Semiclassical wave packet dynamics in Schrodinger equations with periodic potentials

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Abstract. We consider semiclassically scaled Schrödinger equations with an external potential and a highly oscillatory periodic potential. We construct asymptotic solutions in the form of semiclassical wave packets. These solutions are concentrated (both, in space and in frequency) around the effective semiclassical phase-space flow obtained by Peierl's substitution, and involve a slowly varying envelope whose dynamics is governed by a homogenized Schrödinger equation with time-dependent effective mass. The corresponding adiabatic decoupling of the slow and fast degrees of freedom is shown to be valid up to Ehrenfest time scales.

1. Introduction

1.1. **General setting.** We consider the following semiclassically scaled Schrödinger equation:

$$\left\{\begin{array}{c} i\varepsilon\partial_t\psi^\varepsilon + \dfrac{\varepsilon^2}{2}\Delta\psi^\varepsilon = V_\Gamma\left(\dfrac{x}{\varepsilon}\right)\psi^\varepsilon + V(x)\psi^\varepsilon,\ (t,x)\in\mathbb{R}\times\mathbb{R}^d,\\ \psi^\varepsilon_{|t=0} = \psi^\varepsilon_0, \end{array}\right. \tag{1.1}$$

with $d\geqslant 1$, the spatial dimension, and $\psi^\varepsilon = \psi^\varepsilon(t,x)\in\mathbb{C}$. Here, we already have rescaled all physical parameters such that only one semiclassical parameter $\varepsilon>0$ (i.e. the scaled Planck's constant) remains. In the following we shall be interested in the asymptotic description of $\psi^\varepsilon(t,x)$ for $\varepsilon\ll 1$. To this end, the potential $V_\Gamma(y)\in\mathbb{R}$ is assumed to be smooth and *periodic* with respect to some *regular lattice* $\Gamma\simeq\mathbb{Z}^d$, generated by a given basis $\{\eta_1,\ldots,\eta_d\}$, $\eta_\ell\in\mathbb{R}^d$, i.e.

$$V_\Gamma(y+\gamma) = V_\Gamma(y),\quad \forall\, y\in\mathbb{R}^d, \gamma\in\Gamma \tag{1.2}$$

where

$$\Gamma\equiv\Big\{\gamma=\sum_{\ell=1}^d \gamma_\ell\eta_\ell\in\mathbb{R}^d:\ \gamma_\ell\in\mathbb{Z}\Big\}.$$

In addition, the slowly-varying potential $V(x)$ is assumed to satisfy the following:

Assumption 1.1. *The potential V is smooth, real-valued, with at most quadratic growth at infinity, i.e.*

$$V\in C^\infty(\mathbb{R}^d;\mathbb{R})\quad \textit{and}\quad \partial^\gamma V\in L^\infty\left(\mathbb{R}^d\right),\quad \forall|\gamma|\geqslant 2.$$

Equation 1.1 describes the dynamics of quantum particles in a periodic lattice-potential V_Γ under the influence of an external, *slowly varying* driving force $F=-\nabla V(x)$. A typical application arises in solid state physics where (1.1) describes the time-evolution of electrons moving in a crystalline lattice (generated by the ionic cores). The asymptotics of (1.1) as $\varepsilon\to 0_+$ is a natural two-scale problem which is

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well-studied in the physics and mathematics literature. Early mathematical results are based on time-dependent WKB type expansions [3, 14, 33] (see also [6] for a more recent application in the nonlinear case), which, however, suffer from the appearance of caustics and are thus only valid for small times. In order to overcome this problem, other methods based on, e.g., Gaussian beams [9], Wigner measures [12, 13], or space-adiabatic perturbation theory [21, 35] have been developed. These approaches yield an asymptotic description for time-scales of order $\mathcal{O}(1)$.

On the other hand, it is well known that in the case *without periodic potential*, semiclassical approximations which are valid up to *Ehrenfest time* $t \sim \mathcal{O}(\ln 1/\varepsilon)$ can be constructed. These approximations are based on propagating *semiclassical wave packets*, or coherent states, i.e. approximate solutions which are sufficiently concentrated *in space and in frequency* around the classical Hamiltonian phase-space flow

$$\begin{cases} \dot q(t) = p(t), \quad q(0) = q_0, \\ \dot p(t) = -\nabla_x V\left(q(t)\right), \quad p(0) = p_0. \end{cases} \tag{1.3}$$

The basic idea for this type of asymptotic method can be found in the classical works of [15, 26] (see also [4, 28] for a broader introduction). It has been developed further in, e.g., [7, 8, 17, 30, 31, 34] and in addition also proved to be applicable in the case of weakly nonlinear Schrödinger equations [5]. Interestingly enough, though, it seems that so far it has not been extended to include also highly oscillatory periodic potentials $V_\Gamma\left(\frac{x}{\varepsilon}\right)$, and it will be the main task of this work to do so.

To this end, it will be necessary to understand the influence of $V_\Gamma\left(\frac{x}{\varepsilon}\right)$ on the dispersive properties of the solution $\psi^\varepsilon(t,x)$. In particular, having in mind the results quoted above, one expects that in this case the usual kinetic energy of a particle $E = \frac{1}{2}|k|^2$ has to be replaced by $E_m(k)$, i.e. the energy of the m-th Bloch band associated to V_Γ. In physics this is known under the name *Peierl's substitution*. We shall show that under the additional influence of a slowly varying potential $V(x)$, this procedure is in fact asymptotically correct (i.e. for $\varepsilon \ll 1$) up to Ehrenfest time, provided the initial data ψ_0^ε is sufficiently concentrated around $(q_0, p_0) \in \mathbb{R}^{2d}$.

Remark 1.2. Indeed, we could also allow for time-dependent external potentials $V(t,x) \in \mathbb{R}$ measurable in time, smooth in x, and satisfying

$$\partial_x^\gamma V \in L^\infty\left(\mathbb{R}_t \times \mathbb{R}^d_x\right), \quad \forall |\gamma| \geqslant 2.$$

Under this assumptions, it is straightforward to adapt the analysis given below. For the sake of notation, we shall not do so here, but rather leave the details to the reader.

