psi_{n'}^\varepsilon(t))_{\varepsilon>0}$*,* $n,n'\in\mathbb{N}^*$*, and the convergence of the series being understood in the weak-*$*$ *topology of the space of Radon measures on* $\mathbb{R}^{2d}$*.*

(iv) *For all* $n\in\mathbb{N}^*$*, the family* $\psi_n^\varepsilon(t)$ *satisfies*

$$i\varepsilon^2\partial_t\psi_n^\varepsilon = \varrho_n(\varepsilon D)\psi_n^\varepsilon + \varepsilon^2 f_n^\varepsilon(t), \tag{4.11}$$

with

$$f_n^\varepsilon(t,x) := \varphi_n\left(\frac{x}{\varepsilon},\varepsilon D_x\right)\int_{\mathbb{T}^d} \overline{\varphi_n}(y,\varepsilon D_x)(V_{\rm ext}(t,x)U^\varepsilon(t,x,y))dy. \tag{4.12}$$

This corollary motivates the analysis of the Wigner measures associated with the families $(\psi_n^\varepsilon(t))_{\varepsilon>0}$, $n\in\mathbb{N}^*$, that will be performed in the next section and will allow to obtain a complete description of the weak-limits of the density measure $|\psi^\varepsilon(t,x)|^2$ (as stated in Theorem 1.3 when $d=1$).

Proof
(i) 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 (4.1) holds in $L^2(\mathbb{R}^d)$. Besides, in view of (4.6), (4.4), for proving (4.10). 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 4.7 implies that we only have to prove

$$\limsup_{\varepsilon\to 0^+} \left\| \sum_{n>N} P(\varepsilon D_x)^{r/2} P^\varepsilon_{\varphi_n} V^\varepsilon\right\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} + \limsup_{\varepsilon\to 0^+} \left\| \sum_{n>N} \langle\varepsilon D_x\rangle^r P^\varepsilon_{\varphi_n} V^\varepsilon\right\|^2_{L^2(\mathbb{R}^d\times\mathbb{T}^d)} \underset{N\to\infty}{\longrightarrow} 0. \tag{4.13}$$

We thus focus on proving (4.13).

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 (4.9),

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

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

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

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

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

We use three observations.

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

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

To see this note that:

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

due to the definition of the H^s_ε-norm (4.3). 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,

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

This follows from the estimate:

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

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 $J_0, R > 0$,

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

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

$$\xi \longmapsto \sum_{n\in\mathbb{N}^*} |d_n(\xi,j)|^2 = \left\| P(\xi)^{r/2} \mathrm{e}^{2i\pi j\cdot} \right\|^2_{L^2(\mathbb{T}^d)} \in (0,\infty) \tag{4.14}$$

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:

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

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

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

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,

$$\begin{aligned}\limsup_{\varepsilon\to0^+} \sum_{n>N}\sum_{|j|>J_0}\int_{\mathbb{R}^d} |d_n(\varepsilon\xi,j)|^2 |\widehat{V}^\varepsilon_j(\xi)|^2 d\xi &\leq \limsup_{\varepsilon\to0^+} \sum_{|j|>J_0}\int_{\mathbb{R}^d}\sum_{n\in\mathbb{N}^*} |d_n(\varepsilon\xi,j)|^2 |\widehat{V}^\varepsilon_j(\xi)|^2 d\xi \\ &\leq c_r \limsup_{\varepsilon\to0^+} \sum_{|j|>J_0}\int_{\mathbb{R}^d} (1+|\varepsilon\xi|^2+|j|^2)^r |\widehat{V}^\varepsilon_j(\xi)|^2 d\xi < c_r\delta,\end{aligned}$$

using observation (1).

The second term is analyzed using observation (2):

$$\begin{aligned}&\limsup_{\varepsilon\to0^+} \sum_{n>N}\sum_{|j|\leq J_0}\int_{|\varepsilon\xi|>R} |d_n(\varepsilon\xi,j)|^2 |\widehat{V}^\varepsilon_j(\xi)|^2 d\xi \\ &\qquad\leq c_r \limsup_{\varepsilon\to0^+} \sum_{|j|\leq J_0}\int_{|\varepsilon\xi|>R} (1+|\varepsilon\xi|^2+|j|^2)^k |\widehat{V}^\varepsilon_j(\xi)|^2 d\xi < c_r\delta.\end{aligned}$$

Observation (3) ensures that

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

As a consequence of this analysis:

$$\limsup_{N\to+\infty}\limsup_{\varepsilon\to0^+} \sum_{n>N}\sum_{j\in\mathbb{Z}^d}\int_{\mathbb{R}^d} \left| \int_{\mathbb{T}^d} \varrho_n(\varepsilon\xi)^{r/2}\overline{\varphi_n}(z,\varepsilon\xi)\mathrm{e}^{2i\pi j\cdot z}dz\right|^2 |\widehat{V}^\varepsilon_j(\xi)|^2 d\xi < 2c_r\delta.$$

Since δ is arbitrary, the result follows.

(ii) By Point 2 of Proposition 4.1, it is enough to prove that for all $T>0$,

$$\limsup_{\varepsilon\to0^+}\sup_{t\in[0,T]} \|\mathbf{1}_{|\varepsilon D|>R} U^\varepsilon(t)\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} \underset{R\to\infty}{\longrightarrow} 0. \tag{4.15}$$

Because of the choice of $U^\varepsilon_0=\psi^\varepsilon_0\otimes\mathbf{1}_{\mathbb{T}^d}$ and of Remark 2.20 we have

$$\limsup_{\varepsilon\to0^+} \|\mathbf{1}_{|\varepsilon D|>R} U^\varepsilon_0\|_{H^s_\varepsilon(\mathbb{R}^d\times\mathbb{T}^d)} \underset{R\to\infty}{\longrightarrow} 0.$$

We set $U^\varepsilon_R(t,x)=\chi(\varepsilon D/R)U^\varepsilon(t)$ where $\chi\in C^\infty(\mathbb{R}^d)$ is such that $0\leq\chi\leq1$, $\chi(\xi)=1$ for $|\xi|>2$ and $\chi(\xi)=0$ for $|\xi|\leq1$. The family U^ε_R solves

$$i\varepsilon^2\partial_t U^\varepsilon_R = P(\varepsilon D)U^\varepsilon_R + \varepsilon^2 V_{\rm ext}(t,x)U^\varepsilon_R + \varepsilon^2[\chi(\varepsilon D/R),V_{\rm ext}(t,x)]U^\varepsilon \tag{4.16}$$

with initial data $U^\varepsilon_R(0)=\chi(\varepsilon D/R)U^\varepsilon(0)$. Besides, the Using operator $\dfrac{1}{\varepsilon}[\chi(\varepsilon D/R),V_{\rm ext}(t,x)]$ is uniformly bounded in $\mathcal{L}(L^2(\mathbb{R}^d))$ with respect to ε and R, which yields

$$\|U^\varepsilon_R(t)\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}\leq \|U^\varepsilon_R(0)\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}+O(\varepsilon)$$

and gives the result for $s=0$. We then assume $s\in\mathbb{N}^*$ and consider the operators $P(\varepsilon D)^{s/2}$ and $\langle\varepsilon D\rangle^s$. We are going to prove that uniformly with respect to R,

$$\|\langle\varepsilon D\rangle^s U^\varepsilon_R(t)\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}\leq \|\langle\varepsilon D\rangle^s U^\varepsilon_R(0)\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}+O(\varepsilon),$$
$$\|P(\varepsilon D)^{s/2} U^\varepsilon_R(t)\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}\leq \|P(\varepsilon D)^{s/2} U^\varepsilon_R(0)\|_{L^2(\mathbb{R}^d\times\mathbb{T}^d)}+O(\varepsilon).$$

The families $\langle\varepsilon D\rangle^s U^\varepsilon_R(t)$ and $P(\varepsilon D)^{s/2}U^\varepsilon_R(t)$ satisfy an equation similar to (4.16). One observes that the families of operators

$$\frac{1}{\varepsilon}\langle\varepsilon D\rangle^s[\chi(\varepsilon D/R),V_{\rm ext}(t,x)]\langle\varepsilon D\rangle^{-s}\ \text{ and }\ \frac{1}{\varepsilon}P(\varepsilon D)^{s/2}[\chi(\varepsilon D/R),V_{\rm ext}(t,x)]P(\varepsilon D)^{-s/2}$$

are uniformly bounded in $\mathcal{L}(L^2(\mathbb{R}^d\times\mathbb{T}^d))$. And so is the operator $\dfrac{1}{\varepsilon}[\langle\varepsilon D\rangle^s,V_{\rm ext}(t,x)]\langle\varepsilon D\rangle^{s-1}$. These two properties allow to use a recursive argument on s, which gives the expected result for values of s which are in $\mathbb{N}$. One then extends the result to any s by interpolation.

(iii) We proceed to a first extraction to have

$$\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}}\theta(t)a(x,\xi)W^{\varepsilon_\ell}[\psi^{\varepsilon_\ell}](t,x,\xi)dx\,d\xi\,dt\underset{\ell\to\infty}{\longrightarrow}\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}}\theta(t)a(x,\xi)\varsigma^t(dx,d\xi)dt. \tag{4.17}$$

and we keep denoting by ε the resulting subsequence. We put

$$\Psi^\varepsilon_N:=(\psi^\varepsilon_1,\dots,\psi^\varepsilon_N)\in C(\mathbb{R}_t;L^2(\mathbb{R}^d_x,\mathbb{C}^N))$$

and we are left with a vector-valued family as in Section 2.3.4. Any accumulation point of $(W^\varepsilon[\Psi^\varepsilon_N(t)])$ obtained along some subsequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ is a time-dependent family of positive matrix-valued Radon measures μ^t_N. By diagonal extraction, we can find a sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ such that $(W^{\varepsilon_\ell}[\Psi^{\varepsilon_\ell}_N(t)])_{\varepsilon>0}$ converge for every $N\in\mathbb{N}^*$. We denote by $(\mu^t_N)_{N\in\mathbb{N}^*}$ their respective limits and we have for every $n,n'\leq N\leq N'$ one has:

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

where $\mu^t_{n,n'}$ is obtained through (4.19). 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 $a\in C^\infty_c(\mathbb{R}^{2d})$ and $t\in\mathbb{R}$,

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

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

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

Finally, (i) implies that for every $\theta\in L^1(\mathbb{R})$,

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

which in turn guarantees that $\varsigma^t=\sum_{n,n'\in\mathbb{N}^*}\mu^t_{n,n'}$.

(iv) The result comes from the observation that since $\varrho_n(\xi)$ is $2\pi\mathbb{Z}^d$-periodic, L^ε commutes with $\varrho(\varepsilon D_x)$ (cf. point 1 of Proposition 4.1.

4.3. **Semi-classical analysis of Bloch components.** By the definition of $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ (see (4.1)), we deduce from the equation (1.9) that for all $n\in\mathbb{N}^*$, we have the pseudo-differential equation

$$\left\{\begin{array}{l} i\varepsilon^2\partial_t\psi_n^\varepsilon(t,x)=\varrho_n(\varepsilon D_x)\psi_n^\varepsilon(t,x)+\varepsilon^2 f_n^\varepsilon(t,x),\quad (t,x)\in\mathbb{R}\times\mathbb{R}^d,\\ \psi_n^\varepsilon(0,x)=\varphi_n\left(\frac{x}{\varepsilon},\varepsilon D_x\right)\int_{\mathbb{T}^d}\overline{\varphi_n}(y,\varepsilon D_x)\psi_0^\varepsilon(x)dy,\end{array}\right. \tag{4.18}$$

with f_n^ε given by (4.12). By Proposition 4.1 (1), the family $(f^\varepsilon(t))_{\varepsilon>0}$ is bounded in $L^\infty([0,T],L^2(\mathbb{R}^d))$ for all $T>0$.

