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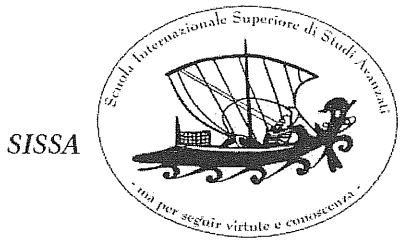

SCUOLA INTERNAZIONALE SUPERIORE DI STUDI AVANZATI
INTERNATIONAL SCHOOL FOR ADVANCED STUDIES

Quantum systems with strong constraining potentials

Thesis submitted for the degree of "Doctor Philosophiæ" in Mathematical Physics
Academic Year 2004–05

Candidate:
Lucattilio Tenuta

Supervisor:
Prof. Gianfausto Dell'Antonio

External referee:
Prof. Peter A. Markowich

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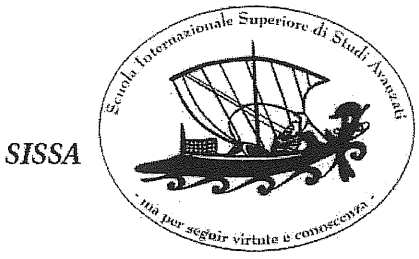

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Chapter 1

Introduction

The aim of this work is to study the motion of a quantum particle in $\mathbb{R}^d$ which is constrained to a submanifold $M \subset \mathbb{R}^d$ of dimension m by a strong potential. More explicitly, by this we mean that the Hamiltonian ruling the dynamics of the particle is given by

$$\widehat{H}(\varepsilon, \hbar) := -\frac{\hbar^2}{2m}\Delta + V(q) + \varepsilon^{-2}W(q), \quad q \in \mathbb{R}^d, \tag{1.1}$$

where ε is a small parameter which eventually goes to zero, and, loosely speaking, the *constraining potential* W is zero on M and strictly positive outside.

We have deliberately avoided to call M a "smooth" submanifold of the configuration space, since an interesting case coming from applications to physics is when M is a graph embedded in $\mathbb{R}^2$ or $\mathbb{R}^3$ and has therefore singular points given by the vertices.

The analysis of the spectrum and the dynamics generated by Hamiltonian (1.1) when $\varepsilon \to 0$ is an old problem in mathematical physics, whose counterpart in classical mechanics is perhaps more widely known because a simple result is quoted in Arnold's textbook to justify the standard treatment of holonomic constraints in Lagrangian mechanics ([Arn], chapter 4; see also [AKN], section 1.6).

From the same point of view, the quantum case has been studied formally by several physicists to get effective equations of motion for a particle living in a proper submanifold of the configuration space, i. e., to "realize holonomic constraints".

In this introduction, we are going to review the main motivations which led to the study of (1.1) both from this traditional aspect and from a more recent one, linked to the effective one dimensional motion of a gas of electrons in modern semiconductor devices, like the so-called quantum circuits. We will also briefly comment on other kinds of partial differential equations (like the elasticity equation in thin domains and the penalized wave equation) which have been analyzed along the same lines of (1.1).

Our aim is to give an account of the existing huge literature in the field, without however the presumption of being exhaustive, but rather of pointing out what we think is missing and deserves more investigation and of highlighting our contribution.

Apart from this introduction, the thesis at hand contains two main parts. In chapter 2 we will study the semiclassical limit of the quantum flow generated by (1.1) under the scaling $\varepsilon = a\hbar$, $a \in \mathbb{R}_+$. The analysis will be carried out for *smooth submanifolds of generic dimension and codimension*, under suitable regularity hypotheses on W (conditions $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$ of subsection 1.1.1). Using a technique developed by Hagedorn [Ha_1, Ha_2] to construct approximate solutions to the Schrödinger equation which are localized along a classical trajectory, we show that the semiclassical limit actually coincides with the limit of the classical flow associated to the Hamiltonian (1.1) when $\varepsilon \to 0$. When the assumptions on the potential are not satisfied, we will give an example where an interesting phenomenon, called *Takens chaos* [Tak] occurs. This will give us also the occasion to make a comparison with the results obtained in classical mechanics using homogenization techniques for ordinary differential equations [Bor].

In chapter 3 we will consider the case where M is a graph embedded in $\mathbb{R}^2$. As it is explained in section 1.2, this case is relevant for applications to nanophysics and theoretical chemistry. In the framework of *adiabatic approximation*, we will consider initial states belonging to *almost invariant subspaces* [Teu] for the total dynamics, and we will deduce an effective dynamics for the motion on the graph in every subspace. For a generic graph, the limit equation will be calculated only outside the vertices, but for a graph with two edges we will propose a different approximation which leads to Dirichlet boundary conditions.

In the end we will discuss open problems and future perspectives, mainly regarding applications to physics.

Even though it will not be stressed sectionwise, it should be emphasized that all the results mentioned above have been obtained in collaboration with my Ph.D. advisor, Gianfausto Dell'Antonio, and a part of them has already appeared in [DeTe].

1.1 A tool to realize holonomic constraints

From a physical viewpoint, one always thinks of a (holonomic) constraint as a complex of forces acting on a system which is then obliged to stay in the vicinity of a given submanifold M of the configuration space.

This gives rise to the distinction between ideal and real constraints (see, e. g., [Gal], chapter 3 and mainly sections 3.6 and 3.10), or, in other words, to the question whether the true motion of the system can be approximated by a simpler one which involves only the variables belonging to M and to which extent the standard mathematical description of constrained motion corresponds to physical reality.

For the sake of clarity, we split our discussion of this point into two parts. We first recall known results in classical mechanics, and then we elaborate on the quantum mechanical case, which presents some characteristic features due mainly to the uncertainty principle.

1.1.1 Classical mechanics

To characterize a real holonomic constraint, we consider the Lagrangian (acting on $\mathbb{R}^d \times \mathbb{R}^d$)

$$L_\varepsilon(q,\dot{q}) := \frac{1}{2}m\dot{q}^2 - V(q) - \varepsilon^2 W(q), \tag{1.2}$$

where V is bounded from below and W models the external forces which constrain the system.[1] Concretely, we suppose that W satisfies the following

Condition W_1. *Let the potential W be non-negative, $W \geq 0$, and let $M := \{q \in \mathbb{R}^d : W(q) = 0\} = \{q \in \mathbb{R}^d : DW(q) = 0\}$ be a smoothly embedded m-dimensional submanifold. Moreover, let us suppose that the Hessian $\mathcal{H}$ of W, defined as a field of linear operators $\mathcal{H} : M \to \mathcal{L}(\mathbb{R}^d)$ by*

$$< \mathcal{H}(q)u, v >= D^2W(q)(u,v) \quad u,v \in \mathbb{R}^d, \quad q \in M, \tag{1.3}$$

($< \cdot, \cdot >$ is the standard scalar product in $\mathbb{R}^d$) has range equal to $T_qM^\perp$,

$$R(\mathcal{H}(q)) = T_qM^\perp, \quad q \in M. \tag{1.4}$$

Essentially, this condition is the precise way of saying that W has a minimum on M, or, in more physical terms, that, sufficiently near to the constraint, the particle feels a strong harmonic restoring force.

Since $\mathcal{H}(q)$ is a self-adjoint operator, we can diagonalize it. We suppose, in addition, that we can do it in a smooth way.

Condition W_2. *Let W be a potential satisfying condition $\boldsymbol{W_1}$. The Hessian of W can be diagonalized smoothly, i. e.,*

$$\mathcal{H}(q) = \sum_{k=1}^{r} \omega_k(q)^2 P_k(q), \quad q \in M, \tag{1.5}$$

where $\omega_k(q)^2$ and $P_k(q)$ represent the smooth *(nonzero) eigenvalues and eigenprojections of the Hessian.*

Since $R(\mathcal{H}(q)) = T_qM^\perp$, we have that $P_k(q) : \mathbb{R}^d \to T_qM^\perp$. Moreover,

$$P_kP_l = \delta_{kl}P_k, \qquad P_k^\dagger = P_k,$$

and

$$P(q) := \sum_{k=1}^{r} P_k(q)$$

[1] When the constraint is a smooth submanifold, as in this section, we suppose that the potentials involved are *smooth functions* too. The smoothness of the constraining potential will be discussed further in chapter 3, where M will be a graph embedded in $\mathbb{R}^2$ or $\mathbb{R}^3$.

is the orthogonal projection from $\mathbb{R}^d$ *onto* $T_qM^\perp$.

Condition $\boldsymbol{W_2}$ could seem a mere technicality, but if it is not satisfied the limit structure described below completely breaks down, as it happens in Takens chaos (see section 2.4).

If we assume that the energy surfaces E_ε = const. are compact submanifold of $\mathbb{R}^d \times \mathbb{R}^d$, then the flow of the Euler-Lagrange equations associated to (1.2) is complete, so that the corresponding initial value problem is solvable for all times. For fixed initial values, $q_\varepsilon(0) = q_*$ and $\dot{q}_\varepsilon(0) = v_*$, and a finite time interval $[0, T]$, there exists then a unique sequence of solutions, $q_\varepsilon(t)$. (It is possible to consider also a sequence of initial values, $q_{\varepsilon,*}$ and $v_{\varepsilon,*}$, converging to q_* and v_*; this generalization is technical and does not change the nature of the problem; we refer the interested reader to [Bor, FrHe, Tak]).

Naively, one could expect that q_ε always converges to a function $q_0 : [0, T] \to M$, but it is fairly simple to construct counterexamples [BoSc] showing that, if the energy

$$E_\varepsilon := \frac{1}{2} m\dot{q}_\varepsilon^2 + V(q_\varepsilon) + \varepsilon^{-2} W(q_\varepsilon) = \frac{1}{2} m v_*^2 + V(q_*) + \varepsilon^{-2} W(q_*)$$

is not uniformly bounded, then, even though the limit can exist, it can be supported outside M. Moreover, solutions of equi-bounded energy have a more evident physical meaning. We will say that they satisfy the

Condition EE (Equi-bounded Energy). *The energy associated to the solution q_ε is uniformly bounded in ε, $E_\varepsilon \leq E_*$. This is equivalent to assume that $q_* \in M$, i. e., that the initial position is on the constraint.*

The first rigorous investigation of solutions obeying to conditions $\boldsymbol{W_1}$, $\boldsymbol{W_2}$ and **EE** was made by Rubin and Ungar at R. Courant's suggestion, [RuUn]. They however considered in detail only the case when M has codimension equal to one. The general case was first studied by Takens [Tak], who pointed out the necessity of some non-resonance condition on the eigenvalues of the Hessian in order to get a limit, when the codimension (*and* the dimension of M) is greater than one. A further generalization to the case where M is a submanifold of a general Riemannian manifold, with applications to molecular dynamics, is given in [Bor].

A different point of view was taken by Froese and Herbst [FrHe], who, aiming at the study of the quantum case, have dealt with the case of *unbounded energies*. Since their approach is motivated by quantum mechanics, we postpone an account of their results to next subsection.

Roughly speaking, the theorems proved by the above authors say that if the potential is "good", the initial condition is correctly chosen and a certain resonance condition is satisfied, then the sequence q_ε converges uniformly to a function q_0 which is the unique solution of the Euler-Lagrange equations corresponding to the Lagrangian

$$L_0(q, \dot{q}) := \frac{1}{2} < \dot{q}, \dot{q} >_M - V(q) - U_{\text{hom}}(q), \quad q \in M, \quad \dot{q} \in T_qM, \tag{1.6}$$

where $< \cdot, \cdot >_M$ is the Riemannian metric induced on M by the standard scalar product in $\mathbb{R}^d$.

If we had followed the usual geometrical approach to describe the motion of a system constrained to M and subject to the external potential V (see, e. g., [Arn]), we would have written instead the Lagrangian

$$L_{\text{geo}} := \frac{1}{2} < \dot{q}, \dot{q} >_M - V(q). \tag{1.7}$$

The additional potential U_{hom} is called the *homogenization* of U with respect to the initial data q_* and v_*. To understand its origin we have to introduce another concept which plays an important role in the analysis of the dynamics generated by (1.1), both in the classical and in the quantum case, that of *adiabatic invariance of the normal actions*.

As we have already said, we model the constraining force essentially like an harmonic oscillator acting in the directions perpendicular to the submanifold. The frequencies are scaled as ε^{-1}, so in the limit $\varepsilon \to 0$ the particle oscillates very fast in the normal directions, while the motion along M is "slow". Therefore, according to the definition of "adiabatic invariants" given, e. g., in [AKN] (chapter 6), we expect that the normal action variables,

$$\vartheta_{\varepsilon,k} := \frac{E^{\perp}_{\varepsilon,k}(t)}{\omega_k(q_{M,\varepsilon}(t))}{}^{1}, \tag{1.8}$$

converge to constant functions (in t) when $\varepsilon \to 0$[2] (this fact has been stressed from a formal point of view in [Koi]).

This is the point where a condition on the normal frequencies enters, because the presence of resonances can spoil the adiabatic invariance of the actions.

To be more precise, we have first to define what we mean by a "resonance".

Definition 1.1. We say that the frequencies $\{\omega_k(q)\}$, $k = 1, \ldots r$, are in a *resonance of order* j if

$$n_1\omega_1 + \ldots + n_r\omega_r = 0, \qquad \sum_{k=1}^{r} |n_k| = j, \tag{1.9}$$

where $n_k \in \mathbb{Z}$.

We can now illustrate the lack of adiabatic invariance in presence of resonances by a very simple example (which is a modified version of an example of Bornemann, [Bor] chapter 1, section 2.6).

[1] We write q in *tubular coordinates*, $q = q_M + q_\perp$, where $q_M \in M$ and $q^\perp \in T_qM^\perp$. The total energy can be decomposed in the same way. A detailed description of this system of coordinates is given on page 10.

[2] Since we suppose that the energy surfaces are compact and we consider finite time intervals, condition W_1 implies that there exists $\omega_* > 0$ such that $\omega_k > \omega_* \ \forall k$, so (1.8) is well defined.

Let us consider a one-dimensional forced harmonic oscillator,

$$\begin{aligned} &\ddot{x} + \frac{\omega^2}{\varepsilon^2} x = \cos\left(\frac{\tilde{\omega}}{\varepsilon} t\right), \\ &x(0) = 0 \qquad \dot{x}(0) = 0. \end{aligned} \tag{1.10}$$

If $\omega \neq \tilde{\omega}$, then the solution is

$$x_\varepsilon(t) = \frac{\varepsilon^2}{\omega^2 - \tilde{\omega}^2} \left[\cos\left(\frac{\omega}{\varepsilon} t\right) - \cos\left(\frac{\tilde{\omega}}{\varepsilon} t\right) \right].$$

It is evident then that $x_\varepsilon \to 0$ uniformly on a finite time interval, and also that

$$E_\varepsilon^\perp(t) := \frac{1}{2} |\dot{x}_\varepsilon(t)|^2 + \frac{\omega^2}{2\varepsilon^2} |x_\varepsilon(t)|^2 = O(\varepsilon^2) \to 0.$$

If $\omega = \tilde{\omega}$ instead, the solution is

$$x_\varepsilon(t) = \frac{\varepsilon}{2\omega} t \sin\left(\frac{\omega}{\varepsilon} t\right). \tag{1.11}$$

So, while it is still true that $x_\varepsilon \to 0$ uniformly on a finite time interval, we have

$$E_\varepsilon^\perp(t) = \frac{1}{8} t^2 + O(\varepsilon) \to \frac{1}{8} t^2 \neq \text{const.} \qquad .$$

Clearly we do not claim that this example gives a proof of the necessity of a resonance condition in order to have adiabatic invariance of the normal actions, but we think it makes it plausible.

To quote the main theorem of this section we need another definition.

Definition 1.2. Let $z : [0, T] \to M$ be a time dependent trajectory lying in constraint's submanifold. We say that z is *non-flatly resonant up to order l* if, for every impact time t_i such that

$$n_1\omega_1(z(t_i)) + \ldots + n_k\omega_k(z(t_i)) = 0 \Rightarrow \frac{d}{dt}[n_1\omega_1(z(t)) + \ldots + n_k\omega_k(z(t))]\Big|_{t=t_i} \neq 0 \tag{1.12}$$

for all resonances whose order is less than or equal to l. If equation (1.9) defines a hypersurface, then the above condition is equivalent to saying that z crosses the hypersurfaces of resonance *transversally*.

Now we can state

Theorem 1.1. *([Bor], chapter 2, theorem 1, or, with more restrictive hypotheses on the resonances, [Tak], theorem 1).*

Given a sequence $\varepsilon \longrightarrow 0$, consider the Lagrangian

$$L_\varepsilon(q,\dot{q}) := \frac{1}{2}m\dot{q}^2 - V(q) - \varepsilon^2 W(q), \quad q \in \mathbb{R}^d.$$

Suppose that the potential W satisfies conditions $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$.

Let q_ε be the unique solution to the Euler-Lagrange equations associated to L_ε on the finite time interval $[0,T]$, with initial conditions $q_\varepsilon(0) = q_*$, $\dot{q}_\varepsilon(0) = v_*$ satisfying condition $\boldsymbol{EE}$ (i. e., $q_* \in M$).

Let $U_{\hom}$ be the homogenization of U with respect to the initial data, defined by

$$U_{\hom}(q) := \sum_{k=1}^{r} \vartheta_{*,k}\omega_k(q), \quad q \in M, \tag{1.13}$$

where

$$\vartheta_{*,k} := \frac{< P_k(q_*)v_*, P_k(q_*)v_* >}{2\omega_k(q_*)}. \tag{1.14}$$

Let q_0 be the unique solution to the Euler-Lagrange equations corresponding to the Lagrangian

$$L_0(q,\dot{q}) := \frac{1}{2} < \dot{q}, \dot{q} >_M - V(q) - U_{\hom}(q), \quad q \in M, \quad \dot{q} \in T_qM, \tag{1.15}$$

with initial conditions $q_0(0) = q_* \in M$ and $\dot{q}_0(0) = (\mathbb{I} - P(q_*))v_* \in T_{q_*}M$.

If q_0 is non-flatly resonant up to order 3, the sequence q_ε converges uniformly to q_0 on $[0,T]$.

Remark 1.1. The constants $\vartheta_{*,k}$ are exactly the limits of the normal actions $\vartheta_{\varepsilon,k}$ defined in (1.8).

Remark 1.2. The theorem tells us that, if the initial velocity of the particle has a component perpendicular to the constraint, then the energy of the normal oscillation changes into a potential energy for the longitudinal motion. In this way, conservation of energy holds also in the limit, in the sense that

$$\begin{aligned} E_0(t) &= \frac{1}{2} < (\mathbb{I} - P(q_*))v_*, (\mathbb{I} - P(q_*))v_* >_M + V(q_*) + U_{\hom}(q_*) = \\ &= \frac{1}{2}|v_*|^2 + V(q_*) = E_* = E_\varepsilon(t). \end{aligned} \tag{1.16}$$

1.1.2 Quantum mechanics

The description of constrained systems has been tackled since the early days of quantum mechanics and several techniques have been created to deal with this matter.

The *intrinsic* approach, which was developed mainly by Dirac [Dir], parallels the geometric treatment of constraints in classical mechanics. The idea is first to remove the redundant degrees of freedom by constructing a consistent Hamiltonian formalism for the classical theory and then to proceed using canonical quantization, i. e., enforcing canonical commutation relations on suitably chosen observables.

As was first noticed by DeWitt however [DeW], when one tries to quantize the classical Hamiltonian, operator ordering ambiguities arise. They are of order $\hbar^2$ and contain terms proportional to the local Gaussian curvature of the constraint, which is the only coordinate-invariant quantity.

A simple example may help to clarify this issue. Let us consider a classical particle constrained to move on a surface Σ embedded in the three-dimensional Euclidean space $\mathbb{R}^3$. According to the standard procedure we can eliminate redundant degrees of freedom introducing Lagrangian coordinates. We get that the system is described by $L = \frac{1}{2} < \dot{q}, \dot{q} >_\Sigma$, where $< \cdot, \cdot >_\Sigma$ is the metric induced on Σ by the Euclidean scalar product. In a local chart the Lagrangian has the form $L = \frac{1}{2} g_{\mu\nu}(q)\dot{q}^\mu \dot{q}^\nu$. Defining the generalized momenta $p_\mu := \frac{\partial L}{\partial \dot{q}^\mu}$ we obtain the Hamiltonian $H := \frac{1}{2} g^{\mu\nu}(q) p_\mu p_\nu$, where $g^{\mu\nu}$ is the inverse of the metric tensor. If we now quantize the theory, we face ordering ambiguities between the multiplication operators corresponding to the q^μ and the differentiation ones corresponding to p_μ, which are not removed even though we require the covariance of the resulting theory under point transformations (see [DeW] for more details). According to the different ordering we choose, we get an operator of the form

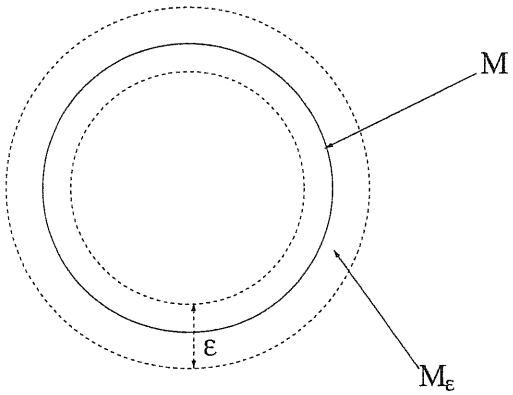
$$\widehat{H} = -\frac{\hbar^2}{2}\Delta + \hbar^2 \alpha R, \tag{1.17}$$

where Δ is the Laplace-Beltrami operator on Σ, R is its *intrinsic* scalar curvature and α is a constant whose value depends on the ordering. If the submanifold is flat, like a one-dimensional curve for example, $R = 0$ and the ambiguity does not arise. Similar problems are encountered in Feynman's path integral approach ([Sch], chapter 24).

To overcome these difficulties, a number of physicists have proposed to replace the intrinsic approach with the constraining potential approach we have already outlined in the classical case. Actually, a more precise statement is necessary. Instead of using a smooth potential W, as we did in (1.1), we could model a constraint considering a free quantum particle which moves in a neighbourhood of M, M_ε, which shrinks in a suitable way to M when $\varepsilon \to 0$.

To have a well defined free Hamiltonian, we have to impose boundary conditions on the Laplacian. In the physics literature the smooth potential or the boundary conditions approach have been used indifferently, but both for conceptual clarity and technical reasons it's better to distinguish them.

Figure 1.1: Example of a rigid constraint



Definition 1.3. Let M be a submanifold of $\mathbb{R}^d$ (or an embedded graph). We say that M is a **soft constraint** for a quantum particle if the Hamiltonian ruling the dynamics of the system is given by (1.1), where the constraining potential W satisfies conditions $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$ [1].

We say instead that M is a **rigid constraint** if there exists a sequence of open neighbourhoods M_ε, $0 < \varepsilon \leq 1$ such that

$$\begin{cases} M_1 \supset M_{\varepsilon_2} \supset M_{\varepsilon_1} & (1 > \varepsilon_2 > \varepsilon_1 > 0), \\ \lim_{\varepsilon \to 0} \bar{M}_\varepsilon = \bigcap_\varepsilon M_\varepsilon = M & \text{(the bar over a set denotes the closure of the set)}, \end{cases}$$

and the Hamiltonian for the particle is given by

$$\widehat{H}_B(\varepsilon, \hbar) := -\frac{\hbar^2}{2} \Delta^B_{M_\varepsilon}, \tag{1.18}$$

where B denotes the boundary condition defining the Laplacian on M_ε.

The choice of B depends on the specific physical phenomenon we want to describe. In next section, we will argue that the most significant choice is given by *Dirichlet boundary conditions*, which we denote by $\boldsymbol{B = D}$. From a technical point of view however, the analysis of the limit with Neumann boundary conditions (which we denote by $\boldsymbol{B = N}$) turns out to be simpler, and it has received much more attention in the literature.

The rigid constraint approach has been exploited mainly for the case when M is a graph embedded in $\mathbb{R}^2$ or $\mathbb{R}^3$ and the emphasis has been put on the *convergence of the*

[1] If M is an embedded graph we have to consider non-smooth constraining potentials; suitable analogs of conditions $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$ will be discussed in chapter 3.

spectrum of $\widehat{H}(\varepsilon,\hbar)$ and *not* of the *dynamics*[1]. For this reason, here in the introduction we limit ourselves to give an account of the soft constraint case, which is actually the one we are more interested in and refer the reader to next section for a review of physical models involving soft or rigid constraints and to chapter 3 for a more detailed account of the rigid constraint case and a comparison with our approach.

One obvious difference between the classical and the quantum case is that since any proper submanifold $M \subset \mathbb{R}^d$ is a subset of zero measure with respect to $d-$dimensional Lebesgue measure, it is not possible to choose a non-zero initial condition which is supported on M. Therefore, due to the Heisenberg principle, the mean value of the Hamiltonian (1.1), taken on an arbitrary non-zero state, will diverge in the limit $\varepsilon \to 0$ (the better we localize the wavefunction on M, the bigger kinetic energy becomes).

Since the energy is not bounded, it is possible that an infinite amount of it is transferred from the normal to the longitudinal motion, resulting in a diverging effective potential (the homogenized potential of the classical case, (1.13)). To avoid this problem, starting from the article of Jensen and Koppe [JeKo], the idea has been to choose constraining potentials whose Hessian has *constant eigenvalues*, i. e., referring to equation (1.5), $\omega_k(q) = \omega_k = const.\ \forall q \in M$. The normal energy is then constant along M and gives rise, in the limit $\varepsilon \to 0$, to a divergent constant which can be *formally* discarded.

One then tries to solve the *time-independent* Schrödinger equation making the Ansatz that the wave function can be separated into a product of a longitudinal part, which belongs to $L^2(M)$, and a normal part, which describes the fast oscillation around the equilibrium position given by M.

To better describe this point, we need to introduce suitable coordinates in $\mathbb{R}^d$, adapted to the submanifold M, called *tubular coordinates*.

