SEMICLASSICAL LIMIT FOR THE SCHRÖDINGER EQUATION WITH A SHORT SCALE PERIODIC POTENTIAL

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ABSTRACT. We consider the dynamics generated by the Schrödinger operator $H = -\frac{1}{2}\Delta + V(x) + W(\varepsilon x)$, where V is a lattice periodic potential and W an external potential which varies slowly on the scale set by the lattice spacing. We prove that in the limit $\varepsilon \to 0$ the time dependent position operator and, more generally, semiclassical observables converge strongly to a limit which is determined by the semiclassical dynamics.

1. Introduction

A basic problem of solid state physics is to understand the motion of electrons in the periodic potential which is generated by the ionic cores. While this problem is quantum mechanical, many electronic properties of solids can be understood already in the semiclassical approximation [2, 16, 26]. One argues that if the wave packet spreads over many lattice spacings, the kinetic energy $(\hbar k)^2/2m$ is modified to the n-th band energy $E_n(k)$. Otherwise the electron responds to external fields, E_{ex}, B_{ex}, as in the case of vanishing periodic potential. Thus the semiclassical equations of motion are

$$\begin{aligned} \dot{r} &= v_n(k) = \nabla_k E_n(k) \\ \hbar\dot{k} &= e(E_{\mathrm{ex}}(r) + v_n(k) \wedge B_{\mathrm{ex}}(r))\,, \end{aligned} \tag{1.1}$$

where r is the position and k the quasimomentum of the electron. Note that there is a semiclassical evolution for each band separately.

The goal of our paper is to understand on a mathematical level how these semiclassical equations arise from the underlying Schrödinger equation. We consider only the case where $B_{\mathrm{ex}} = 0$.

The setup is rather obvious. We start from the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi = H\psi \tag{1.2}$$

with Hamiltonian

$$H = -\frac{1}{2}\Delta + V(x) + W(\varepsilon x). \tag{1.3}$$

The electron moves in $\mathbb{R}^d$ and the solution to (1.2) defines the unitary time evolution $U^\varepsilon(t)\psi(x) = \mathrm{e}^{-itH}\psi(x) = \psi(x,t)$ in $L^2(\mathbb{R}^d)$. We have chosen units such that $\hbar = 1$ and the mass of the particle $m = 1$. $V(x)$ is a periodic potential with average lattice spacing a. The precise conditions on V will be spelled out in the following section, where we also describe the direct fiber integral decomposition for periodic Schrödinger operators. The lattice spacing a defines the microscopic spatial scale. $W(\varepsilon x)$ is an external electrostatic potential with dimensionless scale parameter ε,

$\varepsilon \ll 1$, which means that W is slowly varying on the scale of the lattice. For real metals the condition of slow variation is satisfied even for the strongest external electrostatic fields available, cf. [2], Chapter 13.

The external forces due to W are of order ε and therefore have to act over a time of order ε^{-1} to produce finite changes, which defines the macroscopic time scale. We will mostly work in the microscopic coordinates (x,t) of (1.2). For sake of comparison we note that the macroscopic space-time scale (x',t') is defined through $x = \varepsilon^{-1}x'$ and $t = \varepsilon^{-1}t'$. With this scale change Eqs. (1.2), (1.3) read

$$\begin{aligned} &i\varepsilon\frac{\partial}{\partial t'}\psi = H\psi\,, \\ &H = \left(-\varepsilon^2\frac{1}{2}\Delta' + V(x'/\varepsilon) + W(x')\right) \end{aligned} \tag{1.4}$$

with initial conditions $\psi^\varepsilon(x') = \varepsilon^{-d/2}\psi(x'/\varepsilon)$. If $V = 0$, Eq. (1.4) is the usual semiclassical limit with ε set equal to $\hbar$. Thus our problem is to understand how an additional periodic, but rapidly oscillating potential modifies the standard picture.

The two scale problem (1.2), (1.3) can be attacked along several routes. A first choice would be time dependent WKB [5, 6, 10, 12]. In the limit $\varepsilon \to 0$, for each energy band separately, one obtains a Hamilton-Jacobi equation for the phase and a transport equation for the amplitude of the wave function $\psi(x,t)$. As a main draw-back of this method, generically, the solution to the Hamilton-Jacobi equation develops singularities after some finite macroscopic time. If $V = 0$, it is well understood how to go beyond such caustics by introducing new coordinates on the Lagrangian manifold. For (1.2), (1.3) a corresponding program has not yet been attempted. The results [5, 6, 10, 12] are valid only over a finite macroscopic time span with a duration depending on the initial wave function.

Another variant is to establish the semiclassical limit through the convergence of Wigner functions. In our context one defines a band Wigner function $W_n^\varepsilon(r,k,t)$ depending on the band index n and as a function of the position and quasimomentum. One then wants to prove that in the limit $\varepsilon \to 0$ $W_n^\varepsilon(t)$ converges to $\overline{W}_n(t)$, which is the initial band Wigner function $\overline{W}_n(0)$ evolved according to the semiclassical flow (1.1). Such a result is established in [9, 18] for the case of zero external potential, the general case being left open as a challenging problem.

A third approach to the semiclassical limit for $V = 0$ is the strong convergence of Heisenberg operators [1, 4, 19, 23]. We briefly recall its main features. We define, as unbounded operators on $L^2(\mathbb{R}^d)$,

$$x(t) := \mathrm{e}^{itH}x\mathrm{e}^{-itH},$$

$$p(t) := \mathrm{e}^{itH}p\mathrm{e}^{-itH}, \quad p = -i\nabla_x,$$

where H is the Hamiltonian in (1.3) with $V = 0$. The goal is to establish the strong limit of

$$x^\varepsilon(t)\psi = \varepsilon x(\varepsilon^{-1}t)\psi, \quad p^\varepsilon(t)\psi = p(\varepsilon^{-1}t)\psi$$

as $\varepsilon \to 0$ with ψ in a suitable domain. In the trivial case of free motion, $W = 0$, this amounts to the strong convergence of $x^\varepsilon(t)\psi = (\varepsilon x + pt)\psi$, $p^\varepsilon(t)\psi = p\psi$, which yields $\lim_{\varepsilon\to 0} x^\varepsilon(t) = pt$, $\lim_{\varepsilon\to 0} p^\varepsilon(t) = p$. The general case requires more work

[22]. One obtains the strong limits

$$\lim_{\varepsilon\to 0} x^\varepsilon(t) = r(p,t)\,, \qquad \lim_{\varepsilon\to 0} p^\varepsilon(t) = u(p,t)\,. \tag{1.5}$$

Here $r(p,t)$, $u(p,t)$ are solutions of

$$\dot r = u, \quad \dot u = -\nabla W(r) \tag{1.6}$$

with initial conditions $r_0 = 0$, $u_0 = p$. The initial condition $r_0 = 0$ reflects that $|\psi|^2$ looks like $\delta(r)$ on the macroscopic scale, provided that $\|\psi\|_2 = 1$. For general initial conditions, $r_0 \neq 0$, we would have to shift the initial ψ by $\varepsilon^{-1}r_0$.

The strong operator convergence may look slightly abstract, but all the desired physical information can be deduced. E.g., the initial ψ defines the momentum distribution $|\widehat{\psi}(k)|^2$ independent of ε and the $\delta(r)$ spatial distribution in the limit $\varepsilon \to 0$. Then, according to (1.5), for small ε the position distribution at time t is given by

$$\begin{aligned}\textstyle\int_{\mathbb{R}^d} f(x)|\psi^\varepsilon(x,t)|^2\,dx &= (\psi, f(x^\varepsilon(t))\psi)\\ \simeq (\psi, f(r(p,t))\psi) &= \textstyle\int |\widehat{\psi}(k)|^2 f(r(k,t))\,dk,\end{aligned}$$

which means that the phase space distribution $\delta(r)|\widehat{\psi}(k)|^2\,dr\,dk$ is transported according to the semiclassical flow (1.6). The spatial marginal of this distribution at time t is the desired approximation to the true position distribution $|\psi^\varepsilon(x,t)|^2$. $|\psi^\varepsilon(x,t)|^2$ may oscillate rapidly on small scales and some averaging, as embodied by the test function f, is needed.

In this paper we investigate the semiclassical limit (1.2), (1.3) through the strong convergence of the position operator $x^\varepsilon(t)$. We will show that, in the limit $\varepsilon \to 0$, $x^\varepsilon(t)$ is diagonal with respect to the band index and in each band the structure is analogous to (1.5) with p replaced by the quasimomentum k and (1.6) replaced by (1.1). More generally we will consider the semiclassical limit of the Weyl quantized operators $a^W(\varepsilon x, p)$, whose classical symbol is periodic in p.

To give a short outline: In the following section we collect some properties of periodic Schrödinger operators. In Section 3 we state our main results, which are proved in Sections 5, 6, and 7, respectively. In Section 4 we discuss some implications for the position and quasimomentum distributions, and, more generally, for the band Wigner functions. The difficulties arising from band crossings are explained in Section 9.

2. Periodic Schrödinger operators

For the periodic potential V we will need only some rather minimal assumptions, which we state as

Condition ($\mathrm{C_{per}}$)**.** *Let $\Gamma \simeq \mathbb{Z}^d$ be the lattice generated by the basis $\{\gamma_1, \dots, \gamma_d\}$, $\gamma_i \in \mathbb{R}^d$. Then $V(x+\gamma) = V(x)$ for all $x \in \mathbb{R}^d$, $\gamma \in \Gamma$. Furthermore, we assume V to be infinitesimally operator bounded with respect to H_0. The last condition is satisfied, e.g., if $V \in L^p(M)$, where M is the fundamental domain of Γ, and $p = 2$ for $d \leq 3$ and $p > d/2$ for $d > 3$, respectively.*

($\mathrm{C_{per}}$) will be assumed throughout.

We recall the *Bloch-Floquet* theory for the spectral representation of

$$H_{\mathrm{per}} = \frac{1}{2}p^2 + V(x)\,. \tag{2.1}$$

The reciprocal lattice Γ^* is defined as the lattice generated by the dual basis $\{\gamma_1^*, \dots, \gamma_d^*\}$ determined by $\gamma_i \cdot \gamma_j^* = 2\pi\delta_{ij}$, $i,j = 1,\dots,d$. The fundamental domain of Γ is denoted by M, the one of Γ^* by M^*. M^* is usually referred to as *first Brillouin zone*. If we identify opposite edges of M, resp. M^*, then it becomes a flat d-torus denoted by $\mathbb{T} = \mathbb{R}^d/\Gamma$, resp. $\mathbb{T}^* = \mathbb{R}^d/\Gamma^*$.