Our aim is to obtain information about the measures $\mu_{n,n'}^t$ satisfying for all $\theta\in L^1(\mathbb{R})$, $a\in C_c^\infty(\mathbb{R}^{2d})$,

$$\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}}\theta(t)a(x,\xi)W^{\varepsilon_\ell^{n,n'}}[\psi_n^\varepsilon,\psi_{n'}^\varepsilon](t,x,\xi)dx\,d\xi\,dt\underset{\ell\to\infty}{\longrightarrow}\int_{\mathbb{R}}\int_{\mathbb{R}^{2d}}\theta(t)a(x,\xi)\mu_{n,n'}^t(dx,d\xi))dt, \tag{4.19}$$

Proposition 4.3. *Suppose $V_{\rm per}$ is smooth and $V_{\rm ext}\in C^1(\mathbb{R}^d)$ with $\nabla V_{\rm ext}$ bounded, consider $(\psi_0^\varepsilon)_{\varepsilon>0}$ a bounded family in $H_\varepsilon^s(\mathbb{R}^d)$ for some $s>d/2$. For any $n,n'\in\mathbb{N}^*$, let (ψ_n^ε) and $(\psi_{n'}^\varepsilon)$ be defined by* (4.1) *and let $\mu_{n,n'}^t$ be given by* (4.19)*. Let $\Omega\subseteq\mathbb{R}^d$ be open and invariant by translations by $2\pi\mathbb{Z}^d$. Then the following hold.*

(1) *If $\nabla\varrho_n\in{\rm Lip}(\mathbb{R}^d)$ on Ω and $\nabla_\xi\varrho_n|_\Omega\neq 0$, then $\mu_{n,n}^t(\mathbb{R}^d\times\Omega)=0$ for almost every $t\in\mathbb{R}$.*
(2) *Let $\delta>0$ and suppose that $\Omega\subset\{\xi\in\mathbb{R}^d\,:\,|\varrho_n(\xi)-\varrho_{n'}(\xi)|\geq\delta\}$, then $|\mu_{n,n'}^t|(\mathbb{R}^d\times\Omega)=0$ for almost every $t\in\mathbb{R}$.*

This result shows that $\mu_{n,n}^t$ can only charge the set of critical points of ϱ_n or the sets where ϱ_n has a conical crossing with another Bloch energy (*i.e.* where ϱ_n ceases to be $C^{1,1}(\mathbb{R}^d)$). It also shows that $\Sigma_{n,n'}$ is the only region where the measures $\mu_{n,n'}^t$ can be non-zero. The analysis of these measures will be performed in the following sections by means of a two-scale analysis.

The proof of this proposition uses the calculus of semi-classical pseudo-differential operators with low regularity of Lemma 2.12 and the following result.

Lemma 4.4. *Let $\Omega\subset\mathbb{R}^d$ and $\Phi_s:\mathbb{R}^d\times\Omega\to\mathbb{R}^d\times\Omega$ a flow satisfying: for every compact $K\subset\mathbb{R}^d\times\Omega$ such that K contains no stationary points of Φ there exist constants $\alpha,\beta>0$ such that:*

$$\alpha|s|-\beta\leqslant|\Phi_s(x,\xi)|\leqslant\alpha|s|+\beta,\quad\forall(x,\xi)\in K.$$

Let μ be a finite, positive Radon measure on $\mathbb{R}^d\times\Omega$ that is invariant by the flow Φ_s. Then μ is supported on the set of stationary points of Φ_s.

Proof
It suffices to show that $\mu(K)=0$ for every compact set $K\subset\mathbb{R}^d\times\Omega$ as in the statement of the lemma. By the assumption made on Φ_s, it is possible to find $s_k\to+\infty$ such that $\Phi_{s_k}(K)$, $k\in\mathbb{N}$, are mutually disjoint. The invariance property of μ implies that $\mu(\Phi_{s_k}(K))=\mu(K)$ and therefore, for every $N>0$:

$$\mu\left(\bigcup_{k=1}^N\Phi_{s_k}(K)\right)=N\mu(K).$$

Since μ is finite, we must have $\mu(K)=0$.

Proof
For proving Point 1, we write

$$i\varepsilon^2\frac{d}{dt}(\psi_n^\varepsilon(t),{\rm op}_\varepsilon(a)\psi_n^\varepsilon(t)_{L^2(\mathbb{R}^d)}=(\psi_n^\varepsilon(t),[{\rm op}_\varepsilon(a),\varrho_n(\varepsilon D_x)]\psi_n^\varepsilon(t)_{L^2(\mathbb{R}^d)}+O(\varepsilon^2).$$

By Lemma 2.12 (2), we deduce

$$-\varepsilon\frac{d}{dt}(\psi_n^\varepsilon(t),{\rm op}_\varepsilon(a)\psi_n^\varepsilon(t)_{L^2(\mathbb{R}^d)}=(\psi_n^\varepsilon(t),{\rm op}_\varepsilon(\nabla_\xi\varrho_n\cdot\nabla_x a)\psi_n^\varepsilon(t)_{L^2(\mathbb{R}^d)}+O(\varepsilon).$$

Therefore, for every $\theta \in C_c^\infty(\mathbb{R})$ and $a \in C_c^\infty(\mathbb{R}^d \times \Omega)$,

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

By (4.19), this implies that, for almost every $t \in \mathbb{R}$,

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

or equivalently 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 the measure $\mu_{n,n}^t$ is positive and finite, necessarily it is identically 0, thanks to the Lemma 4.4.

For proving Point 2, we write

$$\begin{aligned} i\varepsilon^2 \frac{d}{dt} &\left(\psi_n^\varepsilon(t), \mathrm{op}_\varepsilon(a)\psi_{n'}^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)} \\ &= \left(\psi_n^\varepsilon(t), \left(\varrho_{n'}(\varepsilon D_x)\mathrm{op}_\varepsilon(a) - \mathrm{op}_\varepsilon(a)\varrho_n(\varepsilon D_x)\right) \psi_{n'}^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)} + \varepsilon^2 R^\varepsilon(t), \end{aligned} \tag{4.20}$$

where $|R^\varepsilon(t)| \leq C\|f_n^\varepsilon(t,\cdot)\|_{L^2(\mathbb{R}^d)}^2$ is locally uniformly bounded in $t \in \mathbb{R}$ for every $\varepsilon > 0$. By Lemma 2.12 (1), 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 (4.20) into

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

Taking limits $\varepsilon \to 0$, which is possible by Remark 2.9, we obtain

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

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

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

5. Two-scale Wigner analysis

We develop in this section a two scale method for analyzing more precisely the concentration of a family on a point of the phase space. The two-scale Wigner measures (or two-scale semi-classical measures) that we describe here, have been first introduced in [17, 40, 41] (see also [18, 19]). The use of two-microlocal semiclassical measures for dispersive equations was initiated in [35], in the context of the Schrödinger equation on the torus. We restrict ourselves to the analysis of concentration on submanifolds of the space of impulsion (the ξ variable).

5.1. Two-scale Wigner measures.

5.1.1. *Two-scale observables.* 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 $\mathbb{S}^{d-1}$ at infinity. The test functions associated with this extended phase space are functions $a \in \mathcal{A}$ where $\mathcal{A}$ is defined as follows.

Definition 5.1. The function $a \in C^\infty(T^*\mathbb{R}^d_{x,\xi} \times \mathbb{R}^d_\eta)$ belongs to the set $\mathcal{A}$ of two-scale observables if it satisfies 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 $(x,\xi) \mapsto a(x,\xi,\eta)$ is a smooth function compactly supported in K;
(2) There exists a smooth function a_∞ defined on $T^*\mathbb{R}^d \times \mathbb{S}^{d-1}$ and $R_0 > 0$ such that, if $|\eta| > R_0$, then $a(x,\xi,\eta) = a_\infty(x,\xi,\eta/|\eta|)$.

In other words, Point 2 means that, in the set $\{|\eta| > R_0\}$, a coincides with a function a_∞ that is homogeneous of degree 0 in η. The data of $a \in \mathcal{A}$, defines a smooth function a_∞ on $\mathbb{R}^{2d} \times \mathbb{S}^{d-1}$ and a function $\underline{a}$ on $\mathbb{R}^{2d} \times \overline{\mathbb{R}}^d$ obtained by setting

$$\underline{a}(x,\xi,\eta) = a(x,\xi,\eta) \text{ if } |\eta| < +\infty \text{ and } \underline{a}(x,\xi,\eta) = a_\infty(x,\xi,\omega) \text{ if } \eta = \infty\,\omega,\ \omega \in \mathbb{S}^{d-1}. \tag{5.1}$$

If $a \in \mathcal{A}$, the compact K of Point 1 of Definition 5.1 is called the support of the symbol a.

The set $\mathcal{A}$ is a subspace of $C^\infty(\mathbb{R}^{3d})$ and of the space of smooth bounded functions with bounded derivatives. Indeed, for any $k \in \mathbb{N}$,

$$\sup_{\beta \in \mathbb{N}^{3d}} \sup_{(x,\xi,\eta) \in \mathbb{R}^{3d}} \left| \partial^\beta_{x,\xi,\eta} a(x,\xi,\eta) \right| < +\infty.$$

We shall consider the semi-norm

$$\widetilde{N}_d(a) := \sup_{\xi,\eta \in \mathbb{R}^d} \sup_{|\beta| \le d+1} \|\partial^\beta_x a(\cdot,\xi,\eta)\|_{L^1(\mathbb{R}^d)} \tag{5.2}$$

that appear in (2.13).

5.1.2. *Quantization of two-scale observables and two-scale Wigner transforms.* We introduce first here a two-scale quantization associated with a point ξ_0 of the space of the impulsions. We denote by ε^κ, for $\kappa \in (0,1]$, the second scale of observation. The two-scale Wigner transform acts on two-scale observables $a \in \mathcal{A}$ according to

$$\langle W^{\varepsilon,\kappa}_{\{\xi=\xi_0\}}[f]\ ,\ a \rangle = \left(f, \mathrm{op}_\varepsilon \left(a(x,\xi,\frac{\xi-\xi_0}{\varepsilon^\kappa}\right) f \right)_{L^2(\mathbb{R}^d)}. \tag{5.3}$$

One then defines the two-scale semi-classical pseudodifferential operator

$$\mathrm{op}^{\{\xi=\xi_0\}}_{\varepsilon,\kappa}(a) := \mathrm{op}_\varepsilon \left(a\left(x,\xi,\frac{\xi-\xi_0}{\varepsilon^\kappa}\right)\right),\quad a \in \mathcal{A},$$

and one has

$$\langle W^{\varepsilon,\kappa}_{\{\xi=\xi_0\}}[f]\ ,\ a \rangle = \left(f, \mathrm{op}^{\{\xi=\xi_0\}}_{\varepsilon,\kappa}(a) f \right)_{L^2(\mathbb{R}^d)},\quad \forall a \in \mathcal{A}.$$

The latter formula shows the zoom effect obtained by adding this new variable η. Indeed, when $|\eta| \le R$ for some $R > 0$, one restricts the domain of a to points (x, ξ) that are at a distance smaller than $R\varepsilon^\kappa$ from the set $\{\xi = \xi_0\}$). When $|\eta| > R$ is large, one considers larger domains, namely rings $\{R\varepsilon^\kappa < |\xi - \xi_0| < M\}$ where the constant M is related with the compact K in which a takes his values. The fact that $|\eta|$ can go to $+\infty$ allows to investigate all the directions and to visit all the compact K.