1.2. **Bloch and semiclassical wave packets.** In order to state our result more precisely, we first recall some well-known results on the spectral theory for periodic Schrödinger operators, cf. [29, 36]:

$$H_{\rm per} := -\frac{1}{2}\Delta_y + V_\Gamma(y).$$

Denote by $Y \subset \Gamma$ the (centered) fundamental domain of the lattice Γ and by $Y^* \simeq \mathbb{T}^d$ the fundamental domain of the corresponding dual lattice (equipped with periodic boundary conditions). The latter is usually referred to as *the Brillouin zone*. Bloch–Floquet theory asserts that $H_{\rm per}$ admits a fiber-decomposition

$$H_{\rm per} = \frac{1}{|Y^*|}\int_{Y^*} H_\Gamma(k)\, dk,$$

where for $k \in Y^*$, we denote

$$H_\Gamma(k) = \frac{1}{2}\left(-i\nabla_y + k\right)^2 + V_\Gamma(y).$$

It therefore suffices to consider the following spectral problem on Y:

$$H_\Gamma(k)\chi_m(\cdot,k) = E_m(k)\chi_m(\cdot,k), \quad k \in Y^*,\ m \in \mathbb{N}, \tag{1.4}$$

where $E_m(k) \in \mathbb{R}$ and $\chi_m(y,k)$, respectively, denote the m-th eigenvalue/eigenvector pair of $H_\Gamma(k)$, parametrized by $k \in Y^*$, the so-called *crystal momentum.* These eigenvalues can be ordered increasingly, such that

$$E_1(k) \leqslant \ldots \leqslant E_m(k) \leqslant E_{m+1}(k) \leqslant \ldots,$$

where each eigenvalue is repeated according to its multiplicity (which is known to be finite). This implies that

$$\operatorname{spec} H_{\mathrm{per}} = \bigcup_{m\in\mathbb{N}} \{E_m(k)\ ;\ k \in Y^*\} \subset \mathbb{R},$$

where $\{E_m(k);\ k \in Y^*\}$ is called the m-th *energy band* (or Bloch band). The associated eigenfunctions $\chi_m(y,k)$ form, for every fixed $k \in Y^*$, a complete orthonormal basis in $L^2(Y)$.

Next, we consider for some $m \in \mathbb{N}$ the corresponding *semi-classical band Hamiltonian*, obtained by Peierl's substitution, i.e.

$$h_m^{\mathrm{sc}}(k,x) = E_m(k) + V(x), \quad (k,x) \in Y^* \times \mathbb{R}^d,$$

and denote the semiclassical phase space trajectories associated to h_m^{sc} by

$$\begin{cases} \dot{q}(t) = \nabla_k E_m\left(p(t)\right), & q(0) = q_0, \\ \dot{p}(t) = -\nabla_x V\left(q(t)\right), & p(0) = p_0. \end{cases} \tag{1.5}$$

This system is the analog of (1.3) in the presence of an additional periodic potential.

Example 1.3 (No external potential)**.** In the case $V(x) = 0$, we simply have

$$p(t) = p_0, \quad q(t) = q_0 + t\nabla_k E_m(p_0), \tag{1.6}$$

that is, a shift with constant speed $\omega = \nabla E_m(p_0)$.

In order to make sure that the system (1.5) is well-defined, we shall from now on impose the following condition on $E_m(k)$.

Assumption 1.4. *We assume that $E_m(p(t))$ is a simple eigenvalue, uniformly for all $t \in \mathbb{R}$, i.e. there exists a $\delta > 0$, such that*

$$|E_m(p(t)) - E_n(k)| \geqslant \delta, \quad \forall n \neq m, t \in \mathbb{R}, k \in Y^*.$$

It is known that if $E_m(k)$ is simple, it is infinitely differentiable and thus the right hand side of (1.5) is well defined. In addition, we also have that $(y,t) \mapsto \chi_m(y,p(t))$ is smooth and bounded together with all its derivatives.

Example 1.5. By compactness of Y^*, Assumption 1.4 is satisfied in either of the following two cases:

(i) If $E_m(k)$ is a simple eigenvalue for all $k \in Y^*$. In particular, in $d = 1$ it is known that every $E_m(k)$ is simple, except possibly at $k = 0$ or at the edge of the Brillouin zone.
(ii) If $V(x) = 0$ and $E_m(k)$ is simple in a neighborhood of $k = p_0$ (which is sufficient in view of Example 1.3).

1.3. **Main result.** With the above definitions at hand, we are now able to state our main mathematical result. To this end, we first define a *semiclassical wave packet* in the m-th Bloch band (satisfying Assumption 1.4) by

$$\varphi^\varepsilon(t,x) = \varepsilon^{-d/4} u\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}\right) \chi_m\left(\frac{x}{\varepsilon}, p(t)\right) e^{i\phi_m(t,x)/\varepsilon} \tag{1.7}$$

with $q(t), p(t)$ given by system (1.5) and $u(t,z) \in \mathbb{C}$, a smooth slowly varying envelope which will determined by an envelope equation yet to be derived (see below). In addition, the ε-oscillatory phase is

$$\phi_m(t,x) = S_m(t) + p(t)\cdot(x-q(t)), \tag{1.8}$$

where $S_m(t) \in \mathbb{R}$ is the (purely time-dependent) semi-classical action

$$S_m(t) = \int_0^t L_m(p(s),q(s))\, ds, \tag{1.9}$$

with L_m denoting the Lagrangian associated to the effective Hamiltonian $h_m^{\rm sc}$, i.e.

$$\begin{aligned} L_m(p(s),q(s)) &= p(s)\cdot\dot q(s) - h_m^{\rm sc}\left(p(s),q(s)\right) \\ &= p(s)\cdot\nabla E_m(p(s)) - h_m^{\rm sc}\left(p(s),q(s)\right), \end{aligned} \tag{1.10}$$

in view of (1.5).

Remark 1.6. Note that this is nothing but the Legendre transform of the effective Hamiltonian $h_m^{\rm sc}$. As in classical mechanics, one associates to a given Hamiltonian $H(p,q)$ a Lagrangian via $L(p,q) = p\cdot\dot q - H(p,q)$.

