A linearized model of quantum transport with interface conditions in the adiabatic regime.

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Abstract

The effects of the local accumulation of charges in resonant tunneling heterostructures have been described using 1D Schrödinger-Poisson Hamiltonians in the asymptotic regime of quantum wells. Taking into account the features of the underlying physical system, the corresponding linearized model is naturally related to the adiabatic evolution of shape resonances on a time scale which is exponentially large w.r.t. an asymptotic parameter \( h \) fixing, in our framework, the quantum scale of the system. According to the complex deformation method, a possible strategy to investigate this adiabatic problem consists in using a complex dilation to identify the resonances with the eigenvalues of a complex deformed operator. Then, the adiabatic evolution for a sheet-density of charges can be reformulated using the deformed dynamical system which, under suitable initial conditions, is expected to evolve following the instantaneous resonant states. After recalling the main technical difficulties related to this approach, we introduce a modified model where \( h \)-dependent artificial interface conditions, occurring at the boundary of the interaction region, allow to obtain adiabatic approximations for the relevant resonant states. Under positivity assumptions on the potential, we show that this modification produces a small perturbation of the dynamics on any time scale. The result extends to the corresponding non-autonomous case, allowing us to consider the adiabatic evolution problem in the modified setting. In this framework, we give an expansion formula for the small-\( h \) asymptotics of the adiabatic variable, where the error introduced on the adiabatic dynamics by the interface conditions is polynomially small w.r.t. \( h \), independently from the adiabatic time scale. This result provides with a rigorous mathematical framework for the interface conditions approach to the analysis of the adiabatic transport problem in the quantum wells regime.

1 Introduction

In the axial transport through resonant tunneling structures (like highly doped p-n semiconductor heterojunctions, multiple barriers or quantum wells diodes) the charge carriers at the resonant levels interact with quantum metastable states and, depending on the geometry of the device, a local accumulation of charges may result. The corresponding repulsive effect, which can strongly modify the transport properties, have been described, in the mean-field approximation, by one-particle quantum Hamiltonians of Hartree-type with Poisson nonlinearity, where a multiple-barriers potential models the conduction band edge-profile (see e.g. in [13], [7]). In this framework, the barriers depth, fixing the time scale for the dispersion of the resonant/metastable states, can be rather large compared to the size of the wave packets. An unitarily equivalent description of this system then consists in replacing the kinetic part of the Hamiltonian with the 'semiclassical' 1D Laplacian, \(-h^2 \partial_x^2\), while the linear part of the potential, \(V^h\), is the superposition of a barrier supported on a bounded interval \([a,b]\) and multiple potential wells with support of size \( h \) inside \((a,b)\). In this particular scaling, usually referred to as quantum wells in a semiclassical island, the parameter \( h \) corresponds to a rescaled Fermi length fixing the quantum scale of the system (see [6]) and, coherently with the features of the physical model, it is assumed to be small. The resulting transport model is described by a double-scale Schrödinger-Poisson Hamiltonian

\[
H_{NL}^h = -h^2 \partial_x^2 + V^h + V_{NL}^h, \tag{1.1}
\]

where the nonlinear potential term, \(V_{NL}^h\), solves a Poisson equation with a source given by the charge density of the system. The corresponding evolution problem is

\[
\begin{align*}
    i \partial_t u^h (\cdot, t) &= H_{NL}^h u^h (\cdot, t), \\
    -\Delta V_{NL}^h &= |u^h (x, t)|^2,
\end{align*}
\tag{1.2}
\]

Resonant energies, produced by the potential \(V^h\), naturally arise in this class of models and play a central role in the description of the quantum tunnelling. The incoming electrons at resonant levels interact with

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resonant states which evolve in time according to a quasi-stationary dynamics. In particular, their $L^2$-mass remains concentrated in a neighborhood of the wells support for a range of time exponentially large w.r.t. $\hbar$. Depending on the position of the wells, this possibly induces a local charging process; then, the nonlinear coupling in (1.2) generates a positive response (depending from the charge in the wells) which modifies the potential profile and reduces the tunneling rate.

This dynamics was considered in the works of G. Jona-Lasinio, C. Presilla and J. Sjöstrand ([13], [19], [20]), within a simplified framework where the Poisson potential is replaced by an affine function multiplied by a nonlinear charge density. Using slowly varying potential assumptions, WKB expansions and a one-mode approximation for the time evolution of the quantum state, the authors discuss the behavior of the sheet density related to the accumulation of electrons in a single well determined by a flat double-barrier potential. Rephrasing the result of their work in our scaling, they show that the relevant time scale of the problem is of the size $\sim e^{1/h}$, corresponding to the imaginary part of the lowest resonance, and provide with an explicit equation for the evolution of the local charge density in the limit $\hbar \to 0$ (eq. 9.7 in [19]).

It is worthwhile to notice that these calculations have been shown to be relevant only in some specific cases. This concerns, in particular, the adiabatic approximation of the nonlinear evolution of the generalized eigenfunctions, which appears to be an essential point of the analysis: the lack of an error bound in the adiabatic formulas for resonant states prevents to control the possible remainder terms in the asymptotic limit. Moreover, the role played by the device’s geometry in the emergence of nonlinear effects still deserves further investigations. This was pointed out by F.Nier, Y.Patel and V.Bonaillie-Nöel, in a series of works devoted to the steady state problem related to (1.2) under far-from-equilibrium assumptions. In [4]-[5], an accurate microlocal analysis of the tunnel effect as $\hbar \to 0$ determines the limit occupation number of resonant states. This analysis leads to a simplified equation for the Poisson problem, where the limit charge density is described by a superposition of delta-shaped distributions.

In the next Section we introduce a linearized problem for the evolution of a quantum observable corresponding to a charge locally accumulating in the interaction region. When the dynamics is driven by resonant states, the complex dilations method leads to an equivalent description of the system where the resonances identify with the spectral points of a deformed operator. The nonselfadjoint perturbation introduced in this framework depends on the deformation’s shape; the simplest choice of a sharp exterior dilation, acting outside the potential support, naturally introduce interface conditions in the description of these phenomena. In the Section 1.2 a class of modified Hamiltonians is considered by using nonselfadjoint point perturbations occurring at the boundary of the potential’s support. These are defined using interface conditions similar to the ones related to the complex dilation. Recalling the results from [5] and [9], we show that a version of the adiabatic theorem for shape resonances holds in this modified setting, providing us with an efficient strategy to obtain reduced equations in the adiabatic limit. A rigorous justification of this strategy requires a comparison between the modified and the ‘physical’ dynamics on the adiabatic time-scale. This problem is stated in the Section 1.3 where we present our main result. The proof is then developed in the Sections 2 and 3.

1.1 A linearized transport problem: the role of the interface conditions

The relevance of the adiabatic approximation, for the Schrödinger-Poisson equation in the regime of quantum wells, suggests to consider as a preliminary step a 'linearized' problem where the nonlinear part of $H^\hbar_{NL}$ is replaced by a potential supported on $(a, b)$ and adiabatically depending on the time; namely we introduce the time dependent family of Schrödinger operators

$$H^\hbar_{0}(t) = -\hbar^2 \partial^2_x + V^\hbar (t) ,$$

where for all $t$ the potential’s shape fulfills the above mentioned prescription (i.e., it is formed by the superposition of a barrier and quantum wells). The adiabatic evolution of an observable $O$ (corresponding to a local charge) is described by the variable $A^\hbar_{0}(t)$ solving the equation

$$
\begin{cases}
A^\hbar_{0}(t) = Tr \left[ O \left( u^\hbar_{0}(\cdot,t) \right) \left( u^\hbar_{0}(\cdot,t) \right) \right] , \\
i \varepsilon \partial_t u^\hbar_{0}(\cdot,t) = H^\hbar_{0}(t) u^\hbar_{0}(\cdot,t) .
\end{cases}
$$

In this framework, the relevant resonant energies for the transport problem are determined by the shape resonances of $H^\hbar_{0}$ (roughly corresponding to those resonances whose real part is below the top of the barrier). In the asymptotic regime of quantum wells ($\hbar \to 0$), it is known that the number of shape resonances is uniformly bounded w.r.t. $\hbar$, while their imaginary parts are of order $e^{-2S_0/\hbar}$ (being $S_0 > 0$ a suitable constant depending on the geometry of the potential and on the particular resonance being considered; for this point we refer to the analysis developed in [10]-[11]). Following [7], this quantity fixes the time scale for the dispersion of the corresponding resonant states. Hence, the effect of the accumulation of charges inside the wells can be investigated by choosing the adiabatic parameter $\varepsilon$, in $e^{2S_0/\hbar}$, of the size $e^{-2S_0/\hbar}$.
The small-$h$ analysis of the linearized problem, involves the following task: clarify, in an energy interval close to the shape resonances, the relation between the evolution of generalized eigenfunctions and of the resonant states in the adiabatic limit. Let us recall that the resonances of a Schrödinger operator correspond (modulo a restriction to a dense subset of dilation-analytic functions) to the poles of the meromorphic extension of its resolvent to the second Riemann sheet (i.e., $\text{Im } \sqrt{z} < 0$). These are detected through the complex deformation method (see [12] for details), which can be adapted to our framework by using the exterior complex scaling: $x \rightarrow xe^{\varphi(\alpha, b)(x)}$; when $\varphi \in \mathbb{R}$, the related deformation is an unitary operator acting on $L^2(\mathbb{R})$ according to

$$U_\varphi u(x) = \begin{cases} e^{\varphi/2u}(e^{\varphi}(x - b) - b), & x > b, \\
 u(x), & (a, b), \\
 e^{\varphi/2u}(e^{\varphi}(x - a) - a), & x < a. \end{cases}$$

The corresponding deformation of a Schrödinger operator $Q = -\Delta + V$, with $\text{supp } V = [a, b]$, is next denoted by $Q(\varphi)$ and explicitly writes as (see e.g. in [3])

$$Q(\varphi) = U_\varphi QU_\varphi^{-1} = -e^{-2\varphi}_{1\mathbb{R}\setminus(a, b)} \Delta_\varphi + V,$$

where $\Delta_\varphi$ is the nonselfadjoint point perturbation of the 1D Laplacian defined by the interface conditions

$$\begin{align*}
e^{-\frac{\varphi}{2}}u(b^+) = u(b^-), & \quad e^{-\frac{\varphi}{2}}u'(b^+) = u'(b^-), \\
e^{-\frac{\varphi}{2}}u(a^-) = u(a^+), & \quad e^{-\frac{\varphi}{2}}u'(a^-) = u'(a^+). \end{align*}$$

Namely, we have

$$\Delta_\varphi : \left\{ D(\Delta_\varphi) = \{ u \in H^2(\mathbb{R}\setminus\{a,b\}) \mid (1.7) \text{ holds} \} \right\},$$

When $\text{Im } \varphi > 0$, this deformation produces a rotation of the essential spectrum in the second Riemann sheet: $\sigma_{ess}(Q(\varphi)) = e^{-2\text{Im } \varphi}_{\mathbb{R}+}$; in the cone spanned by $\mathbb{R}+$ and $\sigma_{ess}(Q(\varphi))$ the resonances of $Q$ identify with the spectral points of $Q(\varphi)$. This important result was obtained at first by J. Aguilar, E. Baslev and J.M. Combes in [1,3], where the case of potentials analytic w.r.t. the uniform complex dilation $x \rightarrow xe^\varphi$ is considered (see also [12, Theorem 16.4]). For potentials which can be complex deformed only outside a compact region, the exterior complex scaling technique appeared in [21] in the singular version that we reconsider here.

**Proposition 1.1** Let $Q = -\Delta + V$, with $\text{supp } V = [a, b]$; the resonances of $Q$ in the cone

$$K_\alpha = \{ \arg z \in (-2\alpha, 0) \}, \quad \text{with } 0 < \alpha < \pi/4,$$

are eigenvalues of the operators $Q(\varphi)$ for all $\varphi$ s.t. $\alpha \leq \text{Im } \varphi$.

As a consequence, the resonant state associated to a resonance $E_{res} \in K_\alpha \cap \sigma Q(\varphi)$ can be defined as an eigenvector of $Q(\varphi)$, with $\alpha \leq \text{Im } \varphi$, and we have

$$\langle Q(\varphi) - E_{res} \rangle \psi_{E_{res}} = 0, \quad \text{in } L^2(\mathbb{R}).$$

It is worth to remark that the resonances in $K_\alpha$ do not depend on the deformation, i.e.: if $E_{res} \in K_\alpha \cap \sigma Q(\varphi)$ for a given $\varphi$, then, $E_{res} \in K_\alpha \cap \sigma Q(\varphi')$ for all $\varphi' > \varphi$. Nevertheless the solution $\psi_{E_{res}}$ of (1.10) possibly depends on $\varphi$ in the exterior region, while the cutoff $1_{(a, b)}(x) \psi_{E_{res}}$ (usually referred to as the quasi-resonant state) is independent from $\varphi$.