Let us introduce the Bloch-Floquet transformation, which should be viewed as a discrete Fourier transform, through

$$(\mathcal{U}\psi)(k,x) := \sum_{\gamma\in\Gamma} \mathrm{e}^{-i(x+\gamma)\cdot k}\psi(x+\gamma), \quad (k,x) \in \mathbb{R}^{2d}\,,$$

for $\psi \in \mathcal{S}(\mathbb{R}^d)$. Clearly,

$$\begin{aligned} (\mathcal{U}\psi)(k,x'+\gamma) &= (\mathcal{U}\psi)(k,x')\,,\\ (\mathcal{U}\psi)(k'+\gamma^*,x) &= \mathrm{e}^{-ix\cdot\gamma^*}(\mathcal{U}\psi)(k',x)\,. \end{aligned} \tag{2.2}$$

Therefore it suffices to specify $\mathcal{U}\psi$ on the set $M^* \times M$ and, if needed, extend it to all of $\mathbb{R}^{2d}$ by (2.2). The linear map $\mathcal{U} : L^2(\mathbb{R}^d) \supset \mathcal{S}(\mathbb{R}^d) \to \mathcal{H} := \int_{M^*}^{\oplus} L^2(M)\,dk$, with dk the normalized Lebesgue measure on M^*, has norm one and can thus be extended to all of $L^2(\mathbb{R}^d)$ by continuity. $\mathcal{U}$ is surjective as can be seen from the inverse mapping

$$(\mathcal{U}^{-1}\phi)(x) := \int_{M^*} \mathrm{e}^{ix\cdot k}\phi(k,x)\,dk,$$

which has norm one. Thus $\mathcal{U} : L^2(\mathbb{R}^d) \to \mathcal{H}$ is unitary.

To transform H_{per} under $\mathcal{U}$, we first note that $\tilde{p} = \mathcal{U}p\mathcal{U}^{-1} = D_x + k$, with $D_x = -i\nabla_x$. Therefore

$$\tilde{H}_{\mathrm{per}} := \mathcal{U}H_{\mathrm{per}}\mathcal{U}^{-1} = \int_{M^*}^{\oplus} H_{\mathrm{per}}(k)\,dk\,,$$

and

$$H_{\mathrm{per}}(k) = \frac{1}{2}(D_x + k)^2 + V(x), \quad k \in \mathbb{R}^d\,.$$

$H_{\mathrm{per}}(k)$ acts on $L^2(M)$ with k-independent domain $D := H^2(\mathbb{T})$. $\psi \in D$ is periodic in x. $H_{\mathrm{per}}(k)$ is a semi-bounded self-adjoint operator, since by condition ($\mathrm{C}_{\mathrm{per}}$) V is infinitesimally operator bounded with respect to $-\Delta$ [7]. In particular, $H_{\mathrm{per}}(k)$ is an entire analytic family of type (B) in the sense of Kato for $k \in \mathbb{C}^d$. Since the resolvent of $H_0(k) = \frac{1}{2}(D_x + k)^2$ is compact, the resolvent $R_\lambda(H_{\mathrm{per}}(k)) := (H_{\mathrm{per}}(k) - \lambda)^{-1}$, $\lambda \neq \sigma(H_{\mathrm{per}}(k))$, is also compact, and $H_{\mathrm{per}}(k)$ has a complete set of (normalized) eigenfunctions $\varphi_n(k) \in H^2(\mathbb{T})$, $n \in \mathbb{N}$, called *Bloch functions*. The corresponding eigenvalues $E_n(k)$, $n \in \mathbb{N}$, accumulate at infinity and we enumerate them according to their magnitude and multiplicity, $E_1(k) \leq E_2(k) \leq \dots$. $E_n(k)$ is called the n-th *band function*. We note that $H_{\mathrm{per}}(k) = \mathrm{e}^{-ix\cdot\gamma^*}H_{\mathrm{per}}(k+\gamma^*)\mathrm{e}^{ix\cdot\gamma^*}$. Therefore $E_n(k)$ is periodic with respect to Γ^*. If $E_{n-1}(k) < E_n(k) < E_{n+1}(k)$ for all $k \in M^*$ (in particular $E_n(k)$ is nondegenerate), then the n-th band is *isolated*. In this case E_n and the corresponding projection operator are real analytic functions as a consequence of analytic perturbation theory [15]. We denote by $\mathcal{I} \subset \mathbb{N}$ the set of indices of isolated bands.

It will be convenient to have also a notation for the spectral subspaces. Let $P_n(k) : L^2(M) \to L^2(M)$ denote the orthogonal projection onto the n-th eigenspace of $H_{\mathrm{per}}(k)$. Similarly, we set $Q_n(k) = \mathbf{1} - P_n(k)$. Their direct fiber integral is denoted by

$$\tilde{P}_n = \int_{M^*}^{\oplus} P_n(k)\, dk\,.$$

$\tilde{P}_n$ projects onto the n-th band subspace in $\mathcal{H}$ and $P_n = \mathcal{U}^{-1}\tilde{P}_n\mathcal{U}$ projects onto the n-th band subspace in $L^2(\mathbb{R}^d)$. We have

$$\begin{aligned}(\tilde{P}_n\psi)(k,\cdot) &= P_n(k)\psi(k,\cdot) = (\varphi_n(k),\psi(k))_{L^2(M)}\varphi_n(k,\cdot)\\ &= \psi_n(k)\varphi_n(k,\cdot)\,.\end{aligned} \tag{2.3}$$

The coefficient functions $\psi_n \in L^2(M^*)$ and are called the *Bloch coefficients* in the n-th band subspace. For the index set $\mathcal{I} \subset \mathbb{N}$ of isolated bands we set $P_{\mathcal{I}} = \sum_{n\in\mathcal{I}} P_n$.

Remark. *To have a concise notation, we will use a tilde for operators acting on $\mathcal{H}$. Thus if A is an operator on $L^2(\mathbb{R}^d)$, then $\tilde{A} = \mathcal{U}A\mathcal{U}^{-1}$. If A has a direct fiber decomposition, then $\tilde{A} = \int_{M^*}^{\oplus} A(k)\, dk$ with $A(k)$ acting on the fiber $L^2(M)$ of $\mathcal{H}$.*

3. Main results

For the potentials we assume ($\mathrm{C}_{\mathrm{per}}$) for V and in addition

Condition (C_{ex})**.** *The external potential $W \in \mathcal{S}(\mathbb{R}^d)$.*

To state the semiclassical limit, we first have to explain the classical dynamics which will serve as a comparison. For each $n \in \mathcal{I}$ the classical phase space is $\mathbb{R}^d \times \mathbb{T}^*$, where $\mathbb{T}^* = \mathbb{R}^d/\Gamma^*$. As n-th band Hamiltonian we have

$$h_n(r,k) = E_n(k) + W(r), \quad (r,k) \in \mathbb{R}^d \times \mathbb{T}^*\,,$$

and the classical dynamics in the n-th band is governed by

$$\dot{r}_n = \nabla_k E_n(k_n), \quad \dot{k}_n = -\nabla_r W(r_n). \tag{3.1}$$

Since we want to prove the strong convergence of the position operator, as in the case $V \equiv 0$, we have to lift (3.1) to operators on $\mathcal{H}$. For this purpose we solve (3.1) with initial condition $r_n(0) = 0$, $k_n(0) = k$. We denote the solution by $(r_n(t;k), k_n(t;k))$, regarded as functions of $k \in \mathbb{T}^*$. For $\psi \in \mathcal{H}$, we define

$$(R(t)\psi)(k,x) = \sum_{n\in\mathcal{I}} r_n(t;k)\tilde{P}_n\psi(k,x)\,,$$

and analogously, for later use,

$$(K(t)\psi)(k,x) = \sum_{n\in\mathcal{I}} k_n(t;k)\tilde{P}_n\psi(k,x)\,.$$

Theorem 3.1. *Let the conditions* ($\mathrm{C}_{\mathrm{per}}$), ($\mathrm{C}_{\mathrm{ex}}$) *be satisfied. Let*

$$x^\varepsilon(t) = \varepsilon U^\varepsilon(-t/\varepsilon)\, x\, U^\varepsilon(t/\varepsilon)\,.$$

Then for every $\psi \in Ran P_{\mathcal{I}} \cap D(|x|) \cap H^2$, with H^2 the second Sobolev space,

$$\lim_{\varepsilon\to 0} x^\varepsilon(t)\psi = \mathcal{U}^{-1}R(t)\mathcal{U}\psi$$

strongly.

Theorem 3.1 will be proved in several steps. First we show that in the semiclassical limit transitions from and to isolated band subspaces are suppressed on the level of the unitary groups. We define $H^n_{\mathrm{diag}} = P_n H P_n + Q_n H Q_n$ and $U^{\varepsilon,n}_{\mathrm{diag}}(t) := \exp(-itH^n_{\mathrm{diag}})$. In Section 5 we will prove

Theorem 3.2. *For any $n \in \mathcal{I}$ we have*

$$\lim_{\varepsilon\to 0}\Big(U^\varepsilon(t/\varepsilon) - U^{\varepsilon,n}_{\mathrm{diag}}(t/\varepsilon)\Big) = 0$$

in $B(H^1, L^2)$, where H^1 is the first Sobolev space.

The position operator is not diagonal with respect to the n-th band subspace and we define its diagonal part by $x^n_{\mathrm{diag}} = P_n x P_n + Q_n x Q_n$ with the time evolution

$$x^{\varepsilon,n}_{\mathrm{diag}}(t) := \varepsilon U^{\varepsilon,n}_{\mathrm{diag}}(-t/\varepsilon) x^n_{\mathrm{diag}} U^{\varepsilon,n}_{\mathrm{diag}}(t/\varepsilon)\,.$$

Our second step is to prove that the off-diagonal part of $x^\varepsilon(t)$ vanishes in the limit $\varepsilon \to 0$.