In the following, we shall use the operator of multiplication by the phase $\mathrm{e}^{-\frac{i}{\varepsilon}\xi_0\cdot x}$

Proposition 5.2. *Let $a \in \mathcal{A}$, we have the following properties.*

(1) *Suppose that the compact K associated to a by Point 1 of Definition 5.1 does not contain ξ_0. Then, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon \in (0, \varepsilon_0)$,*

$$\mathrm{op}_{\varepsilon,\kappa}^{\{\xi=\xi_0\}}(a) = \mathrm{op}_\varepsilon\left(a_\infty\left(x, \xi, \frac{\xi - \xi_0}{|\xi - \xi_0|}\right)\right).$$

(2) *The family of operators $\left(\mathrm{op}_{\varepsilon,\kappa}^{\{\xi=\xi_0\}}(a)\right)_{\varepsilon>0}$ is a bounded family in $\mathcal{L}(L^2(\mathbb{R}^d))$ satisfying*

$$\mathrm{op}_{\varepsilon,\kappa}^{\{\xi=\xi_0\}}(a) = \mathrm{e}^{\frac{i}{\varepsilon}\xi_0\cdot x}\mathrm{op}_{\varepsilon^{1-\kappa}}\left(a(x, \xi_0 + \varepsilon^\kappa\xi, \xi)\right)\mathrm{e}^{-\frac{i}{\varepsilon}\xi_0\cdot x}. \tag{5.4}$$

(3) *There exists $C > 0$ such that for all $f \in \mathcal{S}(\mathbb{R}^d)$*

$$\left|\langle W_{\{\xi=\xi_0\}}^{\varepsilon,\kappa}[f], a\rangle\right| \le C\,\|f\|_{L^2}^2\,\widetilde{N}_d(a),$$

where the semi-norm $\widetilde{N}_d$ is defined in (5.2).

(4) *If $(f^\varepsilon)_{\varepsilon>0}$ is a bounded family in $L^2(\mathbb{R}^d)$, the functionals*

$$a \mapsto \langle W_{\{\xi=\xi_0\}}^{\varepsilon,\kappa}[f^\varepsilon], a\rangle$$

are linear maps on $\mathcal{A}$ that are continuous uniformly in ε for the semi norm $\widetilde{N}_d$.

Proof

Point 1. The first part of the proposition comes from the observation that for such compact K, there exists $\varepsilon_0 > 0$ such that all $\varepsilon \in (0, \varepsilon_0)$, $|\xi - \xi_0| > R_0\varepsilon^\kappa$, where R_0 is associated to a by Point 2 of Definition 5.1. Therefore,

$$a\left(x, \xi, \frac{\xi - \xi_0}{\varepsilon^\kappa}\right) = a_\infty\left(x, \xi, \frac{\xi - \xi_0}{|\xi - \xi_0|}\right)$$

and the result follows.

Point 2 comes from an explicit calculus.

Points 3 and 4 are consequences of Point 2.

Remark 5.3. Equation (5.4) shows a fundamental difference between the case $\kappa \in (0, 1)$ and $\kappa = 1$. Indeed, when $\kappa \in (0, 1)$ and $a \in C_c^\infty(\mathbb{R}^{3d})$, the operator $\mathrm{op}_{\varepsilon,\kappa}^{\{\xi=\xi_0\}}(a)$ is unitarily equivalent to the operator $\mathrm{op}_{\varepsilon^{1-\kappa}}\left(a(x, \xi_0 + \varepsilon^\kappa\xi, \xi)\right)$ that coincides (at leading order) with a semi-classical operator of the same style than those studied in the preceding chapters, but for the scale $\varepsilon^{1-\kappa}$. Indeed one has

$$\mathrm{op}_{\varepsilon^{1-\kappa}}\left(a(x, \xi_0 + \varepsilon^\kappa\xi, \xi)\right) = \mathrm{op}_{\varepsilon^{1-\kappa}}\left(a(x, \xi_0, \xi)\right) + O(\varepsilon^\kappa R), \tag{5.5}$$

where $|\eta| \le R$ on the support of a. This comes from a Taylor estimate: there exists a constant $C > 0$ such that

$$N_d\big(a(x, \xi_0 + \varepsilon^\kappa\xi, \xi) - a(x, \xi_0, \xi)\big) \le \varepsilon^\kappa N_d\left(\int_0^1 x\cdot\nabla_x a(x, \xi_0 + \varepsilon^\kappa s\xi, \xi)ds\right) \le C\,R\,\varepsilon^\kappa.$$

However, if $\kappa = 1$, the latter relation relates the operator $\mathrm{op}_{\varepsilon,1}^{\{\xi=\xi_0\}}(a)$ with the operator $\mathrm{op}_1(a(x, \xi_0, \xi))$ which is no longer a semi-classical operator.

5.1.3. *Two-scale Wigner measures.* We now pass to the limit on the two-scale Wigner transform of a bounded family in $L^2(\mathbb{R}^d)$. We focus here on the scale $\kappa = 1$ and we omit the index 1 in the notation $\mathrm{op}_\varepsilon^{\{\xi=\xi_0\}}$.

Theorem 5.4. *Let $(f^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$, there exists a sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ which tends to 0 when ℓ goes to $+\infty$ and a positive measure ν_∞ on $\mathbb{R}^{2d}_{x,\xi} \times \mathbb{S}^{d-1}$ such that for all $a \in \mathcal{A}$,*

$$\left(f^{\varepsilon_\ell}, \mathrm{op}_{\varepsilon_n}^{\{\xi=\xi_0\}}(a) f^{\varepsilon_\ell}\right)_{L^2(\mathbb{R}^d)} \underset{\ell\to+\infty}{\longrightarrow} \int_{\mathbb{R}^d\times\mathbb{S}^{d-1}} a_\infty(x,\xi_0,\eta)\nu_\infty(d\xi,d\eta) + \left(f, a^W(x,\xi_0,D_x)f\right)_{L^2(\mathbb{R}^d)}$$
$$+ \int_{\mathbb{R}^{2d}\setminus\{\xi=\xi_0\}} a_\infty\left(x,\xi,\frac{\xi-\xi_0}{|\xi-\xi_0|}\right)\mu(dx,d\xi),$$

where μ is a Wigner measure of the family $(f^\varepsilon)_{\varepsilon>0}$ for the scale $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ and f a weak limit in $L^2(\mathbb{R}^d)$ of the family $\left(\mathrm{e}^{-\frac{i}{\varepsilon_\ell}x\cdot\xi_0} f^{\varepsilon_\ell}\right)_{n\in\mathbb{N}}$.

The term $\left(f, a^W(x,\xi_0,D_x)f\right)_{L^2(\mathbb{R}^d)}$ writes

$$\left(f, a^W(x,\xi_0,D_x)f\right)_{L^2(\mathbb{R}^d)} = \mathrm{Tr}(a^W(x,\xi_0,D_x)\mathbf{M}_f)$$

where $\mathbf{M}_f$ is the orthogonal projector on the subspace $\mathrm{Vect}(f)$ of $L^2(\mathbb{R}^d)$. It will be more convenient to use the operator $\mathbf{M}_f$.

Definition 5.5. We call the pair $(\nu_\infty, \mathbf{M}_f)$ a two-scale Wigner measure, or two-scale semi-classical measure, associated with the concentration of $(f^\varepsilon)_{\varepsilon>0}$ on the vector space $\{\xi = \xi_0\}$.

We set for $a \in \mathcal{A}$,

$$I^{\varepsilon_\ell}(a) = \left(f^{\varepsilon_\ell}, \mathrm{op}_{\varepsilon_\ell}^{\{\xi=\xi_0\}}(a) f^{\varepsilon_\ell}\right)_{L^2(\mathbb{R}^d)}.$$

Consider a function $\chi \in C_c^\infty(\mathbb{R}^d,[0,1])$ such that $\chi = 1$ in a neighborhood of 0 and set for $a \in \mathcal{A}$,

$$\left\{\begin{array}{lcl} a^\delta(x,\xi,\eta) & = & a(x,\xi,\eta)\left(1-\chi\left(\frac{\xi-\xi_0}{\delta}\right)\right), \\ a^R_\delta(x,\xi,\eta) & = & a(x,\xi,\eta)\left(1-\chi\left(\frac{\eta}{R}\right)\right)\chi\left(\frac{\xi-\xi_0}{\delta}\right), \\ a_R(x,\xi,\eta) & = & a(x,\xi,\eta)\chi\left(\frac{\eta}{R}\right)\chi\left(\frac{\xi-\xi_0}{\delta}\right). \end{array}\right. \tag{5.6}$$

Then, we have $a = a_R + a^R_\delta + a^\delta$ and

$$\limsup_{\delta\to0}\limsup_{R\to+\infty}\limsup_{\ell\to+\infty} I^\varepsilon(a^R_\delta) = \int_{\mathbb{R}^d\times\mathbb{S}^{d-1}} a_\infty(x,\xi_0,\eta)\nu(d\xi,d\eta),$$
$$\limsup_{\delta\to0}\limsup_{R\to+\infty}\limsup_{\ell\to+\infty} I^\varepsilon(a_R) = \left(f, a^W(x,\xi_0,D_x)f\right)_{L^2(\mathbb{R}^d)},$$
$$\limsup_{\delta\to0}\limsup_{R\to+\infty}\limsup_{\ell\to+\infty} I^\varepsilon(a^\delta) = \int_{\{\xi\neq\xi_0\}\times\mathbb{R}^d} a_\infty\left(x,\xi,\frac{\xi-\xi_0}{|\xi-\xi_0|}\right)\mu(dx,d\xi),$$

We obtain a description of the semi-classical measure above $\xi = \xi_0$

$$\mu(x,\xi)\mathbf{1}_{\xi=\xi_0} = \delta_{\xi_0}(\xi)\otimes\left(|f(x)|^2dx + \int_{\mathbb{S}^{d-1}}\nu_\infty(x,d\eta)\right).$$

The knowledge of the two-scale Wigner measures determine μ above ξ_0.

Example 5.6. Let $\varphi \in \mathcal{S}(\mathbb{R}^d)$, $\xi_0, \eta_0 \in \mathbb{R}^d$, $\beta > 0$ and consider the family

$$u^\varepsilon_\beta(x) = \varphi(x) \mathrm{e}^{\frac{i}{\varepsilon} x\cdot(\xi_0 - \varepsilon^\beta \eta_0)}, \qquad x \in \mathbb{R}^d.$$

Then, the pair $(\nu^{(\beta)}_\infty, f_\beta)$ describing the concentration of $(u^\varepsilon_\beta)_{\varepsilon>0}$ on $\{\xi = \xi_0\}$ is given by

$$\begin{cases} \nu^{(\beta)}_\infty = 0 \;\text{ and }\; f_\beta = \varphi & \text{if } \;\beta > 1, \\ \nu^{(\beta)}_\infty = 0 \;\text{ and }\; f_\beta(x) = \mathrm{e}^{-ix\cdot\eta_0}\varphi(x) & \text{if } \;\beta = 1, \\ \nu^{(\beta)}_\infty(x,\eta) = \delta_{\frac{\eta_0}{|\eta_0|}\infty}(\eta) \otimes |\varphi(x|^2 dx \;\text{ and }\; f_\beta = 0 & \text{if } \;\beta < 1. \end{cases}$$

In the three cases, the semi-classical measure is $\mu(x,\xi) = \delta_{\xi_0}(\xi) \otimes |\varphi(x)|^2 dx$.

Remark 5.7.
(1) As for the standard Wigner measures, the definition of two-scale Wigner measures can be extended to vector-valued families and to time-dependent ones.
(2) The notion can also be extended to the concentration of families on submanifolds of the cotangent space of the form $\mathbb{R}^d \times M$ (see [14]).