The identification of the resonances of $Q(\varphi)$ with the spectral points of the corresponding deformed operator $Q(\varphi)$ suggest an alternative, and possibly more natural, framework to study the adiabatic problem [12,4]. Let us define the observable $O$ according to

$$O \in L^\infty(\mathbb{R}), \quad \text{supp } O \subset (a, b).$$

With this choice, $O$ describes the charge accumulating in a region inside $(a, b)$. Since $O$ commutes with the deformation $U_\varphi$ for all $\varphi$, from the properties of the trace operation it follows

$$A^0_h(t) = \text{Tr} \left[ O \left| u^0_h(\cdot, t, 0) \right\rangle \left\langle u^0_h(\cdot, t, 0) \right| \right] = \text{Tr} \left[ U_\varphi^* OU_\varphi \left| u^0_h(\cdot, t, 0) \right\rangle \left\langle u^0_h(\cdot, t, 0) \right| \right] = \text{Tr} \left[ OU_\varphi \left| u^0_h(\cdot, t, 0) \right\rangle \left\langle u^0_h(\cdot, t, 0) \right| U_\varphi^* \right] = \text{Tr} \left[ O \left| u^0_h(\cdot, t, \varphi) \right\rangle \left\langle u^0_h(\cdot, t, \varphi) \right| \right].$$
where \( u^0_h(\cdot, t, \varphi) \) identifies with the solution of the deformed dynamical system generated by \( H^h_0(t, \varphi) = U_\varphi H^h_0(t) U_\varphi^{-1} \). This allows to rephrase (1.13) in the equivalent form

\[
\begin{align*}
A^h_0(t) &= \text{Tr} \left[ O \left| u^0_h(\cdot, t, \varphi) \right| \left< u^0_h(\cdot, t, \varphi) \right| \right], \\
i \partial_t u^0_h(\cdot, t, \varphi) &= H^h_0(t, \varphi) u^0_h(\cdot, t, \varphi).
\end{align*}
\]

When the undeformed initial state \( u^0_h(\cdot, 0, 0) \) is characterized by energies close to the shape resonances, the relevant informations about the solution \( u^0_h(\cdot, t, \varphi) \) of the adiabatic problem in (1.12) are related to the evolution of the resonant states. To fix this point, assume that, for a suitable choice of the operator \( H^h_0(t) \), the instantaneous resonant state \( \psi(E^h_0(t)) \) solves the eigenvalue equation (1.10) with \( Q(\varphi) = H^h_0(t, \varphi) \). Let \( \hat{u}^h_0(\cdot) \) denotes the generalized Fourier transform of \( u^0_h(\cdot) \) related to the initial and undeformed Hamiltonian; when \( u^0_h(k, t = 0, 0) \) is supported on \( k \) such that: \( k^2 \sim \Re E^h_0(t) \sim \lambda \), it is expected that

\[
1_{(a,b)}(x) u^h_0(x, t, \varphi) \sim 1_{(a,b)}(x) \psi^h_0(t, \varphi),
\]

where \( \psi^h_0(t, \varphi) \) is the solution of the adiabatic evolution problem for the resonance \( E^h_0(0) \)

\[
\begin{align*}
i \partial_t \psi^h_0(t, \varphi) &= H^h_0(t, \varphi) \psi^h_0(t, \varphi), \\
\psi^h_0(0, \varphi) &= \psi(E^h_0(0)).
\end{align*}
\]

Standard results in adiabatic perturbation theory (see e.g. in [18]) would suggests to identify \( \psi^h_0(t, \varphi) \) with the instantaneous resonant state \( \psi(E^h_0(t)) \) (times a suitable modulation factor), with an error of the size \( \sim e^{-1/h} \). Such an adiabatic approximation and the relation (1.13) could then be implemented in (1.12) to study the asymptotic behaviour of \( A^h_0(t) \) as \( h \to 0 \).

The main difficulty in this approach is due to the fact that the complex scaling does not preserves the m-accretivity of the operator, i.e.: the quadratic form associated to \( H^h_0(t, \varphi) \) has an imaginary part with undetermined sign (see the eq. (1.5) in [8]): as a consequence, the deformed dynamics may exhibit an exponential growth w.r.t. \( t \). Since uniform-in-time estimates for the dynamical system are necessary to prove the adiabatic theorem, the lack of this condition in our case, prevents from developing a rigorous approach to the study of (1.14) in the small-\( h \) limit.

**1.2 The modified Hamiltonian**

A possible strategy to overcome the lack of uniform-in-time estimates of the deformed dynamical system consists in modifying the physical Hamiltonian \( H^h_0 \) according to

\[
H^h_0 = -h^2 \Delta_\theta + \mathcal{V}, \quad D(H^h_0) = D(\Delta_\theta),
\]

It is worthwhile to remark that, for \( \theta \neq 0 \), \( H^h_0 \) is neither selfadjoint nor symmetric and identifies with an extension of the symmetric restriction

\[
H^h_{0,0} = H^h_0 \upharpoonright \{ u \in H^2(\mathbb{R}) \mid u(\alpha) = u'(\alpha) = 0, \; \alpha = a, b \}.
\]

In this connection, \( H^h_0 \) is an explicitly solvable model w.r.t. \( H^h_0 \) and relevant quantities, as its resolvent or generalized eigenfunctions, can be expressed in terms of corresponding non-modified quantities, related to the selfadjoint operator \( H^h_0 \), through non-perturbative formulas. This well-known property of point perturbations (see e.g. in [2]) provides with an useful tool for the spectral analysis and allows to consider the pair \( \{ H^h_0, H^h_{0,0} \} \) as a scattering system. A detailed analysis of these modified operators (in a slightly more general framework) has been provided with in [8], [15] and [16].

We next consider a non-autonomous Hamiltonian defined by (1.15) through a time dependent potential \( \mathcal{V}^h(t) \) providing our model with the particular scaling of a quantum well in a semiclassical island for all time, and such that the spectral profile of \( H^h_0(t) \) corresponds to the following picture: \( H^h_0(t) \) has a shape resonance \( E^h_0(t) \) which, for \( \Im \varphi > 0 \) large enough, belong to \( \sigma(H^h_0(t, \varphi)) \), where \( H^h_0(t, \varphi) \) denotes the exterior complex-dilation of \( H^h_0(t) \) through the deformation \( U_\varphi \). Extending the standard semiclassical estimates, holding in the regime of quantum wells, to this modified framework, it has been shown that: \( \Im E^h_0(t) = \mathcal{O}(e^{-2S_0/h}) \), where \( S_0 \) is the Agmon distance between the well and the barrier’s boundary (we refer to [8] Proposition 5.5) for details;
since \( \sigma_{\text{ess}} \left( H^b_0(t, \varphi) \right) = e^{-2\varphi} \mathbb{R}_+ \), \( E^b_0(t) \) can be considered as an isolated part of the spectrum of \( H^b_0(t, \varphi) \), with a spectral gap depending on \( \varphi \), and the adiabatic evolution problem is modified according to

\[
\begin{aligned}
& \left\{ \begin{array}{ll}
    i \varepsilon \partial_t \psi^b_\theta(t, \varphi) = H^b_0(t, \varphi) \psi^b_\theta(t, \varphi), \\
    \psi^b_\theta(0, \varphi) = \psi^{b,0}(0).
\end{array} \right.
\end{aligned}
\]  

(1.17)

If the dynamical system generated by \( H^b_0(t, \varphi) \) allows uniform-in-time estimates, this problem can be analyzed following the standard approach of the adiabatic theorem with spectral gap condition. For a particular choice of the deformation, the modification introduced in (1.15) allows to obtain such a result. Indeed, the deformation \( H^b_0(\varphi) \) is characterized as follows (Lemma 3.1 in [8]).

Lemma 1.2

Let \( \theta = \varphi = i \gamma, \gamma > 0 \). Then: \( i H^b_0(i \gamma) \) is maximal accretive.

According to this result, \( e^{-i s H^b_0(t, i \gamma)} \) is a strongly continuous (w.r.t. \( s \)) semigroup of contractions for each fixed \( t \); then, under suitable time-regularity assumptions on the potential, the non-autonomous Hamiltonian \( H^b_0(t, i \gamma) \) generates a quantum dynamical system of contractions (see [8] Proposition 3.7). In order to minimize the error produced by modification of the Hamiltonian, we next assume \( \gamma \) to be polynomially small w.r.t. \( h \), namely: \( e = h^{N_0} \) for some integer \( N_0 \) possibly large. In this framework, \( E^b_0(t) \) is close to the essential spectrum (located in \( e^{-2h^{N_0} \mathbb{R}_+} \)) and the spectral gap condition depends on \( h \). For \( \theta = \varphi = i h^{N_0} \) and \( \varepsilon = e^{-\tau/h} \) with \( \tau > 0 \) arbitrary, the adiabatic theorem in [8] Theorem 7.1 applies to the solution of the adiabatic problem leading to the expansion

\[
\max_{t \in [0, T]} \left\| \psi_{ih^{N_0}}(t, ih^{N_0}) - u^b_\theta(t) \right\|_{L^2(\mathbb{R})} = \mathcal{O} \left( \varepsilon^{1-\delta} \left\| \psi^{b,0}(0) \right\|_{L^2(\mathbb{R})} \right),
\]  

(1.18)

In particular if: \( \left\| \psi^{b,0}(t) - \psi^{b,0}(t) \right\|_{L^2(\mathbb{R})} \leq \varepsilon^{1-\delta} \), the auxiliary dynamics \( v^b_\theta(t) \) expresses as

\[
v^b_\theta(t) = \mu_\theta(t) e^{-i \delta \int_0^t \psi^{b,0}(s) ds} \psi^{b,0}(t),
\]  

(1.19)

with

\[
\mu_\theta(t) = \exp \left( -i \int_0^t \frac{\psi^{b,0}(s) \partial_s \psi^{b,0}(s)}{\left\| \psi^{b,0}(s) \right\|_{L^2(\mathbb{R})}^2} \right) + \mathcal{O} \left( \varepsilon^{1-\delta} \right).
\]  

(1.20)

(see [9] for the explicit form of the modulation factor).

The linearized adiabatic transport problem corresponding to the modified Hamiltonians \( H^b_0 \) writes as

\[
\begin{aligned}
& \left\{ \begin{array}{ll}
    A^b_\theta(t) = \text{Tr} \left[ O \left| u^b_\theta \right| \left( t \right) \right] \left( u^b_\theta \left( t, \theta \right) \right), \\
    i \varepsilon \partial_t u^b_\theta \left( t, \theta \right) = H^b_0(t, \theta) u^b_\theta \left( t, \theta \right),
\end{array} \right.
\end{aligned}
\]  

(1.21)

and, for \( O \) fulfilling the condition (1.10), the variable \( A^b_\theta(t) \) is related to the complex deformed setting by

\[
\begin{aligned}
& \left\{ \begin{array}{ll}
    A^b_\theta(t) = \text{Tr} \left[ O \left| u^b_\theta \right| \left( t, \varphi \right) \right] \left( u^b_\theta \left( t, \varphi \right) \right), \\
    i \varepsilon \partial_t u^b_\theta \left( t, \varphi \right) = H^b_0 \left( t, \varphi \right) u^b_\theta \left( t, \varphi \right).
\end{array} \right.
\end{aligned}
\]  

(1.22)

In [9], the small-\( h \) behaviour of \( A^b_\theta(t) \) has been investigated for an explicit model where the potential is formed by a flat barrier of height \( V_0 > 0 \) plus an attractive, time-dependent delta interaction acting in \( x_0 \in (a, b) \) and preserving the quantum-well scaling. Explicitly, we consider the model

\[
H^b_0(t) = -h^2 \Delta + V_0 + h \alpha(t) \delta_{x_0}.
\]  

(1.23)

Under suitable assumptions on \( \alpha(t) \), this operator has a single time-dependent shape resonance \( E^b_0(t) \) localized close to a positive energy below \( V_0 \). In this framework a direct computation allows to prove that the conditions hold, while applying the expansion (1.18)-(1.20) applies to the solutions of the dynamical systems in (1.22), in the limit as \( h \to 0 \), \( A^b_\theta(t) \) expands according to

\[
A^b_\theta(t) = a(t) + \mathcal{J}(t) + \mathcal{O} \left( \theta \right).
\]  

(1.24)

Depending on the constraint: \( |x_0 - a| < |x_0 - b| \), the zero order term \( a(t) = \mathcal{O}(1) \) solves an explicit limit equation which, coherently with the reduced model presented in [19], describes the charging process of the well (see eq. (2.24) in [9] and the remarks thereafter), while the first remainder \( \mathcal{J}(t) = \mathcal{O}(h^2) \) is independent from \( \theta \).
1.3 A comparison result

Following the strategy presented in the previous section, the modification introduced by the interface conditions yields an efficient method to obtain reduced equations for the linearized transport problem (1.21), providing with a rigorous control of the remainder terms. The particular example considered in expansion (1.24) suggests that the main contribution to the limit dynamics is not affected by the modification of the model, bringing only physical information. Nevertheless, for a rigorous justification of this approach, the difference \( A^b_{\theta}(t) - A^b_{\theta}(t) \) needs to be carefully estimated on the suitable adiabatic time-scale when both \( h \) and \( \theta \) are small. Our work is devoted to this analysis which will be carried out under generic assumptions on the potential. It is next assumed that

\[
H^b_{\theta}(t) = -h^2 \Delta_{\theta} + V(t) ,
\]

with

\[
V(t) \in C^0([0,T], L^\infty(\mathbb{R}, \mathbb{R})) , \quad \text{supp } V(t) = [a,b] , \quad \text{and } 1_{[a,b]} V(t) > c ,
\]

for some \( c > 0 \). Under this assumption, the small-\( \theta \) behaviour of the quantum dynamical system generated by \( H^b_{\theta}(t) \) is characterized as follows.