Theorem 3.3. *For $n \in \mathcal{I}$*

$$\lim_{\varepsilon\to 0}\Big(x^\varepsilon(t) - x^{\varepsilon,n}_{\mathrm{diag}}(t)\Big) = 0 \tag{3.2}$$

in $B(H^2, L^2)$.

By construction we have $[x^{\varepsilon,n}_{\mathrm{diag}}(t), P_n] = 0$ and it suffices to study the dynamics in the n-th band subspace. This subspace is isomorphic to $L^2(\mathbb{T}^*)$ and, up to errors of higher order, $x^{\varepsilon,n}_{\mathrm{diag}}(t)$ can be replaced by $x^{\varepsilon,n}_{\mathrm{sc}}(t)$ whose time evolution is governed by a Hamiltonian of the form

$$\widetilde{H}^{\varepsilon,n}_{\mathrm{sc}} = E_n(k) + W(-i\varepsilon\nabla_k)\,.$$

At this stage we can apply the standard machinery of semiclassics, except that formally the roles of position and momentum have been interchanged and the new position space is the flat torus rather than $\mathbb{R}^d$.

So far we focused on the position operator, since the electronic density is the most accessible quantity experimentally and it corresponds in essence to a suitable function of the position. On more general grounds one would like to characterize a wider class of semiclassical observables. One further obvious candidate is the momentum p. In the Bloch-Floquet basis we have $\widetilde{p} = k + D_x$. k is semiclassical, as being canonically conjugate to $-i\nabla_k$:

Theorem 3.4. *Let*

$$k^\varepsilon(t) = U^\varepsilon(-t/\varepsilon)\,\mathcal{U}^{-1}\,k\,\mathcal{U}\,U^\varepsilon(t/\varepsilon)\,.$$

Then for every $\psi \in RanP_{\mathcal{I}}$

$$\lim_{\varepsilon\to 0} k^\varepsilon(t)\psi = \mathcal{U}^{-1}K(t)\mathcal{U}\psi \tag{3.3}$$

strongly.

On the other hand, D_x is unbalanced because there is no extra factor of ε. Thus $p(t/\varepsilon)$ has a limit only when averaged over time (compare with Section 6).

It is relatively easy to see (cf. Section 8) that Theorems 3.1 and 3.4 imply the semiclassical limit also for bounded functions of $x^\varepsilon(t)$ resp. of $k^\varepsilon(t)$ (cf. Lemma 8.1). Next note that for Γ^*-periodic functions g, $g(\cdot+\gamma^*) = g(\cdot)$ for all $\gamma^* \in \Gamma^*$, we have $\mathcal{U}g(p)\mathcal{U}^{-1} = g(k)$ and hence, by the functional calculus for self-adjoint operators,

$g(p^\varepsilon(t)) = g(k^\varepsilon(t))$. Therefore we introduce the set $\mathcal{O}(0) \subset C(\mathbb{R}^d \times \mathbb{R}^d, \mathbb{R})$ of bounded and continuous semiclassical symbols which vanish if the first argument approaches infinity and are Γ^*-periodic in their second argument. For $a \in \mathcal{O}(0)$ we introduce its Weyl quantization

$$(a^{\mathrm{W}}\psi)(x) = \frac{1}{(2\pi)^d}\int a\left(\frac{x+y}{2},\xi\right) e^{i(x-y)\cdot\xi}\psi(y)\,d\xi dy \tag{3.4}$$

as a bounded operator on $L^2(\mathbb{R}^d)$. The operator corresponding to the symbol $a(\varepsilon x, \xi)$ will be denoted by $a^{\mathrm{W},\varepsilon}$ and we set, as before,

$$a^{\mathrm{W},\varepsilon}(t) = U^\varepsilon(-t/\varepsilon)a^{\mathrm{W},\varepsilon}U^\varepsilon(t/\varepsilon)\,. \tag{3.5}$$

Theorem 3.5. *Let the conditions* ($\mathrm{C_{per}}$)*,* ($\mathrm{C_{ex}}$) *be satisfied and $a \in \mathcal{O}(0)$. Then for every $\psi \in P_{\mathcal{I}}L^2$ we have*

$$\lim_{\varepsilon\to 0} a^{\mathrm{W},\varepsilon}(t)\psi = \mathcal{U}^{-1}a(R(t),K(t))\mathcal{U}\psi\,.$$

4. Semiclassical distributions

Theorems 3.1 and 3.5 tell us how the quantum distributions behave in the semiclassical limit. Let us first consider the initial $\psi \in P_{\mathcal{I}}\mathcal{H}$. Its scaled position distribution is $\varepsilon^{-d}|\psi(x/\varepsilon)|^2$ which converges to $\delta(x)$ as a measure. The quasimomentum distribution $\sum_{n\in\mathcal{I}}|\psi_n(k)|^2$ is independent of ε. Thus it is natural to chose

$$\rho(dr\,dk) = \sum_{n\in\mathcal{I}}\delta(r)|\psi_n(k)|^2\,dr\,dk\; = \sum_{n\in\mathcal{I}}\rho_n(dr\,dk) \tag{4.1}$$

as initial distribution for the semiclassical flow (3.1). We could consider more general initial measures at the expense of making ψ itself ε-dependent. For example the shifted initial measure $\sum_{n\in\mathcal{I}}\delta(r-r_0)|\psi_n(k)|\,dr\,dk$ is approximated by $\psi(x - \varepsilon^{-1}r_0)$. Under (3.1) $\rho(dr\,dk)$ evolves to $\rho(dr\,dk,t) = \sum_{n\in\mathcal{I}}\rho_n(dr\,dk,t)$. Each ρ_n satisfies weakly the transport equation

$$\frac{\partial}{\partial t}\rho_n = -\nabla E_n(k)\cdot\nabla_r\rho_n + \nabla V(r)\cdot\nabla_k\rho_n \tag{4.2}$$

with initial condition $\rho_n(dr\,dk,0) = \rho_n(dr\,dk)$. We define the position and quasimomentum marginals through

$$\rho(dr,t) = \int_{M^*}\rho(dr\,dk,t)\,,\qquad \rho(dk,t) = \int_{\mathbb{R}^d}\rho(dr\,dk,t)\,. \tag{4.3}$$

To connect with the quantum evolution we consider the quantum mechanical position distribution

$$\rho^\varepsilon(dx,t) = \varepsilon^{-d}|\psi(x/\varepsilon,t/\varepsilon)|^2\,dx \tag{4.4}$$

as a probability measure on $\mathbb{R}^d$. From Theorem 3.1 and Lemma 8.1 we conclude that

$$\lim_{\varepsilon\to 0} f(x^\varepsilon(t))\psi = \mathcal{U}^{-1}f(R(t))\mathcal{U}\psi \tag{4.5}$$

for $f \in C_\infty(\mathbb{R}^d)$. In particular,

$$\lim_{\varepsilon\to 0}\int\rho^\varepsilon(dx,t)f(x) = \lim_{\varepsilon\to 0}(\psi, f(x^\varepsilon(t))\psi) = (\mathcal{U}\psi, f(R(t))\mathcal{U}\psi) \tag{4.6}$$

and we only have to compute the expression on the right hand side. Using that

$$(\mathcal{U}\psi)(x,k) = \sum_{n\in\mathcal{I}} \psi_n(k)\rho_n(x,k)$$

we have

$$(\mathcal{U}\psi, f(R(t))\mathcal{U}\psi) = \sum_{n\in\mathcal{I}} \int_{M^*} |\psi_n(k)|^2 f(r_n(t;k))\, dk = \sum_{n\in\mathcal{I}} \int_M \rho_n(dr,t) f(r)\,. \tag{4.7}$$

Thus the positional distribution $\rho^\varepsilon(dx,t)$ converges weakly as a measure to the incoherent sum $\sum_{n\in\mathcal{I}} \rho_n(dr,t)$.

By the same reasoning, if g is a Γ^*-periodic function, then by Theorem 3.4 and Lemma 8.1

$$\lim_{\varepsilon\to 0} g(p(t/\varepsilon))\psi = \mathcal{U}^{-1} g(K(t))\mathcal{U}\psi\,. \tag{4.8}$$

Therefore, if $\rho^\varepsilon(k,t)\,dk$ denotes the spectral measure for the quasimomentum operator at time t/ε, we have

$$\lim_{\varepsilon\to 0} \rho^\varepsilon(k,t)\,dk = \sum_{n\in\mathcal{I}} \rho_n(dk,t) \tag{4.9}$$

weakly as measures.

More generally for $\psi \in L^2$ we define the scaled Wigner function by

$$W^\varepsilon(x,k,t) = \sum_{\gamma\in\Gamma} \varepsilon^{-d} \psi(\varepsilon^{-1}x - \frac{1}{2}\gamma, \varepsilon^{-1}t)\psi^*(\varepsilon^{-1}x + \frac{1}{2}\gamma, \varepsilon^{-1}t) e^{ik\cdot\gamma} \tag{4.10}$$

with $x \in \mathbb{R}^d$, $k \in M^*$. We think of W^ε as a signed, bounded measure over $\mathbb{R}^d \times M^*$. The Wigner function yields expectations of Weyl quantized operators through

$$\left(\psi, e^{iH^\varepsilon t/\varepsilon} a^{\mathrm{W},\varepsilon} e^{-iH^\varepsilon t/\varepsilon}\psi\right) = \int_{\mathbb{R}^d\times M^*} W^\varepsilon(x,k,t) a(x,k)\, dx\, dk \tag{4.11}$$

with a Γ^*-periodic in its second argument. From Theorem 3.5 we therefore deduce that

$$\lim_{\varepsilon\to 0} W^\varepsilon(r,k,t)\, dr\, dk \; = \rho(dr\, dk, t) \tag{4.12}$$

weakly as measures. The limits (4.6) and (4.9) are the particular cases, where either $a(x,k) = f(x)$ or $a(x,k) = g(k)$.

5. Convergence of the unitary groups

By definition, the time evolution generated by H_{per} leaves invariant the band subspaces $\mathrm{Ran}(P_n)$ for all $n \in \mathbb{N}$. However, $W^\varepsilon(x) = W(\varepsilon x)$ does not respect the Bloch decomposition and it will induce transitions between different bands. Since W^ε is of slow variation, we expect such transitions to have a small amplitude as stated in Theorem 3.2.