Let us now prove Theorem 5.4.

Proof
We use the decomposition $a = a_R + a^R_\delta + a^\delta$ of (5.6). We first observe that if μ is a semiclassical measure of $(f^\varepsilon)_{\varepsilon>0}$ for a subsequence that we denote ε_ℓ, $\ell \in \mathbb{N}$. Then, we have

$$\limsup_{\ell\to+\infty} \left(f^{\varepsilon_\ell}, \mathrm{op}^{\{\xi=\xi_0\}}_{\varepsilon_\ell}(a^\delta) f^{\varepsilon_\ell} \right)_{L^2(\mathbb{R}^d)} \underset{\delta\to 0}{\longrightarrow} \int_{\mathbb{R}^{2d}} a_\infty \left(x, \xi, \frac{\xi-\xi_0}{|\xi-\xi_0|} \right) \mu(dx, d\xi). \tag{5.7}$$

Moreover, by (5.5)

$$\left(f^\varepsilon, \mathrm{op}^{\{\xi=\xi_0\}}_\varepsilon(a_R) f^\varepsilon \right)_{L^2(\mathbb{R}^d)} = \left(\widetilde{f}^\varepsilon, \mathrm{op}_1(a_R(x,\xi_0,\xi)) \widetilde{f}^\varepsilon \right)_{L^2(\mathbb{R}^d)} + O(R\varepsilon)$$

with $\widetilde{f}^\varepsilon = \mathrm{e}^{-\frac{i}{\varepsilon}\xi_0\cdot x} f^\varepsilon$. Since the operator $\mathrm{op}_1(a_R(x,\xi_0,\xi)) = a^W_R(x,\xi_0,D_x)$ is a compact operator, independent of ε, if f is a weak limit in $L^2(\mathbb{R}^d)$ of $\widetilde{f}^\varepsilon$ for the subsequence ε_ℓ, one has

$$\left(\widetilde{f}^{\varepsilon_\ell}, \mathrm{op}_1(a_R(x,\xi_0,\xi)) \widetilde{f}^{\varepsilon_\ell} \right)_{L^2(\mathbb{R}^d)} \underset{\ell\to+\infty}{\longrightarrow} \left(f, a^W_R(x,\xi_0,D_x) f \right)_{L^2(\mathbb{R}^d)}.$$

We deduce

$$\limsup_{\ell\to+\infty} \left(f^{\varepsilon_\ell}, \mathrm{op}^{\{\xi=\xi_0\}}_{\varepsilon_\ell}(a) f^{\varepsilon_\ell} \right)_{L^2(\mathbb{R}^d)} \underset{R\to+\infty}{\longrightarrow} \left(f, a^W(x,\xi_0,D_x) f \right)_{L^2(\mathbb{R}^d)}. \tag{5.8}$$

Finally, we consider the symbol a^R that is supported in the zone $R > |\eta|$. We consider the quantity

$$J_{\varepsilon,R}(a) := \left(\widetilde{f}^\varepsilon, \mathrm{op}_1(a^R(x,\xi_0+\varepsilon\xi,\xi)) \widetilde{f}^\varepsilon \right)_{L^2(\mathbb{R}^d)}.$$

We are interested in the limit where ε goes to 0 first and then R goes to $+\infty$. This quantity is uniformly bounded in $\varepsilon > 0$ and $R > 1$. Besides, for all $a \in \mathcal{A}$, $J_{\varepsilon,R}(a) = J_{\varepsilon,R}(a_\infty)$ as soon as R is large enough. We then deduce by a diagonal extraction argument that one can find two sequences $\varepsilon_\ell \underset{\ell\to+\infty}{\longrightarrow} 0$ and $R_\ell \underset{\ell\to+\infty}{\longrightarrow} +\infty$, and a linear form I defined on $C^\infty(\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{S}^{d-1})$, such that for all $a \in \mathcal{A}$,

$$J_{\varepsilon_\ell, R_\ell}(a) \underset{\ell\to+\infty}{\longrightarrow} J(a_\infty).$$

It remains to prove that $a_\infty \mapsto J(a_\infty)$ is a measure, which will define $\nu \mathbf{1}_{|\eta|=\infty}$. For this, we prove that $a_\infty \mapsto J(a_\infty)$ is a positive distribution. Let us start with the distribution argument: we observe that there exists a constant $C > 0$ such that for all $a \in \mathcal{A}$,

$$J_{\varepsilon_\ell, R_\ell}(a) \leq C \widetilde{N}_d(a^{R_\ell}),$$

and we deduce from $N_d(a^{R_\ell}) \underset{n\to+\infty}{\longrightarrow} N_d(a_\infty)$ that $J(a_\infty) \leq N_d(a_\infty)$. Therefore $a_\infty \mapsto J(a_\infty)$ is a distribution. To prove the positivity, we observe that the operators $a \mapsto \mathrm{op}_1(a^R(x,\xi_0+\varepsilon\xi,\xi)$ satisfy a semi-classical calculus in the parameters ε and $1/R$. Indeed, we have the following observations: for all $a, a_1, a_2 \in \mathcal{A}_d$

(i) $\mathrm{op}_1(a^R(x,\xi_0+\varepsilon\xi,\xi)^* = \mathrm{op}_1(\overline{a}^R(x,\xi_0+\varepsilon\xi,\xi))$,

(ii) in $\mathcal{L}(L^2(\mathbb{R}^d))$,

$$\mathrm{op}_1(a_1^R(x,\xi_0+\varepsilon\xi,\xi)\circ \mathrm{op}_1(a_2^R(x,\xi_0+\varepsilon\xi,\xi)) = \mathrm{op}_1((a_1a_2)^R(x,\xi_0+\varepsilon\xi,\xi)) + O\left(\varepsilon+\frac{1}{R}\right)$$

Therefore, one has the following Gårding inequality

(iii) if $a\geq 0$, then for all $\delta>0$ there exists $C_\delta>0$ such that for all $f\in L^2(\mathbb{R}^d)$,

$$\left(f, \mathrm{op}_1(a^R(x,\xi_0+\varepsilon\xi,\xi)f\right)_{L^2(\mathbb{R}^d)} \geq -\left(\delta + C_\delta\left(\varepsilon+\frac{1}{R}\right)^2\right)\|f\|_{L^2}.$$

One can then conclude to the positivity of the map $a_\infty \mapsto J(a_\infty)$, whence it defines a positive measure on $\mathbb{R}^{2d}\times\mathbb{S}^{d-1}$, that we denote by ν_∞, such that, after extraction of subsequences R_ℓ, ε_ℓ, we have

$$\limsup_{\ell\to+\infty}\left(f^{\varepsilon_\ell}, \mathrm{op}_{\varepsilon_\ell}^{\{\xi=\xi_0\}}(a_\delta^{R_\ell})f^{\varepsilon_\ell}\right)_{L^2(\mathbb{R}^d)} \underset{\delta\to 0}{\longrightarrow} \int_{\mathbb{R}^d\times\mathbb{S}^{d-1}} a_\infty(x_0,\xi,\eta)\nu_\infty(d\xi,d\eta). \tag{5.9}$$

Putting together (5.7), (5.8) and (5.9) concludes the proof.

Let us conclude this paragraph by a comment about the case $\kappa\in(0,1)$, for which one has the following Theorem.

Theorem 5.8. *Let $(f^\varepsilon)_{\varepsilon>0}$ be a bounded family in $L^2(\mathbb{R}^d)$, there exists a sequence $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$ which tends to 0 when n goes to $+\infty$ and a positive measure ν on $\mathbb{R}^d_x\times\overline{\mathbb{R}^d}_\eta$ such that for all $a\in\mathcal{A}$,*

$$\left(f^{\varepsilon_\ell}, \mathrm{op}_{\varepsilon_\ell,\kappa}^{\{\xi=\xi_0\}}(a)f^{\varepsilon_\ell}\right) \underset{\ell\to+\infty}{\longrightarrow} \int_{\mathbb{R}^d\times\overline{\mathbb{R}^d}} \underline{a}(x,\xi_0,\eta)\nu(dx,d\eta) + \int_{\mathbb{R}^{2d}\setminus\{\xi=\xi_0\}} a_\infty\left(x,\xi,\frac{\xi-\xi_0}{|\xi-\xi_0|}\right)\mu(dx,d\xi),$$

where μ is a Wigner measure of the family $(f^\varepsilon)_{\varepsilon>0}$ for the scale $(\varepsilon_\ell)_{\ell\in\mathbb{N}}$.

Thus illustrates the criticality of the concentration at semi-classical scale, as already mentioned in Remark 5.3, in the case $\kappa=1$ some quantum effects remain.

5.2. **Concentration of Bloch components on critical points.** We resume with the families $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ satisfying the equation (4.11). We denote by Λ_n the set of critical points of the Bloch mode ϱ_n.

$$\Lambda_n := \{\xi\in\mathbb{R}^d\setminus\cup_{n'\neq n}\Sigma_{n,n'} \;:\; \nabla\varrho_n(\xi)=0\}. \tag{5.10}$$

According to the analysis of Chapter 3.2, when $d=1$, Λ_n consists in isolated non degenerate critical points. Our aim in this section is to compute the two-scale Wigner measures associated with the concentration of $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ on such a point.

We fix $n>0$ such that ϱ_n is isolated from the remainder of the spectrum in an open subset Ω of $\mathbb{R}^d$ (as in (3.14)). Note that Ω can be chosen so that it does not contain any crossing point of $\Sigma_{n,n'}$. Therefore, by Proposition 4.3, any semi-classical measure of $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ satisfies $\mu_n^t\mathbf{1}_{\xi\in\Omega} = \mu_n^t\mathbf{1}_{\xi\in\Omega\cap\Lambda_n}$.

The equation (4.11) writes

$$i\varepsilon^2\partial_t\psi_n^\varepsilon(t,x) = \varrho_n(\varepsilon D)\psi_n^\varepsilon(t,x) + \varepsilon^2 V_{\mathrm{ext}}(t,x)\psi_n^\varepsilon(t,x) + \varepsilon^2 r_n^\varepsilon(t,x)$$

with $r^\varepsilon(t,x) = L^\varepsilon[V_{\rm ext}(t,x), \Pi_n(\varepsilon D)]U^\varepsilon(t,x,\cdot)$, uniformly bounded in $L^2(\mathbb{R}^d)$. Moreover, since in Ω, the map $\xi \mapsto \Pi_n(\xi)$ is smooth, for all $\theta \in C_c(\Omega)$ and $t \in \mathbb{R}$, $\theta(\varepsilon D) r^\varepsilon(t) = O(\varepsilon)$. Observing that any microlocal symbol $a = a(x,\xi)$ with support in $\mathbb{R}^d \times \Omega$ satisfies ${\rm op}_\varepsilon(a) = {\rm op}_\varepsilon(a)\theta(\varepsilon D) + O(\varepsilon^N)$, in $\mathcal{L}(L^2(\mathbb{R}^d)$ for any function $\theta \in C_c(\Omega)$ such that $\theta = 1$ on the support of a, and for any $N \in \mathbb{N}$, we deduce that for all $a \in \mathcal{A}$ with support in $\mathbb{R}^d \times \Omega$, and uniformly for $t \in [0,T]$, $T > 0$,

$$ {\rm op}_\varepsilon^{\{\xi=\xi_0\}}(a) r^\varepsilon(t) = O(\varepsilon) \;\text{ in }\; L^2(\mathbb{R}^d). $$

The strategy being independent of the dimension of the space, we state the result in any dimension, assuming that Λ_n contains an isolated point ξ_n and we focus on this point.