**Theorem 1.3** Assume: \( h \in (0, h_0) \), \( |\theta| \leq h^{N_0} \), being \( h_0 \) suitably small and \( N_0 \geq 2 \), and let \( H^b_{\theta}(t) \) be defined according to (1.25)-(1.29).

i) The Cauchy problem

\[
\begin{align*}
\begin{cases}
i \partial_t u^b_{\theta}(t) = H^b_{\theta}(t) u^b_{\theta}(t) , & 0 \leq s \leq t \leq T , \\
u^b_{\theta}(s) \in D(H^b_{\theta}) ,
\end{cases}
\end{align*}
\]

is provided with a strongly continuous dynamical system \( U^b_{\theta}(t,s) \), \( 0 \leq s \leq t \leq T \), whose action \( U^b_{\theta}(t,s) u^b_{\theta}(s) \) defines the unique solution of (1.27). In particular, \( U^b_{\theta}(t,s) \) is \( \theta \)-holomorphic and the intertwining relation:

\[
U^b_{\theta}(t,s) W^b_{\theta} = W^b_{\theta} U^b_{\theta}(t,s) ,
\]

holds with

\[
W^b_{\theta} = 1_{L^2(\mathbb{R})} + O(h^{N_0-2}) ,
\]

in the \( L(L^2(\mathbb{R})) \) operator norm sense. Moreover, \( U^b_{\theta}(t,s) \) allows the estimates

\[
\sup_{s,t \in [0,T] , b \in (0,h_0]} \| U^b_{\theta}(t,s) \|_{L(L^2(\mathbb{R}))} \leq M_{a,b,c} ,
\]

and

\[
\sup_{s,t \in [0,T]} \| U^b_{\theta}(t,s) - U^b_{\theta}(t,s) \|_{L(L^2(\mathbb{R}))} \leq C_{a,b,c} h^{N_0-2} ,
\]

where the positive constants \( M_{a,b,c} \) and \( C_{a,b,c} \), possibly depending on the data \( a,b,c \), are independent from \( T \).

ii) Let \( O \in L^\infty(\mathbb{R}, \mathbb{R}) \) and \( V \) defined according to (1.29) with \( T = 1 \). The solution of the adiabatic evolution problem

\[
\begin{align*}
\begin{cases}
A^b_{\theta}(t,\varepsilon) = Tr \left[ O (t) u^b_{\theta,c}(t) \right] , \\
i \varepsilon \partial_t u^b_{\theta,c}(t) = H^b_{\theta}(t) u^b_{\theta,c}(t) , & 0 \leq t \leq 1 , \\
u^b_{\theta,c}(0) = W^b_{\theta} u , & u \in H^2(\mathbb{R}) , \quad \| u \|_{L^2(\mathbb{R})} = 1 ,
\end{cases}
\end{align*}
\]

allows the expansion

\[
A^b_{\theta}(\tau,\varepsilon) = A^b_{\theta}(\tau,\varepsilon) + R(\tau, h, \theta, \varepsilon) , \quad \sup_{\tau \in [0,1]} | R(\tau, h, \theta, \varepsilon) | \leq \tilde{C}_{a,b,c} h^{N_0-2} , \quad \forall \varepsilon > 0 ,
\]

being \( \tilde{C}_{a,b,c} > 0 \) a suitable constant, possibly depending on the data, but independent from \( \varepsilon \).

The second part of the statement has been anticipated as a conjecture in [17], where an expansion of the type (1.32) was suggested. The proof is developed in the next Sections. In the Section 2 following the approach developed in [16], we use a 'Krein-like' formula for the modified generalized eigenfunctions: this allows to obtain a small-\( \theta \) expansion for the stationary wave operators \( W^b_{\theta} \) related to the couple \( \{ H^b_{\theta}, H^b_{\theta} \} \) in the autonomous
assumption (1.26), our result includes the case of modified Hamiltonians with the scaling of quantum wells in
1.4 Notation

a semiclassical island providing, in this connection, with a rigorous mathematical framework for the interface
the adiabatic variable $A$ | conditions, whose size is controlled by $\Omega$ ·

$\Omega$ complex half-plane; 1

The expansion (1.30) is independent from the
time scale, this approximation can still be used in adiabatic case. In the Section 3.1, the small-
$h,\theta$ we get the uniform-in-time estimate (1.29) for the modified dynamical system and its asymptotic behaviour as
quantum propagator without restrictions on the initial state (see (2.87)). In the nonautonomous case, considered
in the assumption (1.29), our result includes the case of modified Hamiltonians with the scaling of quantum wells in
a semiclassical island providing, in this connection, with a rigorous mathematical framework for the interface
conditions approach to the analysis of the adiabatic transport problem in the regime quantum wells.

1.4 Notation

In what follows: $B_\delta(p)$ is the open disk of radius $\delta$ centered in a point $p \in \mathbb{C}$; $\mathbb{C}^\pm$ are the upper and lower
complex half-plane; $1_{\Omega}()$ is the characteristic function of a domain $\Omega$; $d(X, Y)$ is the distance between the sets
$X, Y \subset \mathbb{R}$ or $\mathbb{C}$. $\partial f$, denotes the derivative of $f$ w.r.t. the $j$-th variable; $C^0(U)$ is the set of $C^0$-continuous
functions w.r.t. $x \in U \subset \mathbb{R}$, while $H^j(U)$ is the set of holomorphic functions w.r.t. $z \in D \subset \mathbb{C}$. The notation '$\subseteq$,
appearing in some of the proofs, denotes the inequality: '$\leq C$' being $C$ a suitable positive constant. Moreover, the
generalization of the Landau notation $O(\cdot)$ is defined according to

Definition 1.4 Let be $X$ a metric space and $f, g : X \rightarrow \mathbb{C}$. Then $f = O(g) \iff \forall x \in X$ it holds:
$f(x) = p(x)g(x)$, being $p$ a bounded map $X \rightarrow \mathbb{C}$.

2 Scattering by interface conditions

We consider the modified Schrödinger operators

$$H^b_h : \begin{cases} D (H^b_h) = \{ u \in H^2 (\mathbb{R}) \setminus \{a, b\} \mid (L, \delta) \text{ holds} \} , \\
H^b_h u \} (x) = -h^2 u''(x) + \mathcal{V}(x) u(x) , \quad x \in \mathbb{R} \setminus \{a, b\} .
\end{cases} \quad (2.1)$$

where the potential $\mathcal{V}$ is assumed to be selfadjoint and compactly supported on the bounded interval $[a, b]$. In
particular, we set

$$\mathcal{V} \in L^2(\mathbb{R}, \mathbb{R}) , \quad \text{supp } \mathcal{V} = [a, b] . \quad (2.2)$$

Following the analysis developed in [15, 16], we next resume the main features of these operators focusing on the
scattering couple $\{H^b_h, H^0_h\}$. In the case $h = 1$, it has been shown that the interface conditions [17] do
not modify the spectrum provided that $\theta$ is small (see [15 Proposition 2.6]). In the present case, the dilation:
y $= (x - (b + a) / 2) / h$ transforms the boundary conditions (1.7) into

$$\begin{cases} e^{-\theta/2} u(\beta_n^+) = u(\tilde{\beta}_n^+) , \quad e^{-\theta/2} u' (\beta_n^+) = u'(\tilde{\beta}_n^+) , \\
e^{-\theta/2} u(\alpha_n^-) = u(\tilde{\alpha}_n^-) , \quad e^{-\theta/2} u'(\alpha_n^-) = u'(\tilde{\alpha}_n^-) ,
\end{cases} \quad (2.3)$$

with: $\alpha_n = -(b - a) / 2h$ and $\beta_n = (b - a) / 2h$. The corresponding unitary map on $L^2(\mathbb{R})$ transforms $H^b_h$
into the dilated operator

$$\tilde{H}_\theta : \begin{cases} D (\tilde{H}_\theta) = \{ u \in H^2 (\mathbb{R}) \setminus \{\alpha_n, \beta_n\} \mid (L, \delta) \text{ holds} \} , \\
\tilde{H}_\theta u \} (x) = -u''(x) + \mathcal{V}(x) u(x) , \quad x \in \mathbb{R} \setminus \{\alpha_n, \beta_n\} ,
\end{cases} \quad (2.4)$$

where $\mathcal{V}(x) = \mathcal{V}(hx + (b + a) / 2)$ is compactly supported on $[\alpha_n, \beta_n]$.

Proposition 2.1 Let $h > 0$ fixed and consider the operators $H^b_h$ defined in (2.2), (2.3). For any couple $\theta \in \mathbb{C}$,
the essential part of the spectrum is $\sigma_{ess} (H^b_h) = \mathbb{R}^+$. If, in addition, $\mathcal{V}$ is assumed to be defined positive

$$\langle u, \mathcal{V} u \rangle_{L^2((a, b))} > 0 \quad \forall u \in L^2((a, b)) \text{ s.t. } u \neq 0 , \quad (2.5)$$

it exists $\delta > 0$, possibly depending on $h$, such that: $\sigma (H^b_h) = \mathbb{R}^+$ for all $\theta \in B_\delta (0)$.
Proof. From the Proposition 2.6 in [15], the result holds for \( \hat{H}_\theta \); then it extends to \( H^0_\theta \) due to the unitarily equivalence of the two operators.

Notice The essential spectrum of \( A \) is here defined according to [23] as \( \sigma_{ess}(A) = \mathbb{C} \setminus \mathcal{F}(A) \), being \( \mathcal{F}(A) \) the set of complex \( \lambda \in \mathbb{C} \) s.t. \( (A - \lambda) \) is Fredholm.

The point perturbation model \( H^0_\theta \) can be described as a restriction of the adjoint operator \( (H^0_\theta)^* \) (see [10]) through linear relations on an auxiliary Hilbert space. This construction, achieved in [16] using the ‘boundary equivalence of the two operators.

Proof. \( \nabla \nabla \cdot \mathcal{L} \) as solutions of the boundary value problems

\[
\begin{align*}
\left\{ \begin{array}{l}
(h^2 \partial^2_x + \mathcal{V} - z) G^{\pm}(\cdot, y) = 0, \quad \text{in } \mathbb{R}/\{y\}, \\
G^{\pm}(y^+, y) = G^{\pm}(y^-, y), \quad h^2 (\partial_y G^{\pm}(y^+, y) - \partial_y G^{\pm}(y^-, y)) = -1,
\end{array} \right. \\
\end{align*}
\]

and

\[
\begin{align*}
\left\{ \begin{array}{l}
(h^2 \partial^2_x + \mathcal{V} - z) \mathcal{H}^{\pm}(\cdot, y) = 0, \quad \text{in } \mathbb{R}/\{y\}, \\
h^2 (\mathcal{H}^{\pm}(y^+, y) - \mathcal{H}^{\pm}(y^-, y)) = 1, \quad \partial_y \mathcal{H}^{\pm}(y^+, y) = \partial_y \mathcal{H}^{\pm}(y^-, y),
\end{array} \right.
\end{align*}
\]

Then \( \ker ((H^0_\theta)^* - z) = \text{l.c. } \{\gamma_{h, j}^i, \theta^i_j\}_{j=1}^4 \), with

\[
\gamma_{h, 1} = G^{\pm,h}(x, b), \quad \gamma_{h, 2} = \mathcal{H}^{\pm,h}(x, b), \quad \gamma_{h, 3} = G^{\pm,h}(x, a), \quad \gamma_{h, 4} = \mathcal{H}^{\pm,h}(x, a).
\]

Following [16] eq. (2.19) and (2.26), for all \( z \in \text{res } (H^0_\theta) \) the identity

\[
(H^0_\theta - z)^{-1} - (H^0_\theta - z)^{-1} = -\sum_{i,j=1}^4 \left[ (B_\theta q(z, h) - A_\theta)^{-1} B_\theta \right]_{ij} \langle \gamma_{h, j}, \cdot \rangle_{L^2(\mathbb{R})} \gamma_{h, j},
\]

with

\[
h^2 A_\theta - 1 = \begin{pmatrix} e^{\theta/2} & e^{\theta/2} \\ e^{-\theta/2} & e^{-\theta/2} \end{pmatrix}, \quad B_\theta = \begin{pmatrix} 0 & 1 - e^{\theta/2} \\ e^{\theta/2} & 0 \end{pmatrix},
\]

and \( q(z, h) \) depending on the boundary values of \( G^{\pm,h}, \mathcal{H}^{\pm,h} \) and \( \partial_y \mathcal{H}^{\pm,h} \) according to

\[
q(z, h) = \begin{pmatrix} G^{\pm,h}(b, b) & - (\mathcal{H}^{\pm,h}(b, b) + \frac{1}{2h}) \\ \mathcal{H}^{\pm,h}(b, a) & \mathcal{H}^{\pm,h}(a, a) \end{pmatrix} - \begin{pmatrix} - (\mathcal{H}^{\pm,h}(b, a) + \frac{1}{2h}) \\ - (\mathcal{H}^{\pm,h}(a, a) + \frac{1}{2h}) \end{pmatrix}.
\]