W^ε transforms under $\mathcal{U}$ as

$$\begin{aligned}(\mathcal{U}W^\varepsilon\psi)(k,x) &= \sum_{\gamma\in\Gamma} \mathrm{e}^{-i(x+\gamma)\cdot k} W(\varepsilon(x+\gamma))\psi(x+\gamma)\\ &= \sum_{\gamma\in\Gamma} \mathrm{e}^{-i(x+\gamma)\cdot k}(2\pi)^{-d/2}\int_{\mathbb{R}^d}\widehat{W}(p)\mathrm{e}^{i\varepsilon(x+\gamma)\cdot p}\,dp\,\psi(x+\gamma)\\ &= (2\pi)^{-d/2}\int_{\mathbb{R}^d}\widehat{W}(p)(\mathcal{U}\psi)(k-\varepsilon p,x)\,dp\\ &= (2\pi)^{-d/2}\int_{\mathbb{R}^d}\widehat{W}^\varepsilon(p)(\mathcal{U}\psi)(k-p,x)\,dp =: (\tilde{W}^\varepsilon\mathcal{U}\psi)(k,x)\,,\end{aligned}\tag{5.1}$$

where $\widehat{W}^\varepsilon(p) = \varepsilon^{-d}\widehat{W}(p/\varepsilon)$ and we adopt the quasiperiodic extension (2.2). Since $\widehat{W} \in \mathcal{S}(\mathbb{R}^d)$, the integral (5.1) is well-defined and $\tilde{W}^\varepsilon = \mathcal{U}W^\varepsilon\mathcal{U}^{-1}$ acts on $\mathcal{H}$ as convolution with $\widehat{W}^\varepsilon$ in the fiber parameter k. $\widehat{W}^\varepsilon$ approximates a Dirac delta in the limit $\varepsilon \to 0$ and the shift in (5.1) becomes the identity operator.

In the Bloch-Floquet representation the full Hamiltonian (1.3) becomes

$$(\tilde{H}\psi)(k,\cdot) = H_{\mathrm{per}}(k)\psi(k,\cdot) + (\tilde{W}^\varepsilon\psi)(k,\cdot)\,.$$

We expect the diagonal part of W^ε to be dominant with the off-diagonal piece as a small correction. For such a decomposition it turns out to be convenient to fix the index n of an isolated band and to project along P_n and its complement $Q_n = \mathbf{1} - P_n$. For $n \in \mathcal{I}$ we define the diagonal part H^n_{diag} of H as

$$H^n_{\mathrm{diag}} = P_n H P_n + Q_n H Q_n\,,$$

and the off-diagonal part of the external potential as

$$W^{\varepsilon,n}_{\mathrm{od}} = Q_n W^\varepsilon P_n + P_n W^\varepsilon Q_n\,.$$

Then

$$H = H^n_{\mathrm{diag}} + W^{\varepsilon,n}_{\mathrm{od}} = (H_{\mathrm{per}} + W^{\varepsilon,n}_{\mathrm{diag}}) + W^{\varepsilon,n}_{\mathrm{od}}\,.$$

We note that $W^{\varepsilon,n}_{\mathrm{diag}}$ and $W^{\varepsilon,n}_{\mathrm{od}}$ are bounded operators and set

$$U^\varepsilon(t) = \mathrm{e}^{-itH}, \quad U^{\varepsilon,n}_{\mathrm{diag}}(t) = \mathrm{e}^{-itH^n_{\mathrm{diag}}}\,.$$

To prove Theorem 3.2 we start by writing the difference of the two unitary groups in the Bloch representation as

$$\tilde{U}^\varepsilon(t/\varepsilon) - \tilde{U}^{\varepsilon,n}_{\mathrm{diag}}(t/\varepsilon) = -\,i\varepsilon\int_0^{t/\varepsilon}\tilde{U}^\varepsilon(\varepsilon^{-1}t-s)\left(\varepsilon^{-1}\tilde{W}^{\varepsilon,n}_{\mathrm{od}}\right)\tilde{U}^{\varepsilon,n}_{\mathrm{diag}}(s)\,ds\tag{5.2}$$

and we have to investigate the operator $\tilde{W}^{\varepsilon,n}_{\mathrm{od}}$. By definition, for $\psi \in \mathcal{H}$, we have

$$(\tilde{Q}_n\tilde{W}^\varepsilon\tilde{P}_n\psi)(k) = (2\pi)^{-d/2}\int_{\mathbb{R}^d}\widehat{W}^\varepsilon(p)Q_n(k)P_n(k-p)\psi(k-p)\,dp\,,$$

which vanishes strongly in the limit $\varepsilon \to 0$, since $\widehat{W}^\varepsilon$ localizes around $p = 0$. To control the long times in (5.2) we need uniform convergence of order $o(\varepsilon)$, however. To have a more detailed information on $W^{\varepsilon,n}_{\mathrm{od}}$ we Taylor expand of $P_n(k-p)$ around $P_n(k)$, leading, as we will show, to

$$(\tilde{Q}_n\tilde{W}^\varepsilon\tilde{P}_n\psi)(k) = -\varepsilon(2\pi)^{-d/2}\int_{\mathbb{R}^d}\widehat{F}^\varepsilon(p)Q_n(k)\nabla_k P_n(k)\psi(k-p)\,dp + o(\varepsilon)\,.\tag{5.3}$$

Here $\widehat{F}^\varepsilon(p) := \widehat{W}^\varepsilon(p)\frac{p}{\varepsilon}$ is the Fourier transform of $F^\varepsilon(x) = (D_x W)(\varepsilon x)$ and we will associate to $\widehat{F}^\varepsilon$ the operator $\tilde{F}^\varepsilon$ as in the case of $\widehat{W}^\varepsilon$,

$$(\tilde{F}^\varepsilon\psi)(k) = (2\pi)^{-d/2}\int_{\mathbb{R}^d}\widehat{F}^\varepsilon(p)\psi(k-p)\,dp\,.$$

To justify (5.3) we first need to calculate $\nabla_k P_n(k)$.

Lemma 5.1. *Let $n \in \mathcal{I}$. Then*

$$\begin{aligned}\nabla_k P_n(k) \;&=\; -\,Q_n(k)R_{E_n(k)}(H_{\mathrm{per}}(k))(D_x+k)P_n(k)\\ &\quad -\,P_n(k)(D_x+k)R_{E_n(k)}(H_{\mathrm{per}}(k))Q_n(k)\,,\end{aligned}\tag{5.4}$$

where $R_\lambda(H) = (H-\lambda)^{-1}$ is the resolvent of H. Thus $P_n(\cdot) \in C^\infty(M^*; B(L^2(M)))$.

Proof. Using contour integrals we write

$$\nabla_k P_n(k) = -\frac{1}{2\pi i}\oint_{c_n(k)}\nabla_k R_\lambda(H_{\mathrm{per}}(k))\,d\lambda\,,$$

where $c_n(k)$ is a closed rectifiable curve in the complex spectral plane which encircles $E_n(k)$ only. From

$$\begin{aligned}0 \;&=\; \nabla_k\mathbf{1} = \nabla_k(H_{\mathrm{per}}(k)-\lambda)R_\lambda(H_{\mathrm{per}}(k))\\ &=\; (D_x+k)R_\lambda(H_{\mathrm{per}}(k)) + (H_{\mathrm{per}}(k)-\lambda)\nabla_k R_\lambda(H_{\mathrm{per}}(k))\,,\end{aligned}$$

we infer

$$\nabla_k R_\lambda(H_{\mathrm{per}}(k)) = -R_\lambda(H_{\mathrm{per}}(k))(D_x+k)R_\lambda(H_{\mathrm{per}}(k))\,.$$

Hence we get

$$\begin{aligned}Q_n(k)\nabla_k P_n(k) \;&=\; Q_n(k)\nabla_k P_n(k)(P_n(k)+Q_n(k))\\ &=\; \frac{1}{2\pi i}\oint_{c_n(k)} Q_n(k)R_\lambda(H_{\mathrm{per}}(k))(D_x+k)R_\lambda(H_{\mathrm{per}}(k))P_n(k)\,d\lambda\\ &=\; \frac{1}{2\pi i}\oint_{c_n(k)} R_\lambda(H_{\mathrm{per}}(k))Q_n(k)\frac{1}{E_n(k)-\lambda}\,d\lambda\,(D_x+k)P_n(k)\\ &=\; -R_{E_n(k)}(H_{\mathrm{per}}(k))Q_n(k)(D_x+k)P_n(k)\,,\end{aligned}\tag{5.5}$$

where the term $Q_n(k)\nabla_k P_n(k)Q_n(k)$ vanishes, since in this case the integrand is an analytic function on the whole interior of $c_n(k)$. Note that $P_n(k)$ projects onto a subspace of finite energy, on which $D_x + k$ is bounded. The statement about continuity for this term then follows from the continuity of $P_n(k)$, $E_n(k)$ and the assumption that $E_n(k)$ is isolated from the remainder of the spectrum. An analogous computation for $P_n(k)\nabla_k P_n(k)$ leads to the second term in (5.4).

Finally, $P_n(\cdot) \in C^\infty(M^*; B(L^2(M)))$ follows by induction. □

From $Q_n(k) + P_n(k) = \mathbf{1}$ we conclude that $Q_n(k)$ is differentiable as well and that $\nabla_k Q_n(k) = -\nabla_k P_n(k)$.

Lemma 5.2. *Let $n \in \mathcal{I}$. Then*

$$\tilde{W}^{\varepsilon,n}_{\mathrm{od}} = -\varepsilon\left(\tilde{Q}_n\nabla_k\tilde{P}_n + \tilde{P}_n\nabla_k\tilde{Q}_n\right)\cdot\tilde{F}^\varepsilon + o(\varepsilon)$$

in $B(\mathcal{H},\mathcal{H})$, where $\nabla_k\tilde{P}_n := \int^{\oplus}_{M^*}\nabla_k P_n(k)\,dk$.

Proof. We will treat only the $\tilde{Q}_n\tilde{W}^\varepsilon\tilde{P}_n$ part of $\tilde{W}^{\varepsilon,n}_{\mathrm{od}}$ explicitly, since the argument for the second part is analogous.