Theorem 5.9 ([14]). *Let $n > 0$ such that ϱ_n is isolated from the remainder of the spectrum in an open subset Ω of $\mathbb{R}^d$ (as in* (3.14)*), assume that $\Omega \cap \Lambda_n = \{\xi_n\}$. Then, any pair $(\nu_n^t, \mathbf{M}_n^t)$ of two-microlocal items associated with the concentration of $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ above ξ_n satisfies:*

1. *The operator $\mathbf{M}_n^t$ is the orthogonal projection of $L^2(\mathbb{R}^d)$ along the function $\psi_{\xi_n}^{(n)}(t)$ which solves the Schrödinger equation* (1.12)*, namely*

$$ i\partial_t \psi_{\xi_n}^{(n)}(t,x) = \frac{1}{2} d^2\varrho_n(\xi) D_x \cdot D_x \psi_{\xi_n}^{(n)}(t,x) + V_{\rm ext}(t,x)\psi_{\xi_n}^{(n)}(t,x), $$

with initial data $\psi_{\xi_n}^{(n)}(0)$ which is a weak limit of $\left({\rm e}^{-\frac{i}{\varepsilon}\xi_n\cdot x} L^\varepsilon \Pi_n(\varepsilon D_x)(\psi_0^\varepsilon(x)\mathbf{1}_{y\in\mathbb{T}})\right)_{\varepsilon>0}$.

2. *The measure ν_n^t is invariant by the flow ϕ_n^s,*

$$ \phi_n^s : \; (x,\omega) \mapsto (x + s\, d^2\varrho_n(\sigma)\omega, \omega), $$

which implies by Lemma 4.4, that, if ξ_n is a non degenerate critical point, then $\nu_n^t = 0$.

Note that the operator $\mathbf{M}_n^t$ satisfies the von Neumann equation

$$ i\partial_t \mathbf{M}_n^t = \frac{1}{2}\left[d^2\varrho_n(\xi) D_x \cdot D_x + V_{\rm ext}(t,x), \mathbf{M}_n^t\right]. \tag{5.11} $$

Besides, the map $t \mapsto \mathbf{M}_n^t$ is continuous.

Theorem 5.9 has the following consequence when $d = 1$.

Corollary 5.10. *Assume $d = 1$ and let ξ_n be a critical point of ϱ_n. Then, in Ω*

$$ \mu_{n,n}^t(x,\xi)\mathbf{1}_{\xi\in\Omega} = \delta_{\xi_n}(\xi) \otimes |\psi_{\xi_n}^{(n)}(t,x)|^2 dx $$

where $\psi_{\xi_n}^{(n)}(t)$ solves (1.12)*, with $\xi = \xi_n$.*

Proof
The proof consists in two parts corresponding to the two zones defined by the scale ε around ξ_n. We consider a pair $(\nu_n^t, \mathbf{M}_n^t)$ and we denote by ε the subsequence associated with them.

Part 1: Analysis at finite distance. For computing $\mathbf{M}_n^t$, we analyze for $a \in C_c^\infty(\mathbb{R}^d \times \Omega \times \mathbb{R}^d)$ the time evolution of the quantity $\left\langle W^\varepsilon_{\{\xi=\xi_n\}}[\psi_n^\varepsilon(t)], a\right\rangle$, as defined in (5.3), and omitting the mention of $\kappa = 1$. We have

$$ \begin{aligned} \frac{d}{dt}\left\langle W^\varepsilon_{\{\xi=\xi_n\}}[\psi_n^\varepsilon(t)], a\right\rangle &= \frac{1}{i\varepsilon^2}\left(\psi_n^\varepsilon(t), \left[{\rm op}_\varepsilon^{\{\xi=\xi_n\}}(a), \varrho_n(\varepsilon D)\right]\psi_n^\varepsilon(t)\right) \\ &\quad + \frac{1}{i}\left(\psi^\varepsilon(t)\;,\;\left[{\rm op}_\varepsilon^{\{\xi=\xi_n\}}(a), V_{\rm ext}(t,x)\right]\psi^\varepsilon(t)\right) + O(\varepsilon). \end{aligned} \tag{5.12} $$

Since ϱ_n is smooth in Ω, we can use the standard symbolic calculus for Weyl quantization and we obtain that in $\mathcal{L}(L^2(\mathbb{R}^d))$

$$ \frac{1}{i\varepsilon^2}\left[{\rm op}_\varepsilon^{\{\xi=\xi_n\}}(a), \varrho_n(\varepsilon D)\right] = \frac{1}{\varepsilon}\,{\rm op}_\varepsilon^{\{\xi=\xi_n\}}(\nabla\varrho_n(\xi)\cdot\nabla_x a) + O(\varepsilon). $$

Besides, by Taylor formula and by use of $\nabla\varrho_n(\xi_n)=0$, we have

$$\nabla\varrho_n(\xi)=d^2\varrho_n(\xi_n)\,(\xi-\xi_n)+B(\xi)\,(\xi-\xi_n)\cdot(\xi-\xi_n)\,, \tag{5.13}$$

where $\xi\mapsto B(\xi)$ is a smooth matrix-valued map. This yields

$$\frac{1}{\varepsilon}\nabla\varrho_n(\xi)\cdot\nabla_x a\left(x,\xi,\frac{\xi-\xi_n}{\varepsilon}\right)=b\left(x,\xi,\frac{\xi-\xi_n}{\varepsilon}\right)$$

with

$$b(x,\xi,\eta)=d^2\varrho_n(\xi_n)\eta\cdot\nabla_x a(x,\xi,\eta)+B(\xi)\,(\xi-\xi_n)\cdot\eta\nabla_x a(x,\xi,\eta).$$

At this stage of the proof, we see that $\frac{d}{dt}\left\langle W^\varepsilon_{\{\xi=\xi_n\}}[\psi^\varepsilon_n(t)],a\right\rangle$ is uniformly bounded in ε. Thus using a suitable version of Ascoli's theorem and a standard diagonal extraction argument, we can find a sequence (ε_k) such that the limit exists for all $a\in C_c^\infty(\mathbb{R}^d\times\Omega\times\mathbb{R}^d)$ and all time $t\in[0,T]$ (for some $T>0$ fixed) with a limit that is a continuous map in time. The transport equation that we are now going to prove shall guarantee the independence of the limit from $T>0$ and imply the characterization of $\mathbf{M}^t_n$. Moreover, the continuity of $t\mapsto\mathbf{M}^t_n$ implies that at $t=0$, $\mathbf{M}^0_n$ has to coincide with the projector on a weak limit of $\left({\rm e}^{-\frac{i}{\varepsilon}\xi_n\cdot x}L^\varepsilon\Pi_n(\varepsilon D_x)(\psi^\varepsilon_0(x)\mathbf{1}_{y\in\mathbb{T}})\right)_{\varepsilon>0}$.

It remains to prove the transport equation (5.11). We rewrite (5.12) as

$$\begin{aligned}\frac{d}{dt}\left\langle W^\varepsilon_{\{\xi=\xi_n\}}[\psi^\varepsilon_n(t)],a\right\rangle&=\left(\psi^\varepsilon_n(t),{\rm op}_\varepsilon^{\{\xi=\xi_n\}}(b)\psi^\varepsilon_n(t)\right)\\&\quad+\frac{1}{i}\left(\psi^\varepsilon(t)\;,\;\left[{\rm op}_\varepsilon^{\{\xi=\xi_n\}}(a),V_{\rm ext}(t,x)\right]\psi^\varepsilon(t)\right)+O(\varepsilon),\end{aligned}$$

and pass to the limit. We obtain

$$\begin{aligned}\frac{d}{dt}{\rm Tr}_{L^2(\mathbb{R}^d)}\left(a^W(x,\xi_n,D_x)\mathbf{M}^t_n\right)&={\rm Tr}_{L^2(\mathbb{R}^d)}\left(b^W(x,\xi_n,D_x)\mathbf{M}^t_n\right)\\&\quad+{\rm Tr}_{L^2(\mathbb{R}^d)}\left([a^W(x,\xi_n,D_x),V_{\rm ext}(t,x)]\mathbf{M}^t_n\right).\end{aligned}$$

Moreover

$$b^W(x,\xi_n,D_x)={\rm op}_1\left(d^2\varrho_n(\xi_n)\xi\cdot\nabla_x a(x,\xi_n,\xi)\right)=\frac{1}{2}\left[d^2\varrho_n D_x\cdot D_x,a^W(x,\xi,D_x)\right].$$

We deduce, using the cyclicity of the trace

$$\begin{aligned}&\frac{d}{dt}{\rm Tr}_{L^2(\mathbb{R}^d)}\left(a^W(x,\xi_n,D_x)\mathbf{M}^t_n\right)\\&\quad={\rm Tr}_{L^2(\mathbb{R}^d)}\left(\left[a^W(x,\xi_n,D_x),\frac{1}{2}d^2\varrho_n D_x\cdot D_x+V_{\rm ext}(t,x)\right]\mathbf{M}^t_n\right)\\&\quad={\rm Tr}_{L^2(\mathbb{R}^d)}\left(a^W(x,\xi_n,D_x)\left[\frac{1}{2}d^2\varrho_n D_x\cdot D_x+V_{\rm ext}(t,x),\mathbf{M}^t_n\right]\right),\end{aligned}$$

whence the equation (5.11).

Part 2: Analysis at infinity. Let $a\in\mathcal{A}$ with support in $\mathbb{R}^d\times\Omega\times\mathbb{R}^d$. We use a cut-off function $\chi\in C_c^\infty(\mathbb{R}^d,[0,1])$ identically equal to 1 close to 0, and we set (as in (5.6))

$$a^R_\delta(x,\xi,\eta)=a(x,\xi,\eta)\,\chi\left(\frac{\xi-\xi_n}{\delta}\right)\left(1-\chi\left(\frac{\eta}{R}\right)\right).$$

We introduce the symbol

$$b^R_\delta(s,x,\xi,\eta)=a^R_\delta\left(x+sd^2\varrho_n(\xi)\frac{\eta}{|\eta|},\xi,\eta\right).$$

We have $b_\delta^R \in \mathcal{A}$ and

$$(b_\delta^R)_\infty(s,x,\xi,\omega) = a_\infty \circ \phi_n^s(x,\xi,\omega)\chi\left(\frac{\xi-\xi_n}{\delta}\right).$$

Our aim is to prove that for $\theta \in C_c^\infty(\mathbb{R})$ and $s\in\mathbb{R}$,

$$\limsup_{\delta\to 0}\ \limsup_{R\to+\infty}\ \limsup_{\varepsilon\to 0} \int_{\mathbb{R}} \theta(t)\langle W^\varepsilon_{\{\xi=\xi_n\}}[\psi_n^\varepsilon(t)], b_s^{R,\delta}\rangle dt = 0.$$

We observe

$$\frac{d}{ds} b_\delta^R\left(s,x,\xi,\frac{\xi-\xi_n}{\varepsilon}\right) = \nabla_x a_\delta^R\left(x + sd^2\varrho_n(\xi)\frac{\xi-\xi_n}{|\xi-\xi_n|},\xi,\frac{\xi-\xi_n}{\varepsilon}\right)\cdot d^2\varrho_n(\xi)\frac{\xi-\xi_n}{|\xi-\xi_n|}.$$