The Green’s functions \( G^{\pm,h}, \mathcal{H}^{\pm,h} \) are related to the Jost’s solutions of the equation

\[
(-h^2 \partial^2_z + \mathcal{V}) u = \zeta^2 u, \quad \zeta \in \mathbb{C}^+,
\]

next denoted with \( \chi^{\pm,h}(\cdot, \zeta) \), fulfilling the exterior conditions

\[
\chi^{\pm,h}(\cdot, \zeta)|_{z>b} = e^{i \Phi_z}, \quad \chi^{\pm,h}(\cdot, \zeta)|_{z<a} = e^{-i \Phi_z}.
\]

A detailed analysis of their properties have been given in [24] for generic \( L^1 \)-potentials, while the particular case of a potential barrier is explicitly considered in [15] for \( h = 1 \). The \( h \)-dependent case can be considered as a rescaled problem and the result presented in [15] rephrase as follows

Lemma 2.2 Let \( \mathcal{V} \in L^2(\mathbb{R}, \mathbb{R}) \) s.t.: \( \text{supp } \mathcal{V} = [a, b] \). For any fixed \( h > 0 \), the solutions \( \chi^h_+ \) to the problem (2.12)-(2.15) belong to \( \mathcal{C}^1_2(\mathbb{R}, \mathcal{H}_\zeta(\mathbb{C}^+)) \) and have continuous extension to the real axis.
Proof. With the change of variable: \( y = (x - (b + a)/2)/h \), the problem \( (2.12) - (2.13) \) writes as

\[
\begin{aligned}
\begin{cases}
(-\partial_y^2 + \hat{V}) \hat{x}_\pm^h = \zeta^2 \hat{x}_\pm,
\end{cases} \quad \zeta \in \mathbb{C}^+,
\end{aligned}
\]

(2.14)

where \( \hat{V} \) denotes the dilated potential: \( \hat{V}(y) = V(hy + (b + a)/2) \), supported on \([- (b - a)/2h, (b - a)/2h] \), while \( \hat{x}_\pm^h \) correspond to the rescaled Jost’s functions

\[
\hat{x}_\pm^h(y) = \chi_\pm^h(hy + (b + a)/2)e^{-i\zeta y},
\]

(2.15)

In this framework the Proposition 2.2 in [15] applies; this yield \( \hat{C} \) of the origin.

Let \( \zeta \in \mathbb{C}^+ \) be such that: \( \zeta^2 \in \text{res}(H_0^b) \); rephrasing the relation [24, Chp. 5, eq. (1.10)] in our framework, we get

\[
G^{\zeta, h}(\cdot, y) = \frac{1}{h^2w(\zeta)} \left\{ \begin{array}{ll}
\chi_+^h(\cdot, \zeta) \chi_-^h(y, \zeta), & x \geq y, \\
\chi_-^h(\cdot, \zeta) \chi_+^h(y, \zeta), & x < y,
\end{array} \right.
\]

(2.16)

\[
H^{\zeta, h}(\cdot, y) = \frac{1}{h^2w(\zeta)} \left\{ \begin{array}{ll}
\chi_+^h(\cdot, \zeta) \partial_y \chi_-^h(y, \zeta), & x \geq y, \\
\chi_-^h(\cdot, \zeta) \partial_y \chi_+^h(y, \zeta), & x < y,
\end{array} \right.
\]

(2.17)

where \( w(\zeta) \), depending only on \( \zeta \) and \( V \), denotes the Wronskian associated to the couple \( \{ \chi_+^h(\cdot, \zeta), \chi_-^h(\cdot, \zeta) \} \) (defined by: \( w(f, g) = fg' - f'g \)). Due to the result of the Lemma 2.2, for each \( h > 0 \), the maps \( z \mapsto G^{\zeta, h}(x, y) \), \( z \mapsto H^{\zeta, h}(x, y) \) are meromorphic on \( \mathbb{C} \setminus \mathbb{R}_+ \) with a branch cut along the positive real axis and poles, corresponding to the points in \( \sigma_p(H_0^b) \) located on the negative real axis. Adapting [24, Chp. 5, eq. (1.9)] to the \( h \)-dependent case, the function \( w(k) \) fulfills the identity: \( |w(k)^2| = k^2/h^2 + |w_0^b(k)|^2 \), where \( w_0^b(k) \) is the wronskian associated to the couple \( \{ \chi_+^b(\cdot, -k), \chi_-^b(\cdot, k) \} \). In particular, the inequality

\[
\frac{1}{|w_0^b(k)|} \leq \frac{h}{|k|},
\]

(2.18)

implies that the maps \( z \mapsto G^{\zeta, h}(x, y) \), \( z \mapsto H^{\zeta, h}(x, y) \) continuously extend up to the branch cut, both in the limits \( z \to k^2 \pm i0 \), with the only possible exception of the point \( z = 0 \).

The above characterization and the definition (2.11) imply that \( z \mapsto (B_0 q(z, h) - A_0) \) is meromorphic matrix-valued map on \( \mathbb{C} \setminus \mathbb{R}_+ \) with continuous extension to \( z \to k^2 \pm i0 \) for \( k \neq 0 \). Due to the identity (2.9), the conditions: \( z \in \text{res}(H_0^b) \) and \( 0 \notin \text{res}(B_0 q(z, h) - A_0) \) (i.e.: \( z \) is a pole for the inverse, matrix-valued, function \( z \to (B_0 q(z, h) - A_0)^{-1} \), compel: \( z \in \sigma_p(H_0^b) \). Nevertheless, according to the result of the Proposition 2.1 for defined positive potentials it results: \( \text{res}(H_0^b) = \text{res}(H_0^b) \subset \mathbb{C} \setminus \mathbb{R}_+ \) provided that: \( \theta \in B_0(0) \), for a small \( \delta > 0 \) possibly depending on \( h \). Hence, under these conditions, the inverse \( (B_0 q(z, h) - A_0)^{-1} \) exists in \( \mathbb{C} \setminus \mathbb{R}_+ \) and has continuous extensions to the branch cut both in the limits \( z \to k^2 \pm i0 \), with the only possible exception of the origin.

The generalized eigenfunctions of our model, next denoted with \( \psi_0^h(\cdot, k) \), solve of the boundary value problem

\[
\begin{cases}
(-h^2\partial_y^2 + V) u = k^2 u, \quad x \in \mathbb{R} \setminus \{a, b\}, \quad k \in \mathbb{R}, \\
e^{-\theta/2}u(b^+) = u(b^-), \quad e^{-\theta^3/2}u'(b^+) = u'(b^-), \\
e^{-\theta/2}u(a^-) = u(a^+), \quad e^{-\theta^3/2}u'(a^-) = u'(a^+),
\end{cases}
\]

(2.19)

and fulfill the exterior conditions

\[
\psi_0^h(x, k)|_{x=a} = e^{i\xi x} + R^h(k, \theta)e^{-i\xi x}, \quad \psi_0^h(x, k)|_{x=b} = T^h(k, \theta)e^{i\xi x},
\]

(2.20)

\[
\psi_0^h(x, k)|_{x=a} = T^h(k, \theta)e^{i\xi x}, \quad \psi_0^h(x, k)|_{x=b} = e^{i\xi x} + R^h(k, \theta)e^{-i\xi x},
\]

(2.21)
describing an incoming wave function of momentum \( k \) with reflection and transmission coefficients \( R^h \) and \( T^h \). For \( \theta = 0 \), the generalized eigenfunctions of \( H^h_0 \), \( \psi^h_0(\cdot,k) \), depend on the Jost’s solutions \( \chi^h_{\pm} \) according to

\[
\psi^h_0(x,k) = \begin{cases}
-\frac{2ik}{hw(x)}\chi^h_{\pm}(x,k), & \text{for } k \geq 0, \\
\frac{2ih}{w(-x)}\chi^h_{\pm}(x,-k), & \text{for } k < 0.
\end{cases}
\] (2.22)

Following an approach similar to the one leading to the Krein-like resolvent formula \( (2.9) \), an expansion for the difference: \( \psi^h_0(x,k) - \psi^h_0(x,k) \) as \( \theta \to 0 \) has been provided with In [16, eq. (2.19) and (2.26)]. Let \( G^{k,h} \) and \( H^{k,h} \) be defined by

\[
G^{\pm |k|,h}(\cdot,y) = \lim_{\gamma \to k^\pm \pm 0} G^{\pm,k,h}(\cdot,y), \quad H^{\pm |k|,h}(\cdot,y) = \lim_{\gamma \to k^\pm \pm 0} H^{\pm,k,h}(\cdot,y),
\] (2.23)

and denote with \( g_{k,h,j} \) and \( M^h \) the corresponding limits of \( \gamma_{z,h,j} \) and \( (B_\theta q(z,h) - A_\theta) \) (see the definitions \( 2.8 \), \( 2.11 \) and \( 2.10 \)); namely, we set

\[
g_{\pm |k|,h,j} = \lim_{\gamma \to k^\pm \pm 0} \gamma_{z,h,j}, \quad M^h (\pm |k|, \theta) = \lim_{\gamma \to k^\pm \pm 0} (B_\theta q(z,h) - A_\theta).
\] (2.24)

Due to \( 2.16 \) - \( 2.17 \), \( G^{k,h} \) and \( H^{k,h} \) explicitly write as

\[
G^{k,h}(\cdot,y) = \frac{1}{h^2w^h(k)} \begin{cases}
\chi^h_{\pm}(\cdot,k) \chi^h_{\pm}(y,k), & x \geq y, \\
\chi^h_{\pm}(\cdot,k) \chi^h_{\mp}(y,k), & x < y,
\end{cases}
\] (2.25)

\[
H^{k,h}(\cdot,y) = \frac{-1}{h^2w^h(k)} \begin{cases}
\chi^h_{\pm}(\cdot,k) \partial_1 \chi^h_{\pm}(y,k), & x \geq y, \\
\chi^h_{\pm}(\cdot,k) \partial_1 \chi^h_{\mp}(y,k), & x < y,
\end{cases}
\] (2.26)

while, according to the previous remarks, \( g_{k,h,j} \) and \( M^h(k, \theta) \) are well defined and continuous w.r.t. \( k \in \mathbb{R} \), with the only possible exception of the origin. Denoting with

\[
S^h(\theta) = \left\{ k \in \mathbb{R} \mid \det M^h(k, \theta) = 0 \right\}.
\] (2.27)

the set of the singular points of \( M^h(k, \theta) \), the representation ([16, Proposition 2.2])

\[
\psi^h_0(\cdot,k) = \left\{ \psi^h_0(\cdot,k) - \sum_{i,j=1}^4 \left[ (M^h(k, \theta))^{-1} B_\theta \right]_{ij} \Gamma^h_{k,j} g_{k,h,j}, \quad \text{for } k > 0, \\
\psi^h_0(\cdot,k) - \sum_{i,j=1}^4 \left[ (M^h(-k, \theta))^{-1} B_\theta \right]_{ij} \Gamma^h_{k,j} g_{-k,h,j}, \quad \text{for } k < 0,
\right.\] (2.28)

holds for any fixed \( h > 0, \theta \in \mathbb{C} \) and \( k \in \mathbb{R}^\star \setminus S^h(\theta) \), being \( \Gamma^k,h \) the vector of the boundary values

\[
2\Gamma^k,h = (\psi^h_0(b,k), \partial_1 \psi^h_0(b,k), \psi^h_0(a,k), \partial_1 \psi^h_0(a,k)).
\] (2.29)

2.1 Trace estimates

We aim to control the coefficients at the r.h.s. of \( 2.28 \) when both \( \theta \) and \( h \) are small. This requires accurate estimates for the boundary values of \( g_{k,h,j} \) (occurring in the definition of the matrix \( M^h(k, \theta) \)) and \( \psi^h_0(\cdot,k) \). In [16, eq. (2.19) and (2.26)] these estimates have been provided with, for a finite energy range, when the potential describes quantum wells in a semiclassical island. We next reconsider this problem under a generic condition of positivity for \( 1_{[a,b]} \mathcal{V} \). To this aim, we recall some standard energy estimates; let consider the problem

\[
\begin{cases}
(-h^2\partial_x^2 + \mathcal{V} - \zeta^2) u = 0, & \text{in } (a, b), \\
h \partial_x + i\zeta u(a) = \gamma_a, & h \partial_x - i\zeta u(b) = \gamma_b,
\end{cases}
\] (2.30)

where: \( \mathcal{V} \in L^\infty((a, b), \mathbb{R}), \gamma_a, \gamma_b \in \mathbb{C}, \) and \( h > 0 \).