The function φ^ε given by (1.7) generalizes the usual class of semiclassical wave packets considered in e.g. [15, 26]. Note that in contrast to two-scale WKB approximation considered in [3, 14, 33], it involves a scale of the order $1/\sqrt{\varepsilon}$, i.e. the scale of concentration of the amplitude u. Nevertheless, in comparison to the highly oscillatory Bloch function χ_m, the amplitude is still slowly varying and thus we can expect an adiabatic decoupling between the slow and fast scales to hold on (long) macroscopic time-scales. Indeed, we shall prove the following result:

Theorem 1.7. *Let the Assumptions 1.1, 1.4 hold and let the initial data be given by*

$$\psi_0^\varepsilon(x) = \varepsilon^{-d/4} u_0\left(\frac{x-q_0}{\sqrt{\varepsilon}}\right) \chi_m\left(\frac{x}{\varepsilon}, p_0\right) e^{ip_0\cdot(x-q_0)/\varepsilon},$$

with $q_0, p_0 \in \mathbb{R}^d$ and some given profile $u_0 \in \mathcal{S}(\mathbb{R}^d)$. Then there exists $C>0$ such that the solution of (1.1) *can be approximated by*

$$\|\psi^\varepsilon(t) - \varphi^\varepsilon(t)\|_{L^2(\mathbb{R}^d)} \leqslant C\sqrt{\varepsilon} e^{Ct},$$

where φ^ε is given by (1.7) *and $u \in C(\mathbb{R};\mathcal{S}(\mathbb{R}^d))$ solves the following homogenized Schrödinger equation*

$$i\partial_t u + \frac{1}{2}\mathrm{div}_z\left(\nabla_k^2 E_m\left(p(t)\right)\cdot\nabla_z\right) u = \frac{1}{2}\left\langle z, \nabla_x^2 V\left(q(t)\right) z\right\rangle u, \quad u(0,z) = u_0(z),$$

where ∇^2 denotes the Hessian matrix. In particular there exist $C_0>0$ so that

$$\sup_{0\leqslant t\leqslant C_0 \ln\frac{1}{\varepsilon}} \|\psi^\varepsilon(t) - \varphi^\varepsilon(t)\|_{L^2(\mathbb{R}^d)} \underset{\varepsilon\to 0}{\longrightarrow} 0.$$

This theorem provides an approximate description of the solution to (1.1) up to Ehrenfest time and can be seen as the analog of the results given in [15, 26, 7, 8, 17, 30, 31, 34] where the case of slowly varying potentials $V(x)$ is considered. Note that in contrast to the closely related method of Gaussian beams presented in, e.g., [9], we do not need to include complex-valued phases and in addition, obtain an approximation valid for longer times. Indeed, in the special case where the

initial envelope u_0 is a Gaussian, then its evolution u remains Gaussian, and can be completely characterized; see §4.3.

The homogenized Schrödinger equation given above, features a rather unusual dispersive behavior described by a time-dependent effective mass tensor $M(t) = \nabla_k^2 E_m(p(t))$, i.e. the Hessian of $E_m(k)$ evaluated at $k = p(t)$. To our knowledge, Theorem 1.7 is the first result in which a Schrödinger type equation with *time-dependent* effective mass has been rigorously derived (see also the discussion in Remark 3.1).

Remark 1.8. Let us also mention that the same class of initial data has been considered in [1] for a Schrödinger equation with *locally* periodic potential $V_\Gamma(x, y)$ and corresponding x-dependent Bloch bands $E_m(k; x)$. In this work, the authors derive a homogenized Schrödinger equation, provided that ψ_0^ε is concentrated around a *stationary point* point x_0, p_0 of the semiclassical phase space flow, i.e.

$$\nabla_k E_m(p_0; q_0) = \nabla_x E_m(p_0; q_0) = 0.$$

This implies $q(t) = q_0$ and $p(t) = p_0$, for all $t \in \mathbb{R}$, which the authors interpret as a localization phenomena. Clearly, this is a rather particular situation, which is also included in our result under the condition $V(x) = 0$ and $\nabla_k E_m(k) = 0$ (see Example 1.3).

This work is now organized as follows: In the next section, we shall formally derive an approximate solution to (1.1) by means of a (formal) multi-scale expansion. This expansion yields a system of three linear equations, which we shall solve in Section 3. In particular, we shall obtain from it the homogenized Schrödinger equation. The corresponding Cauchy problem is then analyzed in Section 4, where we also include a brief discussion on the particularly important case of Gaussian profiles (yielding a direct connection to [15]). A rigorous stability result for our approximation, up to Ehrenfest time, is then given in Section 5.

Remark 1.9. We expect that our results can be generalized to the case of (weakly) nonlinear Schrödinger equations (already considered in [5, 6]). This will be the aim of a future work.

2. Formal derivation of an approximate solution

2.1. **Reduction through exact computations.** We seek the solution ψ^ε of (1.1) in the following form

$$\psi^\varepsilon(t, x) = \varepsilon^{-d/4} \mathcal{U}^\varepsilon\left(t, \frac{x - q(t)}{\sqrt{\varepsilon}}, \frac{x}{\varepsilon}\right) e^{i\phi_m(t,x)/\varepsilon}, \tag{2.1}$$

where the phase $\phi(t, x)$ is given by (1.8), the function $\mathcal{U}^\varepsilon = \mathcal{U}^\varepsilon(t, z, y)$ is assumed to be smooth, Γ-periodic with respect to y, and admits an asymptotic expansion

$$\mathcal{U}^\varepsilon(t, z, y) \underset{\varepsilon\to 0}{\sim} \sum_{j\geqslant 0} \varepsilon^{j/2} U_j(t, z, y). \tag{2.2}$$

Note that due to the inclusion of the factor $\varepsilon^{-d/4}$ the $L^2(\mathbb{R}^d)$ norm of the right hand side of (2.1) is in fact uniformly bounded with respect to ε, whereas the $L^\infty(\mathbb{R}^d)$ norm in general will grow as $\varepsilon \to 0$. The asymptotic expansion 2.2 therefore has to be understood in the L^2 sense.

Taking into account that in view of (1.8), $\nabla_x \phi_m(t, x) = p(t)$, we compute:

$$\begin{aligned}
\varepsilon^{d/4} e^{-i\phi_m/\varepsilon} i\varepsilon \partial_t \psi^\varepsilon &= i\varepsilon \partial_t \mathcal{U}^\varepsilon - i\sqrt{\varepsilon}\dot{q} \cdot \nabla_z \mathcal{U}^\varepsilon - \partial_t \phi_m \mathcal{U}^\varepsilon, \\
\varepsilon^{d/4} e^{-i\phi_m/\varepsilon} \varepsilon^2 \Delta \psi^\varepsilon &= \varepsilon \Delta_z \mathcal{U}^\varepsilon + \Delta_y \mathcal{U}^\varepsilon + 2\sqrt{\varepsilon}\,(\nabla_y \cdot \nabla_z)\,\mathcal{U}^\varepsilon - |p|^2 \mathcal{U}^\varepsilon \\
&\qquad + 2i\sqrt{\varepsilon} p \cdot \nabla_z \mathcal{U}^\varepsilon + 2ip \cdot \nabla_y \mathcal{U}^\varepsilon,
\end{aligned}$$

where in all of the above expressions, the various functions have to be understood to be evaluated as follows:

$$\psi^\varepsilon = \psi^\varepsilon(t,x) \quad ; \quad \mathcal{U}^\varepsilon = \mathcal{U}^\varepsilon\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}, \frac{x}{\varepsilon}\right).$$