Since $d^2\varrho_n(\xi)(\xi-\xi_n) = \nabla\varrho_n(\xi) + O(|\xi-\xi_n|^2)$, we have

$$\frac{d}{ds} b_\delta^R\left(s,x,\xi,\frac{\xi-\xi_n}{\varepsilon}\right) = \nabla\varrho_n(\xi)\cdot\nabla x c_\delta^R\left(s,x,\xi,\frac{\xi-\xi_n}{\varepsilon}\right) + \delta\, r_\varepsilon(x,\xi)$$

with

$$c_\delta^R(s,x,\xi,\eta) = \frac{1}{|\xi-\xi_n|} b_\delta^R(s,x,\xi,\eta)$$

and r^ε such that for all $\alpha\in\mathbb{N}^d$, $(x,\xi)\mapsto\partial_x^\alpha r^\varepsilon(x,\xi)$ is bounded uniformly in ε and R. Note that regarding c_δ^R, we have

$$\forall\alpha,\beta\in\mathbb{N}^d,\ \exists C_\alpha>0,\ \forall R>1,\ \forall\delta,\varepsilon\in(0,1),\ \|x^\beta\partial_x^\alpha c_\delta^R\|_{L^\infty} \le \frac{C_\alpha}{R\varepsilon}, \tag{5.14}$$

in particular $\widetilde{N}_d(c_\delta^R) = O(1/(R\varepsilon))$. Let us now conclude the proof. We first write, uniformly in $\varepsilon\in(0,1)$, $R\in[1,+\infty)$ and $s\in\mathbb{R}$

$$\begin{aligned}&\left(\psi_n^\varepsilon(t), \mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(\frac{d}{ds}b_\delta^R(s)\right)\psi_n^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)}\\ &\quad= \left(\psi_n^\varepsilon(t), \frac{i}{\varepsilon}\left[\varrho_n(\varepsilon D), \mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(c_\delta^R(s)\right)\right]\psi_n^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)} + O(\delta).\end{aligned}$$

Then, taking into account equation (4.11), we deduce that uniformly in $\varepsilon\in(0,1)$, $R\in[1,+\infty)$ and $s\in\mathbb{R}$

$$\begin{aligned}\left(\psi_n^\varepsilon(t), \mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(\frac{d}{ds}b_\delta^R(s)\right)\psi_n^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)} &= -\varepsilon\frac{d}{dt}\left(\psi_n^\varepsilon(t), \mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(c_\delta^R(s)\right)\psi_n^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)}\\ &- i\varepsilon\left(\psi_n^\varepsilon(t), \mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(c_\delta^R(s)\right)f_n^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)} + i\varepsilon\left(f_n^\varepsilon(t), \mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(c_\delta^R(s)\right)\psi_n^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)}\\ &+ O(\delta) + O(\varepsilon).\end{aligned}$$

The estimate (5.14) gives $\|\mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(c_\delta^R(s)\right)\|_{\mathcal{L}(L^2(\mathbb{R}^d))} = O\left(\frac{1}{\varepsilon R}\right)$. Therefore, for any $\theta\in C_c^\infty(\mathbb{R})$, we have

$$\int_{\mathbb{R}}\theta(t)\left(\psi_n^\varepsilon(t), \mathrm{op}_\varepsilon^{\{\xi=\xi_n\}}\left(\frac{d}{ds}b_\delta^R(s)\right)\psi_n^\varepsilon(t)\right)_{L^2(\mathbb{R}^d)} dt = O\left(\frac{1}{R}\right) + O(\varepsilon) + O(\delta),$$

which concludes the proof.

5.3. **Concentration above crossing points.** In this section, we analyze the semi-classical measure of $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ above crossing points. Here again, we work in any dimension under the assumption that crossing points are isolated points of the space of impulsions, which is the case when $d=1$. We also assume that for all $n\in\mathbb{N}^*$, 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 $|n-n'|=1$. We write

$$\Sigma_n := \Sigma_{n,n+1}, \quad n\in\mathbb{N}^*. \tag{5.15}$$

We additionally assume that in an open set Ω, we have $\Sigma_n\cap\Omega=\{\sigma_n\}$ and we aim at calculating the two-microlocal semi-classical measures associated with the concentration of $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ above σ_n. All these assumptions are satisfied when $d=1$.

Finally, we assume that the crossing is conical above the point σ_n in the sense that there exists an homogeneous function of degree 1, g_n, such that

$$\forall\xi\in\Omega,\ \ (\varrho_{n+1}-\varrho_n)(\xi)=g_n(\xi-\sigma_n).$$

We set

$$\lambda_n(\xi)=\frac{1}{2}\left(\varrho_{n+1}(\xi)+\varrho_n(\xi)\right).$$

We recall that when $d=1$, $\nabla\lambda_n(\sigma_n)\pm g_n(\omega)\neq 0$ for $\omega\in\{-1,+1\}$ (see Lemma 3.13 (4)).

Theorem 5.11. *Assume $\nabla g_n(\omega)\neq\nabla\lambda_n(\sigma_n)$ for all $\omega\in\mathbb{S}^{d-1}$. Then, with the preceding assumptions, any pair (γ_n^t,Γ_n^t) of two-microlocal semi-classical measures associated with the concentration of $(\psi_n^\varepsilon(t))_{\varepsilon>0}$ on $\{\xi=\sigma_n\}$ is $(0,0)$ dt-almost everywhere.*
If moreover $\nabla g_n(\omega)\neq-\nabla\lambda_n(\sigma_n)$ for all $\omega\in\mathbb{S}^{d-1}$. Then, any pair $(\gamma_{n+1}^t,\Gamma_{n+1}^t)$ of two-microlocal semi-classical measures associated with the concentration of the family $(\psi_{n+1}^\varepsilon(t))_{\varepsilon>0}$ on $\{\xi=\sigma_n\}$ is also $(0,0)$ dt-almost everywhere.

Corollary 5.12. *When $d=1$, the assumptions of Theorem 5.11 are satisfied and, assuming that Ω does not contain any critical points of ϱ_n and ϱ_{n+1} (which is always possible), we have*

$$\mu_{n,n}^t\mathbf{1}_{\xi\in\Omega}=\mu_{n+1,n+1}^t\mathbf{1}_{\xi\in\Omega}=0,\quad \textit{whence}\ \ \mu_{n,n+1}^t\mathbf{1}_{\xi\in\Omega}=0\ \ \textit{as}\ \ \textit{well.}$$

Proof
Here again, we prove Theorem 5.11 in two steps: first we focus on the part of the two-scale Wigner measure that comes from infinity, then we concentrate on the part at finite distance.

Part 1: The two-scale Wigner measure at infinity. Let $a\in\mathcal{A}$ supported in $\mathbb{R}^d\times\Omega\times\mathbb{R}^d$ and $\chi\in C_c^\infty(\mathbb{R}^d,[0,1])$ $\chi\in C_0^\infty(\mathbb{R}^d,[0,1])$ identically equal to 1 close to 0. We set for $R,\delta>0$ (as in (5.6))

$$a_\delta^R(x,\xi,\eta)=a(x,\xi,\eta)\,\chi\left(\frac{\xi-\xi_n}{\delta}\right)\left(1-\chi\left(\frac{\eta}{R}\right)\right).$$

Then, in view of equation (4.18),

$$i\varepsilon\frac{d}{dt}\left\langle W^\varepsilon_{\{\xi=\sigma_n\}}[\psi_n^\varepsilon(t)],a\right\rangle=\varepsilon^{-1}\left(\psi_n^\varepsilon(t),[\mathrm{op}_\varepsilon^{\{\xi=\sigma_n\}}(a_\delta^R),\varrho_n(\varepsilon D)]\psi_n^\varepsilon(t)\right)+O(\varepsilon). \tag{5.16}$$

Using the homogeneity of g_n, we write

$$\varrho_n(\varepsilon D)=\lambda_n(\varepsilon D)-g_n(\varepsilon D-\sigma_n)=\lambda_n(\varepsilon D)-\varepsilon\,\mathrm{op}_\varepsilon^{\{\xi=\sigma_n\}}(g_n).$$

Therefore, we have

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

We apply Lemma 2.12 and we obtain

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

Let $\theta \in C_c^\infty(\mathbb{R})$, equation (5.16) gives, passing to the limits $\varepsilon \to 0$, then $R \to +\infty$, and finally $\delta \to 0$

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

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

$$(x,\sigma,\omega) \mapsto (x + s(\nabla\lambda_n(\sigma) - \nabla g_n(\omega)), \sigma, \omega).$$

As a consequence, by Lemma 4.4, γ_n^t is supported on $\{\nabla\lambda_n(\sigma) - \nabla_\eta g_n(\sigma,\omega) = 0\}$.

Part 2: The two-scaled semiclassical measures coming from finite distance. We now choose $\theta \in C_c^\infty(\mathbb{R})$, $a \in C_c^\infty(\mathbb{R}^d \times \Omega \times \mathbb{R}^d)$. Arguing as in (5.16), we observe

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

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

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

Passing to the limit $\varepsilon \to 0$, we obtain

$$\begin{aligned} 0 &= \int_{\mathbb{R}} \theta(t)\mathrm{Tr}_{L^2(\mathbb{R}^d)} \left((i\nabla\lambda_n(\sigma_n)\cdot\nabla_x a^W(x,\sigma_n,D_x) - [a^W(x,\sigma_n,D_x), g(D_x)])\Gamma_n^t\right) dt = 0 \\ &= \int_{\mathbb{R}} \theta(t)\mathrm{Tr}_{L^2(\mathbb{R}^d)} \left([a^W(x,\sigma_n,D_x), \nabla\lambda_n(\sigma_n)\cdot D_x - g(D_x)]\Gamma_n^t\right) dt \\ &= \int_{\mathbb{R}} \theta(t)\mathrm{Tr}_{L^2(\mathbb{R}^d)} \left(a^W(x,\sigma_n,D_x)\left[\nabla\lambda_n(\sigma_n)\cdot D_x - g(D_x), \Gamma_n^t\right]\right) dt. \end{aligned}$$

We deduce that for almost all $t \in \mathbb{R}$,

$$\left[\nabla\lambda_n(\sigma_n)\cdot D_x - g(D_x), \Gamma_n^t\right] = 0.$$

Recall that the operator Γ_n^t is a rank one projector of $L^2(\mathbb{R}^d)$, $\Gamma_n^t = |\psi_{\sigma_n}(t)\rangle\langle\psi_{\sigma_n}(t)|$. We deduce that there exists a measurable function $t \mapsto c(t) \in \mathbb{C}$ such that

$$(\nabla\lambda_n(\sigma_n)\cdot D_x - g(D_x))\psi_{\sigma_n}(t) = c(t)\psi_{\sigma_n}(t).$$

Therefore the L^2-function $\xi \mapsto \widehat{\psi_{\sigma_n}}(t,\xi)$ is supported on the set $\{\nabla\lambda_n(\sigma_n)\cdot\xi - g(\xi) = c(t)\}$. Since $\nabla\lambda_n(\sigma_n) - g(\xi) \neq 0$ for $\xi \neq 0$, this set is a hypersurface and thus is of Lebesgue measure 0. We deduce $\psi_{\sigma_n}^t = 0$, $dt \otimes dx$-almost everywhere, whence $\Gamma^t = 0$, dt-almost everywhere.

6. CONCLUSION

In this conclusive chapter, we comment how the material displayed till now allow to prove the Theorem 1.3 which was our objective. Then, we discuss the multidimensional case.

6.1. **Effective mass theory in** $1d$. We are now able to prove Theorem 1.3]. By Corollary 4.2 (ii), the family $(\psi^\varepsilon(t))_{\varepsilon>0}$ is ε-oscillating. Thus, (1.13) is a consequence of (1.11). For proving (1.11), we have to determine the semi-classical measures ς^t of $(\psi^\varepsilon(t))_{\varepsilon>0}$.