Let M be a smoothly embedded compact[2] submanifold of $\mathbb{R}^d$ (in the following we identify the image of M under the embedding with M itself as it is customary). At every point $q \in M$ the tangent space $T_q\mathbb{R}^d = \mathbb{R}^d$ decomposes into the direct sum of the tangent space to M, T_qM, and a normal part $T_qM^\perp$. This decomposition, which depends smoothly on q, extends to the restriction to M of the tangent bundle $T\mathbb{R}^d = \mathbb{R}^d \times \mathbb{R}^d$, $T\mathbb{R}^d_{|_M} = TM \oplus TM^\perp$, where TM is the tangent bundle of M and $TM^\perp$ is a bundle over M called *normal bundle*. By the tubular neighbourhood theorem [Lan], it is possible to fix a sufficiently small δ such that there exists a diffeomorphism between

$$\mathcal{U}_\delta := \{q \in \mathbb{R}^d : d(q,M) < \delta\}, \qquad d(q,M) := \inf\{|q-x| : x \in M\}, \tag{1.19}$$

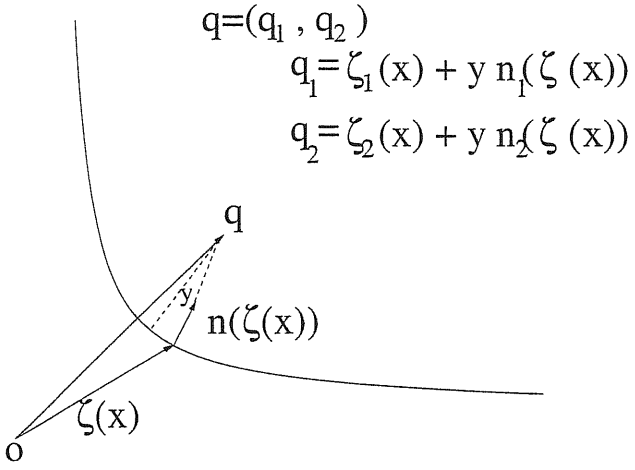
and

$$TM^\perp_\delta := \{(q,n) : q \in M, n \in T_qM^\perp, |n| < \delta\}. \tag{1.20}$$

[1] An exception to this statement is given by [BeMe]. We will comment on this paper at the end of this section.

[2] This compactness hypothesis aims only at streamlining the presentation. The whole discussion holds locally for an arbitrary submanifold.

Figure 1.2: Tubular coordinates for a curve embedded in $\mathbb{R}^2$, of parametric equation given by $\zeta(x)$



The diffeomorphism can be chosen to be

$$f(q,n) := q + n$$

(remember that we have identified every fiber $T_qM^\perp$ with a subspace of $\mathbb{R}^d$).

This means that, given a basis for the normal bundle of M, $\{n_k(q)\}_{k=1}^{l}$ ($l := d-m$), and a local chart $\zeta^{-1} : E \subset M \to \mathbb{R}^m$, we can define a system of coordinates in $\mathcal{U}_\delta$ by

$$q = \zeta(x) + \sum_{k=1}^{l} y_k n_k(\zeta(x)), \quad q \in \mathcal{U}_\delta, \quad x \in \mathbb{R}^m, \quad y \in \mathbb{R}^l, \tag{1.21}$$

($y := (y_1, \ldots, y_l)$). The tubular coordinates of the point q are then given by $z := (x_1, \ldots, x_m; y_1, \ldots, y_l)$.

The *product Ansatz* mentioned above is equivalent to assume that the solution to the Schrödinger equation is, in the limit $\varepsilon \to 0$, the product of a term depending only on the *longitudinal coordinates* $(x_1, \ldots, x_m)$ and a term depending only on the *transverse coordinates* $(y_1, \ldots, y_l)$.

As was first noted by da Costa [daC$_1$, daC$_2$] however, this Ansatz is not always correct. The reason is that, supposing that the wave function is given in a product form, we implicitly suppose that, when $\varepsilon \to 0$, the Hamiltonian can be written as a sum of two terms, one containing only longitudinal variables, the other only normal variables. Even though we choose a constraining potential whose Hessian has constant eigenvalues, this need not be true because the geometry of the constraint M can be such

that the Euclidean metric is not diagonal anymore written in tubular coordinates, and so it is not possible to separate the longitudinal and the transverse motion, which are coupled by a kind of *gauge potential.*

Da Costa eliminated this problem restricting his attention to submanifolds which satisfy a "no twist" condition [Mit], i. e., submanifolds for which the gauge coupling is equal to zero. It can be shown that this is equivalent to require that the normal fundamental form of M, which represents the connection induced by $\mathbb{R}^d$ on the normal bundle $TM^{\perp}$, defined by

$$b_{k,j}[\cdot] :=< n_k, dn_j[\cdot] >_{\mathbb{R}^d}, \tag{1.22}$$

is identically equal to zero. If the dimension of M is equal to one, then we can always make $b_{k,j} = 0$ by a suitable change of basis in the normal bundle, which corresponds to a gauge transformation. Moreover, $b_{k,j}$ is antisymmetric, $b_{k,j} = -b_{j,k}$, so if the codimension of M is equal to one, again $b_{k,j} = 0$, but, apart from these simple cases, the gauge coupling can be non-zero.

In the physical literature there have been subsequently attempts to deal with the general situation using various forms of perturbation theory, [KMH, MaDe, Mar$_1$, Mar$_2$, Mit, ScJa].

The results of these studies can be summarized into two main statements.

First, if the submanifold satisfies da Costa's "no twist" condition, the *formal* limit $\varepsilon \longrightarrow 0$ leads to an effective Hamiltonian for the longitudinal motion given by

$$\widehat{H}_L := -\frac{\hbar^2}{2m}\Delta + \frac{\hbar^2}{4m}R - \frac{\hbar^2}{8m}\eta^2, \tag{1.23}$$

where Δ is the Laplace-Beltrami operator on M, R is the *intrinsic* scalar curvature and η is the mean *extrinsic* curvature of M. Note that, since the mean curvature depends on the embedding of M in $\mathbb{R}^d$, it would be impossible to get a term containing it using Dirac's quantization procedure. Moreover, this additional potential has nothing to do with the homogenized potential of the classical case, which, as we said above, in this case is equal to a constant and is therefore discarded.

Second, in the general case, the effective Hamiltonian contains an additional term[1], which couples the longitudinal motion and the angular momentum in the transverse directions. This term has the form of a minimal gauge coupling and prevents a straightforward separation of longitudinal and transverse motion, which is restored only treating it as a perturbation.

From these brief remarks, it is clear that the quantum mechanical situation seems at first sight very different from the classical one, because of the various kinds of effective potentials involved. This is the reason why a systematic comparison was attempted only recently by Froese and Herbst [FrHe] and Teufel ([Teu], section 2.4).

[1]The complete expression of the effective Hamiltonian will be given in chapter 2.

Froese and Herbst analyze rigorously the case of a constraining potential which is *exactly quadratic* in the transverse coordinates, i. e., whose Taylor expansion near the constraint contains only the second order term, and whose *Hessian* has *constant eigenvalues.*

They consider ε-dependent initial quantum states, ψ_0^ε, whose *position density is more and more localized near* M when $\varepsilon \to 0$. This condition is expressed in the form

$$\|\widehat{H}(\varepsilon,\hbar)\psi_0^\varepsilon\| \leq \frac{C_1}{\varepsilon}, \tag{1.24}$$

where $\widehat{H}(\varepsilon,\hbar)$ is defined in (1.1). This request is natural from an "adiabatic" point of view, as can be seen in a two-dimensional example.

Consider the Hamiltonian

$$\widehat{K}(\varepsilon) := -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2\varepsilon^2}\omega(x)^2 y^2,$$

where $(x,y) \in \mathbb{R}^2$ and ω is a smooth function which is strictly positive, $\omega(x) > \omega_* > 0$.

As in the classical case, we expect that the particle oscillates very fast around the equilibrium position $y = 0$, while the motion along the x direction is comparatively "slow". Then, according to the principles of quantum adiabatic approximation (for an updated review see [Teu]), we can separate the dynamics in almost invariant subspaces, supposing that the fast degrees of freedom immediately adjust themselves to follow the slow evolution. Therefore, it is natural to pick an initial condition which lies in one of these almost invariant subspaces, i. e., which is an eigenstate of the harmonic oscillator in the y variable, with frequency $\omega(x)$ (we denote it by $\Phi_{x,n}^\varepsilon(y)$). It is obvious then that

$$\|\widehat{K}(\varepsilon)f(x)\Phi_{x,n}^\varepsilon(y)\| \leq \frac{C}{\varepsilon},$$

where $f \in H^2(\mathbb{R})$.

In a slightly different framework, without explicitly mentioning the theory of almost invariant subspaces, Froese and Herbst prove that, if the submanifold M satisfies da Costa's "no twist" condition,

$$\sup_{t\in[0,T]} \|\exp\big(-it\widehat{H}(\varepsilon,\hbar)\big)\psi_0^\varepsilon - \exp\big(-it\widehat{H}_{\mathrm{L}}\big)\cdot\exp\big(-it\widehat{H}_{\mathrm{osc}}\big)\psi_0^\varepsilon\| \to 0, \tag{1.25}$$

where $\widehat{H}_{\mathrm{L}}$ is defined in (1.23) and $\widehat{H}_{\mathrm{osc}}$ is the Hamiltonian of the harmonic oscillator with frequencies given by $\frac{\omega_k}{\varepsilon}$, where ω_k are the *constant* eigenvalues of the Hessian.

In the general case, however, they get a formula similar to (1.25), with a longitudinal Hamiltonian which commutes with $\widehat{H}_{\mathrm{osc}}$, but acts on $L^2(TM^\perp)$ and not on $L^2(M)$. Thus it is not possible to interpret the approximate dynamics as a longitudinal motion with superimposed transverse oscillations.

Note again that the homogenized potential of the classical case is absent, because the eigenvalues of the Hessian are constant functions.

A different approach was proposed by Teufel, who noted that, as far as classical dynamics are concerned, it is equivalent to consider strong restoring forces normal to the constraint or weak forces in the non-constraining directions. To illustrate this point, let us suppose for simplicity that $M = \mathbb{R}^m \subset \mathbb{R}^d$, that the constraining potential is strictly harmonic and V depends only on the longitudinal coordinates x:

$$W(x,y) = \frac{1}{2} < y, A(x)y >_{\mathbb{R}^l}, \qquad l = d - m, \qquad q = (x,y) \in \mathbb{R}^m \times \mathbb{R}^l = \mathbb{R}^d$$

Instead of looking at the classical Hamiltonian corresponding to (1.1),

$$H_\varepsilon(q,p) := \frac{1}{2}p^2 + V(x) + \frac{1}{2\varepsilon^2} < y, A(x)y >_{\mathbb{R}^l},$$

we can rescale x and y, $x = \varepsilon\tilde{x}$, $y = \varepsilon\tilde{y}$, and consider

$$\widetilde{H}_\varepsilon(\tilde{q},\tilde{p}) := \frac{1}{2}\tilde{p}^2 + V(\varepsilon\tilde{x}) + \frac{1}{2} < \tilde{y}, A(\varepsilon\tilde{x})\tilde{y} >_{\mathbb{R}^l} .$$

The potentials are now slowly varying in the longitudinal direction, instead of strongly confining along the transverse one.

Rescaling also the time, $t = \varepsilon\tilde{t}$, one can check by direct computation that, if $(\tilde{q}(\tilde{t}), \tilde{p}(\tilde{t}))$ is a solution of the equations of motion generated by $\widetilde{H}_\varepsilon(\tilde{q},\tilde{p})$ then

$$(q(t), p(t)) := \left(\varepsilon\tilde{q}\left(\frac{t}{\varepsilon}\right), \tilde{p}\left(\frac{t}{\varepsilon}\right)\right) \tag{1.26}$$

is a solution of the equations of motion generated by $H_\varepsilon(q,p)$. The motions generated by the two Hamiltonians are related by a rescaling of space-time, so we can study the limit $\varepsilon \to 0$ equivalently in one or the other scale.

On the quantum level however, this equivalence does not hold anymore, i. e., it not possible, rescaling space-time, to pass from the operator

$$\widehat{H}(\varepsilon,\hbar) = -\frac{\hbar^2}{2}\Delta_x - \frac{\hbar^2}{2}\Delta_y + V(x) + \frac{1}{2\varepsilon^2} < y, A(x)y >$$

to the operator (we use the same symbol $\widetilde{H}$ for the classical and the quantum Hamiltonian to avoid to have too many of them)

$$\widetilde{H}(\varepsilon,\hbar) = -\frac{\hbar^2}{2}\Delta_{\tilde{x}} - \frac{\hbar^2}{2}\Delta_{\tilde{y}} + V(\varepsilon\tilde{x}) + \frac{1}{2} < \tilde{y}, A(\varepsilon\tilde{x})\tilde{y} > . \tag{1.27}$$

Therefore, in the quantum case, we have two *different* limit problems.

One advantage of the Hamiltonian $\widetilde{H}(\varepsilon,\hbar)$ is that it does not suffer of the problem of diverging energy which constitutes the main difficulty in treating $\widehat{H}(\varepsilon,\hbar)$. On the other end, since the two problems are *independent*, it is equally legitimate to study the one or the other, as it happens, e. g., in models of field theory, like the massless Nelson model, where classically one can consider the limit of fast photons or the limit of slow particles, while in the corresponding quantum mechanical model the two limits are not equivalent anymore, but both are relevant.

A point of view similar to the one of Teufel is taken by Ben Abdallah and Méhats [BeMe], who have analyzed the limit $\varepsilon \to 0$ of the quantum flow generated by (1.27), in presence of a *time-dependent* external potential, $V^\varepsilon(t,x,y)$, when $M = \mathbb{R}^m$ and the codimension of M is equal to 1. To model the confinement of the particle, however, the authors use a rigid constraint approach, imposing Dirichlet boundary conditions in the strip defined by $0 < y < 1$. Note that the transverse subspace is one-dimensional, and the constraint is flat, therefore, in this case the difficulties linked to the geometric gauge potential do not arise.

The authors perform the limit using Wigner functions, which are a well established tool in semiclassical analysis. Actually, if we rescale the variable $\tilde{x}$ in (1.27), passing to the variable $x = \varepsilon\tilde{x}$, we get (using units in which $\hbar = 1$)

$$\begin{aligned} &\widehat{H}_{\mathrm{BM}} := -\frac{\varepsilon^2}{2}\Delta_x - \frac{1}{2}\Delta_{\tilde{y}} + V^\varepsilon(t,x,\tilde{y}), \qquad \text{(BM=Ben Abdallah, Méhats)} \\ &\psi(y=0) = \psi(y=1) = 0, \qquad \psi(t=0) = \psi_0^\varepsilon \end{aligned} \tag{1.28}$$

so, with this scaling, the limit $\varepsilon \to 0$ resembles a partial semiclassical limit made in the tangential direction only.

They show that, if we split the solution of the time dependent Scrödinger equation along the different transverse subspaces, the Wigner function of the longitudinal components satisfies in the limit a Vlasov equation with potential given by the transverse eigenstate (a nonlinear confining problem, given by a perturbed form of the Scrödinger-Poisson system, is studied in [BAMP], where also a detailed discussion of the scaling employed to arrive at (1.27) is given).

This result is, for the special case $M = \mathbb{R}^m$, codim $M = 1$, analogous to the one we will prove in chapter 2, valid for a manifold of arbitrary dimension and codimension, which is stated in wavefunction, and not Wigner function, language, but with a special class of initial conditions.

Our starting point is however different from the one of the previous authors. We propose to compare the classical and the quantum situation, taking account of the fact that in quantum mechanics there is an *a priori* length scale (in units in which time and mass are of order 1) defined by $\hbar$.

In actual experiments there is always a natural boundary beyond which the particles cannot be further localized. Moreover, in physical systems which can be described with

good accuracy by the Hamiltonian (1.1), like the mesoscopic devices (see next section for more details), the transverse direction cannot become smaller than $\hbar$, which is the order of magnitude of atomic dimensions.

This is the reason why we propose to link the squeezing scale, determined by the constraining potential, to the quantum scale given by $\hbar$ and subsequently study the limit $\hbar \to 0$. This is what is done in chapter 2, which is an expanded version of [DeTe].

1.2 Physical applications: examples from condensed matter physics and theoretical chemistry

The topics discussed above make clear that the study of the dynamics generated by Hamiltonian (1.1) and their link with the corresponding classical flow is important from a conceptual point of view to justify the traditional approach to constrained systems.

There are, however, also many *concrete* physical systems whose dynamical and spectral properties are, with a certain degree of approximation, well described by an Hamiltonian containing a strong confining potential.

Here we give two examples, one concerning semiconductor devices in nanophysics and the other the so called quantum network model for aromatic molecules and periodic solids.

The reader will surely note that the constraints which naturally arise in applications are non-smooth. Specifically, they are given usually by graphs. The study of this kind of constraints poses additional problems to the ones encountered in the smooth case, mainly related to the kind of differential operator one has to define on the graph to describe the motion of the electrons. As stressed in a recent review in the field ([Ku_1], page R16), the method of the confining potential in the case of a graph "has not been explored". We will give some results in this direction in chapter 3, where we will define *quantum graphs* and discuss possible ways of approximating them.

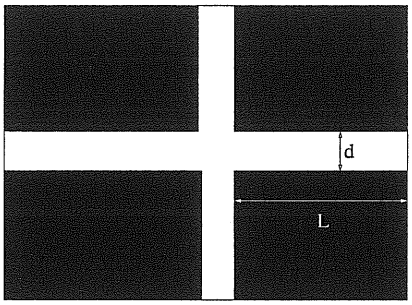
1.2.1 Nanostructures

The operation of many electronic nanostructures, like quantum wires and nanotubes, relies on the formation of a low dimensional electron gas. The electrons are confined in one or two directions, and can freely propagate in the other one(s).

Quantum wires are narrow almost one-dimensional conducting surfaces made of a semiconductor material. They are created using a very thin substrate (which can reach 2 nm of thickness, which amounts to have several atoms only in the transverse cross section) that is subject to a ion bombardment, after having masked a region similar to a waveguide.

The region not covered by the mask becomes not conducting (black area in figure 1.3), so the electrons can move only in the remaining white area. In this way, it is

Figure 1.3: Schematic representation of a quantum wire



possible to "draw" on the substrate various kinds of waveguide-like structures.

Another interesting example is given by nanotubes. They are made up of many atoms situated in cylinder type spatial surfaces. The first kind of nanotube created was the carbon nanotube, which is a variety of fullerenes. Recently, also metal-doped nanotubes have been synthesized.

The main physical properties common to these structures are (see, e.g., [DuEx, LCM] for more details):

1. Small size.

   We have already said that the thickness of quantum wire can reach 2 nm. The transverse length d of figure 1.3 or the diameter of a nanotube are of the same order of magnitude. These quantities are comparable with the de Broglie wavelength $\lambda = 2\pi/k_F \simeq 1$ nm of an electron with energy of the order of the Fermi energy $E_F \simeq 1$ eV, while the longitudinal length L of a quantum wire or a nanotube are much bigger (typically, $L \simeq 100$ nm). This means that we expect quantum effects to play a significant role in the transverse motion, while the longitudinal one can be correctly described in classical terms.

2. Ballistic transport.

   The electron mean free path can be a few μm or even larger, since it is possible to fabricate devices of very high purity, so that the propagation is not disturbed by scattering on impurities.

3. Crystallic structure.

   It is known that, in the first approximation of the strong-coupling method, the dynamics of a particle in a crystal is described by the one particle *free* Hamiltonian, with an effective mass m_*.

4. Confinement.

   The electron is confined inside the nanostructure by a strong potential barrier, which prevents it from escaping outside.

From these remarks it is clear that we can describe the motion of an electron in a nanostructure adding to the free Hamiltonian a constraining potential, whose small parameter ε is linked to the ratio between the transverse and the longitudinal length. If we suppose that the potential barrier confining the electron is infinitely high, we get Dirichlet boundary conditions, as in the rigid constraint approach.

Another model was put forward by Exner [Ex], who considered a δ-type interaction in $\mathbb{R}^2$ (respectively, $\mathbb{R}^3$) with support on a smooth curve (resp., a smooth surface). He studied then the spectral limit when the coupling constant goes to infinity. Since an attractive δ-potential has bound states for negative energies only, this can be an alternative way of taking into account the fact that the confining barrier is not infinitely high. However, if the codimension of the constraint is equal to two or three, the definition of the δ-potential becomes more problematic and if it is greater than three the Hamiltonian with δ-potential cannot be defined as an operator on a Hilbert space [AGHKH].

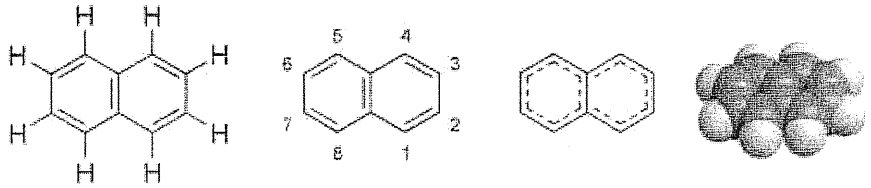
In any case, one should note that realistic quantum wires or nanotubes can have bifurcations, i. e., they can form *branched structures*, like the one in figure 1.3. To implement this feature, one should consider a non-smooth constraint given by a *graph*, where the vertices correspond to the regions where several tubes meet.

1.2.2 Quantum network model

The quantum network model (QNM) has been used in theoretical chemistry to calculate the electronic structure of haromatic molecules and periodic solids.

Its first application was probably given in a famous paper of Ruedenberg and Scherr [RueSc] to analyze systems of conjugated double bonds in organic molecules. They explicitly considered the case of the naphthalene (figure 1.4). Each atom contributes

Figure 1.4: Naphthalene molecule

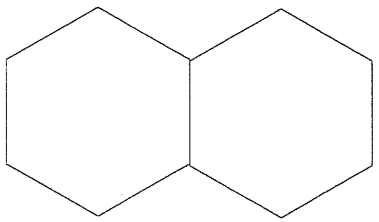


three electrons for the chemical binding of the structure. In a first approximation, one

supposes that two of them, the so called σ-electrons, form bonds which mantain the geometrical arrangement of the molecule, while the third one, the π-electron, moves throughout the whole structure in the potential created by the other ones.

Essentially, the σ-electrons create a "skeleton", to which the π-electrons are confined.

Figure 1.5: Naphthalene molecule's skeleton



In their paper, Ruedenberg and Scherr supposed that the constraining potential was zero on an thin tube containing the bond lines and infinite outside, adopting the rigid contraint point of view. As we have already mentioned before, we think that a smooth potential is a better way to model a real potential barrier which, *a fortiori*, has to be finite.

The quantum network model was afterwards extended to cover other systems of chemical interest, like periodic lattices in metals, by Coulson [Cou], who found a remarkable agreement between his calculations and the spectrum of π-electrons in graphite. Later, Montroll [Mon] studied the case when the vertices of the skeleton contain different atoms, like in the boron nitride crystal. A recent review can be found in [ALM].

1.3 Other models of constrained partial differential equations

The approximation of the dynamics of complex systems by the motion of systems of reduced dimensionality, which describe a sort of "average" motion of the full system, is not restricted to finite-dimensional classical systems nor, in the PDE domain, to the Schrödinger equation. In this section, we give a number of examples which are related to hyperbolic PDEs, both in the soft and in the rigid constraint approach.

The results of Rubin and Ungar, which were mentioned in section 1.1.1, were extended by Ebin [Eb_1] to show that the motion of a slightly compressible inviscid barotropic fluid can be approximated by that of an incompressible one.

Let us suppose for simplicity that the domain filled with the fluid is the n-dimensional

torus $\mathbb{T}^n$, which is equivalent to consider periodic motions in $\mathbb{R}^n$ (for more general domains see [Eb$_2$]).

If $u(t) : \mathbb{T}^n \to \mathbb{R}^n$ is the curve of vector fields describing the fluid velocity (i. e., $u(t)(x)$ is the velocity of the fluid particle which is at position x at time t, where x is usually called *Euler coordinate* of the fluid) and $\varrho : \mathbb{T}^n \to \mathbb{R}^n$ is the fluid density, then, in absence of viscosity, they satisfy

$$\begin{aligned} &\partial_t u + u_j \partial_j u = -\frac{1}{\varrho}\nabla p = -\frac{1}{\varrho}p'(\varrho)\nabla\varrho, \\ &\partial_t \varrho - \operatorname{div}(\varrho u) = 0, \end{aligned} \tag{1.29}$$

where $p(\varrho)$ is a given function, which expresses the pressure of the fluid in terms of the density (this is possible, by definition, in *barotropic* fluids only).

For an *incompressible* fluid, the density is constant, $\varrho_{\text{in}} = \text{const.}$, while the velocity field, denoted by v, satisfies

$$\begin{aligned} &\partial_t v + v_j \partial_j v = 0, \\ &\operatorname{div} v = 0. \end{aligned} \tag{1.30}$$

Apparently, these two systems of hyperbolic equations are unrelated, but, in applications, it is supposed that the solutions of (1.30) approximate the solutions of (1.29), when the compressibility, defined by the reciprocal of $dp/d\varrho$, goes to zero (note that, for physical reasons, $dp/d\varrho$ is always positive).

This is exactly what Ebin proved, reformulating the problem of an incompressible fluid as a constrained motion. In [EbMa], in fact, it is showed that the system of partial differential equations (1.29) can be rewritten as an ordinary differential equation on an infinite dimensional Riemannian manifold, given by the group $\mathcal{G}$ of C^∞ diffeomorphisms of $\mathbb{T}^n$. In the same way, system (1.30) can be rewritten as an ODE on $\mathcal{G}_1$, the group of diffeomorphisms whose Jacobian is equal to one. In this way, considering an incompressible fluid is equivalent to consider an infinite dimensional constrained system.

What Ebin proved is a theorem analogous to theorem 1.1, but he supposed that M is a submanifold of an infinite dimensional Riemannian manifold. He, however, restricted his attention to *tangential initial data* only ($v_* \in T_{q_*}M$, with the notation of 1.1).

A different system of hyperbolic equations, the *wave equation*, was considered by Shatah and Zeng, [ShZe]. They were interested in constructing wave maps, which are maps from Minkowski space $(\mathbb{R}^{n+1}, \eta)$ into an m-dimensional Riemannian manifold (M, g), that satisfy the covariant wave equation. The target manifold M can be isometrically embedded in $\mathbb{R}^{m+l}$, where one considers a penalized wave equation

$$\begin{aligned} &\Box u + V'(u) + \frac{1}{\varepsilon^2}W'(u) = 0, \\ &\Box = \partial_t^2 - \Delta, \qquad u : \mathbb{R}\times\mathbb{R}^n \to \mathbb{R}^{m+l}, \end{aligned} \tag{1.31}$$

where V is a smooth potential and W is the constraining potential. Naturally, this system has a conserved energy,

$$E_\varepsilon(u, \partial_t u) = \int_{\mathbb{R}^n} dx \, \frac{1}{2}|\partial_t u|^2 + \frac{1}{2}|\nabla u|^2 + V(u) + \frac{1}{\varepsilon^2}W(u),$$

so we expect that, if we consider equi-bounded energy solutions, then the penalization term will constrain the solution to M, and, in the limit $\varepsilon \to 0$ we will get a solution of the covariant wave equation on M[1]. This is true if the initial data are tangential to M. When a normal part is present, as in the classical case, additional terms appear in the limit equation for the tangential components. For the case of the wave equation, these terms have been calculated by Keller and Rubinstein [KeRu], who showed that the limit should satisfy a coupled system of transport and wave equations. This, together with the well-posedness of the Cauchy problem, was rigorously proved in [ShZe].

Finally, we would like to conclude this section with an example of an application to hyperbolic PDEs of the rigid constraint method which has been recently employed [DeVWa, DeV] in the study of elastic bodies with one dimension significantly smaller than the others, like long metal beams or rods.