Let $\psi\in\mathcal{H}$. By Lemma 5.1 we are allowed to write the following well-defined identity, setting $e_p = p/|p|$,

$$
\begin{aligned}
&\int \widehat{W^\varepsilon}(p)P_n(k-p)\psi(k-p)\,dp\\
&\quad= \int \widehat{W^\varepsilon}(p)|p|\left(|p|^{-1}(P_n(k-p)-P_n(k)) + e_p\cdot\nabla_k P_n(k)\right)\psi(k-p)\,dp\\
&\qquad + P_n(k)\int \widehat{W^\varepsilon}(p)\psi(k-p)\,dp - \int \widehat{W^\varepsilon}(p)p\cdot\nabla_k P_n(k)\psi(k-p)\,dp\\
&\quad= \varepsilon\int \widehat{W^\varepsilon}(p)\frac{|p|}{\varepsilon}\left(\frac{P_n(k-p)-P_n(k)}{|p|} + e_p\cdot\nabla_k P_n(k)\right)\psi(k-p)\,dp \qquad (5.6)\\
&\qquad + (2\pi)^{d/2}P_n(k)(\tilde{W}^\varepsilon\psi)(k) - \varepsilon(2\pi)^{d/2}\nabla_k P_n(k)\cdot(\tilde{F}^\varepsilon\psi)(k)\,. \qquad (5.7)
\end{aligned}
$$

If in (5.6), (5.7) we apply $Q_n(k)$ from the left, the first term of (5.7) vanishes and it remains to show that (5.6), divided by ε, tends to zero uniformly for all $\psi\in\mathcal{H}$.

We split the integral into two parts. Let $R>0$ be arbitrary, $B_R=\{p\mid |p|\le R\}$. We start with

$$
\begin{aligned}
&\int_{M^*}\left\|\int_{B_R}\widehat{W^\varepsilon}(p)\frac{|p|}{\varepsilon}\left(\frac{P_n(k-p)-P_n(k)}{|p|}\right.\right.\\
&\qquad\qquad\left.\left. + e_p\cdot\nabla_k P_n(k)\right)\psi(k-p)\,dp\right\|_{L^2(M)} dk\\
&\le \sup_{k\in M^*}\sup_{p\in B_R}\left\||p|^{-1}\left(P_n(k-p)-P_n(k)\right) + e_p\cdot\nabla_k P_n(k)\right\|\\
&\qquad\times\int_{B_R}\left|\widehat{W^\varepsilon}(p)\right|\frac{|p|}{\varepsilon}\int_{M^*}\|\psi(k-p)\|_{L^2(M)}\,dk\,dp\\
&\le \|\psi\|_{\mathcal{H}}\left\|\widehat{F^\varepsilon}\right\|_{L^1}\\
&\qquad\times\sup_{k\in M^*,\,p\in B_R}\left\||p|^{-1}(P_n(k-p)-P_n(k)) + e_p\cdot\nabla_k P_n(k)\right\|\,.
\end{aligned}
$$

Since $\|\widehat{F^\varepsilon}\|_{L^1}$ does not depend on ε and since the difference quotient approaches the derivative uniformly on the compact domain M^*, the $\mathcal{H}$-norm of the first part tends to zero uniformly. For the remaining part we have

$$
\begin{aligned}
&\int_{M^*}\left\|\int_{|p|>R}\widehat{W^\varepsilon}(p)\frac{|p|}{\varepsilon}\left(\frac{P_n(k-p)-P_n(k)}{|p|}\right.\right.\\
&\qquad\qquad\left.\left. + e_p\cdot\nabla_k P_n(k)\right)\psi(k-p)\,dp\right\|_{L^2(M)} dk\\
&\le \|\psi\|_{\mathcal{H}}\left\|\widehat{F^\varepsilon}\right\|_{L^1(B_R^c)}\\
&\qquad\times\sup_{k\in M^*,\,p\in\mathbb{R}^d}\left\||p|^{-1}(P_n(k-p)-P_n(k)) + e_p\cdot\nabla_k P_n(k)\right\|\,,
\end{aligned}
$$

which tends to zero uniformly as $\varepsilon \to 0$, since $\|\widehat{F}^\varepsilon\|_{L^1(B_R^c)} \to 0$ for any fixed $R > 0$. □

As a consequence of Lemma 5.2 the difference of the two unitary groups in Eq. (5.2) can be written as

$$\begin{aligned} &\tilde{U}^\varepsilon(t/\varepsilon) - \tilde{U}^{\varepsilon,n}_{\mathrm{diag}}(t/\varepsilon) \\ &= i\varepsilon \int_0^{t/\varepsilon} \tilde{U}^\varepsilon(\varepsilon^{-1}t - s) \Big(\tilde{Q}_n \nabla_k \tilde{P}_n + \tilde{P}_n \nabla_k \tilde{Q}_n\Big) \cdot \tilde{F}^\varepsilon\, \tilde{U}^{\varepsilon,n}_{\mathrm{diag}}(s)\, ds + o(1)\,. \end{aligned} \tag{5.8}$$

We have to estimate the integral without losing one order of ε from the integration over time. As in the proof in [3] of the adiabatic theorem the idea is to rewrite the integrand as a time derivative, i.e. as a commutator of $\tilde{H}^n_{\mathrm{diag}}$ with an appropriately chosen operator A, at least up to an unavoidable error $o(1)$.

Let us define for $n \in \mathcal{I}$

$$B_n(k) = R^2_{E_n(k)}(H_{\mathrm{per}}(k)) Q_n(k)(D_x + k) P_n(k)\,.$$

Lemma 5.3. *For $n \in \mathcal{I}$ we have*

$$\tilde{Q}_n \nabla_k \tilde{P}_n + \tilde{P}_n \nabla_k \tilde{Q}_n = [\tilde{B}_n + \tilde{B}_n^*, \tilde{H}_{\mathrm{per}}]\,.$$

Proof. Using the spectral decomposition and recalling

$$Q_n(k)\nabla_k P_n(k) = -R_{E_n(k)}(H_{\mathrm{per}}(k)) Q_n(k)(D_x + k) P_n(k)$$

from Lemma 5.1, one directly computes

$$\begin{aligned} &B_n(k)H_{\mathrm{per}}(k) - H_{\mathrm{per}}(k)B_n(k) \\ &\quad= -(H_{\mathrm{per}}(k) - E_n(k)) R^2_{E_n(k)}(H_{\mathrm{per}}(k)) Q_n(k)(D_x + k) P_n(k) \\ &\quad= -R_{E_n(k)}(H_{\mathrm{per}}(k)) Q_n(k)(D_x + k) P_n(k) \\ &\quad= Q_n(k)\nabla_k P_n(k)\,. \end{aligned}$$

The lemma then follows from $\tilde{P}_n \nabla_k \tilde{Q}_n = -(\tilde{Q}_n \nabla_k \tilde{P}_n)^*$. □

Lemma 5.4. $\Big[B_n + B_n^*, \tilde{W}^{\varepsilon,n}_{\mathrm{diag}}\Big] \to 0$ *in $B(\mathcal{H}, \mathcal{H})$ as ε tends to zero.*

Proof. To have a concise notation in the following, expressions like $\tilde{W}^{\varepsilon,n}_{\mathrm{diag}} P_n(k)$ are understood in the sense that $\tilde{W}^{\varepsilon,n}_{\mathrm{diag}}$ acts on all k-depending objects on its right hand side. We recall that $\tilde{W}^{\varepsilon,n}_{\mathrm{diag}} = \tilde{P}_n \tilde{W}^\varepsilon \tilde{P}_n + \tilde{Q}_n \tilde{W}^\varepsilon \tilde{Q}_n$. Hence

$$\begin{aligned} &\Big[B_n(k), \tilde{W}^{\varepsilon,n}_{\mathrm{diag}}\Big] \\ &\quad= Q_n(k)\Big[R^2_{E_n(k)}(H_{\mathrm{per}}(k)) Q_n(k)(D_x + k) P_n(k), \tilde{W}^\varepsilon\Big] P_n(k)\,. \end{aligned}$$

We now examine the commutators $[P_n(k), \tilde{W}^\varepsilon]$, $[D_x + k, \tilde{W}^\varepsilon]$ and $[R^2_{E_n(k)} Q_n(k), \tilde{W}^\varepsilon]$ one by one. It follows from the proof of Lemma 5.2 that $[P_n(k), \tilde{W}^\varepsilon]$ vanishes as $\varepsilon \to 0$ and the analogous statement for $[R^2_{E_n(k)} Q_n(k), \tilde{W}^\varepsilon]$ can be shown to hold by a similar argument. Thus it remains to discuss the commutator $[D_x + k, \tilde{W}^\varepsilon]$. For

$\psi \in H^1(\mathbb{R}^d)$ we compute

$$\begin{aligned}
&(2\pi)^{d/2}([D_x + k, \tilde{W}^\varepsilon]\mathcal{U}\psi)(k) \\
&= \int_{\mathbb{R}^d} \widehat{W}^\varepsilon(p)(((D_x + k) - (D_x + k - p))\mathcal{U}\psi)(k-p)\, dp \\
&= \varepsilon \int_{\mathbb{R}^d} \widehat{W}^\varepsilon(p)\varepsilon^{-1} p(\mathcal{U}\psi)(k-p)\, dp \\
&= \varepsilon(\tilde{F}^\varepsilon \mathcal{U}\psi)(k)\,,
\end{aligned}$$

which clearly vanishes uniformly for $\psi \in L^2$ as $\varepsilon \to 0$, since $F \in \mathcal{S}(\mathbb{R}^d, \mathbb{R}^d)$. ☐

In summary we have shown that

$$\left(\tilde{Q}_n \nabla_k \tilde{P}_n + \tilde{P}_n \nabla_k \tilde{Q}_n\right) \cdot \tilde{F}^\varepsilon = \left(\left[\tilde{B}_n + \tilde{B}_n^*, \tilde{H}^n_{\text{diag}}\right] + o(1)\right) \cdot \tilde{F}^\varepsilon\,,$$

and it remains to check

Lemma 5.5. $\left[\tilde{H}^n_{\text{diag}}, \tilde{F}^\varepsilon\right] \to 0$ *in* $B(\mathcal{U}H^1, \mathcal{H})$ *as* ε *tends to zero.*