Thus, ordering equal powers of ε in equation (1.8) we find that

$$\varepsilon^{d/4} e^{-i\phi_m/\varepsilon}\left(i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon - V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon - V(x)\psi^\varepsilon\right) = b_0^\varepsilon + \sqrt{\varepsilon}b_1^\varepsilon + \varepsilon b_2^\varepsilon,$$

with

$$\begin{aligned}
b_0^\varepsilon &= -\partial_t\phi_m\mathcal{U}^\varepsilon + \frac{1}{2}\Delta_y\mathcal{U}^\varepsilon - \frac{1}{2}|p|^2\mathcal{U}^\varepsilon + ip\cdot\nabla_y\mathcal{U}^\varepsilon - V_\Gamma(y)\mathcal{U}^\varepsilon - V(q)\mathcal{U}^\varepsilon,\\
b_1^\varepsilon &= -i\dot{q}\cdot\nabla_z\mathcal{U}^\varepsilon + (\nabla_y\cdot\nabla_z)\,\mathcal{U}^\varepsilon + ip\cdot\nabla_z\mathcal{U}^\varepsilon,\\
b_2^\varepsilon &= i\partial_t\mathcal{U}^\varepsilon + \frac{1}{2}\Delta_z\mathcal{U}^\varepsilon.
\end{aligned}$$

So far, we have neither used the fact that $q(t)$, $p(t)$ are given by the Hamiltonian flow (1.5), nor the explicit dependence of ϕ_m on time. Using these properties, allows us to rewrite $b_0^\varepsilon, b_1^\varepsilon, b_2^\varepsilon$ as follows:

$$\begin{aligned}
b_0^\varepsilon &= \left(h_m^{\mathrm{sc}}(p(t),q(t)) + \nabla V\left(q(t)\right)\cdot(x-q(t))\right)\mathcal{U}^\varepsilon - H_\Gamma\left(p(t)\right)\mathcal{U}^\varepsilon - V(q(t))\mathcal{U}^\varepsilon,\\
b_1^\varepsilon &= i\left(p(t) - \nabla_k E_m\left(p(t)\right)\right)\cdot\nabla_z\mathcal{U}^\varepsilon + (\nabla_y\cdot\nabla_z)\,\mathcal{U}^\varepsilon,\\
b_2^\varepsilon &= i\partial_t\mathcal{U}^\varepsilon + \frac{1}{2}\Delta_z\mathcal{U}^\varepsilon.
\end{aligned}$$

Now, recall that in the above lines, $\mathcal{U}^\varepsilon$ is evaluated at the shifted spatial variable $z = (x-q(t))/\sqrt{\varepsilon}$. Taking this into account, we notice that the above hierarchy has to be modified, and we find:

$$\begin{aligned}
b_0^\varepsilon &= h_m^{\mathrm{sc}}(p(t),q(t))\mathcal{U}^\varepsilon - H_\Gamma\left(p(t)\right)\mathcal{U}^\varepsilon - V\left(q(t)+z\sqrt{\varepsilon}\right)\mathcal{U}^\varepsilon,\\
b_1^\varepsilon &= i\left(p(t) - \nabla_k E_m\left(p(t)\right)\right)\cdot\nabla_z\mathcal{U}^\varepsilon + (\nabla_y\cdot\nabla_z)\,\mathcal{U}^\varepsilon + \left(\nabla V\left(q(t)\right)\cdot z\right)\mathcal{U}^\varepsilon,\\
b_2^\varepsilon &= i\partial_t\mathcal{U}^\varepsilon + \frac{1}{2}\Delta_z\mathcal{U}^\varepsilon.
\end{aligned}$$

Next, we perform a Taylor expansion of V around the point $q(t)$:

$$V\left(q(t)+z\sqrt{\varepsilon}\right) = V\left(q(t)\right) + \sqrt{\varepsilon}\nabla V\left(q(t)\right)\cdot z + \frac{\varepsilon}{2}\left\langle z, \nabla^2 V\left(q(t)\right) z\right\rangle + \mathcal{O}\left(\varepsilon^{3/2}\left\langle z\right\rangle^3\right),$$

since V is at most quadratic in view of Assumption 1.1. Recalling that $h_m^{\mathrm{sc}}(p,q) = E_m(p) + V(q)$, the terms involving $V(q)$ cancel out in b_0^ε, the terms involving $\nabla V(q)$ cancel out in b_1^ε, and thus, we finally obtain:

Lemma 2.1. *Let the Assumptions 1.1, 1.4 hold and ψ^ε be related to $\mathcal{U}^\varepsilon$ through* (2.1)*. Then it holds*

$$\begin{aligned}
i\varepsilon\partial_t\psi^\varepsilon + \frac{\varepsilon^2}{2}\Delta\psi^\varepsilon - V_\Gamma\left(\frac{x}{\varepsilon}\right)\psi^\varepsilon - V(x)\psi^\varepsilon = \\
\frac{e^{i\phi_m/\varepsilon}}{\varepsilon^{d/4}}\left(b_0^\varepsilon + \sqrt{\varepsilon}b_1^\varepsilon + \varepsilon b_2^\varepsilon + \varepsilon^{3/2}r^\varepsilon\right)(t,z,y)\Big|_{(z,y)=\left(\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right)},
\end{aligned}$$

with

$$\begin{aligned}
b_0^\varepsilon &= \left(E_m\left(p(t)\right) - H_\Gamma\left(p(t)\right)\right)\mathcal{U}^\varepsilon,\\
b_1^\varepsilon &= i\left(p(t) - \nabla_k E_m\left(p(t)\right)\right)\cdot\nabla_z\mathcal{U}^\varepsilon + (\nabla_y\cdot\nabla_z)\,\mathcal{U}^\varepsilon,\\
b_2^\varepsilon &= i\partial_t\mathcal{U}^\varepsilon + \frac{1}{2}\Delta_z\mathcal{U}^\varepsilon - \frac{1}{2}\left\langle z, \nabla^2 V\left(q(t)\right) z\right\rangle\mathcal{U}^\varepsilon,
\end{aligned}$$

and a remainder $r^\varepsilon(t,z,y)$ *satisfying*

$$|r^\varepsilon(t,z,y)| \leqslant C\,\langle z\rangle^3\,|\mathcal{U}^\varepsilon(t,z,y)|, \quad \forall (t,z,y)\in\mathbb{R}\times\mathbb{R}^d\times Y,$$

where the constant $C>0$ *is independent of* t,z,y *and* ε.