**Lemma 2.3** Assume \( \zeta \in \mathbb{C}^\star \) such that: \( \mathcal{V} - \text{Re } \zeta^2 > c \) for some \( c > 0 \). The solution of \( 2.30 \) fulfills the estimate

\[
h^{\frac{1}{2}} \sup_{[a,b]} |u| + \|hu\|_{L^2([a,b])} \leq C_{a,b,c} \frac{1}{h^{\frac{1}{2}}} (|\gamma_a| + |\gamma_b|),
\] (2.31)

with \( C_{a,b,c} > 0 \) possibly depending on the data.
Proof. From the equation
\[ \langle u, (-h^2 \partial_x^2 + V - \zeta^2) u \rangle = 0, \]
an integration by parts yields
\[ \|hu'\|_{L^2([a,b])}^2 + \int_a^b (V - \zeta^2) |u|^2 \, dx + h^2 (u^* u'(a) - u^* u'(b)) = 0. \]  
Taking into account the boundary conditions in (2.31), our assumptions \((V - \Re \zeta^2 > c)\) and \(\Im \zeta \geq 0\) imply
\[ \|hu'\|_{L^2([a,b])}^2 + c \|u\|_{L^2([a,b])}^2 \leq h \Re (|u^*(a)| |\gamma_a| - |u^*(b)| |\gamma_b|). \]
The estimate (2.31) then follows from (2.34) by taking into account the Gagliardo-Nirenberg inequality: \(\sup_{[a,b]} |\varphi| \leq C_0 |\varphi'|^2 \|\varphi\|_{L^2([a,b])}^{2/3} \|\varphi\|_{L^2([a,b])}^{1/3}.\)

When the differential operator \((-h^2 \partial_x^2 + V - k^2)\) is defined with a potential \(V \in L^\infty(\R, \R)\) compactly supported on \([a, b]\), the corresponding Green’s functions solve boundary value problems of the type (2.30) and the Lemma 2.2 applies if: \(V - k^2 > c\). Global-in-\(k\) estimates for their boundary values are next considered by combining the explicit representations in terms of the Jost’s solutions, given in (2.25)--(2.26) and (2.22), and energy estimates in the low-energy regime. To this aim, we next assume the potential to be defined according to stronger condition
\[ V \in L^\infty(\R, \R), \quad \sup \operatorname{supp} V = [a, b], \quad 1_{[a,b]} V > c, \]
holding for some \(c > 0\).

**Proposition 2.4** Let \(V\) fulfills the conditions (2.36); the relations
\[ |(1 + k) \psi_0(y, k)| + h |\partial_0 \psi_0(y, k)| \leq |k| C_{a,b,c}, \]
\[ |(1 + k) G^{k,h}(y, y')| + |1_{[a,b]} H^{k,h}(y, y')| + h |k|^{-1} |\partial_0 H^{k,h}(y, y')| \leq C_{a,b,c} h^{-2}, \]
hold for \(y, y' \in [a, b]\) and \(k \in \mathbb{R}\), being \(C_{a,b,c} > 0\) possibly depending on the data and \(h \in (0, h_0]\) with \(h_0 > 0\) small.

Proof. From the result of the Lemma 2.2 the Jost’s solutions \(\chi_{\pm}^k(x, k)\) are \(C^1\)-continuous and the exterior conditions (2.13) can be used for the explicit computation of \(\partial_0 \chi_{\pm}^k(y, k)\) when \(y = a, b\) and \(j = 0, 1\). Then, the relations (2.22), (2.25)--(2.26) allow to obtain (almost) explicit representations of the quantities considered in (2.36)--(2.37). Let start considering the boundary values \(\partial_0 \psi_0(y, k)\); we focus on the case \(y = a\), while similar computations hold for \(y = b\). If \(k < 0\), the representation (2.22) and the exterior conditions (2.13) imply
\[ 1_{\{k < 0\}}(k) \psi_0(a, k) = -\frac{2i k}{h w^h(-k)} e^{i \frac{k}{h} a}, \quad \text{and} \quad 1_{\{k > 0\}}(k) \partial_0 \psi_0(a, k) = -\frac{2k^2}{h w^h(-k)} e^{i \frac{k}{h} a}. \]
Recalling that \(w^h(-k) = (w^h(k))^\ast\), the inequality (2.18) leads to
\[ |1_{\{k < 0\}}(k) \psi_0(a, k)| \leq 2, \quad \text{and} \quad |1_{\{k < 0\}}(k) \partial_0 \psi_0(a, k)| \leq 2 |k|. \]
If \(k \geq 0\), comparing (2.20) with (2.22) and taking into account (2.13), we get the relation
\[ 1_{\{k > 0\}}(k) T^h(k, 0) = -\frac{2ik}{h w^h(k)}, \]
which, using (2.18), leads us to: \(|1_{\{k > 0\}}(k) T^h(k, 0)| \leq 2\). The identity: \(|T^h(k, 0)|^2 + |R^h(k, 0)|^2 = 1\), leads to a similar bound for the reflection coefficients \(R^h(k, 0)\) when \(k \geq 0\); hence, using the representations
\[ 1_{\{k \geq 0\}}(k) \psi_0(a, k) = e^{i \frac{k}{h} a} + R^h(k, 0) e^{-i \frac{k}{h} a}, \quad 1_{\{k \geq 0\}}(k) \partial_0 \psi_0(a, k) = i \frac{k}{h} \left( e^{i \frac{k}{h} a} - R^h(k, 0) e^{-i \frac{k}{h} a} \right), \]
yields
\[ |1_{\{k \geq 0\}}(k) \psi_0(a, k)| \leq 4, \quad |1_{\{k \geq 0\}}(k) \partial_0 \psi_0(a, k)| \leq 4 \frac{k}{h}. \]
From (2.39), (2.41), and from similar computations in the case of \(y = b\), follows
\[ |\psi_0(y, k)| + h |k|^{-1} |\partial_0 \psi_0(y, k)| \leq C_{a,b,c}, \quad y = a, b. \]
The relations (2.37) are next considered for $y' = a$ (when $y' = b$ the result follows from similar computations). According to (2.22), we have
\[
\left|1_{\{k \geq 0\}}(k)(hw(k))^{-1} \partial_i^k \chi^h_+(a,k)\right| + \left|1_{\{k < 0\}}(k)(hw(k))^{-1} \partial_i^k \chi^h_-(b,-k)\right| \leq \left|\frac{a,b,c}{2|k|}\right| \left|\frac{|k|}{h}\right|^j, \quad j = 0,1.
\] (2.44)
with $j = 0,1$. Both these relations easily extend to all $k < 0$ by recalling that: $w^h(-k) = (w^h(k))^*$ and $\partial_i^k \chi^h_+(-, -k) = (\partial_i^k \chi^h_+ , , k)$. Finally, the identities: $\partial_i^k \chi^h_+(b, k) = (\frac{i}{k})^j e^{-i k a}$ and $\partial_i^k \chi^h_+(a, k) = -i \frac{n}{k} e^{-i k a}$ (arising from (2.13)) and the inequality (2.18) allow to generalize this result to all $y = a,b$. This resums as follows
\[
\left|(hw(k))^{-1} \partial_i^k \chi^h_+(y,k)\right| \leq \left|\frac{a,b,c}{2|k|}\right| \left|\frac{|k|}{h}\right|^j, \quad y = a,b, \quad j = 0,1.
\] (2.46)
From the representation (2.29), the boundary values $G^{k|k, h}(y, a)$ write as
\[
G^{k, h}(y, a) = \frac{1}{h^3 w(k)} \chi^h_+(y,k) e^{-i k a}, \quad for \; y \in \{a, b\}.
\] (2.47)
Let $c > 0$ be such that (2.35) holds at consider at first the case $k^2 \geq c$; using (2.46) with $j = 0$, we get
\[
\left|1_{\{k^2 \geq c\}}(k) G^{k, h}(y,a)\right| \leq \left|\frac{a,b,c}{h|k|}\right| \left|\frac{|k|}{h}\right|, \quad y = a, b,
\] (2.48)
for a suitable $\tilde{C}_{a,b,c} > 0$ (depending on $a, b, c$). The function $G^{k|k, h}(\cdot, a)$ solves an equation of the type (2.30) with: $\gamma_1 = -\frac{1}{h}$ and $\gamma_2 = 0$; when $k^2 \leq c$, the lemma (2.3) applies, allowing to control the boundary values $G^{k|k, h}(y, a)$ according to
\[
\left|1_{\{k^2 < c\}}(k) G^{k, h}(y,a)\right| \leq \tilde{C}_{a,b,c} h^{-2}, \quad y = a, b.
\] (2.49)
Hence, (2.48)-(2.49) lead us to
\[
\left|(1 + |k|) G^{k, h}(y,a)\right| \leq \tilde{C}_{a,b,c} h^{-2}, \quad y = a, b.
\] (2.50)
Using the representation (2.20), the exterior condition: $1_{\{x < a\}}(x) \chi^h_+(x, k) = e^{-i k x}$ and the $C_1$-regularity of $\chi^h_+ (\cdot, k)$, it follows
\[
|1_{\{a, b\}} H^{k, h}(y,a)\right| = \frac{i k}{h^3 w(k)} \chi^h_+(y,k) e^{-i k a}, \quad y = a, b,
\] (2.51)
and the inequality (2.46), $j = 0$, yields
\[
\left|H^{k, h}(y,a)\right| \leq \frac{a,b,c}{h^2}, \quad y = a, b.
\] (2.52)
Using once more (2.20), we have
\[
\partial_i H^{k, h}(y,a) = \frac{\partial_i^k}{h^3 w(k)} \partial_i \chi^h_+(y,k) e^{-i k a}, \quad y = a, b.
\] (2.53)
Then, (2.46), $j = 1$, implies
\[
\left|\partial_i H^{k, h}(a,a)\right| \leq \frac{|k|}{h^2}, \quad y = a, b.
\] (2.54)
For $y' = a$, the inequality (2.31) follows from (2.50), (2.52) and (2.54) with a suitable $C_{a,b,c}$.

Finally, we reconsider the bound (2.46); according to (2.20), the relation (2.31) yields
\[
G^{k, h}(b, a) = (h^2 w(k))^{-1} e^{i k (b-a)} = \mathcal{O} \left( h^{-2} \right),
\] (2.55)
uniformly w.r.t. $k \in \mathbb{R}$. It follows: $\inf |w(k)| > c_0$ for a suitable $c_0 > 0$ possibly depending on the data, while, taking into account (2.13), we get: $(w(k))^{-1} = \mathcal{O} \left((1 + k)^{-1}\right)$. Hence, the relations (i)-(2.38), (2.40) and (ii)-(2.41), yield: $|\psi_0^h(a,k)| = \mathcal{O} \left(k (1 + k)^{-1}\right)$; this improves the previous estimates according to (2.38).
Remark 2.5 The result presented in (2.4) stands upon the regularity of the Jost’s solution at the boundaries points \{a, b\}. This property, considered in the Lemma 2.2, generically holds for positive defined and compactly supported potentials, while the trace estimates (2.36)-(2.37) do not depend on \(V\), provided that it fulfills the conditions (2.35).

2.2 Generalized eigenfunctions expansion.

The result of the Proposition 2.4 can be implemented to obtain an expansion of the modified generalized eigenfunctions \(\psi^h_\theta(\cdot, k)\) when both \(\theta\) and \(h\) are small. Using the notation introduced in (2.23) and (2.24), a direct computation leads to

\[
\mathcal{M}^h (k, \theta) = \begin{pmatrix}
\beta (\theta) H^{k,h}\beta(h, b) & -\beta (\theta) \beta_h \beta_h(b, b) & \beta (\partial_h H^{k,h}(b, a)) & -\beta (\partial_h H^{k,h}(b, a)) \\
\beta (\theta) G^{k,h}(b, b) & -\beta (\theta) H^{k,h}(b, b) & \beta (\theta) G^{k,h}(b, a) & -\beta (\theta) H^{k,h}(b, a) \\
\beta (\theta) G^{k,h}(a, b) & -\beta (\theta) H^{k,h}(a, b) & \beta (\theta) G^{k,h}(a, a) & -\beta (\theta) H^{k,h}(a, a) \\
\beta (\theta) G^{k,h}(a, b) & -\beta (\theta) H^{k,h}(a, b) & \beta (\theta) G^{k,h}(a, a) & -\beta (\theta) H^{k,h}(a, a)
\end{pmatrix}
\]

where \(\alpha (\theta)\) and \(\beta (\theta)\) are defined by

\[
\alpha (\theta) = 1 + e^\frac{\theta}{2}, \quad \beta (\theta) = 1 - e^\frac{\theta}{2}.
\]

As consequence of the estimates (2.36)-(2.37), for defined positive potentials the above relation rephrases as

\[
\mathcal{M}^h (k, \theta) = -\frac{1}{h^2} \begin{pmatrix}
\alpha (\theta) & \alpha (\theta) & \alpha (\theta) & \alpha (\theta) \\
\beta (\theta) & \beta (\theta) & \beta (\theta) & \beta (\theta) \\
\beta (\theta) & \beta (\theta) & \beta (\theta) & \beta (\theta) \\
\beta (\theta) & \beta (\theta) & \beta (\theta) & \beta (\theta)
\end{pmatrix}
\]

being the symbols \(\mathcal{O} (\cdot)\) referred to the metric space \(\mathbb{R} \times (0, h_0]\) and defining continuous functions of \(k \in \mathbb{R}\). From the definition of \(\alpha (\theta), \beta (\theta)\), the coefficients of \(\mathcal{M}^h (k, \theta)\) result \(\theta\)-holomorphic and continuous w.r.t. \((k, \theta) \in \mathbb{C} \times \mathbb{R}\) while, using the expansions: \(\alpha (\theta) = 2 + \mathcal{O} (\theta)\) and \(\beta (\theta) = \mathcal{O} (\theta)\), follows

\[
\mathcal{M}^h (k, \theta) = -\frac{2}{h^2} \mathcal{O} (\mathcal{C}^1 + \theta m^h (k, \theta)),
\]

where the remainder term is

\[
m^h (k, \theta) = \begin{pmatrix}
\mathcal{O} (h^{-2}) & \mathcal{O} (|k| h^{-3}) & \mathcal{O} (h^{-2}) & \mathcal{O} (\mathcal{K} |h| h^{-3}) \\
\mathcal{O} (h^{-2}) & \mathcal{O} (h^{-2}) & \mathcal{O} (h^{-2}) & \mathcal{O} (|k| h^{-3}) \\
\mathcal{O} (h^{-2}) & \mathcal{O} (|k| h^{-3}) & \mathcal{O} (h^{-2}) & \mathcal{O} (h^{-2}) \\
\mathcal{O} (h^{-2}) & \mathcal{O} (h^{-2}) & \mathcal{O} (|k| h^{-3}) & \mathcal{O} (h^{-2})
\end{pmatrix},
\]

Hence, \(\mathcal{M}^h (k, \theta)\) is invertible for all \(k\) provided that \(\theta\) is small depending on \(h\), while, from the representation (2.23), an expansion of \(\psi^h_\theta(\cdot, k)\) for small values of \(\theta\) follows.