Proof. The commutator

$$[H_{\text{per}}, F^\varepsilon] = -\frac{1}{2}\varepsilon^2(\Delta F^\varepsilon) - \frac{1}{2}\varepsilon(\nabla F^\varepsilon)\cdot\nabla - \frac{1}{2}\varepsilon(\nabla \cdot F^\varepsilon)\nabla$$

vanishes in $B(H^1, L^2)$ as $\varepsilon \to 0$. The commutator $[\tilde{W}^{\varepsilon,n}_{\text{diag}}, \tilde{F}^\varepsilon]$ vanishes in $B(\mathcal{H}, \mathcal{H})$, since the commutator of $\tilde{P}_n$ and $\tilde{Q}_n$ with $\tilde{F}^\varepsilon$ are both of uniform order $o(1)$ (in $B(\mathcal{H}, \mathcal{H})$) and $[\tilde{W}^\varepsilon, \tilde{F}^\varepsilon]$ vanishes identically. ☐

Defining

$$\tilde{A}_n = \left(\tilde{B}_n + \tilde{B}_n^*\right) \cdot \tilde{F}^\varepsilon\,,$$

it follows that the integrand in (5.8) can be written as

$$\left(\tilde{Q}_n \nabla_k \tilde{P}_n + \tilde{P}_n \nabla_k \tilde{Q}_n\right) \cdot \tilde{F}^\varepsilon = \left[\tilde{A}_n, \tilde{H}^n_{\text{diag}}\right] + o(1)\,,$$

where $o(1)$ is in the norm of $B(\mathcal{U}H^1, \mathcal{H})$. (Note that for $A^\varepsilon \in B(L^2, L^2)$, $\lim_{\varepsilon\to 0} A^\varepsilon = 0$ in $B(L^2, L^2)$ implies, in particular, that also $\lim_{\varepsilon\to 0} A^\varepsilon = 0$ in $B(H^1, L^2)$).

We are now ready for the

Proof of Theorem 3.2. Since $U^{\varepsilon,n}_{\text{diag}}(t) : H^1 \to H^1$ is bounded uniformly in t and ε (cf. Section 6), we obtain for the difference (5.8) of the unitary groups,

$$\begin{aligned}
&\left(\tilde{U}^\varepsilon(t/\varepsilon) - \tilde{U}^{\varepsilon,n}_{\text{diag}}(t/\varepsilon)\right) \\
&= -i\varepsilon \int_0^{t/\varepsilon} \tilde{U}^\varepsilon(\varepsilon^{-1}t - s)\left[\tilde{A}_n, \tilde{H}^n_{\text{diag}}\right]\tilde{U}^{\varepsilon,n}_{\text{diag}}(s)\, ds + o(1)\,.
\end{aligned} \tag{5.9}$$

Abbreviating $X^n(s) = \tilde{U}^\varepsilon(-s)\tilde{U}^{\varepsilon,n}_{\rm diag}(s)$ and $\tilde{A}_n(s) = \tilde{U}^{\varepsilon,n}_{\rm diag}(-s)\tilde{A}_n\tilde{U}^{\varepsilon,n}_{\rm diag}(s)$, we get, using partial integration in (5.9),

$$\begin{aligned}
-i\varepsilon\int_0^{t/\varepsilon} & \tilde{U}^\varepsilon(t/\varepsilon)\, X^n(s)\, \tilde{U}^{\varepsilon,n}_{\rm diag}(-s)\left[\tilde{A}_n, \tilde{H}^n_{\rm diag}\right]\tilde{U}^{\varepsilon,n}_{\rm diag}(s)\, ds \\
&= \varepsilon\, \tilde{U}^\varepsilon(t/\varepsilon)\int_0^{t/\varepsilon} X^n(s)\left(\frac{d}{ds}\tilde{A}_n(s)\right) ds \\
&= \varepsilon\left(\tilde{A}_n\,\tilde{U}^{\varepsilon,n}_{\rm diag}(t/\varepsilon) - \tilde{U}^\varepsilon(t/\varepsilon)\,\tilde{A}_n\right) \\
&\quad - \varepsilon\,\tilde{U}^\varepsilon(t/\varepsilon)\int_0^{t/\varepsilon}\left(\frac{d}{ds}X^n(s)\right)\tilde{A}_n(s)\, ds \\
&= \varepsilon\left(\tilde{A}_n\,\tilde{U}^{\varepsilon,n}_{\rm diag}(t/\varepsilon) - \tilde{U}^\varepsilon(t/\varepsilon)\,\tilde{A}_n\right) \\
&\quad - i\varepsilon\,\tilde{U}^\varepsilon(t/\varepsilon)\int_0^{t/\varepsilon}\tilde{U}^\varepsilon(-s)\,\tilde{W}^{\varepsilon,n}_{\rm od}\,\tilde{A}_n\,\tilde{U}^{\varepsilon,n}_{\rm diag}(s)\, ds\,.
\end{aligned}$$

For $\varepsilon \to 0$ the first term vanishes since $\tilde{A}_n$ is bounded and the second term vanishes, since $W^{\varepsilon,n}_{\rm od}$ tends to zero uniformly according to Lemma 5.2. □

6. Convergence of the position operator

In this section we will study the asymptotics of the position operator $x^\varepsilon(t)$. As in the case of the unitaries we have to establish that the off-diagonal contributions to $x^\varepsilon(t)$ vanish in the limit $\varepsilon \to 0$.

Proof of Theorem 3.3. Let $\psi \in D(|x|) \cap H^2$ and $n \in \mathcal{I}$. Then

$$\begin{aligned}
&\left\|\left(x^\varepsilon(t) - x^{\varepsilon,n}_{\rm diag}(t)\right)\psi\right\| \\
&\leq \left\|\left(x^\varepsilon(t) - U^{\varepsilon,n}_{\rm diag}(-t/\varepsilon)\, x^\varepsilon\, U^{\varepsilon,n}_{\rm diag}(t/\varepsilon)\right)\psi\right\| \qquad (6.1)\\
&\quad + \left\|\left(U^{\varepsilon,n}_{\rm diag}(-t/\varepsilon)\, x^\varepsilon\, U^{\varepsilon,n}_{\rm diag}(t/\varepsilon) - x^{\varepsilon,n}_{\rm diag}(t)\right)\psi\right\|\,. \qquad (6.2)
\end{aligned}$$

In order to estimate (6.1), note that we have

$$x^\varepsilon(t)\psi = \varepsilon x\psi + \varepsilon\int_0^{t/\varepsilon} U^\varepsilon(-s) D_x U^\varepsilon(s)\psi\, ds \qquad (6.3)$$

and

$$\begin{aligned}
U^{\varepsilon,n}_{\rm diag}&(-t/\varepsilon)\, x^\varepsilon\, U^{\varepsilon,n}_{\rm diag}(t/\varepsilon) \\
&= \varepsilon x\psi + \varepsilon\int_0^{t/\varepsilon} U^{\varepsilon,n}_{\rm diag}(-s)\left(D_x + i\left[W^{\varepsilon,n}_{\rm diag}, x\right]\right) U^{\varepsilon,n}_{\rm diag}(s)\psi\, ds \\
&= \varepsilon x\psi + \varepsilon\int_0^{t/\varepsilon} U^{\varepsilon,n}_{\rm diag}(-s) D_x U^{\varepsilon,n}_{\rm diag}(s)\psi\, ds + o(1)\,.
\end{aligned}$$

The last equality holds, since $[W^{\varepsilon,n}_{\rm diag}, x] = o(1)$ in $B(L^2)$, as follows immediately from the fact that $[W^\varepsilon, P_n] = o(1)$ and $[W^\varepsilon, Q_n] = o(1)$, cf. proof of Lemma 5.2.

Hence, using (6.3), the remaining term from (6.1) is

$$\begin{aligned}
&\varepsilon \int_0^{t/\varepsilon} \Big(U^\varepsilon(-s) D_x U^\varepsilon(s) - U^{\varepsilon,n}_{\rm diag}(-s) D_x U^{\varepsilon,n}_{\rm diag}(s) \Big)\, \psi \, ds \\
&= \int_0^t \Big(U^\varepsilon(-s/\varepsilon) - U^{\varepsilon,n}_{\rm diag}(-s/\varepsilon) \Big) D_x U^{\varepsilon,n}_{\rm diag}(s/\varepsilon) \psi \, ds \qquad (6.4) \\
&\quad + \int_0^t U^\varepsilon(-s/\varepsilon) D_x \Big(U^\varepsilon(s/\varepsilon) - U^{\varepsilon,n}_{\rm diag}(s/\varepsilon) \Big)\, \psi \, ds\,. \qquad (6.5)
\end{aligned}$$

Using the fact that V and W are infinitesimally operator bounded with respect to $-\frac{1}{2}\Delta$ and that $\psi \in H^2$, we get for $\psi(s) := U^{\varepsilon,n}_{\rm diag}(s/\varepsilon)\psi$

$$\begin{aligned}
\big\| D_x^2 \psi(s) \big\| &\le \Big\| H^{\varepsilon,n}_{\rm diag} \psi(s) \Big\| + \Big\| (V + W^{\varepsilon,n}_{\rm diag}) \psi(s) \Big\| \\
&\le \Big\| H^{\varepsilon,n}_{\rm diag} \psi \Big\| + c_1 \big\| D_x^2 \psi(s) \big\| + c_2 \, \|\psi\| \,,
\end{aligned}$$

with $c_1 < \frac{1}{2}$ and $c_2 < \infty$. Hence $\|D_x U^{\varepsilon,n}_{\rm diag}(s/\varepsilon)\psi\|_{H^1} \le c\|\psi\|_{H^2}$ with c independent of s and ε and we can apply Theorem 3.2 to conclude that the operator acting on ψ in (6.4) vanishes in $B(H^2, L^2)$ as $\varepsilon \to 0$.

We come to (6.5). Let $\psi(s) = (U^\varepsilon(s/\varepsilon) - U^{\varepsilon,n}_{\rm diag}(s/\varepsilon))\psi$, then, by Cauchy-Schwarz,

$$\| D_x \psi(s) \|^2 = \big(\psi(s), D_x^2 \psi(s) \big) \le \|\psi(s)\| \, \big\| D_x^2 \psi(s) \big\| \,.$$

The first factor tends to zero by Theorem 3.2 whereas the second is uniformly bounded by the same argument as in the treatment of (6.4) a few lines above.