The hyperbolic problem considered is given by

$$\partial_t^2 u = Lu \tag{1.32}$$

where the operator L is defined by

$$Lu := \partial_y\left(a\left(\frac{y}{d}\right)\partial_y u\right) + b\left(\frac{y}{d}\right)\nabla_x \cdot (C(x)\nabla_x u).$$

The problem is posed in a three-dimensional domain, Ω, of thickness d,

$$\Omega := \omega \times (0, \pi d),$$

where ω is a bounded two-dimensional domain of smooth boundary γ. To define it correctly, we have to specify boundary conditions:

$$\begin{aligned} &u = 0 \quad \text{on } \gamma \times (0, \pi d) \times \mathbb{R}, \\ &\partial_n u = 0 \quad \text{on } \mathrm{F}_\pm \times \mathbb{R} \qquad \textit{(Neumann boundary conditions)}, \end{aligned} \tag{1.33}$$

where $\mathrm{F}_\pm$ are the top and the bottom face of Ω, $\mathrm{F}_+ := \{(x, y, z) : (x, y) \in \omega, z = \pi d\}$, $\mathrm{F}_- := \{(x, y, z) : (x, y) \in \omega, z = 0\}$.

DeVille and Wayne show that it is possible to approximate the solutions of the full three-dimensional problem by the solutions to a system of two-dimensional PDEs in the

[1]Note that in this case, as for classical dynamical systems, it is possible to choose initial conditions which give rise to an equi-bounded energy. We have already remarked that this is *not* possible for the Schrödinger equation.

variables (x, y). In particular, they establish a hierarchy of two-dimensional equations whose dynamics model the dynamics of the full plate, and each term of the hierarchy lengthens the time interval over which the approximation holds.

The viewpoint adopted is to think the equation (1.32) as an infinite-dimensional Hamiltonian system. In the phase space of this dynamical system, it is possible to identify an (infinite-dimensional) submanifold which is left invariant by the reduced two-dimensional PDE. Making then a canonical change of variables for the original Hamiltonian, one can show that this invariant manifold is left approximately invariant by the flow of the full three-dimensional PDE.

Actually, using a procedure which is reminiscent of the Nekhoroshev theory of classical mechanics, the authors make a sequence of canonical changes of variables which change the approximately invariant submanifold slightly, leading to more refined effective equations, which approximate the true solution for longer and longer time intervals. This procedure is also formally similar to space-adiabatic perturbation theory [Teu] in the framework of which one can show that the wave function stays for longer and longer times in "tilded" subspaces, constructed starting from the spectral subspaces of the Hamiltonian. In fact, the ratio of the frequency of oscillation of the plate in the "long" directions and in the "thin" direction is a natural adiabatic parameter in the problem.

As a last remark, we would like to stress that the use of Neumann boundary conditions in (1.33) gives rise to a transverse Laplacian whose spectrum has always the same ground state energy, $E = 0$, independently of the thickness of the plate. This fact, which sets the Neumann case apart from the Dirichlet and the smooth potential ones, makes the analysis of the problem somewhat simpler. We will elaborate on this brief remark in chapter 3, when we will speak of the approximation of quantum graphs by fattened graphs employing different kinds of boundary conditions.

Chapter 2

Semiclassical limit in the case of smooth constraints

In this chapter we study the semiclassical limit of the quantum flow associated to Hamiltonian (1.1), under the scaling

$$\varepsilon = a\hbar, \quad a \in \mathbb{R}_+. \tag{2.1}$$

As it has already been stressed in the introduction, we derive an effective Hamiltonian for the classical motion on M, using the technique developed in a series of papers by Hagedorn ([Ha_1, Ha_2] and references therein) to construct approximate solutions to the Schrödinger equation which are localized along a classical trajectory.

To explain the characteristic features of the method we employ, we first analyze in detail a number of explicit cases ($\mathbb{R}^n$ embedded into $\mathbb{R}^{n+m}$, a smooth curve embedded into a plane); we show then how the procedure generalizes to (non-flat) submanifolds of arbitrary dimension and codimension.

We have already stressed that the scaling (2.1) is based on the fact that in quantum mechanics there exists an a priori length scale defined through $\hbar$ (in units in which time and mass are of order one).

In real systems, like the mesoscopic ones mentioned in section 1.2, the transversal directions contain at least some atoms, so any realistic layer cannot become smaller than $\hbar$, which is the order of magnitude of atomic dimensions. Therefore, in our opinion, it is necessary to link the squeezing scale, determined by the constraining potential, to the quantum scale given by $\hbar$.

A simple example

To illustrate this point, we consider the standard two-dimensional example

$$\widehat{H}_\varepsilon = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2} + \frac{1}{2\varepsilon^2}\omega(x)^2 y^2, \qquad \hat{p}_r := -i\hbar\partial_r, \quad r = x, y \tag{2.2}$$

where $\omega : \mathbb{R} \to \mathbb{R}_+$ is an arbitrary smooth function which satisfies $\omega(x) \geq \omega_* > 0$ $\forall x \in \mathbb{R}$.

The squeezing scale is determined by ε, and we want it to be a function of $\hbar$, $\varepsilon = \varepsilon(\hbar)$. Since, as we argued before, ε cannot become smaller than $\hbar$, and it has to go to zero when $\hbar \to 0$ (to achieve the constraining limit), the simplest choice is

$$\varepsilon = a\hbar^\alpha \qquad 0 < \alpha \leq 1 \qquad a \qquad \text{fixed} > 0 \tag{2.3}$$

(there is no loss of generality, since what matters is the behaviour of $\varepsilon(\hbar)$ when $\hbar \to 0$).

With this choice, the Hamiltonian (2.2) becomes

$$\widehat{H}_\hbar = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2} + \frac{1}{2a^2\hbar^{2\alpha}}\omega(x)^2 y^2$$

and we want to examine the limiting behaviour of the dynamics generated by $\widehat{H}_\hbar$, when $\hbar \to 0$.

If we unitarily scale the transversal direction to factorize $\hbar$

$$y \to \hbar^{(\alpha+1)/2} y \qquad \partial_y \to \hbar^{-(\alpha+1)/2}\partial_y,$$

we get

$$\widehat{H}_\hbar \to -\frac{\hbar^2}{2}\partial_x^2 + \hbar^{1-\alpha}\Big[-\partial_y^2 + \frac{1}{2a^2}\omega(x)^2 y^2\Big].$$

If $\alpha \neq 1$, using the same techniques illustrated in the next sections, it can be shown that the influence of the normal motion on the longitudinal one is suppressed, and the effective Hamiltonian is the free one. Therefore, in the following, we consider only the more interesting case $\alpha = 1$.

In the next section we analyze a generalization of (2.2), studying the case of a potential confining to a flat submanifold M of $\mathbb{R}^{n+m}$. We realize the constraining limit through dilations in the direction normal to M, *i. e.*, we put $W^\varepsilon(x,y) = W(x, y/\varepsilon)$. This allows us to consider generic dependence on the transversal variables, unlike what is usually made in the literature [Bor, FrHe, Tak] where the first non zero term in the Taylor expansion of the potential around the constraint is the quadratic one, and so the problem is reduced to the analysis of harmonic motions.

In section 2.2 we consider a two-dimensional example where the constraining limit is realized through the more traditional method of scaling of the coupling constant, *i. e.*, $W^\varepsilon(x,y) = \varepsilon^{-2}W(x,y)$. In the case of a *spectrally smooth* potential confining to a *nondegenerate critical curve* (conditions $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$, page 3) the semiclassical limit motion we get along M is the same as the homogenized classical motion found by Bornemann [Bor].

In section 2.3, we show that an analogous result holds for an n-dimensional nondegenerate critical submanifold embedded into $\mathbb{R}^{n+m}$. We exploit Hagedorn's multiple

scale technique to construct squeezed states whose centre and dispersion take account of the (non-trivial) curved background.

Finally, we address an Hamiltonian showing the phenomenon of *Takens chaos* [Bor, Tak], which is encountered when the constraining potential is not spectrally smooth. In classical mechanics, the motion on the submanifold M is not deterministic anymore, *i. e.*, it is not described by a natural mechanical system on M and the limit set obtained forms a *funnel*. We show that the semiclassical limit offers a natural way to reduce (but however not to eliminate, in general) the degeneracy, linking different trajectories in the funnel to different quantum initial conditions.

2.1 Constraints by normal dilations

Let $M = \mathbb{R}^n$ and $W^\varepsilon(q) = W(x, y/\varepsilon)$, where we split $q \in \mathbb{R}^{n+m}$ as (x, y), $x \in \mathbb{R}^n$, $y \in \mathbb{R}^m$.

We suppose that

$$V, W \in L^2_{\text{loc}} \qquad \text{and are bounded from below,} \tag{2.4}$$

$$\lim_{|y|\to\infty} W(x,y) = \infty \qquad \forall x \in \mathbb{R}^m \qquad \textit{(confining hypothesis).} \tag{2.5}$$

We impose also an implicit smoothness hypothesis on the potentials, through a condition on the resolvent of the reduced Hamiltonian $\widehat{\mathfrak{h}}(x)$, to be defined below.

As argued above, we put $\varepsilon = a\hbar$. Actually, since we have several normal directions, we can choose different $\varepsilon/\hbar$ ratios for each one.

Defining

$$y_a := \left(\begin{array}{ccc} \frac{y_1}{a_1} & \dots & \frac{y_m}{a_m} \end{array} \right) \tag{2.6}$$

equation (2.19) becomes

$$\widehat{H}_\hbar = \frac{|\hat{p}|^2}{2} + V(x) + W(x, y_a/\hbar), \tag{2.7}$$

where, for the sake of simplicity, we suppose that $V(q)$ does not depend on y.

Scaling the transversal directions by the dilation operator

$$(D_\gamma \psi)(x,y) = \gamma^{m/2}\psi(x, \gamma y), \tag{2.8}$$

we get an Hamiltonian of the same form as the Born-Oppenheimer operator, used in molecular physics,

$$\begin{aligned} D^\dagger_{\hbar^{-1}} \widehat{H}_\hbar D_{\hbar^{-1}} &=: \widehat{H}_{BO} = -\frac{\hbar^2}{2}\Delta_x + \widehat{\mathfrak{h}}(x), \\ \widehat{\mathfrak{h}}(x) &= -\frac{1}{2}\Delta_y + W(x, y_a) + V(x). \end{aligned} \tag{2.9}$$

It follows from (2.4), (2.5) that $\widehat{\mathfrak{h}}(x)$ is, for each x, a well defined self-adjoint operator, with compact resolvent and nondegenerate ground state [ReSi$_1$].

We suppose in addition that $\widehat{\mathfrak{h}}(x)$ has a smooth dependence on x, namely that $(\widehat{\mathfrak{h}}(x) - i)^{-1}$ is a C^l function of x, for some $l \geq 2$. This makes its eigenvalues $E(x)$ (which we will call also "transversal" or "normal" energy levels) C^l functions of x away from crossings or absorption in the continuous spectrum.

The behaviour of Born-Oppenheimer Hamiltonian when $\hbar \to 0$ is well understood ([Ha$_1$, Teu] and references therein).

The transversal motion adiabatically decouples from the longitudinal one and stays approximately in a bound state of $\widehat{\mathfrak{h}}(x)$ for a fixed value of x. On the other hand, the longitudinal motion depends on the transversal one because it feels an effective potential which is equal to the normal energy.

Using standard results [Ha$_1$] we can elaborate on this qualitative argument:

Theorem 2.1. *Suppose that there exists an open set $U \subset \mathbb{R}^n$ such that $\widehat{\mathfrak{h}}(x)$ has a nondegenerate eigenvalue $E(x)$ for $x \in U$, with corresponding real normalized C^l eigenfunction $\Phi(x)$.*

Let $a(t)$ and $\eta(t)$ be the solutions of the classical equations of motion with potential $E(x)$ (which exist and are unique since $E(x)$ is $C^l(U)$ and bounded from below)

$$\dot{a}(t) = \eta(t) \tag{2.10}$$

$$\dot{\eta}(t) = -\nabla E(a(t)), \tag{2.11}$$

$$a(0) = a_0 \qquad \eta(0) = \eta_0, \tag{2.12}$$

then, for $t \in [0, T]$,

$$\Big\| \exp\Big(-\frac{it}{\hbar}\widehat{H}_\hbar\Big)\varphi_k(A(0), B(0), \hbar, a(0), \eta(0), x)F(x)D_{\hbar^{-1}}\Phi(x) - \exp\Big(i\frac{S(t)}{\hbar}\Big)\varphi_k(A(t), B(t), \hbar, a(t), \eta(t), x)F(x)D_{\hbar^{-1}}\Phi(x)\Big\|_{L^2(\mathbb{R}^{n+m})} = O(\hbar^{1/2}), \tag{2.13}$$

where $S(t)$ is the classical action, $A(t)$ and $B(t)$ are linked to the dispersions of φ_k in (respectively) position and momentum and F is a cut function which is zero outside a neighbourhood of the classical trajectory $\{a(t) : t \in [0, T]\}$.

Remark 2.1. The functions $\varphi_k(A, B, \hbar, a, \eta, x)$ were introduced by Hagedorn, to whom we refer for the notation [Ha$_2$]. They are a useful tool in studying the semiclassical limit of quantum mechanics and they coincide with the "squeezed states" widely used in quantum optics [Com]. Essentially, they are minimal uncertainty wave packets with different spreads in position and momentum.

Remark 2.2. We will give a proof of a slightly more general version of theorem (2.1) in sections 2.2 and 2.3, where we analyze the Laplace-Beltrami operator in a curved space.

2.1.1 Comments and examples

Let us analyze in greater detail the approximate evolution found in (2.13).

The transversal wave function $D_{\hbar^{-1}}\Phi(x)$ clearly describes a motion confined to the submanifold $M = \mathbb{R}^n$, since

$$\begin{aligned} &< \hat{y} >=< D_{\hbar^{-1}}\Phi(x), yD_{\hbar^{-1}}\Phi(x) >= \hbar < \Phi(x), y\Phi(x) >= O(\hbar), \\ &(\Delta\hat{y}_i)^2 =< D_{\hbar^{-1}}\Phi(x), y_i^2 D_{\hbar^{-1}}\Phi(x) > - < D_{\hbar^{-1}}\Phi(x), y_i D_{\hbar^{-1}}\Phi(x) >^2 = O(\hbar^2), \end{aligned} \tag{2.14}$$

while both $< \hat{p}_y >$ and $< \Delta\hat{p}_y >$ are $O(1)$.

One should note however that we did *not* require W to have a strict minimum on M. Actually this is not needed, since in our scale the average position of the normal motion is always "seen" to be approximately zero, as equation (2.14) shows.

In the standard case where

$$W(x,y) = \frac{1}{2}\sum_{i=1}^{m} \omega_i(x)^2 y_i^2, \tag{2.15}$$

the effective potential for the motion on M will be

$$\begin{aligned} &E_n(x) = \sum_{i=1}^{m} \frac{(n_i + 1/2)}{a_i}\omega_i(x) + V(x) = \sum_{i=1}^{m} \vartheta_i \omega_i(x) + V(x), \\ &n := (n_1, \ldots, n_m), \qquad \vartheta_i := \frac{(n_i + 1/2)}{a_i}. \end{aligned} \tag{2.16}$$

This is exactly the homogenized potential found by Bornemann and Takens (see theorem 1.1), where the ϑ_i are, in the classical case, the adiabatic invariants associated to the normal oscillations (*i. e.*, the energy-frequency ratios).

Varying the squeezing factors a_i, or the transversal wave function $\Phi(x)$, ϑ_i can be made to assume every positive value (the value $\vartheta_i = 0$ can be obtained suppressing the ith mode as we explained in section 2). The harmonic potential is particular in this respect, because, as far as the effective potential is concerned, all normal states are equivalent, since the various choices for $\Phi(x)$ correspond simply to suitable scalings of ε and $\hbar$.

One could even use an x-dependent scale, $\varepsilon = a(x)\hbar$, without altering substantially the structure of equation (2.16).

Such a simple picture cannot be expected when W is not harmonic.

In general, the effective potential will have a non-trivial dependence both on the parameters $\boldsymbol{a} := (a_1, \ldots, a_m)$ and the transversal wave function. This gives a host of

well-defined classical motions on M, whose form, however, cannot be given explicitly as in the harmonic case.

It would be interesting, for instance, to compare the semiclassical effective Hamiltonians produced by a "flat" confining potential, like the sextic harmonic oscillator,

$$W(x,y) = V_4(x)y^4 + V_6(x)y^6 \qquad (x,y) \in \mathbb{R}^2 \qquad V_6(x) \geq V_* > 0 \tag{2.17}$$

with the corresponding homogenized classical motions (if any exists), to see if it is possible to reproduce them in a purely classical way.

Unfortunately, the spectrum of the reduced Hamiltonian associated to (2.17) is known only for particular values of the squeezing parameter a. For example, if $a = 1$ and $V_4(x)^2 = 12V_6(x)^{3/2}$ it is known [SCDS, Ush] that the ground state is

$$E_0(x) = \frac{V_4(x)}{2V_6(x)^{1/2}}, \tag{2.18}$$

but it is not possible to write an explicit expression for all values of a.

2.2 Constraints by scaling of coupling constant: a curve in a plane

In this section we analyze, in a fairly detailed way, a two-dimensional example where $W^\varepsilon = \varepsilon^{-2}W$. It allows to explain the main differences between the curved and the flat case, avoiding technical complications arising from higher codimensions, which are not essential for the result, and will be illustrated in next section.

We suppose, in the same spirit of (2.4), that V and W are C^∞ and non-negative, but, as is customary in classical mechanics [Bor, Tak], we replace (2.5) with the hypothesis that W is a spectrally smooth potential constraining to a nondegenerate critical curve M (condition $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$, page 3).

Our starting Hamiltonian (with the prescription $\varepsilon = a\hbar$) will be then

$$\widehat{H}_\hbar = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2} + V(x,y) + (a\hbar)^{-2}W(x,y). \tag{2.19}$$

Squeezed states are particularly suited to studying this sort of situations, where M is not flat, because, as (2.13) shows, the evolution of a localized state is approximately described (for a bounded time interval) by localized states. This allows us to analyze the motion using one coordinate chart only and therefore local expressions for the operators involved.

Essentially, what we will do here is to adapt the arguments of the last section to a curved case, constructing an approximate solution to the Schrödinger equation which, in suitable coordinates, is still given by a squeezed state in the longitudinal direction and an (harmonic) oscillation in the transversal one.

2.2.1 The Hamiltonian in curvilinear coordinates

We fix a tubular neighbourhood $\mathscr{V}$ of M, and we consider a single chart of tubular coordinates, defined on $\mathscr{U} \subset \mathscr{V}$.

This simply means that, given a local parametric representation of M in terms of its arc length s, $q_M(s) = (x_M(s), y_M(s))$, we can write (for $q \in \mathscr{U}$)

$$q(s,u) = q_M(s) + u\boldsymbol{n}(s), \tag{2.20}$$

where $\boldsymbol{n}(s)$ is the unit normal of M (for more details, we refer the reader to the discussion on page 10 and figure 1.2, page 11).

When q varies over $\mathscr{U}$, s and u vary, respectively, over two intervals I and J.

Lemma 2.1. *The Hilbert space $L^2(\mathscr{U}, dq)$ is isometric to $L^2(I \times J, dsdu)$.*

Proof. This well-known lemma results from two facts.

First, the choice of curvilinear coordinates provides an isometry of $L^2(\mathscr{U}, dq)$ to $L^2(I \times J, g^{1/2}dsdu)$, where

$$g^{1/2} = 1 + k(s)u \tag{2.21}$$

is the Jacobian of the transformation $(x, y) \longrightarrow (s, u)$, and $k(s)$ is the curvature of M.

Second, the multiplication by $g^{1/4}$ is a unitary operator from $L^2(I \times J, g^{1/2}dsdu)$ to $L^2(I \times J, dsdu)$. □

In the following, we will denote the isometry constructed above by $\widehat{U} : L^2(\mathscr{U}, dq) \longrightarrow L^2(I \times J, dsdu)$.

We remark that $\widehat{U}$ maps $C_0^\infty(\mathscr{U})$ onto $C_0^\infty(I \times J)$ and $\widehat{H}_\hbar$ maps $C_0^\infty(\mathscr{U})$ into $C_0^\infty(\mathscr{U})$, so, denoting, with abuse of notation, the restrictions of $\widehat{U}$ and $\widehat{H}_\hbar$ to C_0^∞ functions with the same symbols, we have

$$\begin{aligned}
&\widehat{U}\widehat{H}_\hbar\widehat{U}^\dagger : C_0^\infty(I \times J) \longrightarrow C_0^\infty(I \times J),\\
&\widehat{U}\widehat{H}_\hbar\widehat{U}^\dagger = -\frac{\hbar^2}{2}\frac{1}{(1+k(s)u)^{1/2}}\partial_s\Big(\frac{1}{1+k(s)u}\partial_s\frac{\cdot}{(1+k(s)u)^{1/2}}\Big)+\\
&-\frac{\hbar^2}{2}\partial_u^2 - \frac{\hbar^2}{8}\frac{k(s)^2}{(1+k(s)u)^2} + \tilde{V}(s,u) + (a\hbar)^{-2}\tilde{W}(s,u) =\\
&= -\frac{\hbar^2}{2(1+k(s)u)^2}\partial_s^2 - \frac{\hbar^2\dot{k}(s)u}{(1+k(s)u)^3}\partial_s - \hbar^2 Q(s,u) +\\
&-\frac{\hbar^2}{2}\partial_u^2 + \tilde{V}(s,u) + (a\hbar)^{-2}\tilde{W}(s,u),
\end{aligned} \tag{2.22}$$

where $\tilde{V}$ and $\tilde{W}$ are V and W written in curvilinear coordinates and $\hbar^2 Q$ is the extrapotential of purely quantum origin which we have already discussed in section 1.1.2.

It appears also in mesoscopic physics, and can give rise to interesting phenomena, like bound states, in a quantum waveguide [DuEx]. However, it will not concern us here, since it disappears in the lowest order of semiclassical approximation.

Using again a dilation operator in the transversal direction u,

$$\begin{aligned} D_\gamma : L^2(I \times J_\gamma, dsdu) &\to L^2(I \times J, dsdu) \\ (D_\gamma \psi)(s,u) &= \gamma^{1/2}\psi(s,\gamma u) \\ J_\gamma &:= \{\gamma u : u \in J\}, \end{aligned} \tag{2.23}$$

we get the final form of the Hamiltonian which we will employ in the estimates:

$$\begin{aligned} &\widehat{H}_{BO} : C_0^\infty(I \times J_{\hbar^{-1}}) \to C_0^\infty(I \times J_{\hbar^{-1}}), \\ &\widehat{H}_{BO} := D^\dagger_{\hbar^{-1}} \widehat{U} \widehat{H}_\hbar \widehat{U}^\dagger D_{\hbar^{-1}} = \\ &= -\frac{\hbar^2}{2(1+\hbar k(s)u)^2}\partial_s^2 - \frac{\hbar^3 \dot{k}(s)u}{(1+\hbar k(s)u)^3}\partial_s - \hbar^2 Q(s,\hbar u) + \widehat{\mathfrak{h}}(s), \end{aligned} \tag{2.24}$$

where

$$\widehat{\mathfrak{h}}(s) = -\frac{1}{2}\partial_u^2 + \tilde{V}(s,\hbar u) + (a\hbar)^{-2}\tilde{W}(s,\hbar u). \tag{2.25}$$

Remark 2.3. Note that

$$\begin{aligned} &(a\hbar)^{-2}\tilde{W}(s,\hbar u) = \frac{1}{2a^2}\partial_u^2 \tilde{W}(s,0)u^2 + \frac{\hbar}{6a^2}\partial_u^3 \tilde{W}(s,0)u^3 + \\ &+ \frac{1}{6a^2\hbar^2}\int_0^{\hbar u} dv(\hbar u - v)^3 \partial_u^4 \tilde{W}(s,v) = \frac{1}{2a^2}\omega(s)^2 u^2 + \frac{\hbar}{6a^2}\partial_u^3 \tilde{W}(s,0)u^3 + R_3(\hbar,u), \\ &\tilde{V}(s,\hbar u) = \tilde{V}(s,0) + \hbar u \partial_u \tilde{V}(s,0) + \int_0^{\hbar u} dv(\hbar u - v)\partial_u^2 \tilde{V}(s,v) = \\ &= \tilde{V}(s,0) + \hbar u \partial_u \tilde{V}(s,0) + R_1(\hbar,u). \end{aligned} \tag{2.26}$$

The scaling in the normal direction eliminates the dependence of $\widehat{\mathfrak{h}}$ on $\hbar$ only at the lowest order in the Taylor expansion around the constraint (which is the quadratic one since M is a nondegenerate critical curve).

From now on, we will denote by $\widehat{\mathfrak{h}}^{(2)}(s)$ the harmonic part of $\widehat{\mathfrak{h}}(s)$:

$$\widehat{\mathfrak{h}}^{(2)}(s) := -\frac{1}{2}\partial_u^2 + \frac{1}{2a^2}\omega(s)^2 u^2 + \tilde{V}(s,0). \tag{2.27}$$

2.2.2 The approximate evolution

In this subsection we prove the

Theorem 2.2. *Let $\Phi(s,u)$ be a real normalized eigenstate of $\widehat{\mathfrak{h}}^{(2)}(s)$, considered as an operator on $L^2(\mathbb{R},du)$, with eigenvalue $E(s)$. Let $a(t)$ and $\eta(t)$ be the solutions of the classical equations of motion with potential $E(s)$, and let $F(s,v)$ be a function in $C_0^\infty(I\times J)$ which is equal to 1 for s in a neighbourhood of the trajectory $\{a(t):t\in[0,T]\}$ and v near to 0.*

Then

$$\Big\| \exp\Big(-\frac{it}{\hbar}\widehat{H}_\hbar\Big)\widehat{U}^\dagger D_{\hbar^{-1}}\varphi_k(A(0),B(0),\hbar,a(0),\eta(0),s)F(s,\hbar u)\Phi(s,u) - \exp\Big(\frac{iS(t)}{\hbar}\Big)\widehat{U}^\dagger D_{\hbar^{-1}}\varphi_k(A(t),B(t),\hbar,a(t),\eta(t),s)F(s,\hbar u)\Phi(s,u)\Big\| = O(\hbar^{1/2}), \tag{2.28}$$

where $S(t)$ is the classical action associated to $(a(t),\eta(t))$.

Remark 2.4. The function $\varphi_k(A(t),B(t),\hbar,a(t),\eta(t),s)F(s,\hbar u)\Phi(s,u)$ is in $C_0^\infty(I\times J_{\hbar^{-1}})$, so $\widehat{U}^\dagger D_{\hbar^{-1}}\varphi_k(A(t),B(t),\hbar,a(t),\eta(t),s)F(s,\hbar u)\Phi(s,u)$ belongs to $C_0^\infty(\mathscr{U})$.