2.2. **Introducing the approximate solution.** We now expand $\mathcal{U}^\varepsilon$ in powers of ε, according to (2.2). To this end, we introduce the following (time-dependent) linear operators

$$\begin{aligned} L_0 &= E_m\left(p(t)\right) - H_\Gamma\left(p(t)\right),\\ L_1 &= i\left(p(t) - \nabla_k E_m\left(p(t)\right)\right)\cdot\nabla_z + \nabla_y\cdot\nabla_z,\\ L_2 &= i\partial_t + \frac{1}{2}\Delta_z - \frac{1}{2}\left\langle z, \nabla^2 V\left(q(t)\right) z\right\rangle. \end{aligned}$$

In order to solve (1.1) up to a sufficiently small error term (in L^2), we need to cancel the first three terms in our asymptotic expansion. This yields, the following system of equations

$$\left\{\begin{array}{l} L_0U_0 = 0,\\ L_0U_1 + L_1U_0 = 0,\\ L_0U_2 + L_1U_1 + L_2U_0 = 0. \end{array}\right. \tag{2.3}$$

Assuming for the moment that we can do so, this means that we (formally) solve (1.1) up to errors of order $\varepsilon^{3/2}$ (in L^2), which is expected to generate a small perturbation of the exact solution (in view of the ε in front of the time derivative of ψ^ε in (1.1)).

We consequently define the approximate solution

$$\psi^\varepsilon_{\rm app}(t,x) := \varepsilon^{-d/4}\left(U_0 + \sqrt{\varepsilon}U_1 + \varepsilon U_2\right)\left(t, \frac{x-q(t)}{\sqrt{\varepsilon}}, \frac{x}{\varepsilon}\right) e^{i\phi_m(t,x)/\varepsilon}. \tag{2.4}$$

In view of Lemma 2.1, we thus have the following result (provided we can solve the system (2.3) in a unique way):

Lemma 2.2. *Let* $\psi^\varepsilon_{\rm app}$ *given by* (2.4)*, where* U_0,U_1,U_2 *solve* (2.3)*. Then*

$$\left(i\varepsilon\partial_t + \frac{\varepsilon^2}{2}\Delta - V_\Gamma - V\right)\psi^\varepsilon_{\rm app} = \frac{e^{i\phi_m/\varepsilon}}{\varepsilon^{d/4}}\varepsilon^{3/2}\left(r^\varepsilon + r_1^\varepsilon + r_2^\varepsilon\right)(t,z,y)\Big|_{(z,y)=\left(\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right)},$$

where the remainder terms $r_1^\varepsilon, r_2^\varepsilon$ *are given by*

$$r_1^\varepsilon(t,z,y) = L_2U_1(t,z,y), \quad r_2^\varepsilon(t,z,y) = L_1U_2(t,z,y),$$

and r^ε *satisfies*

$$|r^\varepsilon(t,z,y)| \leqslant C\,\langle z\rangle^3\left|\left(U_0 + \sqrt{\varepsilon}U_1 + \varepsilon U_2\right)(t,z,y)\right|, \quad \forall (t,z,y)\in\mathbb{R}\times\mathbb{R}^d\times Y,$$

where the constant $C>0$ *is independent of* t,z,y *and* ε.

3. Derivation of the homogenized equation

3.1. **Some useful algebraic identities.** Given the form of L_0, the equation $L_0U_0=0$ implies

$$U_0(t,z,y) = u(t,z)\chi_m\left(y,p(t)\right). \tag{3.1}$$

Before studying the other two equations, we shall recall some algebraic formulas related to the eigenvalues and eigenvectors of H_Γ. First, in view of the identity (1.4), we have

$$\nabla_k\left(H_\Gamma - E_m\right)\chi_m + \left(H_\Gamma - E_m\right)\nabla_k\chi_m = 0. \tag{3.2}$$

Taking the scalar product in $L^2(Y)$ with χ_m, we infer

$$\nabla_k E_m = \langle \chi_m, \nabla_k H_\Gamma \chi_m \rangle_{L^2(Y)} + \langle \chi_m, (H_\Gamma - E_m)\, \nabla_k \chi_m \rangle_{L^2(Y)}\,.$$

Since H_Γ is self-adjoint, the last term is zero, thanks to (1.4). We infer

$$\nabla_k E_m(k) = \langle \chi_m, (-i\nabla_y + k)\, \chi_m \rangle_{L^2(Y)}\,. \tag{3.3}$$

Differentiating (3.2) again, we have, for all $j, \ell \in \{1, \ldots, d\}$:

$$\begin{aligned}\partial^2_{k_j k_\ell} (H_\Gamma - E_m)\, \chi_m + \partial_{k_j} (H_\Gamma - E_m)\, \partial_{k_\ell} \chi_m + \partial_{k_\ell} (H_\Gamma - E_m)\, \partial_{k_j} \chi_m \\ + (H_\Gamma - E_m)\, \partial^2_{k_j k_\ell} \chi_m = 0.\end{aligned}$$

Taking the scalar product with χ_m, we have:

$$\begin{aligned}\partial^2_{k_j k_\ell} E_m(k) = \delta_{j\ell} + \left\langle \left(-i\partial_{y_j} + k_j\right) \partial_{k_\ell} \chi_m + (-i\partial_{y_\ell} + k_\ell)\, \partial_{k_j} \chi_m, \chi_m \right\rangle_{L^2(Y)} \\ - \left\langle \partial_{k_\ell} E_m \partial_{k_j} \chi_m + \partial_{k_j} E_m \partial_{k_\ell} \chi_m, \chi_m \right\rangle_{L^2(Y)}\,.\end{aligned} \tag{3.4}$$

3.2. **Higher order solvability conditions.** By Fredholm's alternative, a necessary *and* sufficient condition to solve the equation $L_0 U_1 + L_1 U_0 = 0$, is that $L_1 U_0$ is orthogonal to $\ker L_0$, that is:

$$\langle \chi_m, L_1 U_0 \rangle_{L^2(Y)} = 0. \tag{3.5}$$

Given the expression of L_1 and the formula (3.1), we compute

$$L_1 U_0 = i\,(p(t) - \nabla_k E_m\,(p(t))) \cdot \nabla_z u(t,z) \chi_m\,(y, p(t)) + \nabla_y \chi_m\,(y, p(t)) \cdot \nabla_z u(t,z).$$