Proposition 2.6 Assume \(h \in (0, h_0]\), \(\theta \leq h^2\) and let \(V\) be defined according to (2.35) for some \(c > 0\). For a suitably small \(h_0\), the solutions \(\psi^h_\theta(\cdot, k)\) of the generalized eigenfunctions problem (2.21), (2.22) - (2.24) allow the expansion

\[
\psi^h_\theta (\cdot, k) - \psi^h (\cdot, k) = \mathcal{O} \left( \frac{\theta k}{h} \right) G^{[k, h]} (\cdot, b) + \mathcal{O} \left( \frac{\theta k}{1 + k} \right) H^{[k, h]} (\cdot, b) + \mathcal{O} \left( \frac{\theta k}{h} \right) G^{[k, h]} (\cdot, a) + \mathcal{O} \left( \frac{\theta k}{1 + k} \right) H^{[k, h]} (\cdot, a),
\]
where the symbols \( O(\cdot) \) denote functions of the variables \( \{\theta, k, h\} \in \mathcal{B}_{h^2}(0) \times \mathbb{R} \times (0, h_0] \) holomorphic w.r.t. \( \theta \) and continuous in \( k \).

**Proof.** The coefficients of the remainder \( m^h(k, \theta) \) in (2.59)–(2.60), depending on the variables \( \{\theta, k, h\} \), are \( O(h^{-3}) \); hence, for \( |\theta| \leq h^2 \) and \( h \in (0, h_0] \) with \( h_0 \) suitably small, the expansion (2.60), rephrasing as: \( M^h(k, \theta) = -2h^{-2}1_{C_G} + O(h^{-1}) \), defines an invertible matrix for all \( k \in \mathbb{R} \) and the representation (2.28) globally holds. In particular, from (2.59)–(2.60), a direct computation yields

\[
\det M^h(k, \theta) = h^{-8}(16 + O(h)) ,
\]

and

\[
(M^h(k, \theta))^{-1} = h^2 \begin{pmatrix}
-1/2 + O(h) & O(h) & O(2h) & O(hk) \\
O(h^2(1+k)^{-1}) & -1/2 + O(h) & O(h^2(1+k)^{-1}) & O(h) \\
O(h) & O(h^2(1+k)^{-1}) & -1/2 + O(h) & 0 \\
O(h^2(1+k)^{-1}) & 0 & O(h) & O(h^2(1+k)^{-1}) \\
\end{pmatrix}
\]  

(2.63)

From the relations (2.30) and the definitions (2.10), (2.29), follows

\[
B_{\theta} \Gamma_{k,h} = \left\{ O\left(\frac{\theta k}{h}\right), O\left(\frac{\theta k}{1+k}\right), O\left(\frac{\theta k}{h}\right), O\left(\frac{\theta k}{1+k}\right) \right\} .
\]

(2.64)

where the symbols \( O(\cdot) \) are referred to the metric space \( \mathcal{B}_{h^2}(0) \times \mathbb{R} \times (0, h_0] \). Making use of the above relations, we get

\[
(M^h(k, \theta))^{-1} B_{\theta} \Gamma_{k,h} = \left\{ O\left(\frac{\theta k}{h}\right), O\left(\frac{\theta k}{1+k}\right), O\left(\frac{\theta k}{h}\right), O\left(\frac{\theta k}{1+k}\right) \right\}
\]

(2.65)

Then, the expansion (2.61) follows from the formula (2.28)–(2.29) by taking into account (2.65) and the definition of \( g_{k,h,j} \). 

### 2.3 Stationary wave operators and uniform-in-time estimates for the dynamical system.

Following [15], we next construct a similarity between \( H^b_\psi \) and \( H^b_0 \) by making use of the stationary waves operators related to the scattering system \( \{H^b_\psi, H^b_0\} \). Let us recall that, for potentials defined as in (2.4), the generalized Fourier transform associated to \( H^b_0 \),

\[
(F^b_\psi \varphi)(k) = \int_{\mathbb{R}} \frac{dx}{(2\pi h)^{1/2}} \left( \psi^b_\psi(x,k) \right)^* \varphi(x) , \quad \varphi \in L^2(\mathbb{R}) ,
\]

is a bounded operator on \( L^2(\mathbb{R}) \) with a right inverse coinciding with the adjoint \( (F^b_\psi)^* \)

\[
(F^b_\psi)^* f(x) = \int \frac{dk}{(2\pi h)^{1/2}} \psi^b_\psi(x,k) f(k) ,
\]

(2.67)

and it results: \( F^b_\psi (F^b_\psi)^* = 1_{L^2(\mathbb{R})} \) in \( L^2(\mathbb{R}) \), while the product \( (F^b_\psi)^* F^b_\psi \) defines the projector on the absolutely continuous subspace of \( H^b_0 \) (cf. [24]). In addition, when \( \psi \) is positive defined, \( H^b_0 \) has a purely absolutely continuous spectrum compatible with \( R^+ \); in this case \( F^b_\psi \) is an unitary map with range \( L^2(\mathbb{R}) \) and the representation: \( 1_{L^2(\mathbb{R})} = (F^b_\psi)^* (F^b_\psi) \) holds. According to the above notation, the standard Fourier transform operator, corresponding to the case \( \psi = 0 \), is next denoted with \( F^b_0 \). We consider the maps \( \phi^b_\alpha \) and \( \psi^b_\alpha \), acting on \( L^2(\mathbb{R}) \) as

\[
\phi^b_\alpha(\varphi, f) = \int_{\mathbb{R}} \frac{dk}{(2\pi h)^{1/2}} f(k) G^{(k,h)}(\cdot, \alpha) (F^b_\psi \varphi)(k) , \quad \alpha \in \{a,b\} ,
\]

(2.68)

\[
\psi^b_\alpha(\varphi, f) = \int_{\mathbb{R}} \frac{dk}{(2\pi h)^{1/2}} g(k) H^{(k,h)}(\cdot, \alpha) (F^b_\psi \varphi)(k) , \quad \alpha \in \{a,b\} .
\]

(2.69)

Here \( G^{k,h} \) and \( H^{k,h} \) are the limits of the Green’s functions on the branch cut (see the definition in (2.25)–(2.26)), while \( f \) is an auxiliary function, possibly depending on \( h \) and \( \theta \) aside from \( k \).
Lemma 2.7 Let \( h \in (0, h_0] \) and \( \mathcal{V} \) be defined according to (2.34) with \( h_0 \) suitably small. Assume \( f_j=1,2 \in L^\infty_c(\mathbb{R}) \) such that: \( f = \mathcal{O}(k) \) and \( g \left( \frac{k}{1 + |k|} \right) \). Then it results

\[
h \| \phi^h_\alpha(\cdot, f) \|_{L^2(\mathbb{R})}^2 + \| \psi^h_\alpha(\cdot, g) \|_{L^2(\mathbb{R})}^2 \leq C_{a,b,c}h^{-2},
\]

where \( C_{a,b,c} \) is a positive constant depending on the data.

Proof. We show that each of the maps \( \phi^h_\alpha(\cdot, f) \) and \( \psi^h_\alpha(\cdot, g) \), \( \alpha = a, b, c \), can be expressed as superpositions of terms having the following form

\[
1_{\{x > a\}} \mathcal{T}^{\alpha}_h (\mu_1 + \mathcal{P} \phi \mu_2) \mathcal{F}^h_0 + 1_{\{x < a\}} \mathcal{T}^{\alpha}_h (\mu_3 + \mathcal{P} \phi \mu_4) \mathcal{F}^h_0,
\]

where \( \mu_i \in L^\infty_c(\mathbb{R}) \), \( \mathcal{T}^{\alpha}_h = (\mathcal{F}^h_0)^* \) or \( (\mathcal{F}^h_0)^* \) depending on \( \alpha = a, b, \) while \( \mathcal{P} \) denotes the parity operator: \( \mathcal{P} u(t) = u(-t) \). The estimate (2.70) is a direct consequence of this representation. Let us focus on the case \( \alpha = b \) and explicitly consider \( \phi^h_b(\cdot, f) \). As it follows from (2.25)-(2.22), the functions \( G^{[k,h]}(\cdot, b) \) and \( H^{[k,h]}(\cdot, b) \) allow the representations

\[
G^{[k,h]}(x,b) = 1_{\{x > b\}} (x) \frac{1}{h^2 w^h(|k|)} e^{i \frac{b}{h} x} \chi^h_-(b,|k|) + 1_{\{x < b\}} (x) \left( \frac{-1}{2 i |k|h} \right) \psi^h_0(x, -|k|) e^{i \frac{b}{h} x},
\]

\[
H^{[k,h]}(x,b) = 1_{\{x > b\}} (x) \frac{1}{h^2 w^h(|k|)} e^{i \frac{b}{h} x} \partial_1 \chi^h_+(b,|k|) + 1_{\{x < b\}} (x) \left( \frac{|k|}{2h^2 k} \right) \psi^h_0(x, -|k|) e^{i \frac{b}{h} x}
\]

The condition \( f(k) = \mathcal{O}(k) \) and the estimates (2.46) implies: \( (h^2 w^h(k))^{-1} f(k) \chi^h_+(b,|k|) = \mathcal{O}(h^{-2}) \) and \( 1_{\{x < b\}} f(k) e^{i b x} = \mathcal{O}(h^{-1}) \); thus, using (2.72) for \( x \geq b \) we get

\[
1_{\{x > b\}} \phi^h_b(\varphi, f) = 1_{\{x > b\}} \left( \int_0^{+\infty} \frac{dk}{(2\pi h)^{1/2}} \mathcal{O}(h^{-1}) e^{i \frac{b}{h} x} (\mathcal{F}^h_0 \varphi)(k) + \int_{-\infty}^{0} \frac{dk}{(2\pi h)^{1/2}} \mathcal{O}(h^{-1}) e^{-i \frac{b}{h} x} (\mathcal{F}^h_0 \varphi)(k) \right).
\]

The previous identity rephrases as

\[
1_{\{x > b\}} \phi^h_b(\varphi, f) = 1_{\{x > b\}} (\mathcal{F}^h_0)^* \left[ 1_{\{k > 0\}} (k) (\mathcal{O}(h^{-1}) + \mathcal{P} \mathcal{O}(h^{-1})) \mathcal{F}^h_0 \varphi \right],
\]

where the symbols \( \mathcal{O}(\cdot) \), denoting functions of the variables \( k \) and \( h \), are defined in the sense of the metric space \( \mathbb{R} \times (0, h_0] \). Using (2.72) for \( x < b \) leads to

\[
1_{\{x < b\}} \phi^h_b(\varphi, f) = 1_{\{x < b\}} \left( \int_0^{+\infty} \frac{dk}{(2\pi h)^{1/2}} \mathcal{O}(h^{-1}) \psi^h_0(\cdot, -k) (\mathcal{F}^h_0 \varphi)(k) + \int_{-\infty}^{0} \frac{dk}{(2\pi h)^{1/2}} \mathcal{O}(h^{-1}) \psi^h_0(\cdot, k) (\mathcal{F}^h_0 \varphi)(k) \right),
\]

and, proceeding as before, we get

\[
1_{\{x < b\}} \phi^h_b(\varphi, f) = 1_{\{x < b\}} (\mathcal{F}^h_0)^* \left[ 1_{\{k < 0\}} (k) (\mathcal{P} \mathcal{O}(h^{-1}) + \mathcal{O}(h^{-1})) \mathcal{F}^h_0 \varphi \right].
\]

From (2.75) and (2.77), we get a representation of the type given in (2.71); it follows: \( \| \phi^h_b(\varphi, f) \|_{L^2(\mathbb{R})} \lesssim 1/h \| \varphi \|_{L^2(\mathbb{R})} \). In the case of \( \psi^h_0(\varphi, g) \), the representation (2.78) allows similar computations leading to: \( \| \psi^h_0(\varphi, g) \|_{L^2(\mathbb{R})} \lesssim 1/h^2 \| \varphi \|_{L^2(\mathbb{R})} \), while for \( \alpha = a, \) a representation of the type (2.71) for the maps (2.68)-(2.69) is obtained by a suitably adaptation of the previous arguments.