The proof will follow closely the pattern developed by Hagedorn [Ha$_1$], but the remainder we get is different from that found by him, since $\widehat{\mathfrak{h}}$ contains terms of order $\hbar$ and the kinetic part of (2.24) is not simply $-(\hbar^2/2)\partial_s^2$.

The basic tool we use is a simple application of the fundamental theorem of calculus (also known as Duhamel formula). We give it without proof.

Lemma 2.2. *Suppose $\widehat{H}_\hbar$ is a family of self-adjoint operators for $\hbar>0$. Suppose $\psi(\hbar,t)$ belongs to the domain of $\widehat{H}_\hbar$, is continuously differentiable in t, and approximately solves the Schrödinger equation in the sense that*

$$i\hbar\partial_t\psi(\hbar,t)=\widehat{H}_\hbar\psi(\hbar,t)+\zeta(\hbar,t), \tag{2.29}$$

where $\zeta(\hbar,t)$ satisfies

$$\|\zeta(\hbar,t)\|\le\mu(\hbar,t) \tag{2.30}$$

for $0\le t\le T$. Suppose $\Psi(\hbar,t)$ is the exact solution to the equation

$$i\hbar\partial_t\Psi(\hbar,t)=\widehat{H}_\hbar\Psi(\hbar,t) \tag{2.31}$$

with initial condition $\Psi(\hbar,0)=\psi(\hbar,0)$.

Then, for $0\le t\le T$, we have

$$\|\Psi(\hbar,t)-\psi(\hbar,t)\|\le\hbar^{-1}\int_0^T d\tau\mu(\hbar,\tau). \tag{2.32}$$

Suppose now that $\psi_{\rm ap}(s,u,t) \in C_0^\infty(I \times J_{\hbar^{-1}})$ is an approximate solution to the Schrödinger equation associated to the local Hamiltonian (2.24),

$$i\hbar\partial_t\psi_{\rm ap} = \widehat{H}_{BO}\psi_{\rm ap} + \zeta(\hbar,t) \tag{2.33}$$

with

$$\|\zeta(\hbar,t)\|_{L^2(I\times J_{\hbar^{-1}})} = O(\hbar^{3/2}) \qquad \text{for} \qquad 0 \le t \le T. \tag{2.34}$$

This implies that

$$i\hbar\partial_t\widehat{U}^\dagger D_{\hbar^{-1}}\psi_{\rm ap} = \widehat{H}_\hbar\widehat{U}^\dagger D_{\hbar^{-1}}\psi_{\rm ap} + \tilde{\zeta}(\hbar,t),$$

with $\|\tilde{\zeta}(\hbar,t)\|_{L^2(\mathscr{H})} = O(\hbar^{3/2})$.

Using lemma (2.2) we get finally

$$\Big\| \exp\Big(-\frac{it}{\hbar}\widehat{H}_\hbar\Big)\widehat{U}^\dagger D_{\hbar^{-1}}\psi_{\rm ap}(t=0) - \widehat{U}^\dagger D_{\hbar^{-1}}\psi_{\rm ap}(t)\Big\|_{L^2(\mathbb{R}^2)} = O(\hbar^{1/2}).$$

Therefore, to prove theorem (2.2) we will construct an approximate solution to (2.33), of the form

$$\psi_{\rm ap}(s,u,t) = \psi_0(s,u,t) + \hbar\psi_2^\perp(s,u,t), \tag{2.35}$$

with $\psi_0(s,u,t) = \exp(iS(t)/\hbar)\varphi_k(A(t),B(t),\hbar,a(t),\eta(t),s)F(s,\hbar u)\Phi(s,u)$ (the notation $\psi_2^\perp$ means that the transversal part of this term is orthogonal to Φ).

An educated guess about the form of the remainder $\psi_2^\perp$ can be made employing a multiple scale technique, which allows to split the adiabatic and the semiclassical scale.

We will elaborate on this procedure in the more complicated case of next section, so here we limit ourselves to verify that the right choice is

$$\begin{aligned}\psi_2^\perp(s,u,t) &= \varphi_k(A(t),B(t),\hbar,a(t),\eta(t),s)F(s,\hbar u)\\ \times\hat{r}(s)\Big[&i\eta(t)\partial_s\Phi(s,u) - \eta(t)^2k(s)u\Phi(s,u) - \partial_u\tilde{V}(s,0)u\Phi(s,u)\\ &-\frac{1}{6a^2}\partial_u^3\tilde{W}(s,0)u^3\Phi(s,u)\Big],\end{aligned} \tag{2.36}$$

where $\hat{r}(s)$ is the bounded inverse of the restriction of $[\widehat{\mathfrak{h}}^{(2)}(s) - E(s)]$ to the orthogonal complement of $\Phi(s,u)$ in $L^2(\mathbb{R},du)$.

Estimate (2.34) will follow if we note the following facts:

1. *the terms containing derivatives of F are $O(\hbar^\infty)$.* For instance,

$$\begin{aligned}&\int_{I\times J_{\hbar^{-1}}} dsdu\ |\partial_u F(s,\hbar u)\varphi_k(s)\partial_u\Phi(s,u)|^2 \\ &= \int_{I\times J} dsdv|\partial_v F(s,v)\varphi_k(s)\hbar^{1/2}\partial_u\Phi(s,v\hbar^{-1})|^2 < \exp(-C\hbar^{-1}),\end{aligned} \tag{2.37}$$

since $\partial_v F$ has support away from zero in v, and $\partial_u \Phi(s, v\hbar^{-1})$ is a polynomial times a Gaussian, in $u = v\hbar^{-1}$.

The derivatives with respect to s can be estimated in the same way, since φ_k is a Gaussian in $[s - a(t)]/\hbar^{1/2}$.

2. The term
$$\frac{\hbar^3 \dot{k}(s) u}{(1 + \hbar k(s) u)^3} \partial_s \psi_{\text{ap}}$$
is $O(\hbar^2)$ since $\partial_s \varphi_k$ is $O(\hbar^{-1})$.

3. The term
$$\hbar^2 Q(s, \hbar u) \psi_{\text{ap}}$$
is $O(\hbar^2)$ since $Q(s, u)$ is bounded on the support of F.

4. The last term is
$$\widehat{\mathfrak{h}}(s)\psi_{\text{ap}} = \widehat{\mathfrak{h}}^{(2)}\psi_{\text{ap}} + \frac{\hbar}{6a^2}\partial_u^3 \tilde{W}(s,0)u^3\psi_0 + \hbar u \partial_u \tilde{V}(s,0)\psi_0 + R_3(\hbar, u)\psi_{\text{ap}} + \\ + R_1(\hbar u)\psi_{\text{ap}} + O(\hbar^2) = E(s)\psi_{\text{ap}} + i\hbar\varphi_k(s)F(s, \hbar u)\eta(t)\partial_s \Phi(s, u) + \\ + \hbar\eta(t)^2 k(s) u \psi_0 + O(\hbar^2),$$
since $R_3(\hbar, u)$ and $R_1(\hbar, u)$ are $O(\hbar^2)$ on the support of F.

5. The terms left combine themselves with the kinetic part and the time derivative of ψ_{ap} to give (2.34).

Remark 2.5. The effective motion on M is given by the potential
$$E_n(s) = \frac{(n + 1/2)}{a}\omega(s) + \tilde{V}(s, 0) = \vartheta\omega(s) + \tilde{V}(s, 0), \tag{2.38}$$
and is equal, also in this case, to the homogenized classical motion.

The hypotheses that M is a nondegenerate critical curve and W is spectrally smooth imply that the normal oscillation is harmonic, and so all transversal states are equivalent.

2.2.3 The magnetic trap

Using theorem (2.2) we can analyze the dynamics of a nonrelativistic particle in a strong magnetic field (magnetic trap).

We suppose that the field is "strongly axially symmetric", *i. e.*, that the vector potential is given, in cylindrical coordinates, by
$$\boldsymbol{A}(r, z) = \mathscr{A}(r, z)\boldsymbol{\theta}. \tag{2.39}$$

The Hamiltonian is

$$\widehat{H} = \frac{1}{2m}\Big(\hat{p} - \frac{e}{c}\boldsymbol{A}\Big)^2. \tag{2.40}$$

Since $\mathrm{div}\boldsymbol{A} = 0$, in the subspace with zero angular momentum in the z direction (2.40) becomes

$$\widehat{H}^0 = -\frac{\hbar^2}{2m}\frac{1}{r}\partial_r(r\partial_r) - \frac{\hbar^2}{2m}\partial_z^2 + \frac{e^2}{2mc^2}\mathscr{A}(r,z)^2,$$

or, scaling the wave function by the isometry

$$\widehat{V} : L^2(\mathbb{R}_+ \times \mathbb{R}, rdrdz) \to L^2(\mathbb{R}_+ \times \mathbb{R}, drdz)$$
$$\widehat{V}\psi = r^{1/2}\psi, \tag{2.41}$$

$$\widehat{V}\widehat{H}^0\widehat{V}^\dagger = -\frac{\hbar^2}{2m}\partial_r^2 - \frac{\hbar^2}{8mr^2} - \frac{\hbar^2}{2m}\partial_z^2 + \frac{e^2}{2mc^2}\mathscr{A}(r,z)^2. \tag{2.42}$$

If we put $m = 1$ and consider the case of large electric charge, $c/e = a\hbar$, we get in the end

$$\widehat{H}_\hbar := -\frac{\hbar^2}{2}\partial_r^2 - \frac{\hbar^2}{2}\partial_z^2 - \frac{\hbar^2}{8r^2} + \frac{1}{2a^2\hbar^2}\mathscr{A}(r,z)^2, \tag{2.43}$$

which, except for the centrifugal term, is of the form (2.19), with $W(r,z) = \mathscr{A}(r,z)^2/2$.

Theorem (2.2) tells us that, if we consider an initial state localized away from the origin, the semiclassical motion is constrained along the curve $\mathscr{A}(r,z) = 0$, with effective potential given by

$$E(s) = \vartheta\{\partial_u^2[\tilde{\mathscr{A}}(s,u)]^2/2\}^{1/2}_{|u=0} = \vartheta|\partial_u\tilde{\mathscr{A}}(s,0)| = \vartheta|\boldsymbol{B}(s,0)|, \tag{2.44}$$

where $\boldsymbol{B}$ is the magnetic field strength.

2.3 Constraints by scaling of coupling constant: general case

When the submanifold M has dimension (and codimension) greater than one, the theory developed in foregoing sections has to be generalized essentially in two aspects.

First, if $\dim M > 1$, the metric G_M, induced by the Euclidean metric of $\mathbb{R}^{n+m}$ on M, may not be trivial, so both the classical motion of the centre of the squeezed state and the evolution of the dispersion matrices A and B have to be modified to take this into account. Thinking about the results we got above, it is not difficult to derive the new classical equations; we will simply obtain a motion on a Riemannian manifold with metric $G_M(x)$ in the presence of a potential $E(x)$ which is an eigenvalue of the reduced Hamiltonian. In local coordinates this means (see, for instance, [AbMa])

$$\dot{a}(t) = \eta(t) \tag{2.45}$$

$$\dot{\eta}(t) = -\Gamma(a(t))(\eta,\eta) - G_M^{-1}(a(t))\nabla_x E(a(t)), \tag{2.46}$$

where $\Gamma(\eta,\eta)^i = \Gamma^i_{jk}\eta^j\eta^k$ (Γ^i_{jk} are the Christoffel symbols associated to G_M) and ∇_x denotes the column vector whose coordinates are $\partial^i := \partial^{x_i}$.

The equations for the dispersion matrices are a bit more complicated, but, as we will see below, they can be derived, using Hagedorn's multiple scale method, from the term of order $\hbar$ of the formal expansion of the solution of the Schrödinger equation in powers of $\hbar^{1/2}$.

The second point is that, if $\operatorname{codim} M > 1$, the Euclidean metric written in tubular coordinates is not diagonal anymore.

In a formal expansion of the Hamiltonian $\widehat{H}_\varepsilon$ around the constraint, the off-diagonal terms give rise, as we have already stressed in the introduction, to an induced gauge field which minimally couples the longitudinal and the transversal motion.

At first sight, it might seem that in this case we can no longer split the motion into a tangential and a normal part, even in the semiclassical limit.

Actually this is not true, since, applied to a squeezed state, the gauge coupling is of order $\hbar$, and, due to the antisymmetric character of the normal fundamental form, it maps an eigenstate of the reduced Hamiltonian into a state which is orthogonal to it.

According to the proof of theorem (2.2), this means that, if we start from an initial state which is concentrated along a classical trajectory, and we study its evolution when $\hbar$ goes to zero, the gauge term contributes only to the remainder and not to the leading term of the expansion in powers of $\hbar^{1/2}$, which is again given by a wave packet in the longitudinal variables times an eigenstate of the normal Hamiltonian.

In principle, higher order corrections can be calculated following the procedure developed by Hagedorn [Ha$_1$], even though in the general case the formulae can be cumbersome.

In the following we will give some details of the calculations that justify these claims, even though, given the previous warnings, they are analogous to those of the two-dimensional case.

2.3.1 The Hamiltonian in tubular coordinates

Starting from the expression (1.21), we can calculate the coordinate form of the basis for the tangent space in a point of $\mathscr{E}(\delta)$ simply differentiating with respect to a coordinate x_i or y_k, and then calculate the scalar product of two basis elements to get the local form of the metric.

The result is

$$G(x,y) = \begin{pmatrix} I & N \\ 0 & I \end{pmatrix} \begin{pmatrix} G_M(I-S)^2 & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & N \\ 0 & I \end{pmatrix}^T, \tag{2.47}$$

where

$$N_{i,h}(x,y) = y_k \beta_i^{kh}(x) \qquad \beta_i^{kh} = n_k \cdot \partial^i n_h, \tag{2.48}$$

$$S_{i,j}(x,y) = y_k (G_M^{-1})_{il} \alpha_{lj}^k(x) \qquad \alpha_{lj}^k(x) = n_k \cdot \partial^l t_j, \tag{2.49}$$

and t_l denotes the basis for the tangent space (the index k and h always refer to the normal coordinates, while the other indices refer to the tangential coordinates).

β_i^{kh} and α_{il}^k are called, respectively, *normal fundamental form* and *second fundamental form* of the submanifold M. Together with the metric G_M, they characterize completely the embedding of M into $\mathbb{R}^{n+m}$, up to a Euclidean motion [Spi]. We have already noted that $\beta_i^{hk} = -\beta_i^{kh}$, so, when $\operatorname{codim} M = 1$, β is identically zero.

Using (2.47), we can write the Hamiltonian in tubular coordinates, but, as we did in the two-dimensional case, we have to modify the volume form given by $g(x,y)^{1/2} := [\det G(x,y)]^{1/2}$, in order to get wave functions which have the right normalization when integrated over the submanifold M.

After this, we have to dilate the normal coordinates by $\hbar$, in order to separate the reduced Hamiltonian from the longitudinal part.

This can be achieved by the unitary operator

$$\begin{aligned} &(\widehat{V}\psi)(x,y) = \left(\frac{g_M(x)}{g(x,y)}\right)^{1/4} \hbar^{-m/2}\psi(x, y/\hbar), \\ &\widehat{V} : L^2(\mathscr{E}(\delta/\hbar), g_M(x)^{1/2}dxdy) \to L^2(\mathscr{E}(\delta), g(x,y)^{1/2}dxdy) \end{aligned} \tag{2.50}$$

where $g_M(x) := \det G_M(x)$.

The result in the end is

$$\begin{aligned} &\widehat{H}_{BO} = \widehat{V}^\dagger \widehat{H}_\hbar \widehat{V} = \\ &= -\frac{\hbar^2}{2}\rho_\hbar(x,y)^{-1/4} g_M^{-1/2} \left(\nabla_x^T - \nabla_y^T N^T(x,y), \quad \hbar^{-1}\nabla_y^T \right) g_M^{1/2} \rho_\hbar^{1/2} \cdot \\ &\cdot \begin{pmatrix} [I - \hbar S(x,y)]^{-2} G_M^{-1}(x) & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} \nabla_x - N(x,y)\nabla_y \\ \hbar^{-1}\nabla_y \end{pmatrix} \rho_\hbar^{-1/4} + \\ &+ V(x + \hbar y) + (a\hbar)^{-2} W(x + \hbar y), \end{aligned} \tag{2.51}$$

where

$$\rho_\hbar(x,y) = \frac{g(x, \hbar y)}{g_M(x)} \quad . \tag{2.52}$$

When we further expand the equation (2.51), the terms containing $\rho_\hbar(x,y)$ give rise to additive corrections which depend only on the second derivatives (or the square of the first derivatives) of $\ln \rho_\hbar$. They are of order at least $\hbar^2$. This can be understood if we

note that $S(x,y)$ is linear in y, the second derivatives with respect to x are multiplied by $\hbar^2$ and

$$\ln \rho_\hbar(x,y) = \ln \frac{\det\{G_M[I-\hbar S(x,y)]^2\}}{\det G_M} = 2\ln\det(I-\hbar S(x,y)) = 2\mathrm{Tr}\ln(I-\hbar S)$$
$$= -2\hbar\mathrm{Tr}(S) - \hbar^2\mathrm{Tr}(S^2) + O(\hbar^3) \qquad (2.53)$$

Therefore, in the following, we will put $\rho_\hbar = 1$ without other comments.

Expanding the potentials V and W, we obtain the reduced Hamiltonian

$$\widehat{\mathfrak{h}}^{(2)}(x) = -\frac{1}{2}\Delta_y + \frac{1}{2a^2}y^T H(x)y + V(x), \qquad (2.54)$$

where $H(x)$ is the matrix of the Hessian operator in the basis $\{n_k(\zeta(x))\}$. The hypothesis that W has a smooth spectral decomposition implies that we can choose the n_k to be eigenvectors of H, so we can write $y^T H(x)y = \sum_{\lambda,k_\lambda} \omega_\lambda^2(x) y_{\lambda,k_\lambda}^2$.

We will see in next subsection that, as before, the higher order terms in the Taylor expansion must be included in the remainder.

2.3.2 The approximate evolution

To construct approximate solutions to the Schrördinger equation

$$i\hbar\partial_t\psi = \widehat{H}_{BO}\psi \qquad (2.55)$$

we use the same procedure outlined in previous sections, which is based on the multiple scale expansion developed by Hagedorn [Ha$_1$]. The operator (2.51) is not of the standard form studied in the literature, so we briefly explain the modifications needed to cope with this case.

When all the terms have been spelled out, (2.51) has the form of an elliptic differential operator in x and y, with coefficients which depend on x and y as well as $\hbar$, plus the reduced Hamiltonian, plus a remainder of order $\hbar$, which comes from the Taylor expansion of $V(x+\hbar y)$ and $W(x+\hbar y)$ up to first and third order, respectively.

According to Hagedorn's method, to split the adiabatic and the semiclassical effects, we have to introduce a fictitious new variable

$$\xi := \frac{x-a(t)}{\hbar^{1/2}}, \qquad (2.56)$$

which measures the "deviation" of the quantum evolution from the classical one, and consider ξ as an independent variable in the formal manipulations.

Associated to ξ, there is an auxiliary wave function, $\tilde{\psi}(x,y,\xi;t)$, which satisfies the equation obtained substituting

$$\tilde{\psi}\Big(x,y,\frac{x-a(t)}{\hbar^{1/2}};t\Big)$$

into (2.55), and adding to the right-hand side the term $E(a(t)+\hbar^{1/2}\xi)-E(x)$, which formally equals zero when $\xi=[x-a(t)]/\hbar^{1/2}$, where $E(x)$ is a fixed eigenvalue of $\widehat{\mathfrak{h}}^{(2)}(x)$, with multiplicity 1.

When we perform this substitution, we replace the x dependence in the coefficients of the differential terms with a dependence on $a(t)+\hbar^{1/2}\xi$.

This is justified because when we apply a function of x, $f(x)$, to a squeezed state $\varphi_k(A,B,a,\eta,\hbar,x)$, we can develop $f(x)$ in Taylor series, up to order l, around the centre of the packet, getting a remainder which, in norm, is of order $\hbar^{l/2+1}$ ([Ha$_1$] and references therein).

At this point, we make the Ansatz that

$$\tilde{\psi}(x,y,\xi;t)=\exp\left(iS(t)/\hbar\right)\exp\left[\frac{i\eta(t)^T G_M(a(t))\xi}{\hbar^{1/2}}\right]F(x,\hbar y)$$
$$\times g_M(a(t))^{-1/4}(\tilde{\psi}_0+\hbar^{1/2}\tilde{\psi}_1+\hbar\tilde{\psi}_2+\dots), \tag{2.57}$$

where $a(t)$ and $\eta(t)$ satisfy equation (2.45), $S(t)$ is the associated action

$$S(t)=\int_0^t ds\frac{1}{2}\eta(s)^T G_M(a(s))\eta(s)-E(a(s)) \quad , \tag{2.58}$$

and F is a smooth function which has support in x near the classical trajectory, and in $\hbar y$ near 0.

Substituting this Ansatz in the equation for $\tilde{\psi}$, and keeping terms up to order $\hbar$, we can determine $\tilde{\psi}_0$ and $\tilde{\psi}_2^{\perp}$, which, as shown in [Ha$_1$] are what is needed to solve the Schrödinger equation to lowest order in $\hbar^{1/2}$. The calculations are lengthy and not very interesting, so we give simply the result.

The approximate solution, up to order $\hbar^{1/2}$, of (2.55) is

$$\psi_{\rm ap}(x,y;t)=\exp\left(iS(t)/\hbar\right)\exp\left[\frac{i\eta(t)^T G_M(a(t))\xi}{\hbar^{1/2}}\right]g_M(a(t))^{-1/4}\hbar^{-n/4}$$
$$\times\varphi_k(A(t),B(t),1,0,0,\xi)\Bigg\{\Phi(x,y)+\hat{r}(x)\Bigg[i\eta^T\nabla_x\Phi$$
$$+i\eta(t)^T N(a(t),y)\nabla_y\Phi+\eta(t)^T G_M(a(t))S(a(t),y)\eta(t)\Phi$$
$$+y^T\nabla_y V(x)\Phi+\frac{1}{a}\sum_{|p|=3}\frac{\nabla_y^p W(x)y^p}{p!}\Phi\Bigg]\Bigg\} \quad , \tag{2.59}$$

where ξ is given by (2.56), N and S are defined in (2.48) and (2.49), and $\Phi(x,y)$ is a real eigenstate of $\widehat{\mathfrak{h}}^{(2)}(x)$, with eigenvalue $E(x)$ of multiplicity 1.

As before, $\hat{r}(x)$ is the bounded inverse of the restriction of $[\widehat{\mathfrak{h}}^{(2)}(x)-E(x)]$ to the orthogonal complement of $\Phi(x,y)$ in $L^2(\mathbb{R}^m,dy)$.

Remark 2.6. The evolution of the dispersion matrices $A(t)$ and $B(t)$ can be read from the terms of order $\hbar$ in the expansion, and contains explicitly the metric G_M:

$$\partial_t A(t)_{il} = \eta_k(t)[G_M \partial_j G_M^{-1}]_{ki}(a(t))A(t)_{jl} + i[G_M^{-1}(a(t))B(t)]_{il} \tag{2.60}$$

$$\partial_t B(t)_{il} = \frac{i}{2}\eta(t)^T[G_M(\partial^2_{ij}G_M^{-1})G_M](a(t))\eta(t)A(t)_{jl} + \partial^2_{ij}E(a(t))A(t)_{jl} - \eta_k(t)[G_M\partial_i G_M^{-1}]_{kj}(a(t))B(t)_{jl} \tag{2.61}$$

Remark 2.7. The term coming from the gauge coupling

$$i\eta(t)^T N(a(t), y)\nabla_y \Phi$$

can be written, using creation and destruction operators for the normal oscillations, as

$$i\eta_j \beta_j^{(\lambda,k_\lambda)(\nu,h_\nu)} y_{\lambda,k_\lambda} \frac{\partial}{\partial y_{\nu,h_\nu}}\Phi = \frac{i}{2}\eta_j\beta_j^{(\lambda,k_\lambda)(\nu,h_\nu)}\left[\frac{\omega_\nu}{\omega_\lambda}\right]^{1/2}(a_{\lambda,k_\lambda}a_{\nu,h_\nu} - a_{\lambda,k_\lambda}a^\dagger_{\nu,h_\nu} + a^\dagger_{\lambda,k_\lambda}a_{\nu,h_\nu} - a^\dagger_{\lambda,k_\lambda}a^\dagger_{\nu,h_\nu})\Phi \quad . \tag{2.62}$$

Since β is antisymmetric in $(\lambda, k_\lambda), (\nu, h_\nu)$, the above expression is orthogonal to Φ, as we claimed in the introduction to this section.

2.4 Takens chaos in quantum mechanics

When the constraining potential is not spectrally smooth, that is, roughly speaking, when the eigenvalues or the eigenfunctions of its Hessian are not smooth, the classical motion on the submanifold M shows peculiar features.

In this section we consider the quantum analogue of an example given by Takens ([Tak], see also [Bor]) where W fails to constrain spectrally smooth.

The Hamiltonian we study is

$$H_\varepsilon = \frac{p^2_{x_1} + p^2_{x_2}}{2} + \frac{p^2_{y_1} + p^2_{y_2}}{2} + \frac{1}{2\varepsilon^2} < R(x)y, y >, \tag{2.63}$$

where $q = (x, y) \in \mathbb{R}^4$, $< \cdot, \cdot >$ is the standard scalar product in $\mathbb{R}^2$ and $R(x)$ is the Rellich matrix ([Kat] and references therein)

$$R(x) = \frac{1}{4}\left[\mathbb{I} + \begin{pmatrix} x_1 & x_2 \\ x_2 & -x_1 \end{pmatrix}\right] \quad . \tag{2.64}$$

The eigenvalues of $R(x)$ are

$$\omega_\pm(x)^2 = \frac{1}{4}(1 \pm |x|), \tag{2.65}$$

with corresponding eigenvectors

$$v_+(x) = \begin{pmatrix} \cos(\phi/2) \\ \sin(\phi/2) \end{pmatrix} \qquad v_-(x) = \begin{pmatrix} -\sin(\phi/2) \\ \cos(\phi/2) \end{pmatrix}, \tag{2.66}$$

where $\phi = \tan^{-1}(x_2/x_1)$, and the branch of the inverse tangent is chosen so that $-\pi/2 \leq \phi < 3\pi/2$.

The eigenvectors are discontinuous along the semiaxis $\{x : x_1 = 0, x_2 \leq 0\}$, or better, they exchange place upon crossing the cut.