By Corollary 4.2 (iii), we have

$$\varsigma^t = \sum_{n,n'\in\mathbb{N}^*} \mu^t_{n,n'}, \tag{6.1}$$

where $\mu^t_{n,n'}$ are joint measures of the pair $(\psi^\varepsilon_n(t), \psi^\varepsilon_{n'}(t))_{\varepsilon>0}$, solutions to (4.11). Moreover, if Λ_n is the set of critical points of the Bloch modes ϱ_n and $\Sigma_{n,n'}$ the set of crossing points between ϱ_n and $\varrho_{n'}$, by Proposition 4.3, for $n\in\mathbb{N}^*$,

$$\mu^t_{n,n}(x,\xi) = \mathbf{1}_{\xi\in\widetilde{\Lambda}_n}\mu^t_{n,n}(x,\xi),\ \ \widetilde{\Lambda}_n = \Lambda_n \cup \bigcup_{n'\neq n}\Sigma_{n,n'},$$

and for $n'\neq n$

$$\mu^t_{n,n'}(x,\xi) = \mathbf{1}_{\xi\in\Sigma_{n,n'}}\mu^t_{n,n'}(x,\xi).$$

By Lemma 3.5, $\Lambda_n \subset \pi\mathbb{Z}$ and $\Sigma_n = \pi\mathbb{Z}\setminus\Lambda_n$, in particular, both sets consist in isolated points. The two-microlocal analysis of the concentration of the pair $(\psi^\varepsilon_n(t), \psi^\varepsilon_{n'}(t))_{\varepsilon>0}$ above this point give via Corollaries 5.10 and 5.12

$$\mu^t_{n,n}(x,\xi) = \sum_{\xi\in\Lambda_n}\delta_{\xi_n}(\xi)\otimes|\psi^{(n)}_\xi(t,x)|^2dx,\ \ \mu^t_{n,n'}=0,\ \ n,n'\in\mathbb{N}^*,\ n\neq n',$$

with $\psi^{(n)}_\xi$ solution to (1.12). This terminates the proof.

6.2. **What happens in higher dimension ?** In higher dimension, the precise structure of the sets of critical points and of crossing points are rather open problems. One could have degenerate critical points and manifolds of critical points instead of isolated points. One could also have intersections between Bloch modes on critical points. One then has to exhibit a set of reasonable assumptions, allowing to perform a two-scale semi-classical analysis. Indeed, the approach of Chapter 5 can be extended to analyze the concentration of bounded families in $L^2(\mathbb{R}^d)$ on manifolds. This strategy is developed in [15]. We shortly describe the assumptions made therein and the adaptation to make for obtaining a complete description of the semi-classical measure of the solution $(\psi^\varepsilon(t))_{\varepsilon>0}$ of the Schrödinger equation (1.1).

6.2.1. *Assumptions on the sets of critical and crossing points.* Regarding the set of critical points of the Bloch modes, the following assumption is introduced in [14].

H1 For $n\in\mathbb{N}^*$, we assume that $d^2\varrho_n$ is of constant maximal rank over each connected component of Λ_n.

This assumption has the advantage to be generic. It consists in saying that for all $\xi\in\Lambda_n$,

$$\operatorname{Rank} d^2\varrho_n(\xi) = \operatorname{codim}\Lambda_n$$

or equivalently $\operatorname{Ker} d^2\varrho_n(\xi) = T_\xi\Lambda_n$. It implies in particular that each connected component $X\subseteq\Lambda_n$ is a closed submanifold of $\mathbb{R}^d$, which will give a good setting to perform a two-scale semi-classical analysis above Λ_n.

Regarding the crossing sets between Bloch modes, different sets of assumptions offer a comfortable framework. The assumptions **H2** and **H3** below are introduced in [15].

H2 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 $|n - n'| = 1$.

Hypothesis **H2** is generic, as follows from the variational characterization of the Bloch modes (see (3.3) and (3.4)) As stated, it prevents from having simultaneous crossings of more than two Bloch energies, and higher multiplicities (both scenarii are non-generic). In particular, one can use the normal forms of Lemma 3.13. We introduce moreover a geometric 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 3.12 and for all $\sigma \in \Sigma_n$, $\eta \in N_\sigma \Sigma_n$ with $\eta \neq 0$,

$$\frac{1}{2}\nabla_\xi(\varrho_{n+1} + \varrho_n)(\sigma) \pm \nabla_\eta g_n(\sigma, \eta) \neq 0.$$

Assuming **H2** and **H3** implies that the crossings involve only two modes ϱ_n and ϱ_{n+1} and that the crossing set Σ_n (see (5.15)) is a manifold. Because of the periodicity of the Bloch modes, it is thus the union of connected, closed embedded submanifold of $(\mathbb{R}^d)^*$, which allows the use of a two-microlocal approach on each of these connected components.

We point out that the assumption **H3** may fail and there could be crossings above critical points. Such a situation has been studied in [15], showing that some mass may be trapped above these non conical crossing sets, leading to the presence of non-zero terms $\mu^t_{n,n'}$ in (6.1) with $n \neq n'$.

6.2.2. *Effective mass theory in dimension $d \geq 2$.* The main difference in dimension $d \geq 2$ is the nature of the two-scale Wigner measures involved in the description of the process. 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

$$T^*X := \{(\xi, x) \in X \times \mathbb{R}^d \,:\, x \in T^*_\xi X\}, \tag{6.2}$$

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 $d^2\varrho_n(\xi)D_z \cdot D_z$ acting on $N_\xi \Lambda_n$ for any $\xi \in \Lambda_n$.

Theorem 6.1. [15] *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 is uniformly bounded in $H^s_\varepsilon(\mathbb{R}^d)$ for some $s > \frac{d}{2}$. Then, there exist a subsequence $(\psi_0^{\varepsilon_\ell})_{\ell\in\mathbb{N}}$ 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 $(\mathbf{M}_n)_{n\in\mathbb{N}}$*

$$\mathbf{M}_n : T^*_\xi \Lambda_n(\xi, v) \mapsto \mathbf{M}_n(\xi, v) \in \mathcal{L}^1_+(L^2(N_\xi \Lambda_n)), \;\; \mathrm{Tr}_{L^2(N_\xi\Lambda_n)} \mathbf{M}_n(\xi, v) = 1,$$

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

$$\begin{aligned} &\lim_{\ell\to+\infty} \int_a^b \int_{\mathbb{R}^d} \phi(x)|\psi^{\varepsilon_\ell}(t,x)|^2 dxdt \\ &\quad = \sum_{n\in\mathbb{N}} \int_a^b \int_{T^*\Lambda_n} \mathrm{Tr}_{L^2(N_\xi\Lambda_n)} \left(m_\phi^{\Lambda_n}(\xi, v)\mathbf{M}^t_n(\xi, v)\right) \nu_n(d\xi, dv)dt, \end{aligned} \tag{6.3}$$

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

$$\left\{ \begin{array}{l} i\partial_t \mathbf{M}_n^t(\xi, v) = \left[\frac{1}{2}\, d^2\varrho_n(\xi) D_z \cdot D_z + m^{\Lambda_n}_{V_{\rm ext}}(\xi, v)\ ,\ \mathbf{M}_n^t(\xi, v))\right] \\ \mathbf{M}_n^0 = \mathbf{M}_n. \end{array} \right.$$

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

Theorem 1.3 is a consequence of Theorem 6.1 in the case where critical sets Λ_n consist in isolated points. As Theorem 1.3, Theorem 6.1 tells that conical crossings do not trap energy. We emphasize that $(\mathbf{M}_n)_{n\in\mathbb{N}^*}$ and $(\nu_n)_{n\in\mathbb{N}^*}$ are associated with the initial data. They are two-scale Wigner measures associated with the concentration of $(\psi_0^\varepsilon)_{\varepsilon>0}$ on the manifolds Λ_n.

The main difference with the case of the concentration on a point of $\mathbb{R}^d_\xi$ relies on the structure of the two-scale Wigner measures describing the concentration at finite distance with respect to the second scale ε. Indeed, if $\Lambda_n = \{\xi = \xi_n\}$, $T_{\xi_n}\Lambda = \{0\}$ and $N_{\xi_n}\Lambda_n = \mathbb{R}^d$. Thus, the measure ν_n reduces to a scalar and the trace-class operator $\mathbf{M}_n$ only depends on ξ_n, it is no longer a function. Theorem 5.4 states that in that special case, one can prove that $\mathbf{M}_n$ is a projector.

As a final conclusive remark, one can mention that, regarding the semi-classical analysis of equation (1.1), the main issue consists in the understanding of the behavior of the Bloch modes in dimension $d \geq 1$, which is a problem at the intersection between spectral theory and geometry.

APPENDIX A. KATO-RELLICH'S THEOREM

Kato-Rellich's Theorem offers a way to prove that an operator is self-adjoint by a comparison argument. The reader can refer to [33] or other books about Functional Analysis.

Theorem A.1. *Let A be a self-adjoint operator on its domain $\mathcal{D}(A)$ and B a symmetric operator on $\mathcal{D}(A)$. Let us assume that there exists $0 < \alpha < 1$ and $C > 0$ such that*

$$\forall v \in \mathcal{D}(A), \quad \|Bv\| \leq \alpha\|Av\| + C\|v\|.$$

Then the operator $A + B$ is self-adjoint on $\mathcal{D}(A)$.

As an example, we consider the Hilbert space $L^2([0,1]^d)$ and the operator $-\Delta^{(\xi)}$, which consists in the Laplace operator on the cube $\bar{C} = [0,1]^d$ with boundary conditions

$$f(y+\ell) = \mathrm{e}^{i\xi\cdot\ell} f(y), \quad \partial_n f(y+\ell) = -\partial_n f(y)\mathrm{e}^{i\xi\ell} \quad \forall (y,\ell) \in \partial C \times \mathbb{Z}^d \text{ such that } y+\ell \in \partial C.$$

As mentioned in Section 3.1, this operator is unitarily equivalent to $P_0(\xi)$ and is self-adjoint.

Let us consider potentials V_{per} that are $\mathbb{Z}^d$-periodic and the operator $-\Delta^{(\xi)} + V_{\mathrm{per}}(x)$. We make the assumption:

$$V_{\mathrm{per}} \in L^p(\mathbb{T}^d), \quad \text{with} \begin{cases} p = 2 \text{ if } \ d = 1,2,3, \\ p > 2 \ \text{ if } \ d = 4 \\ p = \frac{d}{2} \ \text{ if } \ d \geq 5 \end{cases} \tag{A.1}$$

Theorem A.2. *Assume that V_{per} satisfies Assumptions A.1. Then, the operator $-\Delta^{(\xi)} + V_{\mathrm{per}}(x)$ is self-adjoint for all $\xi \in \mathbb{R}^d$, and its spectrum is bounded from below. Besides it has a compact resolvent.*

The result comes from the application of Theorem A.1 to the operators $A := -\Delta^{(\xi)}$ and $B := V_{\mathrm{per}}$, the next Lemma shows that the hypothesis of Theorem A.1 are satisfied.

Lemma A.3. *Let V_{per} satisfying Assumptions A.1, then for all $\varepsilon > 0$ there exists a constant $C_\varepsilon > 0$ such that,*

$$\|V_{\mathrm{per}} f\|_{L^2([0,1]^d)} \leq \varepsilon\|\Delta f\|_{L^2([0,1]^d)} + C_\varepsilon\|f\|_{L^2([0,1]^d)}, \quad \forall f \in H^2(]0,1[]^d),$$

$$\left| \int_{[0,1]^d} V_{\mathrm{per}}(y)|f(y)|^2 dy \right| \leq \varepsilon \int_{[0,1]^d} |\nabla f(y)|^2 dy + C_\varepsilon \|f\|^2_{L^2([0,1]^d)}, \quad \forall f \in H^1(]0,1[^d).$$

A potential satisfying this type of property is said to be infinitesimally bounded with respect to the Laplacian. Note that the result is trivial if $V_{\mathrm{per}}(y)$ is bounded. Let us now prove Lemma A.3 when $d = 1,2,3$.