The stationary waves operators \( \mathcal{W}^h_\theta \) are defined by the integral kernel

\[
\mathcal{W}^h_\theta(x,y) = \int_{\mathbb{R}} \frac{dk}{2\pi h} \psi^h_0(x,k) (\psi^h_0(x,k))^*.
\]
Proposition 2.8 Let \( h \in (0, h_0] \), with \( h_0 \) suitably small, \( \mathcal{V} \) be defined according to (2.37) and \( |\theta| \leq h^{N_0} \), with \( N_0 \geq 2 \). Then \( \{ \mathcal{W}_\theta^h \, , \, \theta \in B_{h^{N_0}}(0) \} \) form an analytic family of bounded operators in \( L^2(\mathbb{R}) \) fulfilling the expansion

\[
\mathcal{W}_\theta^h = 1_{L^2(\mathbb{R})} + \mathcal{O} \left( h^{N_0-2} \right),
\]

in the \( L(\mathbb{R}) \) operator norm. For \( \theta \in B_{h^{N_0}}(0) \), the operator \( \mathcal{W}_\theta^h \) maps \( H^2(\mathbb{R}) \) into \( D(H_0^h) \), and it results

\[
H_0^h \mathcal{W}_\theta^h = \mathcal{W}_\theta^h H_0^h.
\]

Proof. Due to our assumptions, \( |\theta| \leq h^2 \), the formula (2.81) applies and the action of \( \mathcal{W}_\theta^h \) on \( \varphi \in L^2(\mathbb{R}) \) writes as

\[
\mathcal{W}_\theta^h \varphi = (\mathcal{F}_\mathcal{V})^* (\mathcal{F}_\mathcal{V}^h \varphi) (k) + \sum_{\alpha = a, b} \int_{\mathbb{R}} \frac{dk}{2\pi h} \left[ \mathcal{O} \left( \frac{\theta k}{h} \right) G^{(k_1)}(\cdot, \alpha) + \mathcal{O} \left( \frac{\theta k}{1+k} \right) H^{(k_1)}(\cdot, \alpha) \right] (\mathcal{F}_\mathcal{V}^h \varphi) (k).
\]

where \( \mathcal{O} (\cdot) \) here denote bounded functions of the variables \( \{ k, \theta, h \} \), holomorphic w.r.t. \( \theta \). With the notation introduced in (2.65)-(2.69), the identities: \( \mathcal{O} (g) = g \mathcal{O} (1) \) (see the definition (1.4)) and \( 1_{L^2(\mathbb{R})} = (\mathcal{F}_\mathcal{V})^* (\mathcal{F}_\mathcal{V}^h \varphi) \) yield

\[
(W_\theta^h - 1_{L^2(\mathbb{R})}) \varphi = \sum_{\alpha = a, b} \left[ \frac{\theta}{h} \phi_\alpha^h (\varphi, \mathcal{O} (k)) + \theta \psi_\alpha^h (\varphi, \mathcal{O} (k (1+k)^{-1})) \right],
\]

Then, the result of the lemma (2.74) applies to the r.h.s. of (2.82) and using \( |\theta| \leq h^{N_0} \), we conclude that

\[
\| W_\theta^h - 1_{L^2(\mathbb{R})} \|_{L(L^2(\mathbb{R}), L^2(\mathbb{R}))} = O \left( h^{N_0-2} \right).
\]

The action of \( \mathcal{W}_\theta^h \) over \( L^2(\mathbb{R}) \) is defined using the expansion (2.82). Each of the maps \( \phi_\alpha^h (\cdot, \mathcal{O} (k)) \) and \( \psi_\alpha^h (\cdot, \mathcal{O} (k (1+k)^{-1})) \), appearing in this formula expresses as a superposition of the form (cf. (2.71))

\[
1_{\{ x \geq \alpha \}} T_\alpha^h (\mu_{1, \alpha} + \mathcal{P} \mu_{2, \alpha}) + 1_{\{ x < \alpha \}} T_\alpha^h (\mu_{3, \alpha} + \mathcal{P} \mu_{4, \alpha}),
\]

\( \mu_{1, \alpha} \) being, in our case, bounded functions of \( \{ k, \theta, h \} \), holomorphic w.r.t. \( \theta \). Thus, \( \phi_\alpha^h (\cdot, \mathcal{O} (k)) \) and \( \psi_\alpha^h (\cdot, \mathcal{O} (k (1+k)^{-1})) \) define holomorphic families of bounded maps on \( L^2(\mathbb{R}) \). This still holds in the case of \( \mathcal{W}_\theta^h \), as it follows by using (2.82).

Let consider the action of \( \mathcal{W}_\theta^h \) on \( H^2(\mathbb{R}) \). As it has been noticed in the Lemma (2.74) the maps \( \phi_\alpha^h (\cdot, f) \) and \( \psi_\alpha^h (\cdot, g) \) are formed by contributions of the type (2.71); since for \( u \in L^\infty(\mathbb{R}) \) the operators \( T_\alpha^h u \mathcal{F}_\mathcal{V}^h \) and \( T_\alpha^h \mathcal{F}_\mathcal{V}^h u \mathcal{F}_\mathcal{V}^h \) map \( H^2(\mathbb{R}) \) into itself, the regularity of these terms is \( H^2(\mathbb{R}) \setminus \{ a,b \} \) and, according to the representation (2.82), \( \mathcal{W}_\theta^h \) maps \( H^2(\mathbb{R}) \) into \( H^2(\mathbb{R}) \setminus \{ a,b \} \), while, due to the definitions (2.19) and (2.78), \( \mathcal{W}_\theta^h \varphi \) fulfills the interface conditions (1.7); then: \( \mathcal{W}_\theta^h \in \mathcal{L}(H^2(\mathbb{R}), D(H_0^h)) \).

Finally, consider the relation (2.80). Let \( \varphi \in H^2(\mathbb{R}) \); using the functional calculus of \( H_0^h \), we have:

\[
(\mathcal{F}_\mathcal{V}^h (\mathcal{W}_\theta^h \varphi)) (k) = k^2 (\mathcal{F}_\mathcal{V} \varphi) (k),
\]

and, from the definition (2.78), the r.h.s. of (2.80) writes as

\[
W_\theta^h H_0^h \varphi = \int_{\mathbb{R}} \frac{dk}{2\pi h} \psi_\theta^h (\cdot, k) k^2 (\mathcal{F}_\mathcal{V} \varphi) (k).
\]

Using once more the definition (2.78) and the relation: \( (H_0^h - k^2) \psi_\theta^h (\cdot, k) = 0 \), the l.h.s. of (2.80) identifies with

\[
H_0^h \mathcal{W}_\theta^h \varphi = \int_{\mathbb{R}} \frac{dk}{2\pi h} \psi_\theta^h (\cdot, k) k^2 (\mathcal{F}_\mathcal{V}^h \varphi) (k).
\]

Remark 2.9 The explicit bounds for the factors \( \mathcal{O} (\cdot) \) appearing in (2.61) depend on the trace estimates provided by the Proposition (2.7). According to the Remark (2.5) these independent from the potential \( \mathcal{V} \) provided that the assumptions are fulfilled. As a consequence, the expansion (2.61), as well as the relations (2.70) and the expansion (2.88) hold uniformly w.r.t. any family of potentials fulfilling the conditions (2.35) for a fixed \( c > 0 \).

Due to the result of the Proposition (2.8), \( \mathcal{W}_\theta^h \) is an invertible map as far as \( h \in (0, h_0) \) and \( |\theta| \leq h^{N_0} \) (with \( N_0 \geq 2 \) and \( h_0 \) small); under these conditions, the intertwining property (2.89) yields a similarity between \( H_0^h \) and \( H_0^h \); this allows to define the quantum dynamics generated by \( H_0^h \) by conjugation.

Theorem 2.10 Let \( h \in (0, h_0) \), with \( h_0 \) suitably small, \( \mathcal{V} \) be defined according to (2.37) and \( |\theta| \leq h^{N_0} \), with \( N_0 \geq 2 \). Then, \( iH_0^h \) generates a strongly continuous group of bounded operators on \( L^2(\mathbb{R}) \). For a fixed \( t \), \( e^{-itH_0^h} \) is \( \theta \)-analytic and allows the expansion

\[
e^{-itH_0^h} = e^{-itH_0^h} = \mathcal{R}(t, \theta), \quad \text{with} \quad \sup_{t \in \mathbb{R}} \| \mathcal{R}(t, \theta) \|_{L(L^2(\mathbb{R}))} = \mathcal{O} \left( h^{N_0-2} \right).
\]
Since $e^{-itH_\theta^0}$ form a strongly continuous group of unitary maps of $L^2(\mathbb{R})$ into itself, and $\mathcal{W}_\theta^0$ is an analytic family w.r.t. $\theta$, the modified propagator $e^{-itH_\theta^0}$ has the same regularity w.r.t. the time and the parameter $\theta$, defining a strongly-continuous-flow on $L^2(\mathbb{R})$. From the identity: $i\partial_t e^{-itH_\theta^0} \psi = H_\theta^0 e^{-itH_\theta^0} \psi$, holding in $L^2(\mathbb{R})$ for any $\psi \in H^2(\mathbb{R})$, it follows

$$i\partial_t \left( e^{-itH_\theta^0} u \right) = H_\theta^0 e^{-itH_\theta^0} u, \quad u \in D \left( H_\theta^0 \right).$$

(2.89)

Then $e^{-itH_\theta^0}$ identifies with the quantum dynamical system generated by $iH_\theta^0$ and the expansion (2.87) follows from (2.79). ■

3 The time dependent case

We consider the time dependent family of modified operators $H_\theta^0 (t)$ defined according to (2.1) when the potential is a continuous function of the time fulfilling the conditions (2.35) uniformly w.r.t. $t$, i.e.

$$\mathcal{V}(t) \in C^0([0, T], L^\infty(\mathbb{R}, \mathbb{R})), \quad \sup \mathcal{V}(t) = [a, b], \quad 1_{[a,b]} \mathcal{V}(t) > c,$$

(3.1)

for a suitable $c > 0$. With this assumption, the operator’s domain does not depend on the time and we have: $D \left( H_\theta^0 (t) \right) = D \left( H_\theta^0 \right)$ for all $t$ (see the definition (2.1)). The corresponding quantum dynamical system is defined by the $\theta$-dependent time propagator $U_{\theta}^h (t, s)$ solving the evolution problem

$$\begin{cases}
    i\partial_t U_{\theta}^h (t, s) u = H_\theta^0 (t) U_{\theta}^h (t, s) u, \\
    U_{\theta}^h (s, s) u = u, \quad u \in D \left( H_\theta^0 \right), \\
    0 \leq s \leq t \leq T.
\end{cases}$$

(3.2)

A standard strategy in the definition of the quantum dynamical system generated by a non-autonomous Hamiltonian, consists in using an approximating sequence whose terms are stepwise products of propagators associated to the ‘instantaneous’ Hamiltonians (cf. [25]). Following this approach for $T > 0$ we introduce the partition $[0, T] = \mathcal{U}_{j=1}^T [t_{j-1}, t_j]$, where $t_j = jT/n$; the step-propagators approximating our dynamics are defined by

$$U_{\theta,n}^h (t, s) = \begin{cases}
    e^{-i(t-s)H_\theta^0 (t_j-1)}, & s, t \in [t_{j-1}, t_j], \\
    U_{\theta,n}^h (t, t_{k+j}) U_{\theta,n}^h (t_{k+j}, t_{k+j+1}) \cdots U_{\theta,n}^h (t_j, s), & s \in [t_{j-1}, t_j], \quad t \in [t_{k+j+1}, t_{k+j}].
\end{cases}$$

(3.3)

Under the assumptions of the Theorem 2.10, $U_{\theta,n}^h (t, s)$ defines, for each $n$, a strongly continuous flow on $L^2(\mathbb{R})$ fulfilling the identities

$$U_{\theta,n}^h (s, s) = 1_{L^2(\mathbb{R})}, \quad U_{\theta,n}^h (t, s) = U_{\theta,n}^h (t, r) U_{\theta,n}^h (r, s), \quad \forall s \leq r \leq t.$$  

(3.4)

**Lemma 3.1** Let $\mathcal{V}(t)$ fulfills the conditions (3.1), $h \in [0, h_0]$, with $h_0$ suitably small, and $|\theta| \leq h^{N_0}$, with $N_0 \geq 2$. There exists $M_{a,b,c} > 0$, possibly depending on the data, such that

$$\sup_{n,h} \left\| U_{\theta,n}^h (t, s) \right\|_{L^2(\mathbb{R})} \leq M_{a,b,c},$$

(3.5)

**Proof.** From the definition (2.88), the modified step propagators $U_{\theta,n}^h (t, s)$ are related to $U_{0,n}^h (t, s)$ by the identity

$$U_{\theta,n}^h (t, s) = \mathcal{W}_\theta^h U_{0,n}^h (t, s) \left( \mathcal{W}_\theta^h \right)^{-1}.$$  

(3.6)

Under our assumptions, $U_{0,n}^h (t, s)$ is unitary for all $n \in \mathbb{N}^+$, $s, t \in [0, T]$ and $h > 0$, while $\mathcal{W}_\theta^h$ and $\left( \mathcal{W}_\theta^h \right)^{-1}$ are bounded uniformly w.r.t. $h \in [0, h_0]$ and $|\theta| \leq h^{N_0}$, with an $L^2$-operator norm possibly depending on $a, b$ and $c$; then (3.4) provide us with the estimate

$$\sup_{h \in [0, h_0]} \left\| U_{\theta,n}^h (t, s) \right\|_{L^2(\mathbb{R})} \leq M_{a,b,c},$$

(3.7)

where $M_{a,b,c}$ is independent from $T$. ■

The definition (3.5) implies: $U_{\theta,n}^h (t, s) u \in D \left( H_\theta^0 \right)$ for any $u \in D \left( H_\theta^0 \right)$, while, introducing: $H_{\theta,n}^h (t) = H_\theta^0 \left( \left\lfloor \frac{t}{n} \right\rfloor \right)$ ($\lfloor \cdot \rfloor$ denotes the floor function), from (2.89) we have

$$i\partial_t U_{\theta,n}^h (t, s) u = H_{\theta,n}^h (t) U_{\theta,n}^h (t, s) u, \quad \forall 0 \leq s \leq t \leq T, \quad u \in D \left( H_\theta^0 \right).$$

(3.8)

We next show that $U_{\theta,n}^h (t, s)$ approximates the the dynamical system $U_\theta^h (t, s)$; the proof adapts the strategy used in [13] Theorem 4.1] to our framework.
Theorem 3.2 Let $\mathcal{V}(t)$ fulfills the conditions (3.7), $h \in (0, h_0]$, with $h_0$ suitably small, and $|\theta| \leq h^{N_0}$, with $N_0 \geq 2$. There exists an unique family of operators $U^h_{\theta}(t, s)$ such that:

i) $U^h_{\theta}(t, s) \in \mathcal{B}(L^2(\mathbb{R}))$, with

$$
\sup_{s, t \in [0, T], \quad h \in (0, h_0]} \|U^h_{\theta}(t, s)\|_{\mathcal{L}(L^2(\mathbb{R}))} \leq M_{a, b, c},
$$

(3.9)

ii) $U^h_{\theta}(t, s)$ is strongly continuous w.r.t. $t$ and $s$, and holomorphic in $\theta$.

iii) $U^h_{\theta}(t, s)$ fulfills the propagator identities (3.3).

iv) $U^h_{\theta}(t, s)$ is the solution of the problem (3.2) for all $u \in D(H^h_{\theta})$.