2.4.1 A brief review of the classical case

To get a confining potential which is bounded from below we restrict the configuration space to

$$\Sigma := \{(x, y) : |x| < 1/2\}. \tag{2.67}$$

With this choice, the Hamiltonian (2.63) constrains the system to the submanifold

$$M := \{(x, y) \in \Sigma : y = 0\}. \tag{2.68}$$

An (almost) complete description of the limit motions when $\varepsilon \to 0$ is given by

Theorem 2.3 ([Tak], theorem 3). *Let*

$$W(q) = \frac{1}{2} < R(x)y, y >,$$

then the solutions of the equations of motion

$$\begin{aligned} &\ddot{q}_\varepsilon(t) = -\frac{1}{\varepsilon^2}\nabla W(q_\varepsilon(t)), \\ &q_\varepsilon(0) = 0 \qquad \dot{q}_\varepsilon(0) \to v_* \end{aligned} \tag{2.69}$$

which satisfy

$$Qv_* \neq 0, \tag{2.70}$$

where $Q : \mathbb{R}^4 \to \mathbb{R}^2$ is the orthogonal projector $Q(x, y) = x$, converge uniformly to the unique *solution of*

$$\begin{aligned} &\ddot{x}(t) = -\nabla U_{\text{hom}}(x(t), t), \\ &x(0) = 0 \qquad \dot{x}(0) = Qv_*, \end{aligned} \tag{2.71}$$

where

$$U_{\text{hom}}(x, t) := \vartheta_+(t)\omega_+(x) + \vartheta_-(t)\omega_-(x). \tag{2.72}$$

The functions $\vartheta_\pm$ are constant for $t \neq 0$ and can have any discontinuity in $t = 0$, provided that $\vartheta_+ + \vartheta_-$ remains constant.

Remark 2.8. If $Qv_* = 0$, the limiting behaviour is *not* known.

2.4.2 A quantum analogue

In the quantum case, we consider the Hamiltonian

$$\widehat{H}_\hbar = -\frac{\hbar^2}{2}(\Delta_x + \Delta_y) + \frac{1}{2a^2\hbar^2} < g(|x|)R(x)y, y >, \tag{2.73}$$

where $g \in C_0^\infty(\mathbb{R})$, $g(z) = 1$ when $|z| < 1/2$, $g(z) = 0$ when $|z| > 3/5$.

We use the same squeezing factor a for both transversal directions so that the eigenvalues of $R(x)$ keep their simple form (2.65).

The quadratic form $< g(|x|)R(x)y, y >$ is non-negative, so $\widehat{H}_\hbar$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^4)$.

Scaling y as we did in the above sections, we get

$$\begin{aligned} \widehat{H}_{BO} &= -\frac{\hbar^2}{2}\Delta_x + \widehat{\mathfrak{h}}(x), \\ \widehat{\mathfrak{h}}(x) &= -\frac{1}{2}\Delta_y + \frac{1}{2a^2} < g(|x|)R(x)y, y > . \end{aligned} \tag{2.74}$$

Let us suppose from now on that $|x| < 1/2$, so that $g(|x|) = 1$ (note that, in theorem (2.1), it is required that $\widehat{\mathfrak{h}}(x)$ has an eigenvalue on an open set only, so this restriction is immaterial).

To calculate the spectrum of $\widehat{\mathfrak{h}}(x)$ we exploit the fact that, for every x, $R(x)$ is a real symmetric matrix, and can be diagonalized by an orthogonal transformation whose form can be derived from (2.66), and is given by

$$Z(x) = \begin{pmatrix} \cos(\phi/2) & -\sin(\phi/2) \\ \sin(\phi/2) & \cos(\phi/2) \end{pmatrix}. \tag{2.75}$$

It shows the same discontinuity of $v_\pm$, but however is defined for all x.

The corresponding unitary operator

$$\begin{aligned} &\widehat{Z}(x) : L^2(\mathbb{R}^2_y) \to L^2(\mathbb{R}^2_y), \\ &[\widehat{Z}(x)\psi](y) = \psi(Z(x)^{-1}y), \end{aligned} \tag{2.76}$$

turns $\widehat{\mathfrak{h}}(x)$ into the Hamiltonian of two uncoupled harmonic oscillators,

$$\widehat{Z}(x)^\dagger \widehat{\mathfrak{h}}(x)\widehat{Z}(x) = -\frac{1}{2}\Delta_y + \frac{1}{2a^2}\omega_+(x)^2 y_1^2 + \frac{1}{2a^2}\omega_-(x)^2 y_2^2. \tag{2.77}$$

The eigenvalues of $\widehat{\mathfrak{h}}(x)$ are then

$$\begin{aligned} E_{n_+,n_-}(x) &= E_{0,0}(x) + \frac{n_+}{a}\omega_+(x) + \frac{n_-}{a}\omega_-(x), \\ E_{0,0}(x) &= \frac{\omega_+(x) + \omega_-(x)}{2a} = \frac{1}{4a}[(1+|x|)^{1/2} + (1-|x|)^{1/2}]. \end{aligned} \tag{2.78}$$

The ground state

The eigenfunction corresponding to $E_{0,0}(x)$ is

$$\Phi_{0,0}(x,y) = [\widehat{Z}(x)\Psi_{0,0}](x,y) = \Psi_{0,0}(x, Z(x)^{-1}y),$$

where $\Psi_{0,0}$ is the eigenfunction of (2.77) with the same eigenvalue.

The result, with a suitable choice of normalization constants, is

$$\Phi_{0,0}(x,y) = \left[\frac{\omega_+(x)\omega_-(x)}{a^2\pi}\right]^{1/4} \exp\Big(-\frac{1}{2a} < R(x)^{1/2}y, y > \Big). \tag{2.79}$$

The equations (2.78) and (2.79) tell us that both the energy and the wave function of the ground state of $\widehat{\mathfrak{h}}(x)$ are C^∞ functions of x for $|x| < 1/2$. Therefore, theorem (2.1) can be used also in this case, and gives us a constrained motion in the cylinder $\{(x,y) : |x| < 1/2, y = 0\}$, with effective potential $E_{0,0}(x)$.

The classical trajectory we obtained is the only one which is associated, in the funnel described by (2.72), to a smooth homogenized potential. The semiclassical limit thus singles out a specific motion, which is linked to the initial normal oscillation.

The excited states

If we consider the excited states of $\widehat{\mathfrak{h}}(x)$, we observe crossings between different eigenvalues in $x = 0$. Unlike what happens in the classical case, however, an incoming semiclassical wave packet splits into two components only, giving rise to a bifurcation of the motion, and not to a funnel.

For the first two excited states, for example, we have

$$E_{0,1}(x) = E_{0,0}(x) + \omega_-(x)/a \tag{2.80}$$
$$E_{1,0}(x) = E_{0,0}(x) + \omega_+(x)/a, \tag{2.81}$$

(when $|x| < 1/2$ we have $\omega_+(x) < 2\omega_-(x)$, so the other eigenvalues remain separated from these).

The corresponding eigenfunctions are

$$\Phi_{0,1}(x,y) = a^{-1/2}\Phi_{0,0}(x,y)[2\omega_-(x)]^{1/2}[-\sin(\phi/2)y_1 + \cos(\phi/2)y_2] \tag{2.82}$$
$$\Phi_{1,0}(x,y) = a^{-1/2}\Phi_{0,0}(x,y)[2\omega_+(x)]^{1/2}[\cos(\phi/2)y_1 + \sin(\phi/2)y_2]. \tag{2.83}$$

Clearly, the two eigenvalues coincide when $x = 0$, and are not differentiable in such point, while the eigenfunctions are not even continuous.

Carrying out a rotation between $\Phi_{0,1}$ and $\Phi_{1,0}$, we can construct a smooth basis in the two-dimensional subspace generated by them.

It is easily seen that

$$\begin{pmatrix} \Phi_{\rm A}(x,y) \\ \Phi_{\rm B}(x,y) \end{pmatrix} := \begin{pmatrix} \sin(\phi/2) & -\cos(\phi/2) \\ \cos(\phi/2) & \sin(\phi/2) \end{pmatrix} \begin{pmatrix} \Phi_{0,1}(x,y) \\ \Phi_{1,0}(x,y) \end{pmatrix} \tag{2.84}$$

are smooth in the origin, since $[2\omega_{\pm}(x)]^{1/2} = (1 \pm |x|)^{1/4} = 1 \pm \frac{1}{4}|x| + O(|x|^2)$, so

$$\Phi_{\rm A}(x,y) = a^{-1/2}\Phi_{0,0}(x,y)\Big\{ -y_1 - \frac{1}{4}y_1x_1 - \frac{1}{4}y_2x_2 + O(|x|^2)\Big\}$$
$$\Phi_{\rm B}(x,y) = a^{-1/2}\Phi_{0,0}(x,y)\Big\{ y_2 + \frac{1}{4}y_1x_2 - \frac{1}{4}y_2x_1 + O(|x|^2)\Big\}.$$

Note that

$$< \Phi_{\rm B}(x,y), \widehat{\mathfrak{h}}(x)\Phi_{\rm A}(x,y) >_{L^2(\mathbb{R}^2_y)} = a^{-1}\sin(\phi/2)\cos(\phi/2)[\omega_-(x) - \omega_+(x)] \tag{2.85}$$
$$= a^{-1}\Big[-\frac{1}{4}x_2 + O(|x|^3)\Big] \neq 0 \qquad \forall x \neq 0. \tag{2.86}$$

Therefore, in Hagedorn's classification [Ha$_1$], this is a crossing of type I. The theory developed by him allows to elaborate on the qualitative features of the propagation we mentioned above.

If the system is initially in a semiclassical state associated to the level $E_{0,1}$ and passes through the region of crossing, $x = 0$, with a non-zero velocity (this assumption of generic crossing was already present in Takens' theorem, (2.70)) the final state is a superposition of two components, one evolving with the potential $E_{0,1}$ and the other with the potential $E_{1,0}$. More precisely we have

Theorem 2.4 ([Ha$_1$], theorem 6.3). *There is an approximate solution $\Psi(\hbar, x, y, t)$ to the Schrödinger equation generated by the Hamiltonian (2.74) that satisfies*

$$\begin{aligned} &\Psi(\hbar,x,y,t) = \Phi_{0,1}(x,y)\exp\big(iS^{(0,1);-}(t)/\hbar\big)\cdot \\ &\cdot \varphi_k(A^{(0,1);-}(t), B^{(0,1);-}(t), \hbar, a^{(0,1)}(t), \eta^{(0,1)}(t), x) + O(\hbar^{1/2}) \end{aligned} \tag{2.87}$$

for $t \in [-T, T_1]$, for any $T_1 > 0$. For $t \in [T_1, T]$, this solution satisfies

$$\begin{aligned} &\Psi(\hbar,x,y,t) = \Phi_{0,1}(x,y)\exp\big(iS^{(0,1);+}(t)/\hbar\big)\times \\ &\times \sum_m d_m^{(0,1)}\varphi_m(A^{(0,1);+}(t), B^{(0,1);+}(t), \hbar, a^{(0,1)}(t), \eta^{(0,1)}(t), x) + \\ &+ \Phi_{1,0}(x,y)\exp\big(S^{(1,0),+}(t)/\hbar\big)\times \\ &\times \sum_{|m|<|k|} d_m^{(1,0)}\varphi_m(A^{(1,0);+}(t), B^{(1,0);+}(t), \hbar, a^{(1,0)}(t), \eta^{(1,0)}(t), x) + \\ &+ O(\hbar^{\alpha/2}), \qquad \textit{for some} \quad \alpha > 0. \end{aligned} \tag{2.88}$$

Chapter 3

Soft approximation of quantum graphs

In the first part of this chapter we will define quantum graphs, and consider different kinds of Hamiltonians which can be defined on them. In particular, we will refer to the work of Kostrykin and Schrader [KoSc$_1$], who classified all the self-adjoint extensions of the Laplacian on a metric graph (see also the detailed review papers by Kuchment [Ku$_1$, Ku$_2$, Ku$_3$]). We will also mention, for comparison's sake, the known results on the rigid approximation of quantum graphs and spectral convergence and the works on the convergence of diffusion processes (see section 3.1.3 for references).

In the second part, we will analyze the convergence of the dynamics for a soft approximation of quantum graphs, i. e., for an Hamiltonian, defined on $L^2(\mathbb{R}^2)$, which contains a potential constraining to a graph Γ. Taking a different perspective compared with the one of last chapter, we will *not* consider anymore highly oscillatory longitudinal solutions, whose wavelength is comparable to the transverse one, but we will deal instead with the case when ε and $\hbar$ are unrelated.

In the case of oscillatory solutions, it is natural to use semiclassical approximation because the longitudinal motion contains a "natural" small parameter given, e. g., by the ratio between the longitudinal wavelength and the characteristic longitudinal length of the tube where the particle moves. To analyze the case when this ratio is not small requires, as we will see, different techniques. We will consider a specific potential, the distance from the graph, discussing how to deal with more general cases and we will obtain a limit equation outside the vertices which is the *free Schrödinger equation.* The behaviour of the limit in the vertices for a generic graph is still unknown.

In the particular case of a graph with two edges, we will discuss a different kind of soft approximation, which is amenable to a complete treatment. Loosely speaking, we will show that, if we approximate the graph with a smooth curve, whose curvature grows in a region which is big with respect to the localization of transverse states, then, in each transverse eigenspace, the limit longitudinal dynamics is given by *Dirichlet boundary*

conditions.

3.1 Quantum graphs

3.1.1 Basic features of quantum graphs

A (finite) graph[1] Γ consists of a finite set of vertices $V = \{v_i\}_{i\in I}$ and a set E of edges connecting the vertices, $E = \{e_j\}_{j\in J}$. We can associate to each edge a pair (v_i, v_k) of vertices, but, if there are loops, this correspondence is obviously not one to one. We suppose that, for each vertex, there exists at least one edge incident to it. This is a reasonable hypothesis thinking to the physical models of section 1.2, where isolated vertices do not play any role.

A graph is said to be a *metric graph* if to each edge e is assigned a length $l_e \in (0, +\infty]$. Edges of infinite length arise naturally if one considers scattering theory on graphs (see, e. g., [MePa] and references therein), which, on the other end, is the first step in calculating the conductivity in mesoscopic devices, via Landauer theory [La].

After having defined the length, we can identify each edge with a finite or infinite interval $[0, l_e]$, with the natural coordinate x_e along it. A metric graph then is naturally a topological space, given by a finite union of intervals, with the quotient topology obtained identifying the ends of the intervals according to the graph structure.

Therefore, a metric graph can be considered, in a purely abstract setting, as a one-dimensional simplicial complex, in which the simplexes (i. e., the edges) have a smooth structure with singularities at the vertices. However, in the applications we are interested in there always exists a natural embedding of the graph in $\mathbb{R}^2$ or $\mathbb{R}^3$ (section 1.2).

Lebesgue measure can be defined in the obvious way on the graph, and then one can define function spaces analogous to the usual ones, with some care concerning the Sobolev spaces.

Definition 3.1.

- The space $L^2(\Gamma)$ is the direct sum of the spaces $L^2(e)$, $e \in E$,

$$L^2(\Gamma) := \bigoplus_{j\in J} L^2(e_j). \tag{3.1}$$

- The space $H^1(\Gamma)$ is made up of all *continuous* functions on Γ that belong to $H^1(e)$ for each edge e. This is equivalent to say that, given a vertex v and the set E_v of all edges incident to it, the restriction, f_e, of a function $f \in H^1(\Gamma)$ to the edge e is in $H^1(e)$ *and* $f_{e_j}(v) = f_{e_k}(v)$ for $e_j, e_k \in E_v$.

[1] In the following, without explicitly mentioning it again, we will consider only *finite* graphs. We refer the reader interested in infinite graphs to [Ku3].

As remarked by Kuchment [Ku$_2$], there does not exist a natural definition of higher order Sobolev spaces, $H^k(\Gamma)$, $k \geq 2$, because, as we will see below, it is necessary to impose boundary conditions at the vertices to have a meaningful free Laplacian on the graph.

A *quantum graph* is a metric graph equipped with a self-adjoint differential or pseudo-differential operator which is called the Hamiltonian of the quantum graph. Standard examples of Hamiltonians include

- the Schrödinger operator,

$$f(x) \to -\frac{1}{2}\frac{d^2 f}{dx^2} + V(x)f(x); \tag{3.2}$$

- the magnetic Schrödinger operator [KoSc$_2$],

$$f(x) \to \frac{1}{2}\left(-i\frac{d}{dx} - A(x)\right)^2 f(x) + V(x)f(x); \tag{3.3}$$

- the Dirac operator [BuTr],

$$\begin{aligned} f(x) &:= \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} \\ f(x) &\to -i\frac{d}{dx} \otimes \sigma_1 f(x) + \mathbb{I} \otimes \sigma_3 f(x), \end{aligned} \tag{3.4}$$

  where σ_1 and σ_3 are the standard Pauli matrices.

Clearly, it is necessary to specify also the domains where these operators are well defined and self-adjoint. We will elaborate on this subject below, for the case of the free Schrödinger operator, which is the one more common in the applications.

3.1.2 Self-adjoint extensions of the free Laplacian on a graph

To give a meaning to the formal expression (3.2) (in the case $V = 0$), we restrict our attention to *local boundary conditions*, i. e., those that involve one vertex only at a time. It is clear then that it is enough to consider a junction with one vertex v and n infinite edges e_j, $j = 1, \ldots, n$.

The Hilbert space of the system is given by

$$\mathcal{H} := \bigoplus_{j=1}^{n} L^2(0, +\infty). \tag{3.5}$$

Each element of $\mathcal{H}$ can be written as an n-tuple $(\psi_1, \ldots, \psi_n)$, $\psi_j \in L^2(0, +\infty)$, $j = 1, \ldots, n$.

On $\mathcal{H}$ we define the symmetric operator

$$\Delta_0\psi := \left(\frac{d^2\psi_1}{dx^2}, \dots, \frac{d^2\psi_n}{dx^2}\right) \tag{3.6}$$

on the domain

$$\mathcal{D}(\Delta_0) = \left\{\psi \in \mathcal{H} : \psi_j \in H^2(0, +\infty), \psi_j(0) = \psi_j'(0) = 0\right\}. \tag{3.7}$$

According to what we have said above, the possible free Hamiltonians for a quantum graph are the self-adjoint extensions of Δ_0. Applying standard von Neumann's theory (see, e. g., [ReSi$_1$] section X.1) one easily obtains that the deficiency indices of Δ_0 are (n, n) and therefore the self-adjoint extensions are parametrized by the unitary group $U(n)$, that is by n^2 real parameters. To get an explicit expression of their domain in terms of boundary conditions however, it is simpler to apply an equivalent description, based on symplectic theory, which we are going to expound.

The adjoint of Δ_0, $\Delta := (\Delta_0)^\dagger$, can be calculated explicitly and is given by the second derivative without any boundary condition,

$$\begin{aligned} \Delta\psi &:= \left(\frac{d^2\psi_1}{dx^2}, \dots, \frac{d^2\psi_n}{dx^2}\right), \\ \mathcal{D}(\Delta) &= \left\{\psi \in \mathcal{H} : \psi_j \in H^2(0, +\infty)\right\}. \end{aligned} \tag{3.8}$$

On $\mathcal{D}(\Delta)$ we define the skew-Hermitian quadratic form Ω by

$$\Omega(\varphi, \psi) := < \Delta\varphi, \psi >_{\mathcal{H}} - < \varphi, \Delta\psi >_{\mathcal{H}} = -\overline{\Omega(\psi, \varphi)}. \tag{3.9}$$

The link between Ω and the self-adjoint extensions of Δ_0 is given by

Proposition 3.1. [1] *There is a one to one correspondence between self-adjoint extensions of Δ_0 and maximal isotropic subspaces of $\mathcal{D}(\Delta)$ (i. e., subspaces where $\Omega = 0$). More specifically, the self-adjoint extensions of Δ_0 are given by the restrictions of Δ to the maximal isotropic subspaces of $\mathcal{D}(\Delta)$ which are closed with respect to the norm $\|\psi\|_\Delta^2 := \|\psi\|^2 + \|\Delta\psi\|^2$.*

Since the functions in H^2 can be integrated by parts, we get

$$\Omega(\varphi, \psi) = \sum_{k=1}^{n} (\bar{\varphi}_k(0)\psi_k'(0) - \bar{\varphi}_k'(0)\psi_k(0)) = \omega([\varphi], [\psi]) := < [\varphi], J[\psi] >_{\mathbb{C}^{2n}},$$

[1] It is a difficult task to trace the history of this proposition. Some hints are given in [KoSc$_1$, Ku$_2$].

where J is the canonical symplectic matrix on $\mathbb{C}^{2n}$,

$$J := \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}, \tag{3.10}$$

and $[\,] : \mathcal{D}(\Delta) \to \mathbb{C}^{2n}$ is the surjective linear map

$$[\psi] := \begin{pmatrix} \psi_1(0) \\ \cdot \\ \cdot \\ \cdot \\ \psi_n(0) \\ \psi_1'(0) \\ \cdot \\ \cdot \\ \cdot \\ \psi_n'(0) \end{pmatrix} = \begin{pmatrix} \psi(0) \\ \psi'(0) \end{pmatrix}. \tag{3.11}$$

The form ω is called an *Hermitian symplectic form*[1], because the complex conjugate in its definition makes it different from the standard symplectic form in $\mathbb{C}^{2n}$. In this way, the problem of finding the maximal isotropic subspaces of $\mathcal{D}(\Delta)$ is equivalent to the problem of finding the Lagrangian planes of the Hermitian symplectic form ω. This can be done using a procedure entirely analogous to the one employed for Euclidean forms.

The results can be summarized by

Proposition 3.2. *[KoSc$_1$] Let the subspace $\mathcal{M}(A,B) \subset \mathcal{D}(\Delta)$ be defined by the equation*

$$A\psi(0) + B\psi'(0) = 0,$$

where A and B are two $n \times n$ matrices. Then $\mathcal{M}(A,B)$ is a maximal isotropic subspace of $\mathcal{D}(\Delta)$ if and only if

$$\begin{aligned} &\textit{the } n \times 2n \textit{ matrix } (A,B) \textit{ has maximal rank} \\ &\textit{and} \\ &AB^\dagger \textit{ is self-adjoint.} \end{aligned} \tag{3.12}$$

In this way we get a complete characterization of the self-adjoint extensions of Δ_0 in terms of boundary conditions.

Some simple examples satisfying (3.12) are[2]

[1] [KoSc$_1$]. This notion, together with the one of Hermitian symplectic spaces is thoroughly analyzed in [Har].

[2] In the following the derivatives along the edges are always taken in the *directions away from the vertex.*

- δ-type conditions.

$$\begin{cases} f(x) \quad \text{continuous on} \quad \Gamma, \\ \text{at each vertex } v, \quad \sum_{e \in E_v} \frac{df}{dx_e}(v) = \alpha_v f(v). \end{cases}$$

- Kirchhoff conditions.

$$\begin{cases} f(x) \quad \text{continuous on} \quad \Gamma, \\ \text{at each vertex } v, \quad \sum_{e \in E_v} \frac{df}{dx_e}(v) = 0. \end{cases}$$

  If there are only two edges incident to a vertex v, the Kirchhoff conditions say that the vertex has no effect on the motion of the wavefunction, so, in a sense, they correspond to an absence of interaction between the particle and the vertex itself.

- δ'-type conditions.

  These conditions are similar to the δ-type ones, but with the role of functions and derivatives reversed at each vertex.

  Let f_e denote the function f restricted to edge e.

$$\begin{cases} \text{The value of the derivative} \frac{df_e}{dx_e}(v) \text{is the same for all edges } e \in E_v, \\ \sum_{e \in E_v} f_e(v) = \alpha_v \frac{df}{dx}(v). \end{cases}$$

- Dirichlet conditions.

$$f_e(v) = 0 \quad \forall e \in E_v.$$

  In this case the Hamiltonian *completely decouples* into the direct sum of Dirichlet Hamiltonians in each edge so that there is no communication between them.

3.1.3 Rigid approximation of quantum graphs

The above discussion shows that the requirement of self-adjointness alone does not single out an Hamiltonian for a quantum graph. We have seen in section 1.2 however, that quantum graphs typically appear as simplified models to describe electron motion in nanophysics and theoretical chemistry. Therefore, a natural question arises: can we eliminate the ambiguity and select between the n^2 parameters self-adjoint extensions one that is the limit of a more realistic model?

This formulation of the problem requires to specify a physically sound model whose dynamical and spectral characteristics are well approximated by a quantum graph in certain regimes, i. e., for example, for a certain class of initial conditions or for the calculation of physically relevant quantities like the conductivity.

In the models we described in section 1.2 the electron is confined inside a branched waveguide by the interaction with other particles (a crystal, the σ-electrons...), so we think that it is possible to get a suitable description of its motion employing a constraining potential.

Another appropriate choice is to consider a "thickened graph" composed of thin tubes which have the same topology as the original graph and reduce to it in the limit of vanishing tube radius. It is reasonable to suppose that the motion of the electron in this thickened structure is free, but one needs to specify boundary conditions to get a well-defined Laplacian. The most natural choice is to use Dirichlet boundary conditions, which correspond to an infinite constraining potential barrier. Some light on this case has been shed only very recently [Po$_1$].

For technical reasons however, much more attention has been devoted to the case of Neumann boundary conditions, which is by now well understood.

Since we think that it is interesting to compare our results concerning soft approximations with the ones already known for rigid approximations we give a brief account of them, concentrating on the differences between the Neumann boundary conditions case on one side and the Dirichlet and the constraining potential case on the other side. Actually, as we will see in section 3.3, in certain situations these last two cases are interchangeable.

As a last remark, we would like also to stress that all the results obtained so far on the rigid approximation of quantum graphs concern the *spectral convergence* and the *convergence of diffusion processes* on graphs whose *edges have finite length*, while we are interested instead in the convergence of the dynamics in the spirit of adiabatic perturbation theory and eventually to scattering theory.

Neumann boundary conditions

Let us consider a graph Γ embedded in $\mathbb{R}^2$, whose *edges have finite length*. For simplicity, we suppose that the edges of the graph are straight lines, but in the references we quote below the reader will find the generalization to the case where each edge is a finite segment of a C^2 curve.

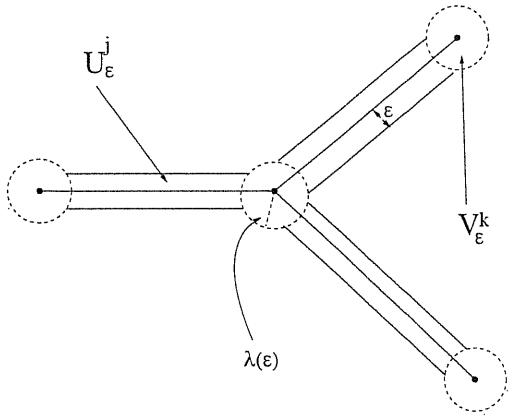
Let M_ε be a domain consisting of narrow tubes U_ε^j surrounding the edges and small neighbourhoods V_ε^k of the vertices,

$$M_\varepsilon := \Big(\cup_{j\in J} U_\varepsilon^j \Big) \bigcup \Big(\cup_{k\in K} V_\varepsilon^k \Big). \tag{3.13}$$

We assume for brevity that the cross-sections of the tubes are intervals with centers on Γ, and that the neighbourhoods of the vertices are balls in $\mathbb{R}^2$.