Next we rewrite (6.2) as

$$\varepsilon U^{\varepsilon,n}_{\rm diag}(-t/\varepsilon)\, x^n_{\rm od}\, U^{\varepsilon,n}_{\rm diag}(t/\varepsilon)$$

with $x^n_{\rm od} := Q_n x P_n + P_n x Q_n$. This certainly vanishes as $\varepsilon \to 0$ if $x^n_{\rm od}$ can be shown to be a bounded operator. To see this, note that in Bloch representation x acts as $i\nabla_k$. Hence

$$(\mathcal{U} Q_n x P_n \psi)(k) = i Q_n(k) \nabla_k P_n(k) (\mathcal{U}\psi)(k) = i Q_n(k) (\nabla_k P_n(k)) (\mathcal{U}\psi)(k)$$

and thus $\|Q_n x P_n\| = \|\tilde{Q}_n \nabla_k \tilde{P}_n\|$. Finally also $P_n x Q_n$ is bounded, since it is the adjoint of $Q_n x P_n$. □

7. Semiclassical equations of motion for the position operator

As we have shown, on the macroscopic scale the position and quasimomentum operators commute with the projection on isolated bands. Thus it remains to investigate the semiclassical limit for each isolated band separately. For this purpose we note that any $\psi \in \tilde{P}_n \mathcal{H}$ is of the form $\psi_n(k)\varphi_n(x,k)$ with $\psi_n \in L^2(M^*)$. Since φ_n already satisfies (2.2), we have to extend the Bloch coefficients periodically. We determine now how $H^{\varepsilon,n}_{\rm diag}$ acts on $L^2(M^*)$. We have $[H_{\rm per}, \tilde{P}_n] = 0$ and therefore $H_{\rm per}$ acts as multiplication by $E_n(k)$. For $W^{\varepsilon,n}_{\rm diag}$ we have

$$\begin{aligned}
&\Big(\tilde{P}_n \tilde{W}^\varepsilon \tilde{P}_n \mathcal{U} \psi \Big)(k,x) \\
&\quad = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \widehat{W^\varepsilon}(p) \big(\varphi_n(k), \varphi_n(k-p) \big)_{L^2(M)} \psi_n(k-p)\, dp\, \varphi_n(k,x) \\
&\quad =: (\tilde{W}^{\varepsilon,n} \psi_n)(k) \varphi_n(x,k)\,. \qquad (7.1)
\end{aligned}$$

Thus $H^{\varepsilon,n}_{\rm diag}$ restricted to $\tilde{P}_n \mathcal{H}$ is unitarily equivalent to $H^{\varepsilon,n} := E_n(k) + \tilde{W}^{\varepsilon,n}$.

To be able to use techniques from semiclassics we next approximate $\tilde{W}^{\varepsilon,n}$ by the operator $\tilde{W}^{\varepsilon,n}_{\mathrm{sc}} = W(-i\varepsilon\nabla_k)$, where ∇_k is understood with periodic boundary conditions on $\mathbb{R}^d/\Gamma^*$.

Lemma 7.1. *For any $n \in \mathcal{I}$*

$$\tilde{W}^{\varepsilon,n} = \tilde{W}^{\varepsilon,n}_{\mathrm{sc}} + o(\varepsilon) \tag{7.2}$$

in $B(L^2(M^*))$.

Proof. By definition we have

$$\left(\tilde{W}^{\varepsilon,n}_{\mathrm{sc}}\psi\right)(k) = (2\pi)^{-d/2}\int_{\mathbb{R}^d} \widehat{W}^{\varepsilon}(p)\psi_n(k-p)\,dp\,,$$

and therefore

$$\begin{aligned}\left(\left(\tilde{W}^{\varepsilon,n} - \tilde{W}^{\varepsilon,n}_{\mathrm{sc}}\right)\psi\right)(k) &= \\ &= (2\pi)^{-d/2}\int_{\mathbb{R}^d} \widehat{W}^{\varepsilon,n}(p)\Big(\big(\varphi_n(k),\varphi_n(k-p)\big)_{L^2(M)} - 1\Big)\psi(k-p)\,dp\,. \end{aligned} \tag{7.3}$$

As to be shown, there exists a constant c such that

$$\left|\big(\varphi_n(k),\varphi_n(k-p)\big)_{L^2(M)} - 1\right| \le c|p|^2 \tag{7.4}$$

for Lebesgue almost all k. Therefore we conclude

$$\begin{aligned}\left\|\left(\tilde{W}^{\varepsilon,n} - \tilde{W}^{\varepsilon,n}_{\mathrm{sc}}\right)\psi\right\|_{L^2(M^*)} &\le c\varepsilon^2\left\|\int\left|\widehat{W}^{\varepsilon}(p)\frac{|p|^2}{\varepsilon^2}\right||\psi(k-p)|\,dp\right\|_{L^2(M^*)} \\ &\le c'\varepsilon^2\|\psi\|_{L^2(M^*)}\,.\end{aligned}$$

To show (7.4) note that one can chose $\varphi_n(k)$ such that the map $k \mapsto \varphi_n(k) \in L^2(M)$ is smooth Lebesgue almost everywhere. This is because according to Lemma 5.1 the projections $P_n(k)$ depend smoothly on k and hence one can locally define $\varphi_n(k) = P_n(k)\varphi_n(k_0)/\|P_n(k)\varphi_n(k_0)\|$. Now we can cover M^* by finitely many open disjoint sets U_i such that $M^* \setminus \cup_i U_i$ is a set of Lebesgue measure zero and $\varphi_n(k)$ can be defined on the closure of each U_i in the way described above. One obtains a family $\varphi_n(k)$ of eigenfunctions which is smooth except at the boundaries between the sets, where we pick $\varphi_n(k)$ with an arbitrary phase. Wherever $\varphi_n(k)$ is smooth, Taylor expansion yields $\varphi_n(k-p) = \varphi_n(k) - p\cdot\nabla_k\varphi_n(k) + \frac{1}{2}p\cdot\mathbb{H}(\varphi_n)(k')p$, where $\mathbb{H}(\varphi_n)$ denotes the Hessian and $\frac{1}{2}p\cdot\mathbb{H}(\varphi_n)(k')p$ is the Lagrangian remainder. In view of $(\varphi_n(k),\nabla_k\varphi_n(k))_{L^2(M)} = 0$, which follows from comparing (5.4) with

$$(\nabla_k P_n\psi)(k) = (\varphi_n(k),\psi(\cdot,k))\nabla_k\varphi_n(k) + (\nabla_k\varphi_n(k),\psi(\cdot,k))\varphi_n(k)\,,$$

we obtain

$$\left|\big(\varphi_n(k),\varphi_n(k-p)\big)_{L^2(M)} - 1\right| \le c(k)|p|^2\,.$$

Here $c(k) = \frac{1}{2}\sum_{i,j}|(\varphi_n(k'),\partial_{k_i}\partial_{k_j}\varphi_n(k'))|$. However, $c(k)$ is bounded uniformly in k, since $\varphi_n(k)$ is smooth on each compact $\bar{U_i}$. □

We define now the semiclassical Hamiltonian $H^{\varepsilon,n}_{\mathrm{sc}}$

$$H^{\varepsilon,n}_{\mathrm{sc}} = E_n(k) + W(-i\varepsilon\nabla_k) \tag{7.5}$$

acting on $L^2(M^*)$. Then Lemma 7.1 shows that the difference $H^{\varepsilon,n} - H^{\varepsilon,n}_{\mathrm{sc}}$ is of order $o(\varepsilon)$ uniformly in $B(L^2(M^*))$ and hence (cf. Section 5) the difference of the corresponding unitary groups approaches zero as $\varepsilon \to 0$.

Corollary 7.2. *Let* $U_{\mathrm{sc}}^{\varepsilon,n}(t) = \mathrm{e}^{-itH_{\mathrm{sc}}^{\varepsilon,n}}$ *and* $U^{\varepsilon,n}(t) = \mathrm{e}^{-itH^{\varepsilon,n}}$*, then*

$$\lim_{\varepsilon\to 0}\big(U^{\varepsilon,n}(t/\varepsilon) - U_{\mathrm{sc}}^{\varepsilon,n}(t/\varepsilon)\big) = 0$$

in $B(L^2(M^*))$.

The semiclassical limit for $U_{\mathrm{sc}}^{\varepsilon,n}(t/\varepsilon)$ on $L^2(\mathbb{T}^*)$ is well studied. We refer to [8, 14, 22]. As a consequence the strong limits

$$\lim_{\varepsilon\to 0} U_{\mathrm{sc}}^{\varepsilon,n}(-t/\varepsilon)\,(-i\varepsilon\nabla_k)\,U_{\mathrm{sc}}^{\varepsilon,n}(t/\varepsilon) \;=\; r_n(t;k)\,, \tag{7.6}$$

$$\lim_{\varepsilon\to 0} U_{\mathrm{sc}}^{\varepsilon,n}(-t/\varepsilon)\,k\,U_{\mathrm{sc}}^{\varepsilon,n}(t/\varepsilon) \;=\; k_n(t;k) \tag{7.7}$$

exist on $H^1(\mathbb{T}^*)$. r_n and k_n act as multiplication operators and are defined as in (3.1) with initial conditions $(r_n(0), k_n(0)) = (0, k)$.