In view of (3.3), we infer that (3.5) is automatically fulfilled. We thus obtain

$$U_1(t,z,y) = u_1(t,z) \chi_m\,(y, p(t)) + u_1^\perp(t,z,y),$$

where $u_1^\perp$, the part of U_1 which is orthogonal to $\ker L_0$, is obtained by inverting an elliptic equation:

$$u_1^\perp = -L_0^{-1} L_1 U_0.$$

Note that the formula for $L_1 U_0$ can also be written as

$$L_1 U_0 = -i\nabla_k \left(E_m\,(p(t)) - H_\Gamma\,(p(t))\right) \chi_m\,(y, p(t)) \cdot \nabla_z u(t,z),$$

thus taking into account (3.2), we simply have:

$$u_1^\perp(t,z,y) = -i \nabla_k \chi_m\,(y, p(t)) \cdot \nabla_z u(t,z).$$

At this stage, we shall, for simplicity choose $u_1 = 0$, in which case U_1 becomes simply a function of u:

$$U_1(t,z,y) = -i \nabla_k \chi_m\,(y, p(t)) \cdot \nabla_z u(t,z). \tag{3.6}$$

As a next step in the formal analysis, we must solve

$$L_0 U_2 + L_1 U_1 + L_2 U_0 = 0.$$

By the same argument as before, we require

$$\langle \chi_m, L_1 U_1 + L_2 U_0 \rangle_{L^2(Y)} = 0. \tag{3.7}$$

With the expression (3.6), we compute

$$L_1 U_1 = \sum_{j,\ell=1}^{d} \left(\left(p(t) - \nabla_k E_m\,(p(t))\right)_j \partial_{k_\ell} \chi_m\,(y, p(t)) - i \partial^2_{y_j k_\ell} \chi_m\,(y, p(t)) \right) \partial^2_{z_j z_\ell} u,$$

and we also have

$$\begin{aligned}L_2 U_0 = \left(\left(i\partial_t + \frac{1}{2}\Delta_z - \frac{1}{2} \left\langle z, \nabla^2 V\,(q(t))\, z \right\rangle \right) u \right) \chi_m\,(y, p(t)) \\ + i u\, \dot p(t) \cdot \nabla_k \chi_m\,(y, p(t))\,.\end{aligned}$$

Recalling that $\|\chi_m\|_{L^2(Y)} = 1$, we have $\langle \chi_m, \nabla_k \chi_m \rangle_{L^2(Y)} = 0$, we find:

$$\langle \chi_m, L_1U_1 + L_2U_0 \rangle_{L^2(Y)} = \left(i\partial_t + \frac{1}{2}\Delta_z - \frac{1}{2}\left\langle z, \nabla^2 V\left(q(t)\right) z \right\rangle \right) u \\ - \sum_{j,\ell} \left\langle \chi_m, \partial_{k_j} E_m\left(p(t)\right) \partial_{k_\ell} \chi_m + i\partial^2_{y_j k_\ell} \chi_m \right\rangle_{L^2(Y)} \partial^2_{z_j z_\ell} u$$

By making the last sum symmetric with respect to j and ℓ, and using (3.4), we finally obtain the homogenized Schrödinger equation with time-dependent effective mass:

$$i\partial_t u + \frac{1}{2}\mathrm{div}_z\left(\nabla_k^2 E_m\left(p(t)\right) \cdot \nabla_z\right) u = \frac{1}{2}\left\langle z, \nabla^2 V\left(q(t)\right) z \right\rangle u. \tag{3.8}$$

This is equation models a quantum mechanical time-dependent harmonic oscillator, in which the time dependence is present both in the differential operator, and in the potential.

Remark 3.1. In the case where $V(x) = 0$ and thus $p(t) = p_0$ (in view of Example 1.3), Equation (3.8) simplifies to an equation with a *time-independent* effective mass tensor:

$$i\partial_t u + \frac{1}{2}\mathrm{div}_z\left(\nabla_k^2 E_m\left(p_0\right) \cdot \nabla_z\right) u = 0.$$

This equation has been derived in [2], see also [32, 19, 22] for similar results. Note, however, that in the quoted works the scaling of the original equation (1.1) is different (i.e. not in semiclassical form).

Assuming for the moment that we can solve (3.8), we can write

$$U_2(t,z,y) = u_2(t,z)\chi_m\left(y, p(t)\right) + u_2^\perp(t,z,y),$$

where

$$u_2^\perp = -L_0^{-1}\left(L_1U_1 + L_2U_0\right).$$

Like we did for u_1, we shall from now on also impose $u_2 \equiv 0$ and thus $U_2 = u_2^\perp$. For the upcoming analysis, we define the following class of energy spaces

$$\Sigma^k = \left\{ f \in L^2(\mathbb{R}^d)\ ;\ \|f\|_{\Sigma^k} := \sum_{|\alpha|+|\beta|\leqslant k} \left\| x^\alpha \partial_x^\beta f \right\|_{L^2(\mathbb{R}^d)} < \infty;\ k \in \mathbb{N} \right\}.$$

Proposition 3.2. *Let Assumption 1.4 hold and let $u \in C(\mathbb{R}; \Sigma^k)$ solve (3.8). Set*

$$\begin{aligned} U_0(t,z,y) &= u(t,z)\chi_m\left(y, p(t)\right), \\ U_1(t,z,y) &= -i\nabla_k \chi_m\left(y, p(t)\right) \cdot \nabla_z u(t,z), \\ U_2(t,z,y) &= -L_0^{-1}\left(L_1U_1(t,z,y) + L_2U_0(t,z,y)\right). \end{aligned}$$

Then $U_j \in C(\mathbb{R}; \Sigma_z^{k-j} \times W^{\infty,\infty}(Y))$, for $j = 0,1,2$ and (U_0, U_1, U_2) solves (2.3).

4. The envelope equation

We examine the Cauchy problem for (3.8), with special emphasis on the large time control of u.