Let ε be the radius of the tubes surrounding the edges and $\lambda(\varepsilon)$ the radius of the balls centered at the vertices (see figure 3.1), where $\lim_{\varepsilon\to 0} \lambda(\varepsilon) = 0$. The Neumann

Figure 3.1: Example of a thickened graph



Laplacian on M_ε, Δ_N^ε, is defined in the standard way as the unique self-adjoint operator associated to the quadratic form (see, e. g., [Dav], chapter 7)

$$\begin{aligned} Q_N^\varepsilon(f) &:= -\int_{M_\varepsilon} dq\ |\nabla f(q)|^2, \\ \mathcal{D}(Q) &= H^1(M_\varepsilon). \end{aligned} \tag{3.14}$$

The behaviour of the spectrum $\sigma(-\Delta_N^\varepsilon)$ (which, since M_ε is a compact set, is *purely discrete*) in the limit $\varepsilon \to 0$ has been investigated by Rubinstein and Schatzman [RubSc] and by Kuchment and Zeng [KuZe$_1$, KuZe$_2$], who considered also the case of the magnetic Neumann Laplacian. Later, Exner and Post [ExPo] studied much more general "thickened graphs" considering abstract edges and vertices neighbourhoods, U_ε^j and V_ε^k, given by manifolds whose diameter shrinks to zero. Their approach, which is more geometric, does not depend on the particular embedding and contains the previous results as particular case. A weak form of resolvent convergence (which somewhat resembles what we do in section 3.2 for the time evolution) was studied by Saito [Sai$_1$], who analyzed also less usual thickened graphs, given by fractal domains [EvSa, Sai$_2$].

The convergence of diffusion processes was studied instead by Freidlin and Wentzell ([FrWe], [Fr] chapter 7) who considered the problem of determining the behaviour of the solution of the equation

$$\begin{aligned} &\frac{\partial u_\varepsilon(t,q)}{\partial t} = \frac{1}{2}\Delta u_\varepsilon(t,q), \qquad t>0, \quad q \in M_\varepsilon, \\ &u_\varepsilon(0,q) = g(q), \qquad \left.\frac{\partial u_\varepsilon(t,q)}{\partial n(q)}\right|_{t>0, q\in\partial M_\varepsilon} = 0, \end{aligned} \tag{3.15}$$

as $\varepsilon \to 0$, where $g(q)$ is a continuous bounded function and $n(q)$ is the normal to the boundary at $q \in \partial M_\varepsilon$.

The results which have been obtained can be summarized as follows:

1. Suppose $\lambda(\varepsilon) = \varepsilon^\alpha$, with $1/2 < \alpha \leq 1$, then

   - if we denote by $\mu_l(\varepsilon)$, $l \in \mathbb{N}$, the eigenvalues of $-\Delta_N^\epsilon$ written in increasing order and repeated according to multiplicity,

     $$\mu_l(\varepsilon) \to \mu_l(0), \tag{3.16}$$

     where $\mu_l(0)$ are the eigenvalues of (minus) the Laplacian on the graph with Kirchhoff boundary conditions.

   - if we denote by $\pi(q)$ the point of Γ closest to q (if it is not unique, we take any of them), then

     $$\sup_{q \in M_\varepsilon} |u_\varepsilon(t,q) - u_0(t,\pi(q))| \to 0, \quad \varepsilon \to 0, \tag{3.17}$$

     where u_0 is the unique solution to the equation

     $$\begin{aligned} &\frac{\partial u_0(t,x)}{\partial t} = \frac{1}{2}\frac{\partial^2 u_0(t,x)}{\partial x^2}, \qquad t > 0, \quad x \in \Gamma \backslash \{v_k\}_{k \in K}, \\ &u_0(0,x) = g(x), \end{aligned} \tag{3.18}$$

     with Kirchhoff boundary conditions at the vertices.

2. Suppose $\lambda(\varepsilon) = \varepsilon^\alpha$, with $0 < \alpha < 1/2$, then $\mu_l(\varepsilon) \to \mu_l(0)$, where $\mu_l(0)$ are the eigenvalues of the operator

   $$\widehat{H}_0 := \bigoplus_{j \in J} -\Delta_D^{e_j} \oplus \mathbf{0}, \tag{3.19}$$

   acting on the Hilbert space

   $$\mathcal{H}_0 := L^2(\Gamma) \oplus \mathbb{C}^K, \tag{3.20}$$

   where $\Delta_D^{e_j}$ is the Laplacian with Dirichlet boundary conditions on the edge e_j, $\mathbf{0}$ is the zero operator acting on $\mathbb{C}^K$ and K is the number of vertices in the graph.

   In other words, since in this case the vertex neighbourhoods are much bigger than the edge neighbourhoods, the particle sees them as an insuperable obstacle and it does not succeed in going through. However, there is an additional eigenmode for each vertex, corresponding to the lowest eigenvalue of the Neumann Laplacian in the big ball.

An analogous theorem, which can be found in the references given above, holds for equation (3.15). In terms of diffusion processes, one can say that each vertex becomes a trap for the limiting process, i. e., if a trajectory enters a vertex it stays there forever and cannot come out.

3. Suppose $\lambda(\varepsilon) = \varepsilon^{1/2}$, the borderline case. As in the previous examples, it is possible to show that $\mu_l(\varepsilon) \to \mu_l(0)$, where $\mu_l(0)$ are the eigenvalues of a positive self-adjoint operator $\widehat{H}_0$ which acts on the extended graph space of case 2, $\mathcal{H}_0 = L^2(\Gamma) \oplus \mathbb{C}^K$.

   The quadratic form associated to $\widehat{H}_0$ is

$$Q_0(f,a) := \sum_j \int_{e_j} dx_j \; |f'_{e_j}|^2, \tag{3.21}$$

   with domain $\mathcal{D}(Q_0) \subset H^1(\Gamma) \oplus \mathbb{C}^K$ given by elements $(f,a) \in H^1 \oplus \mathbb{C}^K$ such that $a_r = \sqrt{\frac{\pi}{2}} f(v_r)$ for each $r = 1, \ldots, K$.

   By direct calculation one can prove that $\widehat{H}_0$ acts on elements $(f,a) \in \mathcal{D}(\widehat{H}_0)$ as

$$\widehat{H}_0(f,a) = \left(-\frac{d^2 f}{dx_j^2}, c \right), \quad x_j \in e_j,$$

   where $c \in \mathbb{C}^K$ is defined by

$$c_k := \sqrt{\frac{2}{\pi}} \sum_{v_k \in e_j} f'_{e_j}(v_k), \quad k = 1, \ldots, K.$$

   The eigenvalue problem $\widehat{H}_0(f,a) = \mu(f,a)$ can then be rewritten as

$$\begin{cases} -\frac{d^2 f}{dx^2} = \mu f & \text{for } x \in e_j \\ f \text{ is continuous} & \text{at each vertex } v_k, \quad k = 1, \ldots, K, \\ \sum_{v_k \in e_j} f'_{e_j}(v_k) = \frac{\mu\pi}{2} f(v_k) & \text{at each vertex } v_k, \quad k = 1, \ldots, K. \end{cases} \tag{3.22}$$

   In this formulation of the spectral problem the extra variables in $\mathbb{C}^K$ are eliminated, and there is some similarity between equation (3.22) and the eigenvalue equation for delta boundary conditions (page 50). The difference is that the coupling constant α in this case depends on the eigenvalue itself, i. e., we have a sort of energy dependent delta interaction.

As we have briefly remarked at the end of chapter 1, one should stress that the convergence results stated above are reasonable because the infimum of the spectrum of the operator $-\Delta_N^\varepsilon$ is 0, *independently of* ε, while if one uses Dirichlet boundary

conditions or a constraining potential the infimum of the spectrum of the Hamiltonian goes to infinity when $\varepsilon \to 0$, so it is necessary, in some sense, to "renormalize" it in order to get a finite answer in the limit.

Secondly, in the works we mentioned, to pass from M_ε to Γ, the authors project the functions in M_ε onto the first eigenfunction of the Neumann Laplacian in the transverse direction. We expect, however, that an adiabatic decoupling takes place for all the transverse eigenstates, not only for the lowest one, and then that an effective Hamiltonian can be obtained in every almost invariant subspace (i.e., in every transverse subspace). The problem with this formulation is that near each vertex the different transverse subspaces relative to each edge mix, and so it is conceivable that there is a transition between orthogonal subspaces at the leading order.

In next section, 3.2, we will show that this is not possible for energy conservation reasons, if we propagate a state which is localized away from the vertices.

Dirichlet boundary conditions

Rigid approximations of quantum graphs by Dirichlet boundary conditions have been tackled only recently by Post [Po$_1$]. He considered, as it is customary in rigid approximation framework, a graph embedded in $\mathbb{R}^2$ whose edges have finite length, and a thickened graph M_ε similar to the one drawn in figure 3.1, but with *small vertex neighbourhood.* For the precise meaning of "small" we refer the reader to the original paper, but, just to give a rough idea, we can say that vertex neighbourhoods have to be *strictly smaller* than the standard ε-neighbourhood defined by the distance from the graph,

$$V_{\varepsilon,\mathrm{dist}} := \{q \in \mathbb{R}^2 : \mathrm{dist}(q,\Gamma) := \inf_{x\in\Gamma} |q-x| < \varepsilon\}. \tag{3.23}$$

He then proved that, if $\mu_l(\varepsilon)$ is the lth eigenvalue of the Dirichlet Laplacian on M_ε, $-\Delta_D^\varepsilon$, (counted with respect to multiplicity) then

$$\mu_l(\varepsilon) - \frac{\mu_1}{\varepsilon^2} \to \mu_l(0), \qquad \varepsilon \to 0, \tag{3.24}$$

where $\mu_l(0)$ denotes the lth eigenvalue of

$$\bigoplus_{j\in J} -\Delta_D^{e_j 1}, \tag{3.25}$$

the direct sum of Dirichlet Laplacians on the edges, and μ_1 is the first transverse eigenvalue.

This result tells us that, using the more realistic Dirichlet conditions, the edges decouple already when the vertex neighbourhoods are small, unlike what happens with

[1] In the case of curved edges, according to the heuristic calculations of Da Costa, equation (1.23), an additional term containing the curvature appears, [Po$_1$].

the Neumann ones, where this occurs only when they are big. It also explicitly shows the need of renormalizing the Hamiltonian to get convergence.

The cases we will analyze below can be considered in some sense dual to Post's ones, because we concentrate on an Hamiltonian with a constraining potential given by the distance from the graph, which is the case excluded by his treatment. Moreover, we have already stressed that we are interested in an approximate time evolution for a suitable class of initial conditions, and we will show that, subtracting the corresponding transverse eigenvalue, it is possible to get it in every almost invariant subspace, not only in the subspace corresponding to the transverse ground state.

3.2 Convergence outside the vertices for a generic graph

In this section we consider, according to the definitions of section 3.1.1, a finite metric graph embedded in $\mathbb{R}^2$, Γ, whose edges, however, can have infinite length.

We approximate the dynamics on the graph using an Hamiltonian, acting on $L^2(\mathbb{R}^2)$, with a constraining potential given by the square of the distance from Γ:

$$\begin{aligned} \widehat{H}(\varepsilon) &= -\frac{1}{2}\Delta + \frac{1}{2\varepsilon^2} d_\Gamma^2, \\ d_\Gamma(q) &:= \inf_{x\in\Gamma} |q - x|, \end{aligned} \tag{3.26}$$

choosing units in which the (effective) mass of the particle and $\hbar$ are equal to 1.

Remark 3.1. Note that ε and $\hbar$ are unrelated. Moreover, in the following we will consider longitudinal initial conditions which are independent of ε. This means that we look at a situation, different from that of chapter 2, where longitudinal wave packets have a wavelength much bigger than the characteristic wavelength of the transverse motion. In the actual experimental setting, external fields can be employed which cause the wave function to vary rapidly in the longitudinal direction too. This can be an interesting further field of study.

Remark 3.2. When the constraint is a smooth submanifold, the square of the distance from it represents the prototype of a constraining potential satisfying conditions $\boldsymbol{W_1}$ and $\boldsymbol{W_2}$ (page 3). Thus, in the context of graphs, it is natural to analyze first a model which uses it. Actually, the results we will prove can be generalized to more general constraining potentials, which are not quadratic near the graph, but whose Taylor expansion near the graph contains higher order terms (note however that we only suppose the potential to be smooth away from the vertices, since d_Γ is C^0, but not C^1 near the vertices). The important hypothesis is that the *Hessian of the potential is constant along the graph.* In last chapter we saw that, if we consider highly oscillating

longitudinal wave packets, whose wavelength is comparable to the transverse one, then the energy of oscillation changes into a potential energy for the longitudinal motion. In this case, however, the potential energy would be of the form $\omega(x)/\varepsilon$, so, in the limit $\varepsilon \to 0$, we would get again a constraining problem and the wavefunction would concentrate around the minima of $\omega(x)$ (a phenomenon of this kind was studied for classical trajectories by Hellfer and Sjöstrand in the context of "mini-puits", mini-wells, [HeSj], see also [FrHe]). To avoid this type of problems, we restrict ourselves to potentials with constant Hessian, and we analyze explicitly d_Γ^2.

We denote by $\widehat{U}_t(\varepsilon)$ the unitary evolution associated to Hamiltonian (3.26),

$$\widehat{U}_t(\varepsilon) := \exp(-it\widehat{H}(\varepsilon)), \tag{3.27}$$

and we apply it to an initial state which, in physicists' language, lies in a subband, i. e., in a fixed transverse mode, localized *inside one edge*. As we have already stressed in last chapter, these are the states which are thought to convey the propagation of the particles in semiconductor structures.

We have then

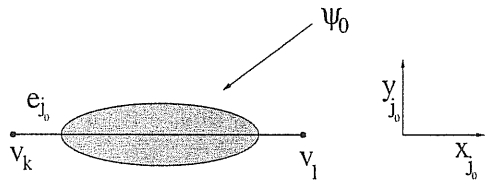
$$\psi_0(x_{e_{j_0}}, y_{e_{j_0}}) = f(x_{j_0})\Phi_n^\varepsilon(y_{j_0}), \tag{3.28}$$

where $f \in C_0^\infty(0, l_{e_{j_0}})$ and, as in chapter 2, Φ_n^ε is an eigenstate of the harmonic oscillator,

$$\begin{aligned} &\left(-\frac{1}{2}\frac{\partial^2}{\partial y^2} + \frac{1}{2\varepsilon^2}y^2 \right)\Phi_n^\varepsilon(y) = \frac{E_n}{\varepsilon}\Phi_n^\varepsilon(y), \\ &E_n = n + \frac{1}{2}. \end{aligned} \tag{3.29}$$

$x_{e_{j_0}}$ is the natural coordinate along the edge e_{j_0} and $y_{e_{j_0}}$ is the corresponding coordinate in the orthogonal direction. $x_{e_{j_0}}$ varies in the interval $[0, l_{e_{j_0}}]$ (or $[0, +\infty)$ if the edge has infinite length) and, since the edges are straight lines, y_{j_0} is well defined and assumes values between $-\infty$ and $+\infty$.

Figure 3.2: Schematic representation of the initial state



Applying $\widehat{U}_t(\varepsilon)$ to ψ_0 we expect the appearance of a strongly oscillating factor, given by $\exp(-iE_nt/\varepsilon)$. To cope with this fact, we subtract it from the Hamiltonian, and we

consider the corresponding modified unitary group:

$$\begin{aligned} \widetilde{H}(\varepsilon) &:= \widehat{H}(\varepsilon) - \frac{E_n}{\varepsilon}, \\ \psi_t^\varepsilon &:= \widetilde{U}(\varepsilon)\psi_0 := \exp(-it\widetilde{H}(\varepsilon))\psi_0. \end{aligned} \tag{3.30}$$

To analyze the adiabatic decoupling, we split ψ_t according to the different transverse components in each edge:

$$s_j^m(t, x_j; \varepsilon) := \int dy_j \; \Phi_m^\varepsilon(y_j)^* \psi_t^\varepsilon(x_j, y_j)^1, \tag{3.31}$$

where x_j is the natural coordinate along e_j and y_j is orthogonal to it.

Proposition 3.3. *Let P_j^m the operator from $\mathcal{S}(\mathbb{R}^2)$ to $H^k(\mathbb{R}^2)$ defined by*

$$P_j^m \psi(x_j) := \int_{\mathbb{R}} dy_j \; \Phi_m^\varepsilon(y_j)^* \psi(x_j, y_j), \tag{3.32}$$

then P_j^m extends to a unique operator (of norm 1) from $H^k(\mathbb{R}^2)$ to $H^k(\mathbb{R}^2)$, for every $k \in \mathbb{N}$, $k \geq 0$.

Proof. Given $\psi \in \mathcal{S}(\mathbb{R}^2)$ it is clear that

$$\begin{aligned} &\partial_x^l (P_j^m \psi)(x) = \int_{\mathbb{R}} dy \; \Phi_m(y)^* \partial_x^l \psi(x, y) = < \Phi_m, \partial_x^l \psi >_{L^2(\mathbb{R}_y)} \\ &\Rightarrow |\partial_x^l (P_j^m \psi)(x)|^2 \leq \|\Phi_m\|^2_{L^2(\mathbb{R})} \cdot \int dy |\partial_x^l \psi(x, y)|^2 \\ &\Rightarrow \int dx |\partial_x^l (P_j^m \psi)(x)|^2 \leq \|\Phi_m\|^2_{L^2(\mathbb{R})} \cdot \|\partial_x^l \psi\|^2_{L^2(\mathbb{R}^2)} \end{aligned}$$

$$\Rightarrow \|P_j^m \psi\|^2_{H^k(\mathbb{R})} = \sum_{l=0}^{k} \|\partial_x^l P_j^m \psi\|^2_{L^2(\mathbb{R})} \leq \|\Phi_m\|^2 \sum_{l=0}^{k} \|\partial_x^l \psi(x, y)\|^2_{L^2(\mathbb{R}^2)}. \tag{3.33}$$

□

Corollary 3.1. *The components $s_j^m(t, x_j; \varepsilon)$ are well defined, belong to $H^1(\mathbb{R})$ in the variable x_j and satisfy*

$$\sup_{t \in [0,T]} \|s_j^m(t, \cdot; \varepsilon)\|_{L^2(\mathbb{R})} \leq \textit{const.} \tag{3.34}$$

[1] With an abuse of notation, we denote by $\psi_t^\varepsilon(x_j, y_j)$ the function ψ_t^ε written in coordinates (x_j, y_j). Since the different systems of coordinates associated to each edge are linked to one another by a rigid motion of the plane, this does not modify the differentiability or integrability properties of ψ_t^ε. Note, instead, that $\Phi_m^\varepsilon(y_j)$ is an eigenfunction of the harmonic oscillator in the variable y_j.

Proof. The domain of the quadratic form associated to $\widetilde{H}(\varepsilon)$ is given by

$$Q(\widetilde{H}(\varepsilon)) := H^1(\mathbb{R}^2) \cap Q(d^2) \quad , \tag{3.35}$$

where $Q(d^2) := \{\psi \in L^2(\mathbb{R}^2) : d_\Gamma(x,y)\psi \in L^2(\mathbb{R}^2)\}$. ψ_0 belongs to $Q(\widetilde{H}(\varepsilon))$, so ψ_t^ε is in $H^1(\mathbb{R}^2)$. □

Lemma 3.1.

$$\|\widetilde{H}(\varepsilon)\psi_0\| \leq C \quad (\textit{independent of} \quad \varepsilon). \tag{3.36}$$

Proof. Since the Laplacian is invariant by rotations and translations, we have (for simplicity we drop the index j_0 in x and y)

$$\begin{aligned}
\widetilde{H}(\varepsilon)\psi_0 &= -\frac{1}{2}\partial_x^2 f \cdot \Phi_n - \frac{1}{2} f \cdot \partial_y^2 \Phi_n + \frac{1}{2\varepsilon^2} d_\Gamma^2 f \cdot \Phi_n - \frac{E_n}{\varepsilon} f \cdot \Phi_n = \\
&= -\frac{1}{2}\partial_x^2 f \cdot \Phi_n + \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2) f \cdot \Phi_n - \frac{1}{2} f \cdot \partial_y^2 \Phi_n + \\
&+ f \frac{1}{2\varepsilon^2} y^2 \cdot \Phi_n - \frac{E_n}{\varepsilon} f \cdot \Phi_n = \\
&= -\frac{1}{2}\partial_x^2 f \cdot \Phi_n + \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2) f \cdot \Phi_n.
\end{aligned}$$

Let a be the infimum of the support of f, and $b > a$ the supremum. Since f is supported inside the edge e_{j_0} and near each edge the distance from the graph is equal to $|y_j|$, the function $\frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2) f \cdot \Phi_n$ will be zero when $|y| < D$, where D, depending on the support of f, can be small, but it is strictly positive. Therefore we have

$$\|\frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2) f \cdot \Phi_n\|^2 = \int_a^b dx \int_{|y|>D} dy \, \frac{1}{4\varepsilon^4}(d_\Gamma^2 - y^2)^2 |f(x)\Phi_n^\varepsilon(y)|^2. \tag{3.37}$$

Now we use the following two properties:

- d_Γ^2 is equal to a polynomial of second order in the variables (x,y);
- Φ_n^ε is equal to a polynomial in $y/\varepsilon^{1/2}$ times $\exp(-y^2/2\varepsilon)$.

The norm (3.37) contains then terms of the form (P and Q are polynomials)

$$\begin{aligned}
&\int_a^b dx \, |f(x)|^2 \int_{|y|>D} dy \, P(x,y) Q(x, y/\varepsilon^{1/2}) \exp\left(-\frac{y^2}{\varepsilon}\right) = \\
&= \int_a^b dx \, |f(x)|^2 \int_{|y|>D} dy \, P(x,y) Q(x, y/\varepsilon^{1/2}) \exp\left[-\left(\frac{1}{\varepsilon} - M\right) y^2\right] \exp(-My^2) \leq \\
&\leq \exp\left[-\left(\frac{1}{\varepsilon} - M\right) D^2\right] \int_a^b dx \, |f(x)|^2 \int_{|y|>D} dy \, P(x,y) Q(x, y/\varepsilon^{1/2}) \exp(-My^2) = \\
&= O(e^{-c/\varepsilon}).
\end{aligned}$$

This implies that

$$\|\frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)f \cdot \Phi_n\|^2 = O(e^{-c/\varepsilon}), \tag{3.38}$$

and therefore the thesis is proved. □

Corollary 3.2. *For every system of coordinates (x_j, y_j) associated to an edge e_j we have*

$$\frac{1}{2}\|\partial_{x_j}\psi_t^\varepsilon\|^2 + \frac{1}{2}\|\partial_{y_j}\psi_t^\varepsilon\|^2 + \frac{1}{2\varepsilon^2}\|d_\Gamma\psi_t^\varepsilon\|^2 \leq \frac{C}{\varepsilon}. \tag{3.39}$$

Corollary 3.3. *Let $F_{d_\Gamma \geq \delta}$ be the characteristic function of the set $\{(x,y) : d_\Gamma(x,y) \geq \delta\}$, where δ is any positive number, then*

$$\sup_{t\in[0,T]} \|F_{d_\Gamma\geq\delta}\ \psi_t^\varepsilon\|_{L^2(\mathbb{R}^2)} = O(\varepsilon^{1/2}). \tag{3.40}$$

Proof. Last term in (3.39) gives

$$\frac{1}{2}\|d_\Gamma\psi_t^\varepsilon\|^2 \leq C\varepsilon.$$

Therefore we get

$$\delta^2 \cdot < \psi_t^\varepsilon,\ F_{d_\Gamma\geq\delta}\ \psi_t^\varepsilon > \leq < d_\Gamma\ \psi_t^\varepsilon,\ F_{d_\Gamma\geq\delta}\ d_\Gamma\ \psi_t^\varepsilon > \leq\ 2C\varepsilon.$$

□

We are now ready to prove

Theorem 3.1. *For $m \neq n$ and $j \in J$*

$$s_j^m(t, x_j; \varepsilon) \overset{*}{\rightharpoonup} 0, \quad \varepsilon \to 0, \tag{3.41}$$

where the convergence is in the weak topology of $L^\infty((0,T), L^2(\mathbb{R}))$.*

Proof. For convenience of the reader, we recall that a *bounded* sequence f_ε of functions in $L^\infty((0,T), L^2(\mathbb{R}))$ converges to a limit $f_0 \in L^\infty((0,T), L^2(\mathbb{R}))$ in the weak* topology if and only if

$$\int_0^T dt\ \varphi(t) < \chi(\cdot), f_\varepsilon(t,\cdot) >_{L^2(\mathbb{R})} \to \int_0^T dt\ \varphi(t) < \chi(\cdot), f_0(t,\cdot) >_{L^2(\mathbb{R})}$$

for every function $\varphi \in L^1(0,T)$ and every function $\chi \in L^2(\mathbb{R})$.

It is a standard fact about weak* topology that it is enough to prove convergence only for φ and χ in dense subsets of $L^1((0,T))$ and $L^2(\mathbb{R})$ respectively (see, e. g., [Bor], Appendix B or [Rud], theorems 3.15 and 3.16).

Let us then show first that

$$\sup_{t\in[0,T]} |< \chi(\cdot), s_j^m(t,\cdot;\varepsilon) >_{L^2(\mathbb{R})}| \to 0, \quad \varepsilon \to 0, \tag{3.42}$$

for every function $\chi \in C_0^\infty(\mathbb{R}\backslash\{0, l_{e_j}\})$ if the edge e_j has finite length and for every $\chi \in C_0^\infty(\mathbb{R}\backslash\{0\})$ if e_j has infinite length. We consider explicitly only the latter case, the former being analogous.

If the support of χ is contained in $(-\infty, 0)$ then

$$|< \chi, s_j^m >_{L^2(\mathbb{R})}| = |< \chi \cdot \Phi_m^\varepsilon, \psi_t^\varepsilon >_{L^2(\mathbb{R}^2)}| = |< \chi \cdot \Phi_m^\varepsilon, F_\chi\, \psi_t^\varepsilon >| \le \|\chi \cdot \Phi_m^\varepsilon\| \cdot \|F_\chi\, \psi_t^\varepsilon\| =$$
$$= O(\varepsilon^{1/2}),$$

where F_χ is the characteristic function of the support of χ and we have used corollary 3.3.