Since the restriction of $\varepsilon x_{\mathrm{diag}}^n$ to the n-th band subspace is unitarily equivalent to $-i\varepsilon\nabla_k$ on $L^2(\mathbb{T}^*)$, we can, in view of Theorem 3.3, conclude the proof of Theorem 3.1 by showing

Lemma 7.3. *In* $B(L^2(M^*))$ *we have*

$$\lim_{\varepsilon\to 0}\big(U^{\varepsilon,n}(-t/\varepsilon)(-i\varepsilon\nabla_k)U^{\varepsilon,n}(t/\varepsilon) - U_{\mathrm{sc}}^{\varepsilon,n}(-t/\varepsilon)(-i\varepsilon\nabla_k)U_{\mathrm{sc}}^{\varepsilon,n}(t/\varepsilon)\big) = 0\,. \tag{7.8}$$

Proof. The proof of (7.8) is analogous to the proof of Theorem 3.3 in Section 5, however, simpler. As in (6.3) we have

$$U_{\mathrm{sc}}^{\varepsilon,n}(-t/\varepsilon)(-i\varepsilon\nabla_k)U_{\mathrm{sc}}^{\varepsilon,n}(t/\varepsilon) = -i\varepsilon\nabla_k + \varepsilon\int_0^{t/\varepsilon} U_{\mathrm{sc}}^{\varepsilon,n}(-s)\big[-i\nabla_k, H_{\mathrm{sc}}^{\varepsilon,n}\big]U_{\mathrm{sc}}^{\varepsilon,n}(s)\,ds$$

and

$$\begin{aligned} &U^{\varepsilon,n}(-t/\varepsilon)(-i\varepsilon\nabla_k)U^{\varepsilon,n}(t/\varepsilon) = \\ &= -i\varepsilon\nabla_k + \varepsilon\int_0^{t/\varepsilon} U^{\varepsilon,n}(-s)\big[-i\nabla_k, H^{\varepsilon,n}\big]U^{\varepsilon,n}(s)\,ds \\ &= -i\varepsilon\nabla_k + \varepsilon\int_0^{t/\varepsilon} U^{\varepsilon,n}(-s)\Big(\big[-i\nabla_k, H_{\mathrm{sc}}^{\varepsilon,n}\big] + \big[-i\nabla_k, \Delta\tilde{W}^{\varepsilon,n}\big]\Big)U^{\varepsilon,n}(s)\,ds\,, \end{aligned}$$

where $\Delta\tilde{W}^{\varepsilon,n} := \tilde{W}^{\varepsilon,n} - \tilde{W}_{\mathrm{sc}}^{\varepsilon,n}$. Now $[-i\nabla_k, H_{\mathrm{sc}}^{\varepsilon,n}] = -i\nabla_k E_n(k)$ is bounded, and (7.8) follows from Corollary 7.2 if we can show that $[-i\nabla_k, \Delta\tilde{W}^{\varepsilon,n}] = o(1)$ in $B(L^2(M^*))$. Noting that $(\Delta\tilde{W}^{\varepsilon,n}\psi)(k)$ is given by (7.3), this can be shown by an argument similar to the one in Lemma 7.1.

□

8. Semiclassical equations of motion for general observables

We proceed to more general semiclassical observables. First note that Theorem 3.4 follows immediately from the results obtained so far (Theorem 3.2, Corollary 7.2 and (7.7)), since multiplication with k in Bloch representation is bounded. Hence we now have that

$$\lim_{\varepsilon\to 0}\|x^\varepsilon(t)\psi - \mathcal{U}^{-1}R(t)\mathcal{U}\psi\| = 0 \tag{8.1}$$

for all $\psi \in \mathrm{Ran}P_{\mathcal{I}} \cap D(|x|) \cap H^2$ and that

$$\lim_{\varepsilon\to 0}\|k^\varepsilon(t)\psi - \mathcal{U}^{-1}K(t)\mathcal{U}\psi\| = 0 \tag{8.2}$$

for all $\psi \in \mathrm{Ran} P_{\mathcal{I}}$. We next consider bounded continuous functions of $x^\varepsilon(t)$ and $k^\varepsilon(t)$:

Lemma 8.1. *Let $f \in C_\infty(\mathbb{R}^d)$ and $g \in C(M^*)$. Then for all $\psi \in \mathrm{Ran} P_{\mathcal{I}}$ we have*

$$\lim_{\varepsilon\to 0} \| \big(f(x^\varepsilon(t)) - \mathcal{U}^{-1} f(R(t)) \mathcal{U}\big)\,\psi\| = 0 \tag{8.3}$$

and

$$\lim_{\varepsilon\to 0} \| \big(g(k^\varepsilon(t)) - \mathcal{U}^{-1} g(K(t)) \mathcal{U}\big)\,\psi\| = 0\,. \tag{8.4}$$

Proof. We will sketch the proof for $x^\varepsilon(t)$. First note that $\bar{R}(t) := \mathcal{U}^{-1} R(t) \mathcal{U}$ is a bounded self-adjoint operator and commutes with $P_{\mathcal{I}}$. Hence the sets $D_\pm := (\bar{R}(t) \pm i)(\mathrm{Ran} P_{\mathcal{I}} \cap D(|x|) \cap H^2)$ are dense in $P_{\mathcal{I}}$ (Since R and x^ε are vectors of operators in $\mathbb{R}^d$, note that this and the following statements hold component wise). For $\psi \in D_\pm$ we have

$$\left[(x^\varepsilon(t) \pm i)^{-1} - (\bar{R}(t) \pm i)^{-1}\right] \psi = (x^\varepsilon(t) \pm i)^{-1} (\bar{R}(t) - x^\varepsilon(t)) \varphi \tag{8.5}$$

for $\varphi = (\bar{R}(t) \pm i)^{-1} \psi \in \mathrm{Ran} P_{\mathcal{I}} \cap D(|x|) \cap H^2$. Thus, by Theorem 3.2, (8.5) strongly approaches zero as $\varepsilon \to 0$ and, since $D_\pm$ are dense in $P_{\mathcal{I}}$, $(x^\varepsilon(t) \pm i)^{-1}$ strongly approach $(\bar{R}(t) \pm i)^{-1}$ on $P_{\mathcal{I}}$.

Using the fact that polynomials in $(x_j \pm i)^{-1}$, $j = 1, \ldots, d$, are dense in $C_\infty(\mathbb{R}^d)$ one concludes that the convergence $x^\varepsilon(t) \to \bar{R}(t)$ on $\mathrm{Ran} P_{\mathcal{I}}$ in the "strong resolvent sense" implies

$$\lim_{\varepsilon\to 0} \| \big(f(x^\varepsilon(t)) - f(\bar{R}(t))\big)\,\psi\| = 0$$

for all $f \in C_\infty(\mathbb{R}^d)$ and $\psi \in \mathrm{Ran} P_{\mathcal{I}}$ (cf. Theorem VIII.20 in [20]). However, by the functional calculus for self-adjoint operators we have $f(\mathcal{U}^{-1} R(t) \mathcal{U}) = \mathcal{U}^{-1} f(R(t)) \mathcal{U}$ and (8.3) follows.

Clearly (8.4) follows analogously. □

Proof of Theorem 3.5. Let $a \in \mathcal{O}(0)$. Referring again to the general Stone-Weierstraß theorem we can uniformly approximate $a(x,\xi)$ by a sum of products, i.e. $a(x,\xi) = \sum_{i=0}^\infty a_i f_i(x) g_i(\xi)$ with $f_i \in C_\infty(\mathbb{R}^d)$, $g_i \in C(M^*)$, $\sum |a_i| < \infty$ and $\sup_{i\in\mathbb{N}, x\in\mathbb{R}^d, \xi\in M^*} |f_i(x) g_i(\xi)| < \infty$. Hence in order to prove Theorem 3.5 we are left to show that for arbitrary $f \in C_\infty(\mathbb{R}^d)$ and $g \in C(M^*)$ we have

$$\big(f(x) g(\xi)\big)^{W,\varepsilon}(t) \to \mathcal{U}^{-1} f(R(t)) g(K(t)) \mathcal{U} \tag{8.6}$$

strongly on $\mathrm{Ran} P_{\mathcal{I}}$. To see this recall the so called product rule for quantum observables (cf. [22]). It states, in particular, that for two symbols $A, B \in \mathcal{O}(0)$

$$\lim_{\varepsilon\to 0} \left\| \big((AB)^{W,\varepsilon} - A^{W,\varepsilon} B^{W,\varepsilon}\big)\,\psi \right\| = 0\,.$$

Applied to our case this yields

$$\big(f(x) g(\xi)\big)^{W,\varepsilon}(t) \to \big(f(x)^{W,\varepsilon} g(\xi)^{W,\varepsilon}\big)(t) = f(x^\varepsilon(t)) g(k^\varepsilon(t))\,.$$

Finally, since f and g are bounded, Lemma 8.1 implies (8.6) and thus Theorem 3.5. □

9. Band crossings

We proved the semiclassical limit for isolated bands only. In principle, there are two distinct mechanisms of how this assumption could be violated. First of all a band could be isolated but have a constant multiplicity larger than one. This occurs, e.g., for the Dirac equation where because of spin the electron and positron bands are both two-fold degenerate. A systematic study is only recent [9, 24] and leads to a matrix valued symplectic structure for the semiclassical dynamics. For periodic potentials degeneracies are the exception. They form a real analytic subvariety of the Bloch variety $B = \{(k,\lambda) \in \mathbb{R}^d \times \mathbb{R} \mid \exists f \in L^2(M) : H_{\mathrm{per}}(k)f = \lambda f\}$ and have a dimension at least one less than the dimension of B [17, 25]. Thus points of band crossings have a k-Lebesgue measure zero. From the study of band structures in solids one knows that band crossings indeed occur. Thus it is of interest to understand the extra complications coming from band crossings.

There are two types of band crossings. The first one is removable through a proper analytic continuation of the bands. In a way, removable band crossings correspond to a wrong choice of the fundamental domain. E.g. for $V = 0$ we may artificially introduce a lattice Γ. The bands touch then at the boundary of M^*. Upon analytic continuation we recover the single band $E_1(k) = k^2/2$ with $M^* = \mathbb{R}^d$. In one dimension all band crossings can be removed [21]. Thus, with the adjustment discussed, our result fully covers the case $d = 1$. For $d \geq 2$ generically band crossings cannot be removed.

It is then of great physical interest to understand how a wave packet tunnels into a neighboring band through points of degeneracy (or almost degeneracy). For a careful asymptotic analysis in particular model systems we refer to the monumental work of G. Hagedorn [13]. Gerard [11] considers a model system with two bands in two dimensions, i.e., the role of $-\frac{1}{2}\Delta + V$ is taken by $\begin{pmatrix} k_1 & k_2 \\ k_2 & -k_1 \end{pmatrix}$. He investigates the semiclassical limit and proves that the particle may tunnel to the other band with a probability which depends on how well the initial wave packet is concentrated near a semiclassical orbit hitting the singularity.

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