4.1. **The general Cauchy problem.** Equation 3.8 can be seen as the quantum mechanical evolutionary problem corresponding to the following time-dependent Hamiltonian,

$$H(t,z,\zeta) = \frac{1}{2}\left\langle \zeta, \nabla_k^2 E_m\left(p(t)\right)\zeta\right\rangle + \frac{1}{2}\left\langle z\nabla^2 V\left(q(t)\right)z\right\rangle. \tag{4.1}$$

Under Assumptions 1.1 and 1.4, this Hamiltonian is self-adjoint, smooth in time, and quadratic in (z,ζ) (in fact, at most quadratic would be sufficient). Using the results from [23], inspired by [10, 11] (see also [24]), we directly infer the following existence result:

Lemma 4.1 (From [23])**.** *For $d \geqslant 1$ and $u_0 \in L^2(\mathbb{R}^d)$, consider the equation*

$$i\partial_t u + \frac{1}{2}\sum_{1\leqslant j,k\leqslant d} a_{jk}(t)\partial_{jk}^2 u = \frac{1}{2}\sum_{1\leqslant j,k\leqslant d} b_{jk}(t)x_j x_k u \quad ; \quad u_{|t=0} = u_0. \tag{4.2}$$

If the coefficients a_{jk} and b_{jk} are continuous and real-valued, such that the matrices $(a_{jk})_{j,k}$ and $(b_{jk})_{j,k}$ are symmetric for all time, then (4.2) has a unique solution $u \in C(\mathbb{R};L^2(\mathbb{R}^d))$. It satisfies

$$\|u(t)\|_{L^2(\mathbb{R}^d)} = \|u_0\|_{L^2(\mathbb{R}^d)}, \quad \forall t\in\mathbb{R}. \tag{4.3}$$

Moreover, if $u_0 \in \Sigma^k$ for some $k\in\mathbb{N}$, then $u\in C(\mathbb{R};\Sigma^k)$.

In particular, if $u_0 \in \Sigma^k$, then (3.8) has a unique solution $u \in C(\mathbb{R};\Sigma^k)$ such that $u_{|t=0} = u_0$.

Remark 4.2. It may happen that the functions a_{jk} are zero on some non-negligible set. In this case, (4.2) ceases to be dispersive. Note that the standard harmonic oscillator is dispersive, *locally in time* only, since it has eigenvalues. We shall see that this is not a problem in our analysis though.

4.2. **Exponential control of the envelope equation.** To prove Theorem 1.7, we need to control the error present in Lemma 2.2 for large time. In general, i.e. without extra geometric assumptions on the wave packet, exponential growth in time must be expected:

Proposition 4.3. *Let $u_0 \in \Sigma^k$, $k\in\mathbb{N}$. Then the solution u to (3.8) satisfies $u\in C(\mathbb{R};\Sigma^k)$, and there exists $C>0$ such that*

$$\|u(t,\cdot)\|_{\Sigma^k} \leqslant Ce^{Ct}, \quad t\geqslant 0.$$

Proof. The result can be established by induction on k. The constant C must actually be expected to depend on k, as shown by the case of

$$i\partial_t u + \frac{1}{2}\Delta_z u = -\frac{|z|^2}{2}u \quad ; \quad u_{|t=0} = u_0.$$

There, the fundamental solution is explicit (generalized Mehler formula, see e.g. [20]), and we check that $\|u(t)\|_{\Sigma^k}$ behaves like e^{kt}.

For $k=0$, the result is obvious, since in view of Lemma 4.1, the L^2-norm is conserved. The case $k=1$ illustrates the general mechanism of the proof, and we shall stick to this case for simplicity. The key remark is that even though the operators z and ∇_z (involved in the definition of Σ^1) do not commute with the Hamiltonian (4.1), the commutators yield a closed system of estimates. First, multiplying (3.8) by z, we find

$$\left(i\partial_t - H\right)zu = -\left[H,z\right]u = \nabla_k^2 E_m\left(p(t)\right)\nabla_z u.$$

The L^2 estimate (4.3) then yields

$$\begin{aligned}\|zu(t)\|_{L^2} &\leqslant \|zu_0\|_{L^2} + \int_0^t \left\|\nabla_k^2 E_m\left(p(s)\right)\nabla_z u(s)\right\|_{L^2} ds \\ &\leqslant \|zu_0\|_{L^2} + C\int_0^t \|\nabla_z u(s)\|_{L^2}\, ds,\end{aligned}$$

for some C independent of t, since $\nabla_k^2 E_m$ is bounded on Y^* which is compact. Similarly,

$$\left(i\partial_t - H\right)\nabla_z u = -\left[H, \nabla_z\right] u = \nabla^2 V\left(q(t)\right) zu,$$

and, in view of Assumption 1.1,

$$\|\nabla_z u(t)\|_{L^2} \leqslant \|\nabla_z u_0\|_{L^2} + C\int_0^t \|zu(s)\|_{L^2}\, ds.$$

Summing over the two inequalities and using the conservation of mass, we infer

$$\|u(t)\|_{\Sigma^1} \leqslant \|u_0\|_{\Sigma^1} + C\int_0^t \|u(s)\|_{\Sigma^1}\, ds,$$

and Gronwall's lemma yields the proposition in the case $k = 1$. By induction, applying (z, ∇_z) to (3.8) k times, the defects of commutation always yield the same sort of estimate, and the proposition follows easily. □

4.3. **Gaussian wave packets.** In the case where the initial datum in (3.8) is a Gaussian, we can compute its evolution and show that it remains Gaussian, by following the same strategy as in [15] (see also [16, 17]). As a matter of fact, the order in which we have proceeded is different from the one in [15], since we have isolated the envelope equation (3.8) before considering special initial data. As a consequence, we have fewer unknowns. Consider (3.8) with initial datum

$$u(0,z) = \frac{1}{(\det A)^{1/2}} \exp\left(-\frac{1}{2}\left\langle z, BA^{-1}z\right\rangle\right), \tag{4.4}$$

where the matrices A and B satisfy the following properties:

$$A \text{ and } B \text{ are invertible;} \tag{4.5}$$

$$BA^{-1} \text{ is symmetric} : BA^{-1} = M_1 + iM_2, \text{ with } M_j \text{ real symmetric;} \tag{4.6}$$

$$\operatorname{Re} BA^{-1} \text{ is strictly positive definite;} \tag{4.7}$$

$$\left(\operatorname{Re} BA^{-1}\right)^{-1} = AA^*. \tag{4.8}$$

Proposition 4.4. *Let u solve* (3.8)*, with initial datum* (4.4)*, where the matrices A and B satisfy* (4.5)–(4.8)*. Then for all time, $u(t,z)$ is given by*

$$u(t,z) = \frac{1}{(\det A(t))^{1/2}} \exp\left(-\frac{1}{2}\left\langle z, B(t)A(t)^{-1}z\right\rangle\right), \tag{4.9}$$

where the matrices $A(t)$ and $B(t)$ evolve according to the differential equations

$$\begin{cases} \dot{A}(t) = i\nabla_k^2 E_m\left(p(t)\right) B(t) \quad ; \quad A(0) = A, \\ \dot{B}(t) = i\nabla_x^2 V\left(q(t)\right) A(t) \quad ; \quad B(0) = B. \end{cases} \tag{4.10}$$