If the support of χ in contained in $(0, +\infty)$, then, following the proof of lemma 3.1 we can show that

$$\widetilde{H}(\varepsilon)[\chi(x_j)\Phi_m^\varepsilon(y_j)] = (\text{we drop the index } j) \quad -\frac{1}{2}\partial_x^2\chi \cdot \Phi_m^\varepsilon +$$
$$+\frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi \cdot \Phi_m^\varepsilon + \frac{E_m - E_n}{\varepsilon}\chi \cdot \Phi_m^\varepsilon.$$

Since χ is supported away from the vertex (located at $x_j = 0$), an equation similar to (3.38) holds:

$$\|\frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi \cdot \Phi_m^\varepsilon\|^2 = O(e^{-c/\varepsilon}).$$

Since $m \neq n$, we have then

$$\chi\Phi_m^\varepsilon = \frac{\varepsilon}{m-n}\left\{\widetilde{H}(\varepsilon)[\chi(x_j)\Phi_m^\varepsilon(y_j)] + \frac{1}{2}\partial_x^2\chi \cdot \Phi_m^\varepsilon\right\} + O(e^{-c/\varepsilon}).$$

This implies

$$< \chi(\cdot), s_j^m(t,\cdot;\varepsilon) >=< \chi(\cdot)\Phi_m^\varepsilon, \psi_t^\varepsilon > = \frac{\varepsilon}{m-n} < \chi(\cdot)\Phi_m^\varepsilon, \widetilde{H}(\varepsilon)\psi_t^\varepsilon > +$$
$$+\frac{\varepsilon}{m-n} < \frac{1}{2}\partial_x^2\chi \cdot \Phi_m^\varepsilon, \psi_t^\varepsilon > + O(e^{-c/\varepsilon}) =$$
$$= \text{(lemma 3.1) } O(\varepsilon).$$

Now, if $\varphi \in L^1((0,T))$, we get

$$\left| \int_0^T dt\ \varphi(t) < \chi(\cdot), s_j^m(t,\cdot;\varepsilon) >_{L^2(\mathbb{R})} \right| \le \|\varphi\|_{L^1} \cdot \sup_{t\in[0,T]} |< \chi(\cdot), s_j^m(t,\cdot;\varepsilon) >|,$$

but we have just shown that the right-hand side goes to zero for $\chi \in C_0^\infty(\mathbb{R}\backslash\{0\})$ (or $C_0^\infty(\mathbb{R}\backslash\{0, l_{e_j}\})$ for an edge of finite length) which is dense in $L^2(\mathbb{R})$. □

Theorem 3.1 shows that, although in a weak sense, there is indeed adiabatic separation between the different transverse states even in the presence of vertices, if the initial state is localized in two senses: first, it has to be localized inside one edge to avoid mixing between the different transverse states associated to each edge and second, it has to be in one (or a finite number of) transverse band(s).

Since the limit of s_j^m for $m \neq n$ is zero, to analyze in a complete way the (limit) evolution of ψ_0 we have to determine the behaviour of s_j^n, $j \in J$.

Theorem 3.2. *There exists a weak* convergent subsequence of $s_j^n(t, x_j; \varepsilon)$ in $L^\infty((0,T), L^2(\mathbb{R}))$ (which, making an abuse of notation, we denote again by the same symbol), whose limit $s_j^n(t, x_j; 0) \in L^\infty((0,T), L^2(\mathbb{R}))$ satisfies*

$$i\partial_t s_j^n(t, x_j; 0) = -\frac{1}{2}\partial_x^2 s_j^n(t, x_j; 0) \quad \text{in} \quad \mathcal{D}'((0,T) \times (0, l_{e_j})). \tag{3.43}$$

Remark 3.3. By corollary 3.1, $s_j^n(t, x_j; \varepsilon)$ is a bounded sequence in $L^\infty((0,T), L^2(\mathbb{R}))$. Since the balls in $L^\infty((0,T), L^2(\mathbb{R}))$ are compact metric spaces with respect to the weak* topology (see the theorems in the book of Rudin quoted above), a weak* convergent subsequence certainly exists.

Moreover, if one shows that all the weak* convergent subsequences converge to a limit independent of the sequence itself, then this implies that the sequence itself converges.

The equation satisfied by the limit in theorem 3.2 is clearly independent of the subsequence, but it does not determine the behaviour of the limit in the vertices, so we cannot conclude from it the convergence of the sequence, but this is the strategy we have in mind, which has been successfully applied by Bornemann [Bor] in the classical case.

We split the proof of the theorem into a number of lemmas.

Lemma 3.2. *$s_j^n(t, x_j; \varepsilon)$ belongs to $\mathrm{C}^1([0,T], L^2(\mathbb{R}))$ and moreover it is an equicontinuous sequence of function from $[0,T]$ to $L^2(\mathbb{R})$.*

Proof. Let us denote by $\tilde{s}_j^n(t, x_j; \varepsilon) \in \mathrm{C}^0([0,T], L^2(\mathbb{R}))$ the function

$$P_j^n[-i\widetilde{H}(\varepsilon)\psi_t^\varepsilon].$$

Using proposition 3.3 we have that

$$\left\| \frac{s_j^n(t+h, \cdot; \varepsilon) - s_j^n(t, \cdot; \varepsilon)}{h} - \tilde{s}_j^n(t, \cdot; \varepsilon) \right\|_{L^2(\mathbb{R})} = \left\| P_j^n \left[\frac{\widetilde{U}_{t+h}(\varepsilon) - \widetilde{U}_t(\varepsilon)}{h} + i\widetilde{U}_t(\varepsilon)\widetilde{H}(\varepsilon) \right] \psi_0 \right\|$$

$$\leq \left\| \left[\frac{\widetilde{U}_{t+h}(\varepsilon) - \widetilde{U}_t(\varepsilon)}{h} + i\widetilde{U}_t(\varepsilon)\widetilde{H}(\varepsilon) \right] \psi_0 \right\| \to 0.$$

This proves that

$$i\partial_t s_j^n(t,x_j;\varepsilon) = \tilde{s}_j^n(t,x_j;\varepsilon) = P_j^m[-i\widetilde{U}_t(\varepsilon)\widetilde{H}(\varepsilon)\psi_0]. \tag{3.44}$$

Since $\|\widetilde{H}(\varepsilon)\psi_0\|$ is bounded (lemma 3.1), $\|\tilde{s}_j^m(t,x_j;\varepsilon)\|$ is bounded, therefore

$$\|s_j^m(t,\cdot;\varepsilon) - s_j^m(t',\cdot;\varepsilon)\|_{L^2(\mathbb{R})} = \left\| \int_t^{t'} d\tau\ \partial_\tau s_j^m(\tau,\cdot;\varepsilon) \right\|$$
$$\leq \int_t^{t'} d\tau\ \|\partial_\tau s_j^m(\tau,\cdot;\varepsilon)\| \leq C|t-t'|,$$

showing that $s_j^m(t,x_j;\varepsilon)$ is an equicontinuous sequence. □

Corollary 3.4. *There exists a subsequence $s_j^m(t,x_j;\varepsilon)$ which satisfies:*

1. *$s_j^m(t,x_j;\varepsilon)$ converges, in the weak topology of $L^2(\mathbb{R})$, uniformly in t, to a limit $s_j^m(t,x_j;0) \in L^2(\mathbb{R})$. Moreover, the limit is continuous in t in the weak topology of L^2.*

2. *$\partial_t s_j^m(t,x_j;\varepsilon) \overset{*}{\rightharpoonup} \partial_t s_j^m(t,x_j;0)$ in $L^\infty(\,(0,T),L^2(\mathbb{R}))$, where the derivative $\partial_t s_j^m(t,x_j;0)$ is to be interpreted as derivative in $\mathcal{D}'((0,T)\times\mathbb{R}_x)$.*

Proof. The sequence $s_j^m(t,x_j;\varepsilon)$ is contained in a ball in $L^2(\mathbb{R})$. This ball is a compact metric space with respect to the weak topology. Since the sequence is equicontinuous with respect to the strong topology, it will be equicontinuous with respect to the weak topology too. Therefore, the theorem of Ascoli-Arzelà (see, e. g., [Roy], theorem 10.40) proves the first point.

Equation (3.44) implies that $\partial_t s_j^m(t,x_j;\varepsilon)$ is a bounded sequence in $L^\infty(\,(0,T),L^2(\mathbb{R}))$, so, extracting possibly another subsequence, we have that there exists $g_j^m \in L^\infty(\,(0,T),L^2(\mathbb{R}))$ such that (again, we denote the subsequence with the same symbol as the sequence itself)

$$\partial_t s_j^m(t,x_j;\varepsilon) \overset{*}{\rightharpoonup} g_j^m,$$

but this implies that $\forall\ \varphi \in C_0^\infty((0,T))$, $\forall\ \chi \in C_0^\infty(\mathbb{R})$,

$$\int_0^T dt \int_{\mathbb{R}} dx\ g_j^m(t,x)\varphi(t)\chi(x) =$$
$$= \int_0^T dt\ \varphi(t) < \chi(\cdot), g_j^m(t,\cdot) >_{L^2(\mathbb{R})} \leftarrow \int_0^T dt\ \varphi(t) < \chi, \partial_t s_j^m(t,\cdot;\varepsilon) >=$$
$$= \int_0^T dt\ \varphi(t)\partial_t < \chi, s_j^m(t,\cdot;\varepsilon) >=$$
$$= -\int_0^T dt\ \partial_t\varphi < \chi, s_j^m(t,\cdot;\varepsilon) > \rightarrow -\int_0^T dt\ \partial_t\varphi < \chi, s_j^m(t,\cdot;0) >=$$
$$= \int_0^T dt \int_{\mathbb{R}} dx\ s_j^m(t,x;0)\partial_t\varphi(t)\chi(x),$$

$$\Rightarrow g_j^m = \partial_t s_j^m(t, x_j; 0) \text{ in } \mathcal{D}'((0,T) \times \mathbb{R}_x).$$

□

We can now prove theorem 3.2.

Proof. We suppose that edge e_j has infinite length. The proof for an edge of finite length is analogous.

Corollary 3.3, together with the proof of the first part of the proof of theorem 3.1 implies that

$$\sup_{t\in[0,T]} | < \chi, s_j^m(t, \cdot; \varepsilon) > | = O(\varepsilon^{1/2}),$$

for all $j \in J$ and for all $\chi \in \mathrm{C}_0^\infty(-\infty, 0)$, but the first point of corollary 3.4 gives

$$< \chi, s_j^m(t, \cdot; 0) >_{L^2(\mathbb{R})} = \lim_{\varepsilon \to 0} < \chi, s_j^m(t, \cdot; \varepsilon) > = 0.$$

Equation (3.44) allows us to write, for all $\chi \in \mathrm{C}_0^\infty(0, +\infty)$,

$$\begin{aligned}
&< \chi, i\partial_t s_j^m(t, \cdot; \varepsilon) >_{L^2(\mathbb{R})} = < \chi \cdot \Phi_n^\varepsilon, \widetilde{H}(\varepsilon)\psi_t^\varepsilon >_{L^2(\mathbb{R}^2)} = < \widetilde{H}(\varepsilon)\chi \cdot \Phi_n^\varepsilon, \psi_t^\varepsilon > = \\
&= < -\frac{1}{2}\partial_x^2 \chi \cdot \Phi_n^\varepsilon, \psi_t^\varepsilon > + < \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi \cdot \Phi_n^\varepsilon, \psi_t^\varepsilon > = < -\frac{1}{2}\partial_x^2 \chi, s_j^m(t, \cdot; \varepsilon) >_{L^2(\mathbb{R})} + \\
&+ < \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi \cdot \Phi_n^\varepsilon, \psi_t^\varepsilon >
\end{aligned}$$

Since χ is supported in $(0, +\infty)$, equation (3.38) holds also in this case, therefore

$$\| \frac{1}{2\varepsilon^2}(d_\Gamma^2 - y^2)\chi \cdot \Phi_n^\varepsilon \|^2 = O(e^{-c/\varepsilon}).$$

We have then, for all $\varphi \in \mathrm{C}_0^\infty(0, T)$, and for all $\chi \in \mathrm{C}_0^\infty(0, +\infty)$,

$$\begin{aligned}
&\int_0^T dt\ \varphi(t) < \chi, i\partial_t s_j^n(t, \cdot; 0)) >_{L^2(\mathbb{R})} \leftarrow \int_0^T dt\ \varphi(t) < \chi, i\partial_t s_j^n(t, \cdot; \varepsilon) >_{L^2(\mathbb{R})} = \\
&= \int_0^T dt\ \varphi(t) < -\frac{1}{2}\partial_x^2 \chi, s_j^n(t, \cdot; \varepsilon) >_{L^2(\mathbb{R})} + O(e^{-c/\varepsilon}) \|\varphi\|_{L^1(0,T)} \\
&\to \int_0^T dt\ \varphi(t) < -\frac{1}{2}\partial_x^2 \chi, s_j^n(t, \cdot; 0) >_{L^2(\mathbb{R})},
\end{aligned}$$

$$\Rightarrow i\partial_t s_j^n(t, x_j; 0) = -\frac{1}{2}\partial_x^2 s_j^n(t, x_j; 0) \text{ in } \mathcal{D}'((0,T) \times (0, +\infty)). \tag{3.45}$$

□

3.3 Full treatment of a graph with two edges

In this section, we are going to put forward a different kind of soft approximation for a graph with one vertex and two infinite edges. Even though the geometry of the graph is very simple, this model illustrates clearly a possible mechanism by which the adiabatic decoupling between the different transverse states takes place. In particular, it shows that the bound states localized near the vertex which can arise (and indeed do arise for a rigid approximation of a quantum graph, [CLMM$_1$, CLMM$_2$, GoJa]) do not interfere with the propagation of product states localized inside one of the edges at the leading order, because their spectral distance becomes infinite in the limit.

We denote the graph by Γ_ϑ, where ϑ is the angle made by the two edges, $0 < \vartheta < \pi$.

As we have already mentioned in the introduction to this chapter, we do not consider directly Γ_ϑ, but we approximate it by smooth curves, $\Gamma_{\vartheta,\delta}$, whose curvature becomes bigger and bigger in a region whose width, given by δ, goes to zero and we consider a potential constraining to this family curves.

More precisely, to specify the approximating curves we need only to specify their curvature, k_δ, because, as it is well known, this specifies the curve up to rigid motions of the plane. Naturally, we want that, when δ goes to zero, the curves tend to the graph. This in particular implies that the turning angle has to become equal to ϑ when $\delta \longrightarrow 0$.

A simple choice which satisfies these requests is (s is the arc length parameter)

$$\begin{aligned} &k_\delta(s) := \frac{\vartheta}{\delta} k\left(\frac{s}{\delta}\right), \quad \int_{\mathbb{R}} ds\ k(s) = 1, \\ &k \in \mathrm{C}_0^\infty(-1,1), \quad \begin{cases} k = 1 & |s| < 1/2 \\ k = 0 & |s| > 3/4, \end{cases} \end{aligned} \tag{3.46}$$

which amounts to deformate the graph in a neighbourhood of the vertex replacing it with an arc of a circle. Note that the δ scaling is fixed by the request that the turning angle of the approximating curves be ϑ,

$$\int_{\mathbb{R}} ds\ \frac{\vartheta}{\delta} k\left(\frac{s}{\delta}\right) = \vartheta.$$

We consider the Hamiltonian

$$\widehat{H}(\varepsilon, \delta(\varepsilon)) = -\frac{1}{2}\Delta + \frac{1}{\varepsilon^2} W_{\delta(\varepsilon)}, \quad \delta(\varepsilon) \longrightarrow 0 \text{ when } \varepsilon \longrightarrow 0,$$

where, for simplicity, we suppose that

$$W_{\delta(\varepsilon)}(x,y) = \frac{1}{2} d^2_{\delta(\varepsilon)}(x,y) = \frac{1}{2} \mathrm{dist}[(x,y), \Gamma_{\vartheta,\delta(\varepsilon)}]^2.$$

Remark 3.1, about the possibility to generalize the analysis to potentials with constant Hessian, applies here too. As in the previous section, we are interested in the time evolution of a product state which is initially localized away from the vertex.

Naturally, we expect that the particle oscillates very fast along the direction normal to the curve, and, since we are considering the case of a curve embedded in $\mathbb{R}^2$ we expect tubular coordinates, defined on page 10, to be the most suitable for the analysis of the motion, since the problems related to the existence of a gauge coupling do not appear in the codimension one case.

However, tubular coordinates are defined only in the region

$$\{(x,y) \in \mathbb{R}^2 : d_\delta(x,y) < \varrho\}, \tag{3.47}$$

where ϱ is the radius of curvature of $\Gamma_{\vartheta,\delta}$. When k_δ is different from zero, this quantity is proportional to δ itself, so, by hypothesis, it goes to zero when $\varepsilon \to 0$.

To get rid of the region $\{(x,y) : d_\delta(x,y) > \delta\}$ we will use a theorem, proved first by Froese and Herbst in the more general context of a potential constraining to a submanifold (proposition 8.1 in [FrHe]), which basically says that if one starts from an initial state more and more localized near the constraint, then all that matters for the time evolution is a small region near the constraint itself. We repeat the proof of Froese and Herbst because we need to keep track of the dependence of all the constants in the estimates on δ, to apply them to the region $\{(x,y) \in \mathbb{R}^2 : d_\delta(x,y) < \delta(\varepsilon)\}$.

Theorem 3.3. *Let $\psi \in L^2(\mathbb{R}^2)$, $\|\psi\| = 1$ and $\|\widehat{H}(\varepsilon,\delta)\psi\| \leq \frac{C_1}{\varepsilon}$ (C_1 independent of δ). Then,*

$$\|F_{d_\delta \geq \delta} e^{-it\widehat{H}(\varepsilon,\delta)}\psi\| \leq (2C_1)^{1/2}\frac{\varepsilon^{1/2}}{\delta}. \tag{3.48}$$

F indicates the characteristic function of the region indicated.

Moreover, let $\widehat{H}_D(\varepsilon,\delta)$ be the Hamiltonian $\widehat{H}(\varepsilon,\delta)$ with Dirichlet boundary conditions on the set $\{(x,y) \in \mathbb{R}^2 : d_\delta(x,y) = \delta\}$.

Let us suppose that $\delta = \delta(\varepsilon)$, $\lim_{\varepsilon\to 0}\delta(\varepsilon) = 0$. Taking into account (3.48), let us also assume that

$$\lim_{\varepsilon\to 0}\frac{\varepsilon^{1/2}}{\delta(\varepsilon)} = 0. \tag{3.49}$$

Then, for all $t \in [0,T]$, we have

$$\|F_{d_\delta<\delta}e^{-it\widehat{H}(\varepsilon,\delta)}\psi - e^{-it\widehat{H}_D(\varepsilon,\delta)}F_{d_\delta<\delta}\psi\| \leq C_2(C_1,T)\left(\frac{\varepsilon^{1/4}}{\delta^{5/2}} + \frac{\varepsilon^{1/2}}{\delta^3}\right). \tag{3.50}$$

Remark 3.4. The theorem implies that if we choose a $\delta(\varepsilon)$ such that

$$\lim_{\varepsilon\to 0}\frac{\varepsilon^{1/10}}{\delta(\varepsilon)} = 0 \tag{3.51}$$

then we can restrict ourselves to analyze the Dirichlet Hamiltonian $\widehat{H}_D(\varepsilon, \delta(\varepsilon))$, which is localized inside the region where tubular coordinates are defined. This, however, means that we have to consider a "tube" encircling the graph whose diameter is much bigger than the localization of the transverse states, which for an harmonic oscillator is $\varepsilon^{1/2}$.

Remark 3.5. As already observed in [FrHe], the estimate (3.50) is not optimal.

Proof. Let us first prove (3.48).

Since $\|\widehat{H}(\varepsilon,\delta)\psi\| \leq \frac{C_1}{\varepsilon}$, we have from Schwarz inequality

$$< \psi, \widehat{H}(\varepsilon,\delta)\psi > \leq \frac{C_1}{\varepsilon}.$$

This implies immediately that

$$\frac{C_1}{\varepsilon} \geq < \widehat{H}^{1/2}\psi, \widehat{H}^{1/2}\psi > = \frac{1}{2}\|\nabla\psi\|^2 + \frac{1}{2\varepsilon^2}\|d_\delta\psi\|^2 \Rightarrow \|d_\delta\psi\|^2 \leq 2C_1\varepsilon. \tag{3.52}$$

It follows then

$$\delta^2 < F_{d_\delta\geq\delta}\psi, F_{d_\delta\geq\delta}\psi > \leq < d_\delta F_{d_\delta\geq\delta}\psi, d_\delta F_{d_\delta\geq\delta}\psi > \leq \|d_\delta\psi\|^2 \leq 2C_1\varepsilon. \tag{3.53}$$

The same argument can applied also to $e^{-it\widehat{H}(\varepsilon,\delta)}\psi$, so (3.48) is proved.

We need now to prove an estimate on the behaviour of the gradient of ψ away from the graph.

Let $\tilde{\chi} \in \mathrm{C}_0^\infty(\mathbb{R})$ be 1 when $1/4 < |x| < 3/4$ and 0 when $|x| \leq 1/8$ or $|x| \geq 7/8$, then the function

$$\chi(u) := \tilde{\chi}\left(\frac{1}{2(\alpha-\lambda_1)}|u| + \frac{1}{4} - \frac{\lambda_1}{2(\alpha-\lambda_1)}\right)$$

will be 1 when $\lambda_1 < |u| < \alpha$ and 0 for $|u|$ near zero. If we choose λ_1 and α such that $0 < \lambda_1 < \alpha < \delta$, then χ is well defined (and $\in \mathrm{C}_0^\infty(\mathbb{R})$) when u is the coordinate along the direction normal to the curve $\Gamma_{\vartheta,\delta}$ (see figure 1.2, page 11).

We have then

$$\|F_{\lambda_1<d_\delta<\alpha}\nabla\psi\| = \|F_{\lambda_1<d_\delta<\alpha}\nabla(\chi\psi)\| \leq \|\nabla(\chi\psi)\|.$$

Using again the Schwarz inequality and the fact that $\chi\psi \in \mathcal{D}(\Delta)$ (the potential is bounded on the support of χ) we get

$$\|\nabla(\chi\psi)\| \leq \|\Delta(\chi\psi)\|^{1/2}\|\chi\psi\|^{1/2},$$

so, to estimate $\|F_{\lambda_1<d_\delta<\alpha}\nabla\psi\|$ we need to get an estimate on $\|\Delta(\chi\psi)\|$. To obtain it, we use an energy estimate of second order, i. e., we calculate the quadratic form associated to $\widehat{H}(\varepsilon,\delta)^2$.

$$\widehat{H}(\varepsilon,\delta)^2 = \frac{1}{4}|p|^4 + \left(\frac{1}{2\varepsilon^2}d_\delta^2\right)^2 + \sum_j p_j \frac{1}{2\varepsilon^2} d_\delta^2 p_j - \frac{1}{2\varepsilon^2}\Delta d_\delta^2, \tag{3.54}$$

where $p = -i\nabla$. The first three terms are positive operators, while if we take the mean value of the last one with respect to the state $\chi\psi$ we get

$$< \chi\psi, \Delta d_\delta^2 \chi\psi >= \int_{d_\delta<\delta} dxdy\, |\chi\psi|^2 \Delta d_\delta^2 = \int_{|u|<\delta} dsdu\, [1+uk_\delta(s)]\, |\chi\psi|^2\, [1+uk_\delta(s)]^{-1} \cdot$$
$$\cdot\, \partial_u\{[1+uk_\delta(s)]2u\} = \int_{|u|<\delta} dsdu\, [1+uk_\delta(s)]\, |\chi\psi|^2 \cdot 2 + \int_{|u|<\delta} dsdu\, |\chi\psi|^2\, 2uk_\delta(s) \leq$$
$$\leq C\|\chi\psi\|^2,$$

where the change to curvilinear coordinates has been described in last chapter (page 2.2.1) and in the last step we have used the fact that

$$\sup_{|u|<\delta} |uk_\delta(s)| \leq \delta k_\delta(s) = \vartheta k\left(\frac{s}{\delta}\right) \leq const. \text{ (independent of } \delta) \quad .$$

Taking the mean value of (3.54) with respect to $\chi\psi$ we obtain then

$$\|\frac{1}{2}\Delta(\chi\psi)\|^2 \leq \|\widehat{H}(\varepsilon,\delta)(\chi\psi)\|^2 + \frac{C}{\varepsilon^2},$$

which can be written equivalently as

$$\frac{1}{2}\|\Delta(\chi\psi)\| \leq \frac{C^{1/2}}{\varepsilon} + \|\widehat{H}(\varepsilon,\delta)\psi\| + \frac{1}{2}\|[\Delta,\chi]\psi\|.$$

The last term is equal to

$$[\Delta,\chi]\psi = (\Delta\chi)\psi + \nabla\chi\cdot\nabla\psi,$$

and we can estimate its norm changing to curvilinear coordinates,

$$\nabla\chi = \partial_x\tilde{\chi}(x(u))\frac{1}{2(\alpha-\lambda_1)}\frac{u}{|u|}\boldsymbol{n}(s),$$
$$\Delta\chi = (1+k_\delta u)^{-1}\partial_u[(1+k_\delta u)\partial_u\chi] = \partial_u^2\chi + (1+k_\delta u)^{-1}k_\delta\partial_u\chi =$$
$$= \partial_x^2\tilde{\chi}(x(u))\frac{1}{2(\alpha-\lambda_1)^2} + \partial_x\tilde{\chi}(x(u))\frac{1}{2(\alpha-\lambda_1)}\frac{u}{|u|}\frac{k_\delta}{1+k_\delta u}.$$

Using (3.52) to estimate $\|\nabla\psi\|$, we have then

$$\|[\Delta,\chi]\psi\| \leq \frac{C}{\varepsilon^{1/2}(\alpha-\lambda_1)} + \frac{C}{(\alpha-\lambda_1)^2} + \frac{C}{\delta(\alpha-\lambda_1)}. \tag{3.55}$$

In what follows, we will need to choose α and λ_1 proportional to δ. Assumption (3.49) implies then that all terms in (3.55) are *at most* of order ε^{-1}.

To sum up, we have

$$\|\Delta(\chi\psi)\| \leq \frac{C}{\varepsilon}, \tag{3.56}$$

from which it follows that (assuming that α and λ_1 are proportional to δ and that $\delta(\varepsilon)$ satisfies (3.49))

$$\|F_{\lambda_1<d_\delta<\alpha}\nabla\psi\| \leq C\varepsilon^{-1/2}\frac{\varepsilon^{1/4}}{\delta^{1/2}} = \frac{C}{\varepsilon^{1/4}\delta^{1/2}}. \tag{3.57}$$

Let now $\tilde{\xi}$ be a function in $\mathrm{C}_0^\infty(\mathbb{R})$ such that $\tilde{\xi}(x) = 1$ when $|x| < 1/4$ and $\tilde{\xi}(x) = 0$ when $|x| > 1/2$. We define the function ξ by the equation $\xi(u) := \tilde{\xi}(u/\delta)$, where u is the curvilinear coordinate normal to the curve.