Proof. From (3.8), the relation

$$(U^h_{\theta,n}(t, s) - U^h_{\theta,m}(t, s)) u = -i \int_0^t U^h_{\theta,n}(t, t') (H^h_{\theta,n}(t') - H^h_{\theta,m}(t')) U^h_{\theta,m}(t', s) u \, dt',
$$

(3.10)

holds for $u \in D(H^h_{\theta})$ and, using the result of the Lemma 3.1, this leads us to the estimate

$$
\|U^h_{\theta,n}(t, s) - U^h_{\theta,m}(t, s)\|_{L^2(\mathbb{R})} \leq M_{a, b, c} \int_0^T \|H^h_{\theta,n}(t') - H^h_{\theta,m}(t')\|_{\mathcal{L}(L^2(\mathbb{R}))} \|u\|_{L^2(\mathbb{R})} \, dt'.
$$

(3.11)

The difference at the r.h.s. writes as

$$
H^h_{\theta,n}(t') - H^h_{\theta,m}(t') = \mathcal{V} \left(\frac{T}{n} \left[\frac{nt}{T}\right]\right) - \mathcal{V} \left(\frac{T}{m} \left[\frac{mt}{T}\right]\right).
$$

(3.12)

and the regularity of $\mathcal{V}(t)$ yields

$$
\lim_{n, m \to \infty} \sup_{h \in (0, h_0]} \|H^h_{\theta,n}(t') - H^h_{\theta,m}(t')\|_{\mathcal{L}(L^2(\mathbb{R}))} = \lim_{n, m \to \infty} \left|\mathcal{V} \left(\frac{T}{n} \left[\frac{nt}{T}\right]\right) - \mathcal{V} \left(\frac{T}{m} \left[\frac{mt}{T}\right]\right)\right|_{L^\infty(\mathbb{R})} = 0.
$$

Hence, for any $u \in D(H^h_{\theta})$, $U^h_{\theta,n}(t, s) u$ forms a Cauchy sequence in $L^2(\mathbb{R})$, uniformly w.r.t. $t, s \in [0, T]$ and $h \in (0, h_0]$. As a consequence, $U^h_{\theta,n}(t, s) u$ uniformly converges to a limit $U^h_{\theta}(t, s) u$ allowing the bound

$$
\sup_{s, t \in [0, T], \quad h \in (0, h_0]} \|U^h_{\theta,n}(t, s) u\|_{L^2(\mathbb{R})} \leq \sup_{t, s, h \in (0, h_0]} \|U^h_{\theta,n}(t, s)\|_{\mathcal{L}(L^2(\mathbb{R}))} \|u\|_{L^2(\mathbb{R})} \leq M_{a, b, c} \|u\|_{L^2(\mathbb{R})}.
$$

(3.13)

Then, using the density of $D(H^h_{\theta})$ in $L^2(\mathbb{R})$ we conclude that $U^h_{\theta,n}(t, s)$ converges to $U^h_{\theta}(t, s)$ in the $\mathcal{L}(L^2(\mathbb{R}))$ topology, uniformly w.r.t. $t, s \in [0, T]$ and $h \in (0, h_0]$. In particular, due to the uniform character of the convergence, the holomorphicity in $\theta$ and the strongly continuity in $t$ and $s$ of $U^h_{\theta,n}(t, s)$ extend to the limit operator $U^h_{\theta}(t, s)$, as well as the identities (3.3). The last point of the statement finally follows by using the Proposition 4.3 in [14] (for this this point we refer to the second part of the the proof of the Theorem 4.1 in [14]). ■

The uniform convergence of $U^h_{\theta,n}(t, s)$ and the relation (3.8) imply

$$
U^h_{\theta}(t, s) = W^h_0 U^h_{0}(t, s) \left(W^h_0\right)^{-1}.
$$

(3.14)

Then, using the expansion (2.7), it easily follows

$$
\sup_{s, t \in [0, T]} \|U^h_{\theta}(t, s) - U^h_{0}(t, s)\|_{\mathcal{L}(L^2(\mathbb{R}))} \leq C_{a, b, c} h^{N_0 - 2},
$$

(3.15)

where $C_{a, b, c}$ is independent from $T$.

### 3.1 The adiabatic evolution problem

According to the expansion (3.8), the dynamical systems $U^h_{\theta}(t, s)$ and $U^h_{0}(t, s)$ are close uniformly-in-time, and independently from the time scale, provided that $|\theta|$ is small enough. This allows us to consider the adiabatic evolution problem corresponding to (3.2).

Lemma 3.3 Assume: $\varepsilon > 0$, $h \in (0, h_0]$ and $|\theta| \leq h^{N_0}$, being $h_0$ suitably small and $N_0 \geq 2$. Let $\mathcal{V}$ fulfill the conditions (3.7), with $T = 1$ and $H_{\theta, \varepsilon}(t)$ denote the time dependent operator defined by (3.3) with the potential: $\mathcal{V}^\varepsilon(t) = \mathcal{V}(\varepsilon t)$. For $u, v \in L^2(\mathbb{R})$ the corresponding time evolution operator $U^h_{\theta, \varepsilon}(t, s)$ fulfills the relation

$$
U^h_{\theta, \varepsilon}(t, 0) u = U^h_{0, \varepsilon}(t, 0) v + u_{\varepsilon, \varepsilon}(t, h, \theta, \varepsilon),
$$

(3.16)
with
\[
\sup_{t \in [0,1/\varepsilon]} \| r_{u,v}(t, h, \theta, \varepsilon) \|_{L^2(\mathbb{R})} \leq K_{a,b,c} \left( \| v \|_{L^2(\mathbb{R})} h^{N_0 - 2} + \| u - v \|_{L^2(\mathbb{R})} \right), \quad \forall \varepsilon > 0,
\]
(3.17)
where \(K_{a,b,c} > 0\) (possibly depending on the data) is independent from \(\varepsilon\).

**Proof.** Under our assumptions, the Theorem 3.22 and the expansion (3.15) apply with \(T = 1/\varepsilon\); in particular, the estimates (3.9) and (3.15) rephrase as
\[
\sup_{s, t \in [0,1/\varepsilon], h \in (0,h_0]} \left\| U_{\theta,\varepsilon}^h (t, s) \right\|_{L^2(\mathbb{R})} \leq M_{a,b,c}, \quad \forall \varepsilon > 0,
\]
(3.18)
and
\[
\sup_{s, t \in [0,1/\varepsilon]} \left\| U_{\theta,\varepsilon}^h (t, s) - U_{0,\varepsilon}^h (t, s) \right\|_{L^2(\mathbb{R})} \leq C_{a,b,c} h^{N_0 - 2}, \quad \forall \varepsilon > 0,
\]
(3.19)
(being \(M_{a,b,c}\) and \(C_{a,b,c}\) independent from \(\varepsilon\)). Then, we have
\[
\left\| U_{\theta,\varepsilon}^h (t, 0) u - U_{0,\varepsilon}^h (t, 0) v \right\|_{L^2(\mathbb{R})} = \left\| U_{\theta,\varepsilon}^h (t, 0) (v + (u - v)) - U_{0,\varepsilon}^h (t, 0) v \right\|_{L^2(\mathbb{R})}
\]
\[
\leq \left\| (U_{\theta,\varepsilon}^h (t, 0) - U_{0,\varepsilon}^h (t, 0)) v \right\|_{L^2(\mathbb{R})} + \left\| U_{\theta,\varepsilon}^h (t, 0) (u - v) \right\|_{L^2(\mathbb{R})},
\]
(3.20)
Using the relations (3.15)-(3.19), we get
\[
\sup_{s, t \in [0,1/\varepsilon]} \left\| U_{\theta,\varepsilon}^h (t, 0) u - U_{0,\varepsilon}^h (t, 0) v \right\|_{L^2(\mathbb{R})} \leq C_{a,b,c} \| v \|_{L^2(\mathbb{R})} h^{N_0 - 2} + M_{a,b,c} \| u - v \|_{L^2(\mathbb{R})}, \quad \forall \varepsilon > 0.
\]
(3.21)
Let \(V\) fulfill the conditions (3.1) with \(T = 1\) and \(H^0_\theta (\tau)\) denote the corresponding time dependent Hamiltonian; the solution of the adiabatic problem
\[
\begin{align*}
&\{ i\varepsilon \partial_\tau \psi_{\theta,\varepsilon}^h (\tau) = H^0_\theta (\tau) \psi_{\theta,\varepsilon}^h (\tau), \quad 0 \leq \tau \leq 1, \\psi_{\theta,\varepsilon}^h (0) = W^0_\theta u, \quad u \in H^2(\mathbb{R}), \}
&\end{align*}
\]
(3.22)
is related to the dynamics \(U_{\theta,\varepsilon} (t, 0)\) through the scaling: \(\psi_{\theta,\varepsilon}^h (\tau) = U_{\theta,\varepsilon}^h (\tau/\varepsilon, 0) W^0_\theta u\). In this framework, the above result rephrases as
\[
\psi_{\theta,\varepsilon}^h (\tau) = \psi_{0,\varepsilon}^h (\tau) + \tilde{r} (\tau, h, \theta, \varepsilon),
\]
(3.23)
with
\[
\sup_{\tau \in [0,1]} \| \tilde{r} (\tau, h, \theta, \varepsilon) \|_{L^2(\mathbb{R})} \leq K_{a,b,c} \left( \| v \|_{L^2(\mathbb{R})} h^{N_0 - 2} + \| (W^0_\theta - 1) u \|_{L^2(\mathbb{R})} \right), \quad \forall \varepsilon > 0,
\]
(3.24)
and, taking into account the expansion (2.79), it follows
\[
\sup_{\tau \in [0,1]} \| \tilde{r} (\tau, h, \theta, \varepsilon) \|_{L^2(\mathbb{R})} \leq K_{a,b,c} \| u \|_{L^2(\mathbb{R})} h^{N_0 - 2}, \quad \forall \varepsilon > 0,
\]
(3.25)
provided that \(h_0\) is small enough. Let \(O \in L^\infty (\mathbb{R}, \mathbb{R})\) be a quantum observable and consider the adiabatic evolution problem for its expected values starting from an initial state \(W^0_\theta u\)
\[
\begin{align*}
&\{ A^h_\theta (\tau, \varepsilon) = \text{Tr} \left[ O \left| \psi_{\theta,\varepsilon}^h (\tau) \right\rangle \left\langle \psi_{\theta,\varepsilon}^h (\tau) \right| \right] \} \\
&i\varepsilon \partial_\tau \psi_{\theta,\varepsilon}^h (\tau) = H^0_\theta (\tau) \psi_{\theta,\varepsilon}^h (\tau), \quad 0 \leq \tau \leq 1, \\psi_{\theta,\varepsilon}^h (0) = W^0_\theta u, \quad u \in H^2(\mathbb{R}), \quad \| u \|_{L^2(\mathbb{R})} = 1.
&\end{align*}
\]
(3.26)
Using the expansion (3.23)-(3.25), a straightforward computation shows that
\[
A^h_\theta (\tau, \varepsilon) = A^h_0 (\tau, \varepsilon) + R (\tau, h, \theta, \varepsilon), \quad \sup_{\tau \in [0,1]} \| R (\tau, h, \theta, \varepsilon) \| \leq \tilde{C}_{a,b,c} h^{N_0 - 2}, \quad \forall \varepsilon > 0,
\]
(3.27)
being \(\tilde{C}_{a,b,c} > 0\) a suitable constant, possibly depending on the data, but independent from \(\varepsilon\).
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