In addition, for all time $t \in \mathbb{R}$, $A(t)$ and $B(t)$ satisfy (4.5)–(4.8)*.*

Proof. The argument is the same as in [15] (see also [16, 17]): One easily checks that if $A(t)$ and $B(t)$ evolve according to (4.10), then u given by (4.9) solves (3.8). On the other hand, it is clear that (4.10) has a global solution. Finally, since $\nabla_k^2 E_m\left(p(t)\right)$ and $\nabla_x^2 V\left(q(t)\right)$ are symmetric matrices, it follows from [15, Lemma 2.1] that for all time, $A(t)$ and $B(t)$ satisfy (4.5)–(4.8). □

5. Stability of the approximation up to Ehrenfest time

As a final step we need to show that the derived approximation $\psi^\varepsilon_{\rm app}(t)$ indeed approximates the exact solution $\psi^\varepsilon(t)$ up to Ehrenfest time.

Proposition 5.1. *Let Assumptions 1.1 and 1.4 hold and $u_0 \in \Sigma^5$. Then there exists $C > 0$ such that*

$$\|\psi^\varepsilon(t) - \psi^\varepsilon_{\rm app}(t)\|_{L^2(\mathbb{R}^d)} \leqslant C\sqrt{\varepsilon}e^{Ct},$$

where $\psi^\varepsilon_{\rm app}(t,x)$ is given by (2.4) *with $u(t,z)$ solving* (3.8) *with $u_{|t=0} = u_0$, and U_0, U_1, U_2 given by Proposition 3.2.*

Proof. First, note that ψ^ε and $\psi^\varepsilon_{\rm app}$ do not coincide at time $t = 0$, since elliptic inversion has forced us to introduce U_1 and U_2 which are not zero initially. Setting $w^\varepsilon = \psi^\varepsilon - \psi^\varepsilon_{\rm app}$, and using (1.1) and Lemma 2.2, we see that the error solves

$$\left(i\varepsilon\partial_t + \frac{\varepsilon^2}{2}\Delta - V_\Gamma - V\right) w^\varepsilon = -\frac{e^{i\phi_m/\varepsilon}}{\varepsilon^{d/4}}\varepsilon^{3/2}\left(r^\varepsilon + r_1^\varepsilon + r_2^\varepsilon\right)(t,z,y)\Big|_{(z,y)=\left(\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right)},$$
$$w^\varepsilon(0,x) = \varepsilon^{-d/4}\left(\sqrt{\varepsilon}U_1 + \varepsilon U_2\right)\left(0, \frac{x-q_0}{\sqrt{\varepsilon}}, \frac{x}{\varepsilon}\right)e^{i\phi_m(0,x)/\varepsilon}.$$

The a-priori L^2 estimate yields

$$\|w^\varepsilon(t)\|_{L^2} \leqslant \sqrt{\varepsilon}\|U_1(0)\|_{L^2_z L^\infty_y} + \varepsilon\|U_2(0)\|_{L^2_z L^\infty_y}$$
$$+ \sqrt{\varepsilon}\int_0^t \left(\|r^\varepsilon(s)\|_{L^2_z L^\infty_y} + \|r_1^\varepsilon(s)\|_{L^2_z L^\infty_y} + \|r_2^\varepsilon(s)\|_{L^2_z L^\infty_y}\right) ds.$$

The assertion then follows from Lemma 2.2 (establishing the needed properties for the functions r^ε, r_1^ε and r_2^ε), Proposition 3.2, and Proposition 4.3. With this approach, we need to know that r^ε is in L^2_z, so U_0, U_1 and U_2 have three momenta in L^2_z: in view of Proposition 3.2 and Proposition 4.3, this amounts to demanding $u_0 \in \Sigma^5$. □

This asymptotic stability result directly yields the assertion of Theorem 1.7.

End of the proof of Theorem 1.7. To conclude, it suffices to notice that

$$\varphi^\varepsilon(t,x) = \psi^\varepsilon_{\rm app}(t,x) - \left(\sqrt{\varepsilon}U_1 + \varepsilon U_2\right)(t,z,y)\Big|_{(z,y)=\left(\frac{x-q(t)}{\sqrt{\varepsilon}},\frac{x}{\varepsilon}\right)},$$

so Proposition 3.2 and Proposition 4.3 imply

$$\|\varphi^\varepsilon(t) - \psi^\varepsilon_{\rm app}(t)\|_{L^2} \leqslant C\sqrt{\varepsilon}e^{Ct}.$$

This estimate and Proposition 5.1 yield Theorem 1.7. □

Remark 5.2. The construction of the approximate solution $\psi^\varepsilon_{\rm app}$ has forced us to introduce non-zero correctors U_1 and U_2, given by elliptic inversion. Therefore, we had to consider well-prepared initial data for $\psi^\varepsilon_{\rm app}$. This aspect is harmless as long as one is interested only in the leading order behavior of ψ^ε as $\varepsilon \to 0$. As a consequence, our approach would not allow us to construct arbitrary accurate approximations for ψ^ε (in terms of powers of ε), unless well-prepared initial data are considered, i.e. data lying in so-called *super-adiabatic subspaces*, in the terminology of [27] (after [25]). This is due to the spectral analysis implied by the presence of the periodic potential V_Γ, and shows a sharp contrast with the case $V_\Gamma = 0$.

Of course the above given stability result immediately generalizes to situations where, instead of a single φ^ε, a superposition of finitely many semiclassical wave packets is considered,

$$\psi_0^\varepsilon(x) = \varepsilon^{-d/4} \sum_{n=1}^{N} u_n \left(\frac{x - q_n}{\sqrt{\varepsilon}} \right) \chi_{m_n} \left(\frac{x}{\varepsilon}, p_n \right) e^{ip_n \cdot (x-q_n)/\varepsilon}.$$

Since the underlying semiclassical Schrödinger equation (1.1) is linear, each of these initial wave packets will evolve individually from the rest, as in Theorem 1.7. Up to some technical modifications, it should be possible to consider even a *continuous* superposition of wave packets, yielding a semiclassical approximation known under the name "frozen Gaussians", see [18].

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