Because of (3.48), to prove (3.50) is enough to show that

$$\|e^{it\widehat{H}_D(\varepsilon,\delta)}\xi e^{-it\widehat{H}(\varepsilon,\delta)}\psi - \xi\psi\| \leq C_2(C_1,T)\left(\frac{\varepsilon^{1/4}}{\delta^{5/2}} + \frac{\varepsilon^{1/2}}{\delta^3}\right)$$

for $t \in [0,T]$. Let

$$\phi_{t,\varepsilon,\delta} := e^{it\widehat{H}_D(\varepsilon,\delta)}\xi e^{-it\widehat{H}(\varepsilon,\delta)}\psi - \xi\psi.$$

Integrating the derivative we have

$$\begin{aligned}\phi_{t,\varepsilon,\delta} &= i\int_0^t ds\; e^{is\widehat{H}_D(\varepsilon,\delta)}[\widehat{H}_D(\varepsilon,\delta)\xi - \xi\widehat{H}(\varepsilon,\delta)]e^{-is\widehat{H}(\varepsilon,\delta)}\psi = \\ &= \int_0^t ds\; e^{is\widehat{H}_D(\varepsilon,\delta)}[\nabla\xi\cdot p - (i/2)\Delta\xi]e^{-is\widehat{H}(\varepsilon,\delta)}\psi,\end{aligned}$$

therefore

$$\|\phi_{t,\varepsilon,\delta}\|^2 = \int_0^t ds\; < e^{-is\widehat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}, [\nabla\xi\cdot p - (i/2)\Delta\xi]e^{-is\widehat{H}(\varepsilon,\delta)}\psi > .$$

Let now $\tilde{\zeta}$ be a $\mathrm{C}_0^\infty(\mathbb{R})$ function which is 1 on the support of $\partial_x\tilde{\xi}$ and 0 when $|x|$ is near zero. As above, we denote by $\zeta(u) := \tilde{\zeta}(u/\delta)$. We can then write

$$\begin{aligned}&\|\phi_{t,\varepsilon,\delta}\|^2 \leq \int_0^t ds\; \|\zeta e^{-is\widehat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}\|(\|\nabla\xi\cdot pe^{-is\widehat{H}(\varepsilon,\delta)}\psi\| + \|(1/2)\Delta\xi e^{-is\widehat{H}(\varepsilon,\delta)}\psi\|) \leq \\ &\leq C\left(\frac{1}{\delta^{3/2}\varepsilon^{1/4}} + \frac{1}{\delta^2}\right)\int_0^t ds\; \|\zeta e^{-is\widehat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}\|,\end{aligned} \tag{3.58}$$

where we have used (3.57) and the definition of ξ.

Now

$$< \phi_{t,\varepsilon,\delta}, \widehat{H}_D(\varepsilon,\delta)\phi_{t,\varepsilon,\delta} > \ \leq \ 2 < \xi e^{-it\widehat{H}(\varepsilon,\delta)}\psi, \widehat{H}_D(\varepsilon,\delta)\xi e^{-it\widehat{H}(\varepsilon,\delta)}\psi > +$$
$$+ 2 < \xi\psi, \widehat{H}_D(\varepsilon,\delta)\xi\psi >= 2 < \xi e^{-it\widehat{H}(\varepsilon,\delta)}\psi, \left[-\frac{1}{2}\Delta\xi - i\nabla\xi\cdot p + \xi\widehat{H}_D(\varepsilon,\delta)\right] e^{-it\widehat{H}(\varepsilon,\delta)}\psi > +$$
$$+ 2 < \xi\psi, \left[-\frac{1}{2}\Delta\xi - i\nabla\xi\cdot p + \xi\widehat{H}_D(\varepsilon,\delta)\right]\psi > .$$

Using again equation (3.57) and the definition of ξ, we get

$$|< \xi\ \psi, -\frac{1}{2}\Delta\xi\ \psi >| \leq \frac{C}{\delta^2},$$
$$|< \xi\ \psi, -i\nabla\xi\cdot p\ \psi >| \leq \frac{C}{\varepsilon^{1/4}\delta^{3/2}},$$
$$|< \xi\ \psi, \xi\widehat{H}_D(\varepsilon,\delta)\ \psi >| \leq \frac{C}{\varepsilon},$$

and corresponding equations with $e^{-it\widehat{H}(\varepsilon,\delta)}\psi$ instead of ψ. If we suppose that the sequence $\delta(\varepsilon)$ satisfies (3.49), then all the terms grow at most as ε^{-1}, so we obtain in the end

$$< \phi_{t,\varepsilon,\delta}, \widehat{H}_D(\varepsilon,\delta)\phi_{t,\varepsilon,\delta} >\leq \frac{C}{\varepsilon}.$$

Repeating the proof of (3.48), we can then show that

$$\|\zeta e^{-is\widehat{H}_D(\varepsilon,\delta)}\phi_{t,\varepsilon,\delta}\| \leq \frac{C\varepsilon^{1/2}}{\delta},$$

and substituting this back in (3.58) we get

$$\|\phi_{t,\varepsilon,\delta}\|^2 \leq C\left(\frac{1}{\delta^{3/2}\varepsilon^{1/4}} + \frac{1}{\delta^2}\right)\frac{\varepsilon^{1/2}}{\delta} = C\left(\frac{\varepsilon^{1/4}}{\delta^{5/2}} + \frac{\varepsilon^{1/2}}{\delta^3}\right). \tag{3.59}$$

□

Now, let us fix a sequence $\delta(\varepsilon)$ satisfying (3.51). As in last section, we consider the time evolution of a product state localized inside one of the two edges, away from the vertex,

$$\begin{aligned} \psi_t^\varepsilon &= e^{-it\widehat{H}(\varepsilon,\delta(\varepsilon))}\psi_0, \\ \psi_0(x,y) &= f(x)\Phi_n^\varepsilon(y), \end{aligned} \tag{3.60}$$

where (x,y) is the system of coordinates associated to one of the edges, $f \in \mathrm{C}_0^\infty(\mathbb{R})$ and Φ_n^ε has been defined in (3.29). If we choose ε sufficiently small, the tubular coordinates

associated to the curve $\Gamma_{\vartheta,\delta}$, (s_δ, u_δ), coincide with (x, y) apart from a small neighbourhood of the vertex. The state ψ_0 is then well defined and independent of δ. The limit $\varepsilon \to 0$ gives us therefore the leading behaviour of an initial state which propagates through a tube which curves slowly with respect to the transverse wavelength.

Equation (3.48) allows us to discard $F_{d_{\delta(\varepsilon)}>\delta(\varepsilon)}\psi_t^\varepsilon$, while (3.50) allows us to approximate $F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_t^\varepsilon$ with $e^{-it\widehat{H}_D(\varepsilon,\delta(\varepsilon))}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_0$.

We can now prove

Proposition 3.4. *Let ψ_t^ε be given by* (3.60)*, then, for $t \in [0, T]$,*

$$\begin{aligned}&\|\exp[-it\widehat{H}_D(\varepsilon,\delta(\varepsilon))]F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_0+\\&-\exp[-it\widehat{K}(\delta(\varepsilon))-itE_n/\varepsilon](f)\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\Phi_n^\varepsilon(u_{\delta(\varepsilon)})\|\to 0,\quad \varepsilon\to 0,\end{aligned} \tag{3.61}$$

where

$$\widehat{K}(\delta(\varepsilon)) = -\frac{1}{2}\partial_s^2 - \frac{k_\delta(s)^2}{8} \quad . \tag{3.62}$$

Proof. The proof is an application of Duhamel formula, lemma 2.2,

$$\begin{aligned}&\|\exp[-it\widehat{H}_D(\varepsilon,\delta(\varepsilon))]F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\psi_0+\\&-\exp[-it\widehat{K}(\delta(\varepsilon))-itE_n/\varepsilon](f)\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}\Phi_n^\varepsilon(u_{\delta(\varepsilon)})\| =\\&=\|\{\exp[it\widehat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\widehat{K}(\delta(\varepsilon))-itE_n/\varepsilon]-\mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^\varepsilon(u_{\delta(\varepsilon)})+\\&+F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^\varepsilon(u_\delta)-F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^\varepsilon(y)\|\le\\&\le\|\{\exp[it\widehat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\widehat{K}(\delta(\varepsilon))-itE_n/\varepsilon]-\mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^\varepsilon(u_\delta)\|+\\&+\|F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^\varepsilon(u_\delta)-F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f(x)\Phi_n^\varepsilon(y)\| =\\&=\|\{\exp[it\widehat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\widehat{K}(\delta(\varepsilon))-itE_n/\varepsilon]-\mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^\varepsilon(u_\delta)\|,\end{aligned}$$

because the second term is zero if ε (and therefore δ) is sufficiently small.

Applying now Duhamel formula[1], we have that

$$\begin{aligned}&\|\{\exp[it\widehat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\widehat{K}(\delta(\varepsilon))-itE_n/\varepsilon]-\mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^\varepsilon(u_\delta)\|\le\\&\le\int_0^t ds\ \|[\widehat{H}_D(\varepsilon,\delta(\varepsilon))-\widehat{K}(\delta(\varepsilon))-E_n/\varepsilon]\cdot\\&\cdot\exp[-is\widehat{K}(\delta(\varepsilon))-isE_n/\varepsilon]F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^\varepsilon(u_\delta)\|.\end{aligned} \tag{3.63}$$

[1]For every fixed δ, the domain of $\widehat{K}(\delta)$ is $H^2(\mathbb{R})$, so $\exp[-it\widehat{K}(\delta)](f)\cdot F_{d_\delta<\delta}\Phi(u_\delta)$ is in the domain of $\widehat{H}_D(\varepsilon,\delta)$.

The Hamiltonian $\widehat{H}_D(\varepsilon,\delta(\varepsilon))$ in curvilinear coordinates, acting on $L^2(\mathbb{R}\times[0,\delta],dsdu)$, is given by equation (2.22),

$$\widehat{H}_D(\varepsilon,\delta(\varepsilon)) = -\frac{1}{2}\frac{1}{[1+uk_\delta(s)]^2}\frac{\partial^2}{\partial s^2} + \frac{1}{[1+uk_\delta(s)]^3}uk'_\delta(s)\frac{\partial}{\partial s} + V(s,u) + \\ - \frac{1}{2}\frac{\partial^2}{\partial u^2} + \frac{1}{2\varepsilon^2}u^2,$$

where V is the geometric potential,

$$V(s,u) = \frac{1}{2}\Big\{ - \frac{k_\delta^2}{4[1+uk_\delta]^2} + \frac{uk''_\delta}{2[1+uk_\delta]^2} - \frac{5}{4}\frac{u^2(k'_\delta)^2}{[1+uk_\delta]^2}\Big\}. \tag{3.64}$$

Making a unitary dilation by the factor $\varepsilon^{1/2}$ along u, we get an operator acting on $L^2(\mathbb{R}\times[0,\delta(\varepsilon)/\varepsilon^{1/2}],dsdu)$, given by

$$D_{\varepsilon^{1/2}}\widehat{H}_D(\varepsilon,\delta(\varepsilon))D^\dagger_{\varepsilon^{1/2}} = -\frac{1}{2}\frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^2}\frac{\partial^2}{\partial s^2} + \frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^3}\varepsilon^{1/2}uk'_\delta(s)\frac{\partial}{\partial s} + \\ + V(s,\varepsilon^{1/2}u) - \frac{1}{2\varepsilon}\frac{\partial^2}{\partial u^2} + \frac{1}{2\varepsilon}u^2, \tag{3.65}$$

where

$$D_{\varepsilon^{1/2}}\psi(u) = \varepsilon^{1/4}\psi(\varepsilon^{1/2}u).$$

Therefore, equation (3.63) becomes

$$\|\{\exp[it\widehat{H}_D(\varepsilon,\delta(\varepsilon))]\exp[-it\widehat{K}(\delta(\varepsilon)) - itE_n/\varepsilon] - \mathbb{I}\}F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)}f\cdot\Phi_n^\varepsilon(u_\delta)\| \le \\ \le \int_0^t ds\ \|[D_{\varepsilon^{1/2}}\widehat{H}_D(\varepsilon,\delta(\varepsilon))D^\dagger_{\varepsilon^{1/2}} - \widehat{K}(\delta(\varepsilon)) - E_n/\varepsilon]\cdot \\ \cdot\exp[-is\widehat{K}(\delta(\varepsilon)) - isE_n/\varepsilon]f\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\| \quad .$$

Therefore, it is clear from previous equations that

$$\|[V(s,\varepsilon^{1/2}u) + k_\delta^2/8]\exp[-is\widehat{K}(\delta(\varepsilon)) - isE_n/\varepsilon]f\cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\| = \\ = O(\varepsilon^{1/2}/\delta^3)\to 0, \quad \varepsilon\to 0,$$

$$\Big\|\Big(-\frac{1}{2\varepsilon}\frac{\partial^2}{\partial u^2} + \frac{1}{2\varepsilon}u^2 - \frac{E_n}{\varepsilon}\Big)\exp[-is\widehat{K}(\delta(\varepsilon)) - isE_n/\varepsilon]f\cdot \\ \cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot\Phi_n^{\varepsilon=1}(u_\delta)\Big\| \to 0, \quad \varepsilon\to 0,$$

so we need to control only the terms containing the derivative with respect to s in (3.65).

Using lemma 3.3, proved below, we have that

$$\left\| \frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^3}\varepsilon^{1/2}uk'_\delta(s)\frac{\partial}{\partial s}\exp[-it\widehat{K}(\delta(\varepsilon)) - itE_n/\varepsilon]f(s)\cdot \right.$$
$$\left. \cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot \Phi_n^{\varepsilon=1}(u_\delta)\right\| \leq (\varepsilon^{1/2}\|k'_\delta\|_{L^\infty}\cdot\|\partial_s f\|_{L^2} + |t|\cdot\varepsilon^{1/2}\|k_\delta\|_{L^\infty}\|k'_\delta\|^2_{L^\infty}\|f\|_{L^2})\cdot$$
$$\cdot \|u\Phi_n^{\varepsilon=1}(u)\| = O(\varepsilon^{1/2}/\delta^5)\to 0, \quad \varepsilon\to 0.$$

In the same way we have also that

$$\left\| -\frac{1}{2}\left\{\frac{1}{[1+\varepsilon^{1/2}uk_\delta(s)]^2} - 1\right\}\frac{\partial^2}{\partial s^2}\exp[-it\widehat{K}(\delta(\varepsilon)) - itE_n/\varepsilon]f(s)\cdot \right.$$
$$\left. \cdot F_{d_{\delta(\varepsilon)}<\delta(\varepsilon)/\varepsilon^{1/2}}\cdot \Phi_n^{\varepsilon=1}(u_\delta)\right\| \leq C\varepsilon^{1/2}\|k_\delta\|_\infty[\|\partial_s^2 f\| + |t|\cdot$$
$$\cdot (2\|k_\delta\|_\infty\cdot\|k'_\delta\|_\infty\|\partial_s f\| + \|k'_\delta\|^2_\infty\|f\| + \|k_\delta\|_\infty\|k''_\delta\|_\infty\|f\|)] = O(\varepsilon^{1/2}/\delta^5)\to 0, \quad \varepsilon\to 0.$$

□

Lemma 3.3. *Let $\widehat{H}$ be the one-dimensional Hamiltonian $\widehat{H} = -\frac{1}{2}\partial_x^2 + V$, where V is a potential bounded together with its first two derivatives, then, given $\psi \in H^1(\mathbb{R})$, we have*

$$\|\partial_x \exp(-it\widehat{H})\psi\|_{L^2(\mathbb{R})} \leq \|\partial_x\psi\|_{L^2(\mathbb{R})} + |t|\cdot\|\partial_x V\|_{L^\infty}\cdot\|\psi\|_{L^2(\mathbb{R})}, \tag{3.66}$$

and, given $\varphi \in H^2(\mathbb{R})$,

$$\begin{aligned}\|\partial_x^2 \exp(-it\widehat{H})\varphi\|_{L^2(\mathbb{R})} &\leq \|\partial_x^2\varphi\|_{L^2(\mathbb{R})} + \\ &+ |t|(2\|\partial_x V\|_{L^\infty}\cdot\|\partial_x\varphi\|_{L^2(\mathbb{R})} + \|\partial_x^2 V\|_{L^\infty}\cdot\|\varphi\|_{L^2(\mathbb{R})})\end{aligned} \tag{3.67}$$

Proof. Since V is bounded, the domain of the quadratic form associated to $\widehat{H}$ is $H^1(\mathbb{R})$, and the time evolution sends it into itself. It makes therefore sense to write, for $\psi \in H^1(\mathbb{R})$,

$$[-i\partial_x, e^{-it\widehat{H}}]\psi = e^{-it\widehat{H}}\int_0^t ds\ \partial_s e^{is\widehat{H}}(-i\partial_x)e^{-is\widehat{H}}\psi =$$
$$= ie^{-it\widehat{H}}\int_0^t ds\ e^{is\widehat{H}}[\widehat{H}, -i\partial_x]e^{-is\widehat{H}}\psi = e^{-it\widehat{H}}\int_0^t ds\ e^{is\widehat{H}}\ \partial_x V\ e^{-is\widehat{H}}\psi,$$

but this implies immediately

$$-i\partial_x e^{-it\widehat{H}}\psi = e^{-it\widehat{H}}(-i\partial_x)\psi + [-i\partial_x, e^{-it\widehat{H}}]\psi$$
$$\Rightarrow \|-i\partial_x e^{-it\widehat{H}}\psi\| \leq \|-i\partial_x\psi\| + \int_0^t ds\ \|\partial_x V e^{-is\widehat{H}}\psi\|,$$

which gives (3.66).

Following the same path and noticing that

$$[\widehat{H}, -\partial_x^2] = -\partial_x^2 V - 2\partial_x V \cdot \partial_x \tag{3.68}$$

we get (3.67). □

Remark 3.6. The request that the time evolution of the Hamiltonian with a constraining potential be approximated by the Hamiltonian with Dirichlet boundary conditions forces us, as stressed above, to choose a "big" tube. Proposition 3.4 says that this choice gives the same result as doing first the limit $\varepsilon \to 0$, i. e., as constraining first the particle to the curve, and then doing the limit $\delta \to 0$, i. e., changing the curve into the graph.

To complete the analysis of this case we need to study the limit of the dynamics $\exp[-it\widehat{K}(\delta(\varepsilon))]$ when $\varepsilon \to 0$.

The limit of one-dimensional Hamiltonians containing rescaled potentials has been studied in detail in the context of the approximation of singular interactions, like the delta coupling, by short range smooth potentials ([AGHKH] and references therein). The scaling used by us in (3.62) however, is not covered in the results presented in [AGHKH], but it can be analyzed using exactly the same techniques.

The idea is to show convergence in norm of the resolvent of $\widehat{K}(\delta(\varepsilon))$ to the resolvent of the Hamiltonian with Dirichlet boundary conditions in $s = 0$. As it is well known ([ReSi$_1$], theorem VIII.21) this implies strong convergence of the corresponding unitary group.

One could expect convergence to Dirichlet boundary conditions because the potential $-k_\delta^2/8$ is a strongly attractive well, which becomes deeper and deeper, but whose range is shorter and shorter. As explained in [EnSe] in a different context, we expect this to give rise to Dirichlet boundary conditions. This in particular says that the strong convergence of the unitary group (or the norm resolvent convergence) does not capture the behaviour of the eigenvalues which go to $-\infty$ when $\delta \to 0$, because, even though the ground state of $\widehat{K}(\delta(\varepsilon))$ tends to $-\infty$, its resolvent converges to that of a semibounded operator. This phenomenon has already been illustrated in [Ges].

We can now prove

Theorem 3.4. *Let $[\widehat{K}(\delta(\varepsilon)) - z^2]^{-1}$ be the resolvent of $\widehat{K}(\delta(\varepsilon))$, where $\Im z > 0$, then*

$$[\widehat{K}(\delta(\varepsilon)) - z^2]^{-1} \to [\widehat{K}_D - z^2]^{-1}, \quad \varepsilon \to 0, \tag{3.69}$$

in the norm of bounded operators on $L^2(\mathbb{R})$, where K_D is the free Laplacian on $L^2(\mathbb{R})$ with Dirichlet boundary conditions in $s = 0$.

Proof. The potential $Q(s) := -k^2/8$ is in $L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$, so we can apply the dilation technique described in [AGHKK] (see also [AGHKH]). Applying lemma A.1 of [AGHKK] we get

$$[\widehat{K}(\delta(\varepsilon)) - z^2]^{-1} = G_z - A_\delta(z)[\delta + B_\delta(z)]^{-1}C_\delta(z), \qquad \Im z > 0, \tag{3.70}$$

where G_z is the free resolvent, with kernel $g_z(w)$,

$$\begin{aligned} G_z &:= (\widehat{H}_0 - z^2)^{-1}, \qquad g_z(w) := \frac{i}{2z} e^{iz|w|} \\ \widehat{H}_0 &:= -\frac{\partial^2}{\partial s^2}, \qquad D(\widehat{H}_0) = H^2(\mathbb{R}), \end{aligned} \tag{3.71}$$

while $A_\delta(z)$, $B_\delta(z)$ and $C_\delta(z)$ are Hilbert-Schmidt operators with kernels

$$\begin{aligned} A_\delta(z,s,r) &= g_z(s-\delta r)|Q(r)|^{1/2}, \\ B_\delta(z,s,r) &= -|Q(s)|^{1/2} g_z[\delta(s-r)]|Q(r)|^{1/2}, \\ C_\delta(z,s,r) &= -|Q(s)|^{1/2} g_z(\delta s - r). \end{aligned} \tag{3.72}$$

It is not difficult to see (lemma 2.3 [AGHKK]) that

$$\begin{aligned} A_\delta &\to A_0, \\ B_\delta &\to B_0, \\ C_\delta &\to C_0, \end{aligned} \tag{3.73}$$

in Hilbert-Schmidt norm, where A_0, B_0 and C_0 have kernels

$$\begin{aligned} A_0(z,s,r) &= g_z(s)|Q(r)|^{1/2}, \\ B_0(z,s,r) &= -g_z(0)|Q(s)|^{1/2}|Q(r)|^{1/2}, \\ C_0(z,s,r) &= -|Q(s)|^{1/2} g_z(-r). \end{aligned} \tag{3.74}$$

The operator B_0 is not invertible on the whole Hilbert space, but it is clear from the expression of the kernel that it actually acts on the one-dimensional subspace, denoted by $\mathcal{H}_Q$, generated by the vector φ_Q given by

$$\varphi_Q(s) := \frac{|Q(s)|^{1/2}}{\| \, |Q(s)|^{1/2} \, \|_{L^2(\mathbb{R})}} = \frac{|Q(s)|^{1/2}}{\|Q(s)\|_{L^1(\mathbb{R})}^{1/2}} \quad . \tag{3.75}$$

So we can write

$$B_0 = -g_z(0)\|Q(s)\|_{L^1(\mathbb{R})} \varphi_Q < \varphi_Q, \cdot > . \tag{3.76}$$

On $\mathcal{H}_Q$, B_0 is invertible and the inverse is given by

$$B_0^{-1} = -\frac{1}{g_z(0)\|Q(s)\|_{L^1(\mathbb{R})}} \varphi_Q < \varphi_Q, \cdot > . \tag{3.77}$$

Since the operator C_0 has range equal to $\mathcal{H}_Q$ and A_0 acts non trivially only on $\mathcal{H}_Q$, we get that

$$[\widehat{K}(\delta(\varepsilon)) - z^2]^{-1} \to G_z - A_0 B_0^{-1} C_0,$$

which has a kernel given by

$$g_z(s-r) - \frac{g_z(s)g_z(-r)}{g_z(0)}, \tag{3.78}$$

which is the kernel of the resolvent of the Dirichlet Hamiltonian. □

Conclusions and future developments

We have been motivated to study the problem of quantum systems with strong constraining potentials essentially by two reasons.

The first is to understand how it is possible to recover the known classical results in the subject performing a suitable semiclassical limit on the quantum Hamiltonian (1.1). Our interested was aroused by the fact that, as we have explained in detail in the introduction, there seems to be a contradiction between the theorems proved in classical mechanics and the results (many of which are in a non rigorous form) known in quantum mechanics.

The main discrepancy is the presence, in the classical theorems, of the homogenized potential (theorem 1.1) which does not appear in the quantum case. This is due above all to the hypothesis, made in most of the published works, that the the constraining potential (or better, its Hessian) is constant on the constraint. In chapter 2 we have shown (theorem 2.2 and section 2.3) that, using a suitable scaling justified by physical considerations, the motion on the submanifold is ruled, in the semiclassical limit, by an Hamiltonian which contains exactly the same homogenized potential of theorem 1.1. We have also shown, using a non standard perspective, that semiclassical limit can offer new insights in dealing with the phenomenon of Taken chaos.

The second reason is that almost one or two-dimensional motions caused by the action of a confining potential are relevant to explain the physical features of many electronic nanostructures, like quantum wires, and have also been used in theoretical chemistry as simple models to calculate complex band structures in solids. The essential new feature, analyzed in chapter 3, is the presence in these structures of branching regions, which, in the limit of constrained motion give rise to singular structures, the "quantum graphs".

We have shown (section 3.2) that, because of adiabatic decoupling, it is possible to get an effective equation for the motion along the graph, outside of the vertices, in every transverse subspace. This is, as expected, the free Schrödinger equation. Even though our result is not complete, in the sense that the behaviour in the vertex is not described, we would like to stress that all the results published in the context of the

rigid approximation of quantum graphs and spectral convergence use the projection on the transverse ground state. We think that this is due only to technical reasons, because one expects, as we proved, decoupling in each transverse subspace.

In the same context, we have proposed to approximate a graph with two edges by a smooth curve, making its curvature bigger and bigger in a region of decreasing width. We have shown then that the limit motion on the graph is described by Dirichlet boundary conditions.

To prove this result we have revisited a theorem of Froese and Herbst, to approximate the time evolution of an Hamiltonian with a constraining potential with the one generated by an Hamiltonian with Dirichlet boundary conditions. With the estimates available, this is possible only when the Dirichlet tube is much bigger than the localization of the transverse states. It would be worthwhile to examine in which sense the Hamiltonian with a constraining potential and the one with Dirichlet conditions are equivalent for a different range of the parameters.

Another interesting related field of research would be the analysis of the convergence of the time evolution for rigid approximations of quantum graphs, which, till now, have been investigated considering (almost) only spectral convergence. Some results in this direction have been recently announced [Po_2].

The reader will have noticed, passing from chapter 2 to chapter 3, that the behaviour of the longitudinal states we consider is not homogeneous[1], in the sense that they can oscillate with a wavelength which is comparable to the transverse one or, in the opposite case, vary slowly. The methods for dealing with these cases are different, but it would be worthwhile to have a description for all these different classes of initial conditions, which are not just of academic interest, but can be actually found in the experiments.

A related topic is the introduction, besides the constraining potential, which varies on a scale of order ε, of another potential, varying on a scale of order $\varepsilon^{1/2}$ for example, to model differently the interaction near the vertices. This could give rise to different boundary conditions in the limit.

As a final remark, we would like to emphasize that this subject is actually linked to the issue, which should certainly be studied in greater detail, of the connection between our mathematical model and the actual physical devices we want to describe. First of all, our model contains only one body interactions. One can argue that a more realistic description, especially near the vertices, should contain at least two-body interactions, like in the scattering model proposed in [MePa]. Second, we have completely neglected the spin of the electrons, even though it has been recently proposed to use nanotubes for spin control purposes [EnMa], adding a spin-orbit term to (1.1).

[1]This concept has been stressed in [BDT].

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