Proof
Assume $d = 1,2,3$ and $V_{\mathrm{per}} \in L^2(\mathbb{T}^d)$. Consider $\chi \in C_c^\infty(\mathbb{R}^d)$ such that $0 \leq \chi \leq 1$, $\chi = 1$ on $[0,1]^d$ and $\mathrm{supp}(\chi) \subset [-1,2]^d$. We associate with any $f \in H^2(]0,1[^d)$ the function $f_\chi = \chi f$ which is in $H^2(\mathbb{R}^d)$, and thus in $L^\infty(\mathbb{R}^d)$ since $2 > d/2$. Note that V_{per} can be extended to $\mathbb{R}^d$ by periodicity.

$$\begin{aligned} \|V_{\mathrm{per}} f\|_{L^2([0,1]^d)} &\leq \|V_{\mathrm{per}} f_\chi\|_{L^2(\mathbb{R}^d)} \\ &\leq \|f_\chi\|_{L^\infty(\mathbb{R}^d)} \|V_{\mathrm{per}} 1_{[-1,2]^d}\|_{L^2(\mathbb{R}^d)} \\ &\leq C_d \|f_\chi\|_{L^\infty(\mathbb{R}^d)} \|V_{\mathrm{per}}\|_{L^2([0,1]^d)}, \end{aligned}$$

The constant C_d depends on the numbers of cells which are included in $[-1,2]^d$ and next to $[0,1]^d$. We then uses the inverse Fourier transform to evaluate $\|f_\chi\|_{L^\infty(\mathbb{R}^d)}$:

$$\|f_\chi\|_{L^\infty(\mathbb{R}^d)} \leq (2\pi)^{-d} \int_{\mathbb{R}^d} |\widehat{f}_\chi(\xi)| d\xi.$$

We choose $\beta \in \left]\frac{d}{2}, 2\right[$ and use Cauchy-Schwartz inequality to write

$$\|f_\chi\|_{L^\infty(\mathbb{R}^d)} \leq (2\pi)^{-d} \left(\int_{\mathbb{R}^d} \frac{d\xi}{(1+|\xi|^2)^\beta}\right)^{1/2} \left(\int_{\mathbb{R}^d} (1+|\xi|^2)^\beta |\widehat{f}_\chi(\xi)|^2 d\xi\right)^{1/2}.$$

For all $\varepsilon > 0$, we can find $C_\varepsilon > 0$ such that

$$\forall \xi \in \mathbb{R}^d, \ \ (1+|\xi|^2)^\beta \leq \varepsilon(1+|\xi|^2)^2 + C_\varepsilon.$$

Therefore, we have

$$\begin{aligned} \|f_\chi\|_{L^\infty(\mathbb{R}^d)} &\leq \varepsilon\|(1-\Delta)f_\chi\|_{L^2(\mathbb{R}^d)} + C_\varepsilon\|f_\chi\|_{L^2(\mathbb{R}^d)} \\ &\leq \varepsilon\|\Delta f_\chi\|_{L^2(\mathbb{R}^d)} + (C_\varepsilon + \varepsilon)\|f_\chi\|_{L^2(\mathbb{R}^d)} \end{aligned}$$

Besides, by the properties of χ,

$$\|\Delta f_\chi\|_{L^2(\mathbb{R}^d)} \leq \|\Delta f\|_{L^2([0,1]^d)} + 2\|\nabla f\|_{L^2([0,1]^d)}\|\nabla\chi\|_{L^2(\mathbb{R}^d)} + \|\Delta\chi\|_{L^2(\mathbb{R}^d)}\|f\|_{L^2(\mathbb{R}^d)}$$

which gives the result.

Appendix B. Compact operators and operators with compact resolvent

We close this elements of spectral theory with a few words about compact operators, that are used in this book. Recall that $A \in \mathcal{L}(\mathcal{H})$ is said to be a compact operator if for any bounded family $(f_n)_{n\in\mathbb{N}}$ of $\mathcal{H}^\mathbb{N}$, the sequence (Af_n) has a limit point. Compact operators enjoy lots of properties. In particular, the structure of their spectrum is very rigid. The next Theorem is classic and proved in any book of functional analysis.

Theorem B.1. *Assume $\mathcal{H}$ is of infinite dimension. Let A be a compact self-adjoint operator, then its spectrum consists in isolated eigenvalues of finite multiplicity, $(\lambda_n)_{n\in\mathbb{N}}$, which admits the only limit point 0. Moreover, there exists an orthonormal basis $(\varphi_n)_{n\in\mathbb{N}}$ of $\mathcal{H}$ consisting of eigenvectors of A.*

As a consequence of this result, we have the following description of the spectrum of self-adjoint operators with compact resolvent.

Proposition B.2. *Let $A : \mathcal{D}(A) \to \mathcal{H}$ a self-adjoint operator the resolvent of which, $(A_\lambda)^{-1}$ is compact for some $\lambda \in \mathbb{C}$. Then, there exists an orthonormal basis $(\varphi_n)_{n\in\mathbb{N}}$ and a sequence $(\varrho_n)_{n\in\mathbb{N}} \in \mathbb{R}^\mathbb{N}$ such that $\varrho_n \underset{n\to+\infty}{\longrightarrow} +\infty$ and*

$$A\varphi_n = \varrho_n\varphi_n, \ \ \forall n \in \mathbb{N}.$$

Proof
By hypothesis, there exists $(\varphi_n)_{n\in\mathbb{N}}$ and $(\lambda_n)_n \in \mathbb{N}$ with $\lambda_n \underset{n\to+\infty}{\longrightarrow} 0$ such that

$$(A-\lambda)^{-1}\varphi_n = \lambda_n\varphi_n, \ \ \forall n \in \mathbb{N}.$$

Besides, $\lambda_n \neq 0$. Then, a simple computation gives $\varphi_n = \lambda_n^{-1}(A-\lambda)\varphi_n$, whence

$$A\varphi_n = \lambda_n^{-1}(\lambda_n\lambda + 1)\varphi_n.$$

We thus obtain the result with $\varrho_n = \lambda + \lambda_n^{-1}$. The fact that $\varrho_n \in \mathbb{R}$ for all $n \in \mathbb{N}$ comes from the self-adjointness of A.

APPENDIX C. MIN-MAX FORMULA

We give here a MinMax characterization of the eigenvalues $\varrho_n(\xi)$ of the operators $P(\xi)$. This comes from the links between self-adjoint operator and quadratic forms. We associate with $P(\xi)$ the positive quadratic form

$$Q_\xi(f) = \frac{1}{2}\|(D_y+\xi)f\|^2_{L^2(\mathbb{T}^d)} + (V_{\mathrm{per}}f, f)_{L^2(\mathbb{T}^d)} + K\|f\|^2_{L^2(\mathbb{T}^d)}.$$

where K is chosen such that for all $\xi \in \mathcal{B}$, the spectrum of $P(\xi)$ is included in $]-K+1, +\infty[$. The quadratic form Q_ξ is associated with the operator $P(\xi)+K$, in the sense that for all f in the domain of $P(\xi)$ (which is included in the domain of Q_ξ)

$$Q_\xi(f) = ((P(\xi)+K)f, f)_{L^2(\mathbb{T}^d)}\,.$$

The domain of the quadratic form Q_ξ is $H^1(\mathbb{T}^d)$ and Q_ξ is coercive since

$$Q_\xi(f) \geq \|f\|_{L^2(\mathbb{T}^d)},\ \ \forall f \in L^2(\mathbb{T}^d)$$

and thus defines a norm $f \mapsto \sqrt{Q_\xi(f)}$ on $H^1(\mathbb{T}^d)$. The form Q_ξ and the operator $P(\xi)+K$ are linked by Riesz-Friedrichs theorem: $A_\xi = P(\xi)+K$ is the unique self-adjoint operator with domain $\mathcal{D}(A_\xi) \subset \mathcal{D}(Q_\xi)$ and such that $(A_\xi f, f) = Q_\xi(f)$ for all $f \in \mathcal{D}(A_\xi)$. This is another way to define $P(\xi)$ as $A_\xi - K$ where A_ξ is the self adjoint operator associated with the form Q_ξ.

Proposition C.1. *The family of eigenvalues $(\varrho_n(\xi))_{n\in\mathbb{N}}$ are given by the Courant-Fischer formula (also called Min-Max formula),*

$$\lambda_1(\xi) := \varrho_1(\xi) + K = \min_{\|f\|=1} Q_\xi(f), \tag{C.1}$$

and, for $n \in \mathbb{N}\setminus\{1\}$,

$$\lambda_n(\xi) := \varrho_n(\xi) + K = \min_{\mathrm{dim}M=n,\ M\subset H^1(\mathbb{T}^d)}\ \max_{f\in M,\ \|f\|=1} Q_\xi(f). \tag{C.2}$$

Note that the real numbers $\lambda_n(\xi)$ are non negative for all $\xi \in \mathbb{R}^d$.

Proof

Let us prove the Courant-Fischer formula. Recall that for any $f \in L^2(\mathbb{T}^d)$ such that

$$Q_\xi(f) = \sum_{n\in\mathbb{N}} \lambda_n(\xi)|\langle f, \varphi_n(\xi)\rangle|^2.$$

Therefore, since the $\lambda_n(\xi)$ are non negative, one gets that if $\|f\|_{L^2(\mathbb{T}^d)} = 1$, one has

$$Q_\xi(f) \geq \lambda_1(\xi)\sum_{n\in\mathbb{N}} |\langle f, \varphi_n(\xi)\rangle|^2 = \lambda_1(\xi) = Q_\xi(\varphi_1(\xi)),$$

which proves (C.1).

For proving (C.2), we consider the sets $M_n = \mathrm{Vect}\,(\varphi_1(\xi), \cdots, \varphi_n(\xi))$ for $n \in \mathbb{N}^*$. We first deduce

$$\min_{\mathrm{dim}M=n,\ M\subset H^1(\mathbb{T}^d)}\ \max_{f\in M,\ \|f\|=1} Q_\xi(f) \leq \max_{f\in M_n,\ \|f\|=1} Q_\xi(f) = \lambda_n(\xi).$$

Let us now consider a vector space $M \subset L^2(\mathbb{T}^d)$ of dimension n. Since $\dim M_{n-1} = n-1$,

$$\dim M \cap M_{n-1}^\perp = \dim M - \dim M \cap M_{n-1} \geq n - (n-1) = 1$$

and $M \cap M_{n-1}^\perp \neq \emptyset$. Let $f \in M \cap M_{n-1}^\perp$ with $\|f\|_{L^2(\mathbb{T}^d)} = 1$, then f has only components on $\varphi_p(\xi)$ for $p \geq n$ and

$$Q_\xi(f) = \sum_{p\geq n} \lambda_p(\xi)|\langle f, \varphi_p(\xi)\rangle|^2 \geq \lambda_n(\xi)\sum_{p\geq n} |\langle f, \varphi_p(\xi)\rangle|^2 = \lambda_n(\xi).$$

Therefore, for any vector space $M \subset L^2(\mathbb{T}^d)$ of dimension n

$$\max_{f\in M,\ \|f\|=1} Q_\xi(f) \geq \lambda_n(\xi)$$

and we obtain

$$\min_{\dim M=n,\ M\subset H^1(\mathbb{T}^d)} \ \max_{f\in M,\ \|f\|=1} Q_\xi(f) \geq \lambda_n(\xi),$$

which concludes the proof of (C.2).

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